



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 AM GMT

PDB ID : 2Q3U
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At5g08170, agmatine iminohydrolase
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-30
Resolution : 1.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

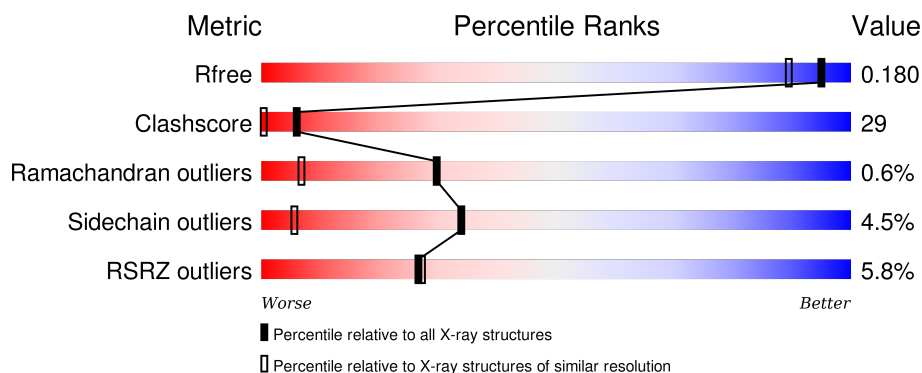
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1555 (1.56-1.52)
Clashscore	102246	1627 (1.56-1.52)
Ramachandran outliers	100387	1594 (1.56-1.52)
Sidechain outliers	100360	1592 (1.56-1.52)
RSRZ outliers	91569	1555 (1.56-1.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	383	<div> <div>4%</div> <div>52% 36% 7% • 5%</div> </div>
1	1-B	383	<div> <div>8%</div> <div>56% 34% • • 5%</div> </div>
1	2-A	383	<div> <div>4%</div> <div>53% 34% 7% • 5%</div> </div>
1	2-B	383	<div> <div>8%</div> <div>55% 34% 5% • 5%</div> </div>
1	3-A	383	<div> <div>4%</div> <div>54% 34% 6% • 5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	3-B	383	
1	4-A	383	
1	4-B	383	
1	5-A	383	
1	5-B	383	
1	6-A	383	
1	6-B	383	
1	7-A	383	
1	7-B	383	
1	8-A	383	
1	8-B	383	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	1-A	901	-	-	-	X
3	EDO	1-A	902	-	-	-	X
3	EDO	1-A	903	-	-	-	X
3	EDO	1-A	906	-	-	-	X
3	EDO	1-A	908	-	-	-	X
3	EDO	1-B	904	-	-	-	X
3	EDO	1-B	911	-	-	-	X
3	EDO	1-B	913	-	-	-	X
3	EDO	2-A	901	-	-	-	X
3	EDO	2-A	902	-	-	-	X
3	EDO	2-A	903	-	-	-	X
3	EDO	2-A	906	-	-	-	X
3	EDO	2-A	908	-	-	X	X
3	EDO	2-B	904	-	-	-	X
3	EDO	2-B	911	-	-	X	X
3	EDO	2-B	913	-	-	-	X
3	EDO	3-A	901	-	-	-	X
3	EDO	3-A	902	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	3-A	903	-	-	-	X
3	EDO	3-A	906	-	-	-	X
3	EDO	3-A	908	-	-	X	X
3	EDO	3-B	904	-	-	-	X
3	EDO	3-B	911	-	-	X	X
3	EDO	3-B	913	-	-	-	X
3	EDO	4-A	901	-	-	-	X
3	EDO	4-A	903	-	-	-	X
3	EDO	4-A	906	-	-	-	X
3	EDO	4-A	908	-	-	-	X
3	EDO	4-B	904	-	-	-	X
3	EDO	4-B	911	-	-	X	X
3	EDO	4-B	913	-	-	-	X
3	EDO	5-A	901	-	-	-	X
3	EDO	5-A	902	-	-	-	X
3	EDO	5-A	903	-	-	-	X
3	EDO	5-A	906	-	-	-	X
3	EDO	5-A	908	-	-	X	X
3	EDO	5-B	904	-	-	-	X
3	EDO	5-B	911	-	-	X	X
3	EDO	5-B	913	-	-	-	X
3	EDO	6-A	901	-	-	-	X
3	EDO	6-A	902	-	-	-	X
3	EDO	6-A	903	-	-	-	X
3	EDO	6-A	908	-	-	X	X
3	EDO	6-B	904	-	-	-	X
3	EDO	6-B	911	-	-	X	X
3	EDO	6-B	913	-	-	-	X
3	EDO	7-A	901	-	-	-	X
3	EDO	7-A	903	-	-	-	X
3	EDO	7-A	906	-	-	-	X
3	EDO	7-A	908	-	-	X	X
3	EDO	7-B	904	-	-	-	X
3	EDO	7-B	911	-	-	X	X
3	EDO	7-B	913	-	-	-	X
3	EDO	8-A	901	-	-	-	X
3	EDO	8-A	902	-	-	-	X
3	EDO	8-A	903	-	-	X	X
3	EDO	8-A	906	-	-	-	X
3	EDO	8-A	908	-	-	X	X
3	EDO	8-B	904	-	-	-	X
3	EDO	8-B	911	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	8-B	913	-	-	-	X
4	MPO	1-A	9000	-	-	-	X
4	MPO	2-A	9000	-	-	-	X
4	MPO	3-A	9000	-	-	-	X
4	MPO	4-A	9000	-	-	-	X
4	MPO	5-A	9000	-	-	-	X
4	MPO	6-A	9000	-	-	-	X
4	MPO	7-A	9000	-	-	-	X
4	MPO	8-A	9000	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 53040 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Agmatine deiminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	2-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	3-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	4-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	5-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	6-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	7-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	8-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	1-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	2-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	3-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	4-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	5-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	6-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	7-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	8-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
A	15	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
A	49	GLY	ASP	VARIANT	UNP Q8GWW7
A	85	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
A	87	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
A	159	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
A	190	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
A	228	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
A	284	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
B	15	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
B	49	GLY	ASP	VARIANT	UNP Q8GWW7
B	85	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
B	87	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
B	159	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
B	190	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
B	228	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7
B	284	MSE	MET	MODIFIED RESIDUE	UNP Q8GWW7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

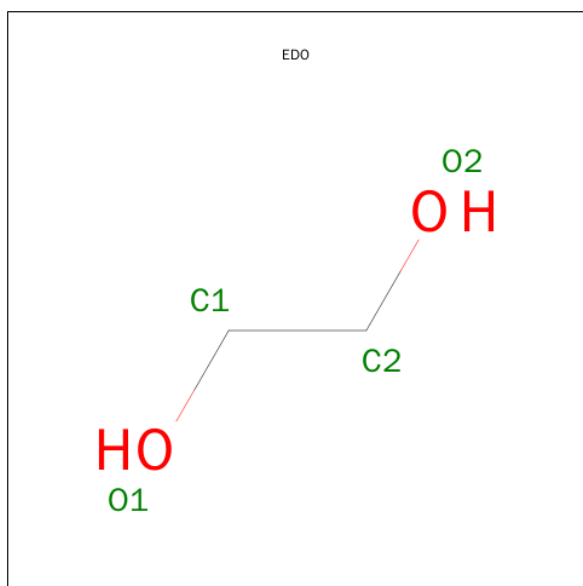
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	7-B	1	Total Mg 1 1	0	0
2	3-A	1	Total Mg 1 1	0	0
2	8-B	1	Total Mg 1 1	0	0
2	3-B	1	Total Mg 1 1	0	0
2	5-B	1	Total Mg 1 1	0	0
2	4-A	1	Total Mg 1 1	0	0
2	1-B	1	Total Mg 1 1	0	0
2	5-A	1	Total Mg 1 1	0	0
2	6-B	1	Total Mg 1 1	0	0
2	8-A	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	1	Total 1	Mg 1	0	0
2	6-A	1	Total 1	Mg 1	0	0
2	2-B	1	Total 1	Mg 1	0	0
2	2-A	1	Total 1	Mg 1	0	0
2	4-B	1	Total 1	Mg 1	0	0
2	7-A	1	Total 1	Mg 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

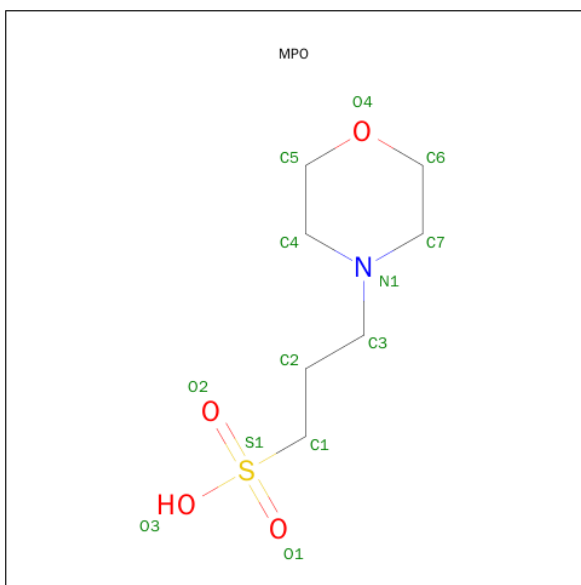
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	2-B	1	Total	C	O	0	0
			4	2	2		
3	3-B	1	Total	C	O	0	0
			4	2	2		
3	4-B	1	Total	C	O	0	0
			4	2	2		
3	5-B	1	Total	C	O	0	0
			4	2	2		
3	6-B	1	Total	C	O	0	0
			4	2	2		
3	7-B	1	Total	C	O	0	0
			4	2	2		
3	8-B	1	Total	C	O	0	0
			4	2	2		
3	1-B	1	Total	C	O	0	0
			4	2	2		
3	2-B	1	Total	C	O	0	0
			4	2	2		
3	3-B	1	Total	C	O	0	0
			4	2	2		
3	4-B	1	Total	C	O	0	0
			4	2	2		
3	5-B	1	Total	C	O	0	0
			4	2	2		
3	6-B	1	Total	C	O	0	0
			4	2	2		
3	7-B	1	Total	C	O	0	0
			4	2	2		
3	8-B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C₇H₁₅NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	1-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	2-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	3-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	4-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	5-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	6-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	7-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	8-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	404	Total	O	0	0
			404	404		
5	2-A	409	Total	O	0	0
			409	409		
5	3-A	404	Total	O	0	0
			404	404		
5	4-A	410	Total	O	0	0
			410	410		

Continued on next page...

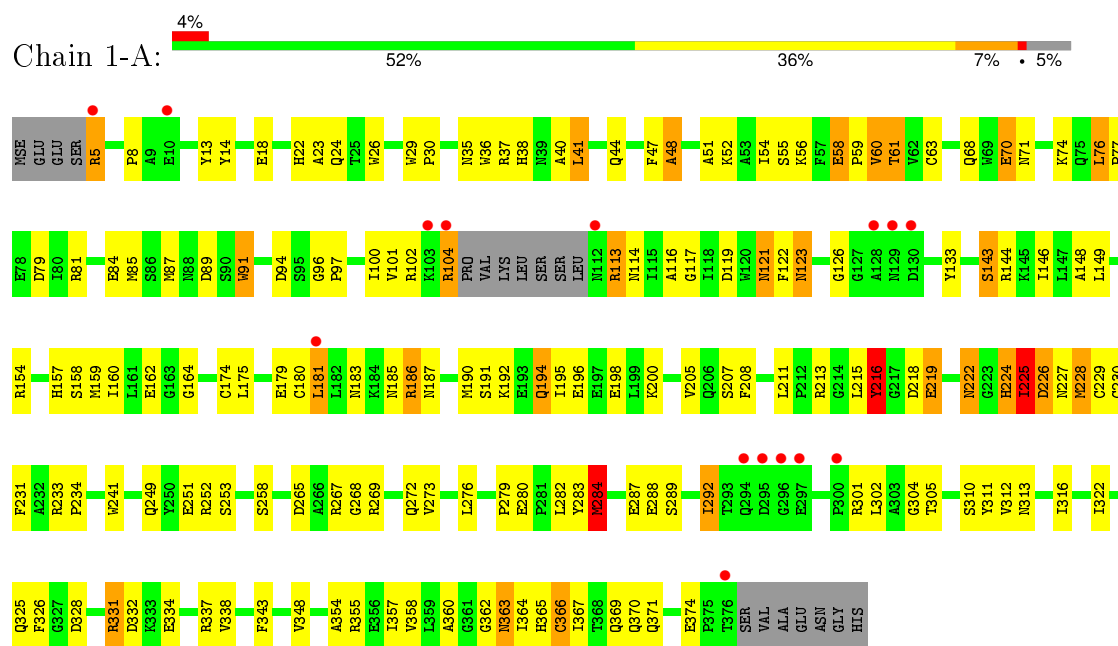
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	5-A	407	Total 407	O 407	0	0
5	6-A	403	Total 403	O 403	0	0
5	7-A	405	Total 405	O 405	0	0
5	8-A	409	Total 409	O 409	0	0
5	1-B	375	Total 375	O 375	0	0
5	2-B	370	Total 370	O 370	0	0
5	3-B	375	Total 375	O 375	0	0
5	4-B	369	Total 369	O 369	0	0
5	5-B	372	Total 372	O 372	0	0
5	6-B	376	Total 376	O 376	0	0
5	7-B	374	Total 374	O 374	0	0
5	8-B	370	Total 370	O 370	0	0

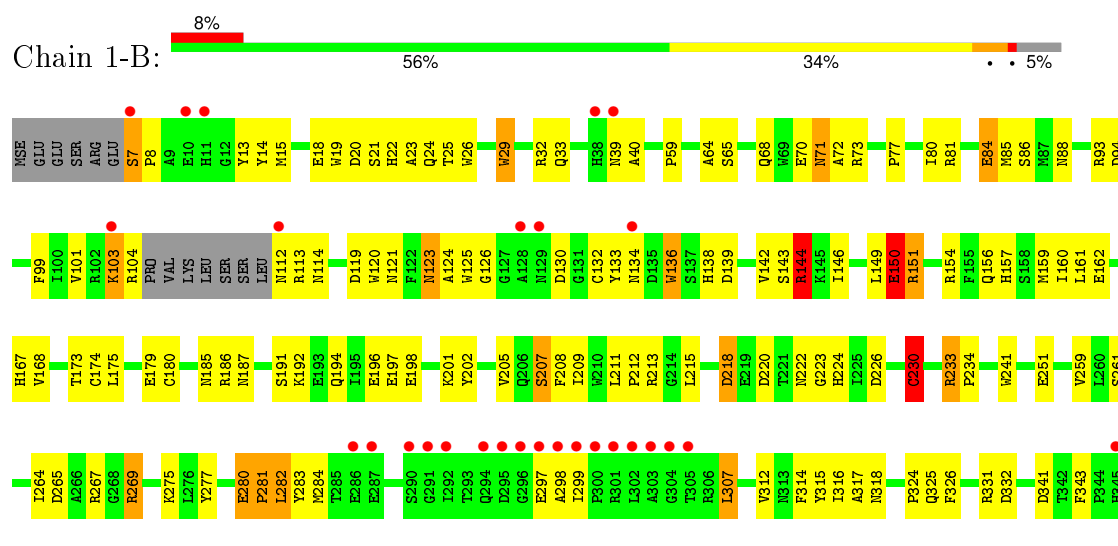
3 Residue-property plots

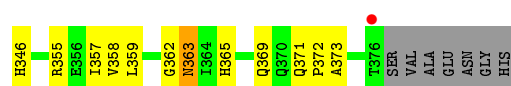
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Agmatine deiminase

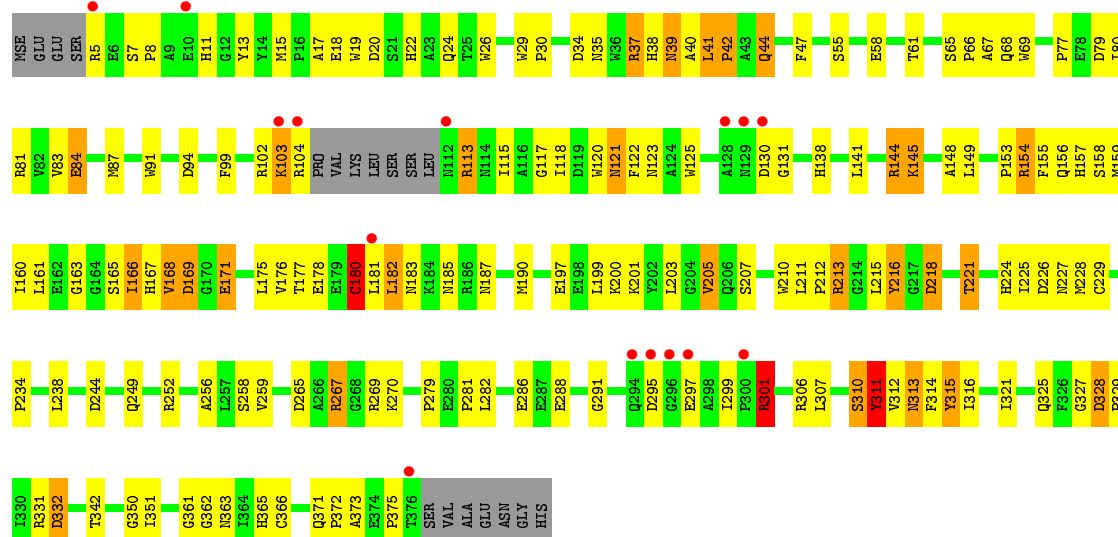


• Molecule 1: Agmatine deiminase

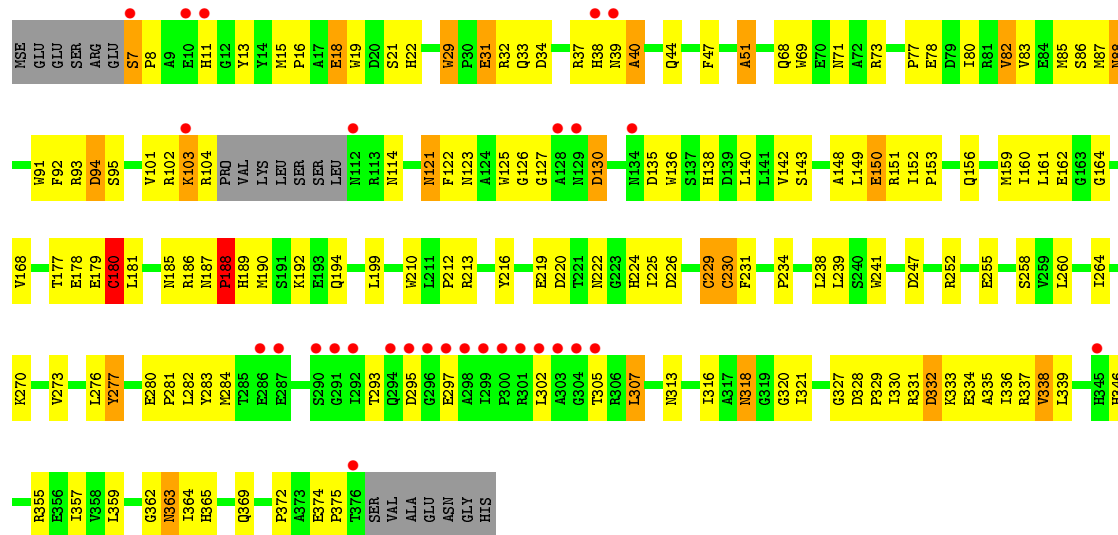




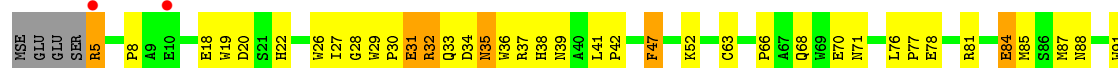
- Molecule 1: Agmatine deiminase

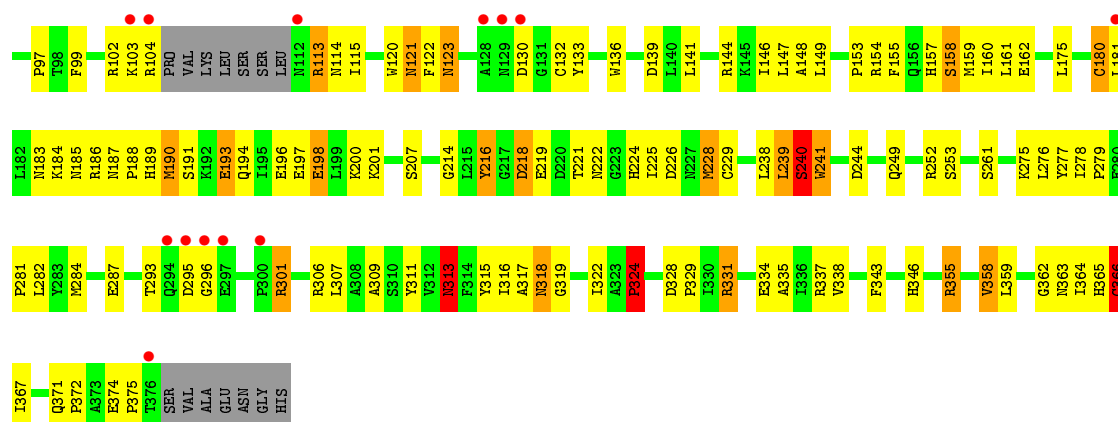


- Molecule 1: Agmatine deiminase

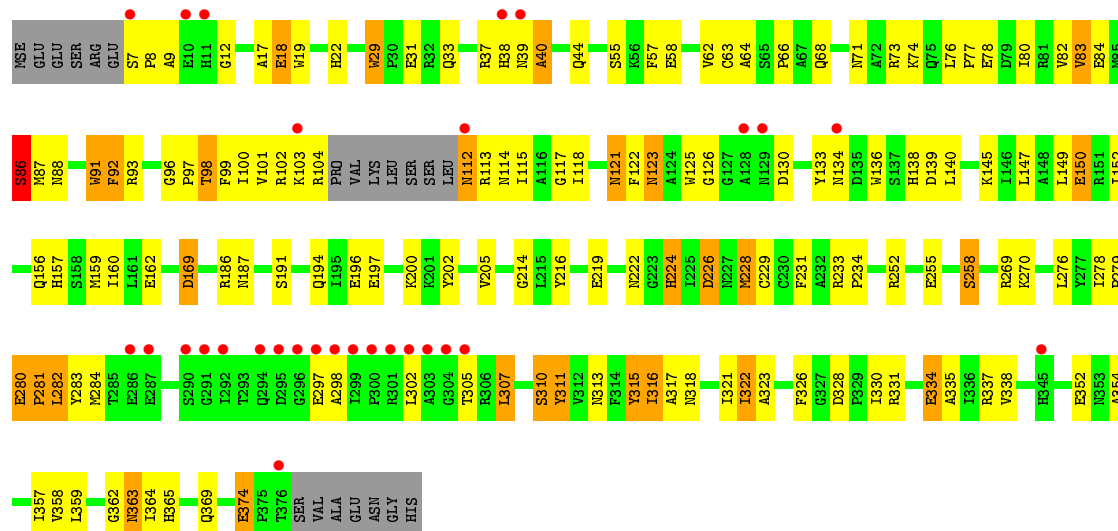


- Molecule 1: Agmatine deiminase

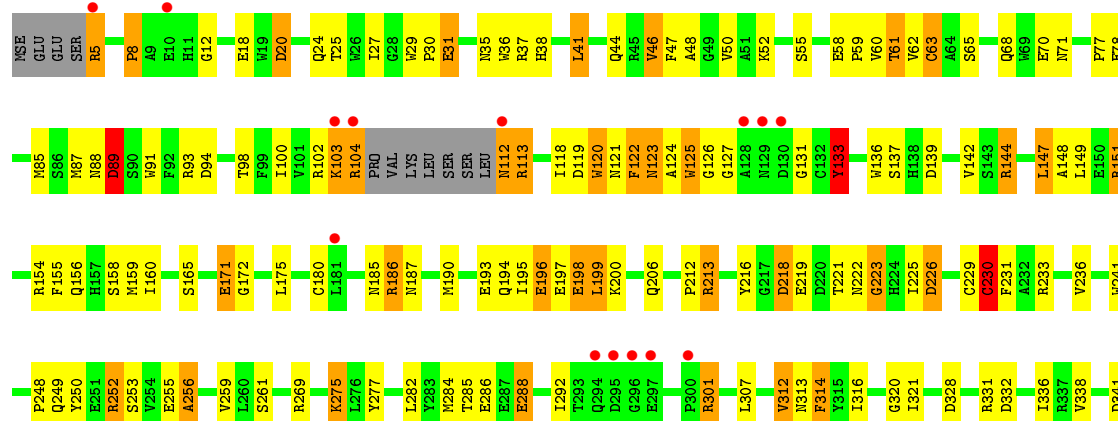


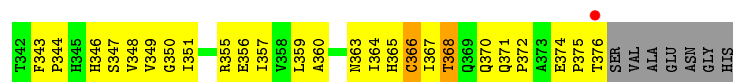


• Molecule 1: Agmatine deiminase

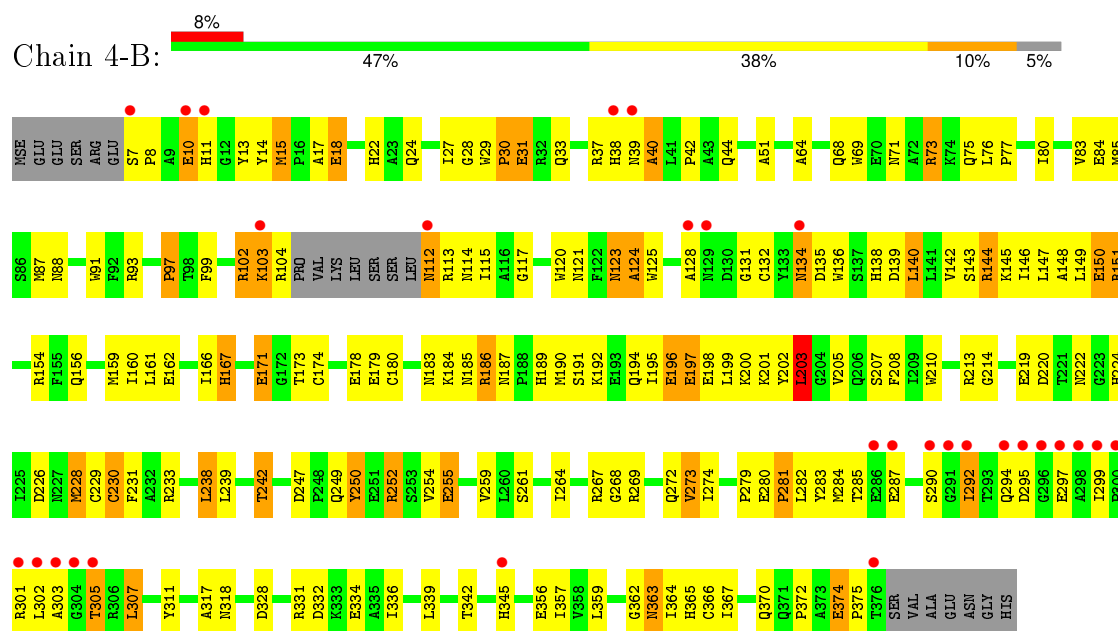


• Molecule 1: Agmatine deiminase

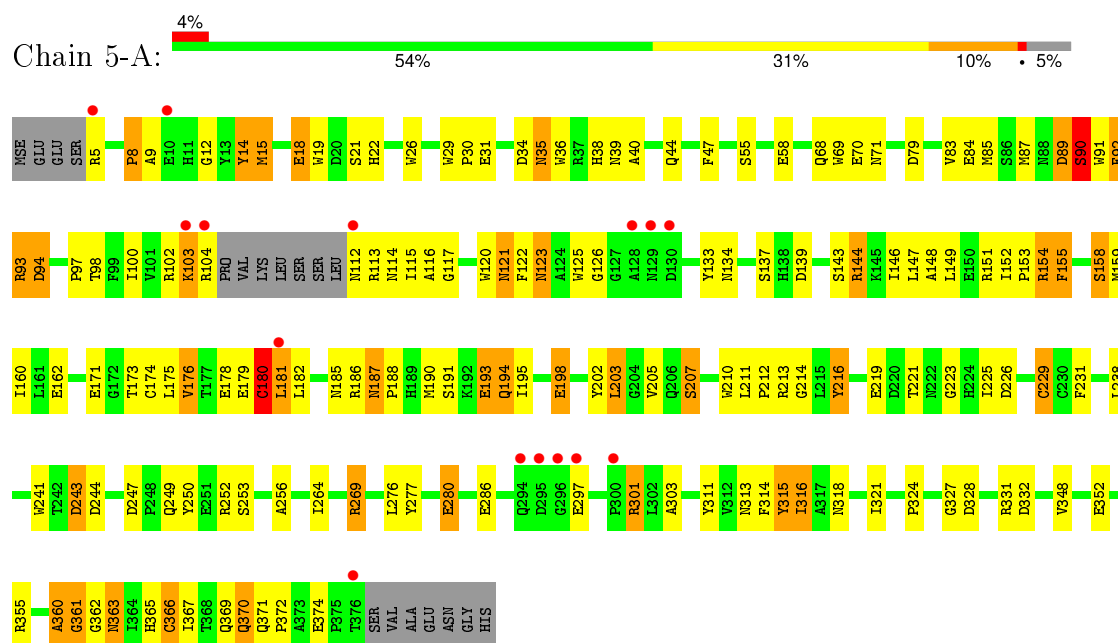




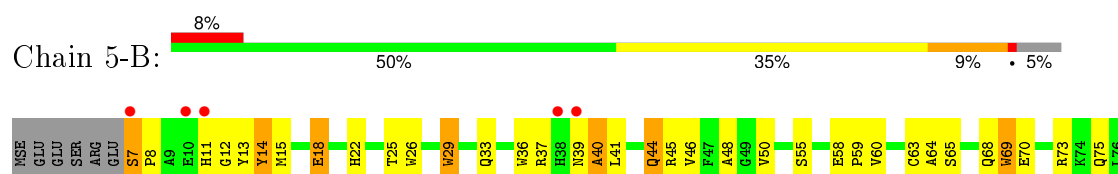
• Molecule 1: Agmatine deiminase

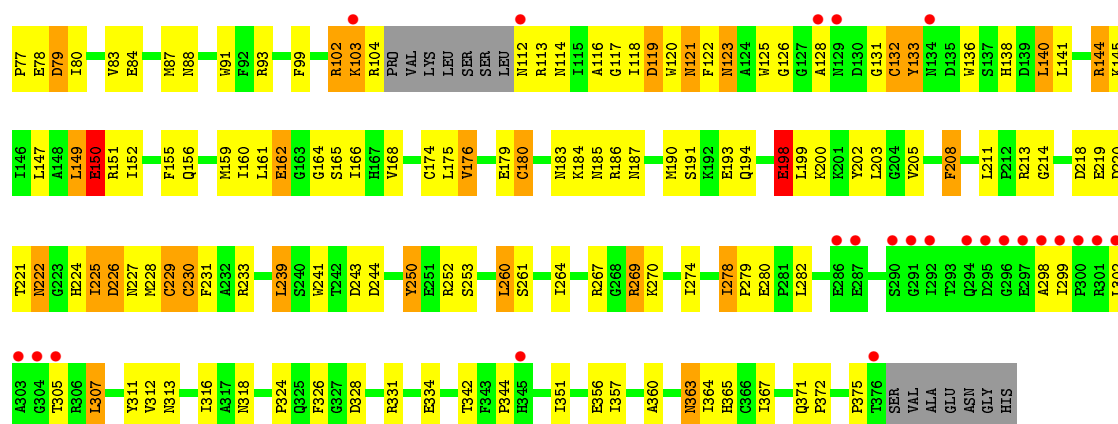


• Molecule 1: Agmatine deiminase

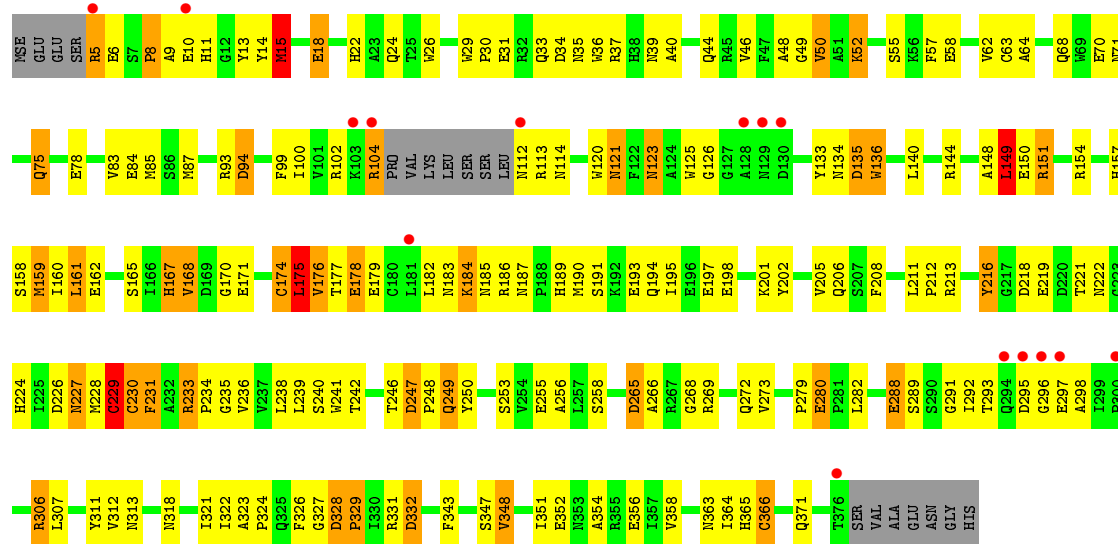


• Molecule 1: Agmatine deiminase

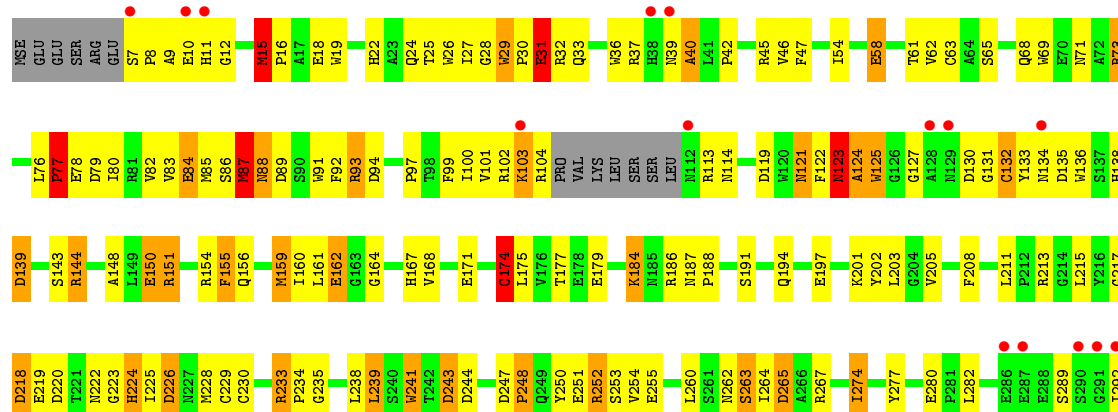
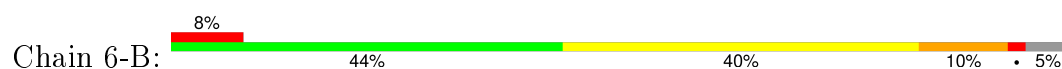


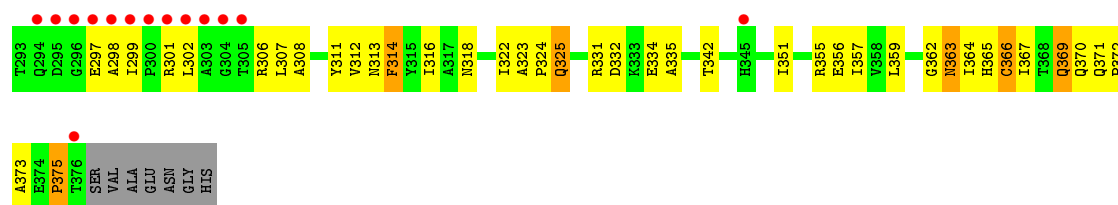


• Molecule 1: Agmatine deiminase

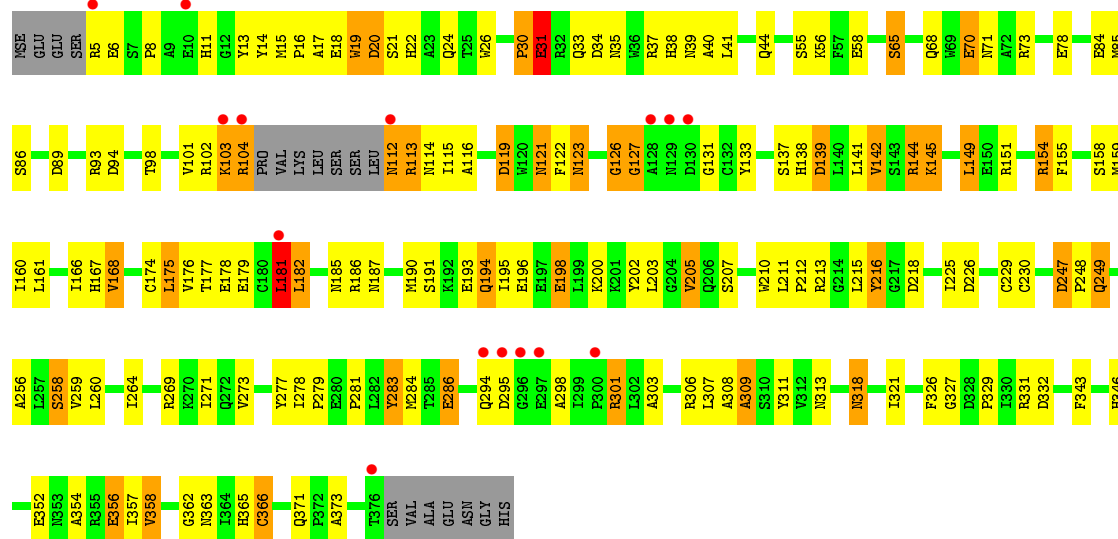


• Molecule 1: Agmatine deiminase

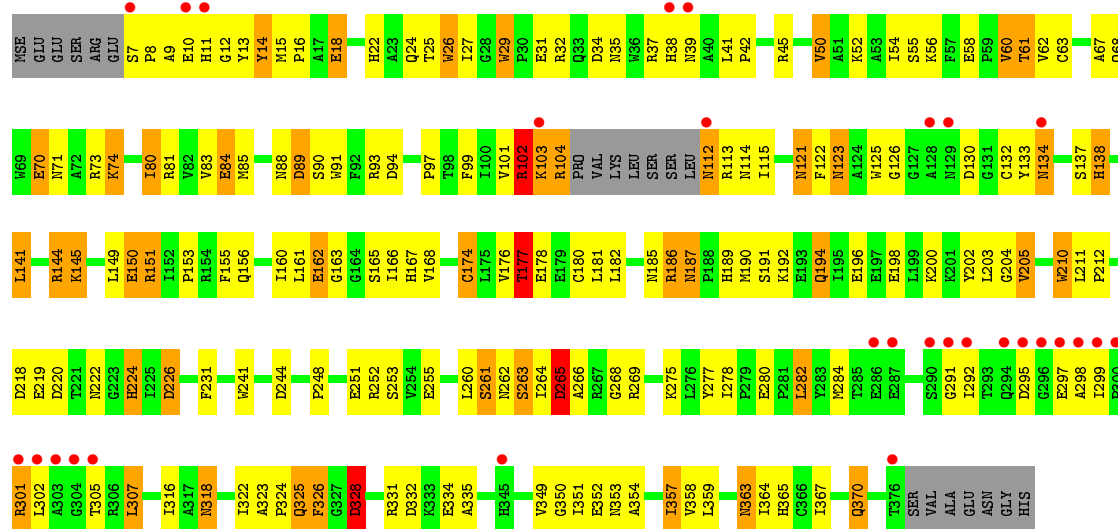




- Molecule 1: Agmatine deiminase

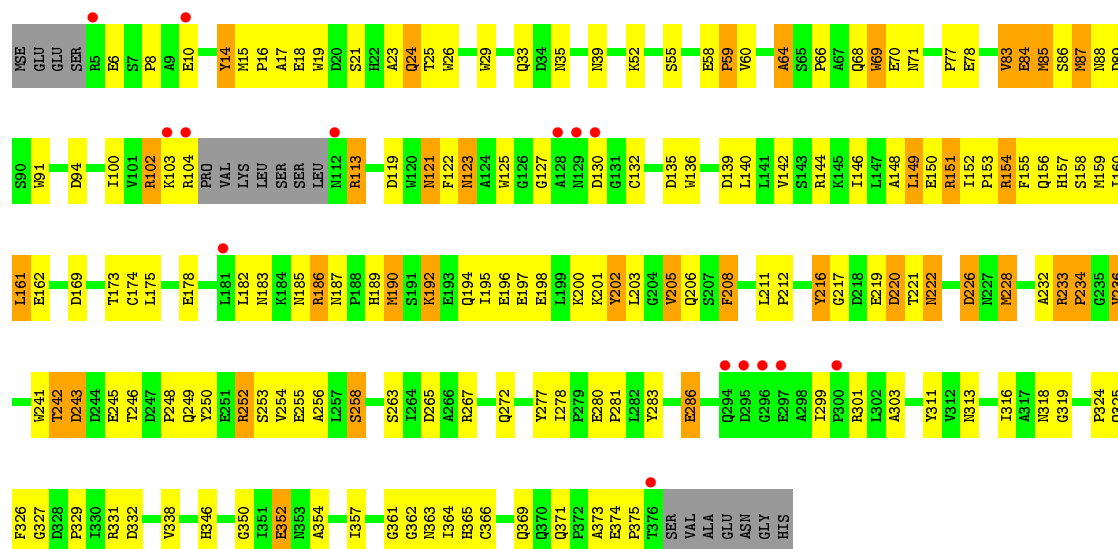


- Molecule 1: Agmatine deiminase

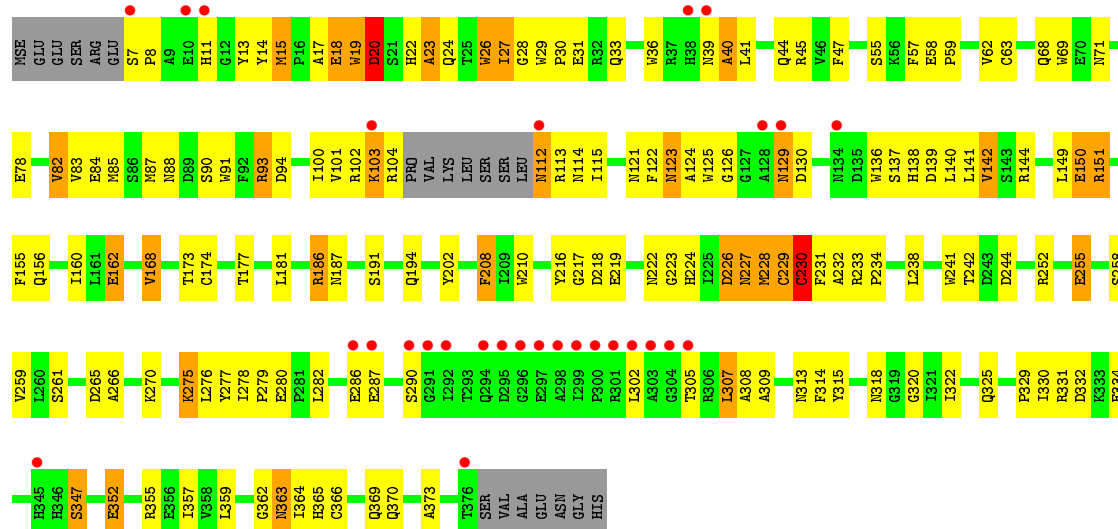


- Molecule 1: Agmatine deiminase





• Molecule 1: Agmatine deiminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.02Å 115.81Å 66.63Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	19.87 – 1.53 19.87 – 1.53	Depositor EDS
% Data completeness (in resolution range)	91.8 (19.87-1.53) 91.9 (19.87-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 1.53Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.135 , 0.171 0.147 , 0.180	Depositor DCC
R_{free} test set	6038 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 119958 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53040	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPO, MG, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1-A	1.58	20/2968 (0.7%)	1.40	28/4021 (0.7%)
1	1-B	1.52	15/2948 (0.5%)	1.32	19/3995 (0.5%)
1	2-A	1.59	28/2968 (0.9%)	1.36	21/4021 (0.5%)
1	2-B	1.57	19/2948 (0.6%)	1.31	13/3995 (0.3%)
1	3-A	1.52	18/2968 (0.6%)	1.39	28/4021 (0.7%)
1	3-B	1.49	20/2948 (0.7%)	1.27	12/3995 (0.3%)
1	4-A	1.61	28/2968 (0.9%)	1.43	27/4021 (0.7%)
1	4-B	1.59	37/2948 (1.3%)	1.36	20/3995 (0.5%)
1	5-A	1.71	39/2968 (1.3%)	1.48	28/4021 (0.7%)
1	5-B	1.69	22/2948 (0.7%)	1.45	28/3995 (0.7%)
1	6-A	1.78	47/2968 (1.6%)	1.56	28/4021 (0.7%)
1	6-B	1.71	40/2948 (1.4%)	1.48	29/3995 (0.7%)
1	7-A	1.71	35/2968 (1.2%)	1.50	34/4021 (0.8%)
1	7-B	1.71	43/2948 (1.5%)	1.45	20/3995 (0.5%)
1	8-A	1.74	45/2968 (1.5%)	1.51	31/4021 (0.8%)
1	8-B	1.69	39/2948 (1.3%)	1.35	9/3995 (0.2%)
All	All	1.64	495/47328 (1.0%)	1.42	375/64128 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	1-B	0	2
1	2-A	0	1
1	3-B	0	1
1	4-A	0	2
1	5-A	0	2
1	5-B	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	6-B	0	1
1	7-A	0	2
1	7-B	0	2
1	8-A	0	2
1	8-B	0	1
All	All	0	19

All (495) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	230	CYS	CB-SG	-18.60	1.50	1.82
1	8-B	230	CYS	CB-SG	18.04	2.12	1.82
1	5-B	174	CYS	CB-SG	-17.96	1.51	1.82
1	4-B	230	CYS	CB-SG	-17.44	1.52	1.82
1	2-B	230	CYS	CB-SG	15.05	2.07	1.82
1	1-B	230	CYS	CB-SG	-13.85	1.58	1.82
1	5-A	180	CYS	CB-SG	-12.98	1.60	1.82
1	6-A	15	MSE	CG-SE	-12.50	1.52	1.95
1	5-B	63	CYS	CB-SG	11.06	2.01	1.82
1	8-B	229	CYS	CB-SG	-10.88	1.63	1.82
1	2-A	216	TYR	CD2-CE2	10.78	1.55	1.39
1	4-B	202	TYR	CD1-CE1	-10.60	1.23	1.39
1	1-B	198	GLU	CB-CG	10.53	1.72	1.52
1	5-B	14	TYR	CE2-CZ	10.51	1.52	1.38
1	3-B	86	SER	CB-OG	-10.50	1.28	1.42
1	2-A	311	TYR	CD2-CE2	-10.46	1.23	1.39
1	7-A	230	CYS	CB-SG	-10.38	1.64	1.82
1	4-A	63	CYS	CB-SG	10.14	1.99	1.82
1	8-B	277	TYR	CD2-CE2	10.09	1.54	1.39
1	4-A	60	VAL	CB-CG1	9.95	1.73	1.52
1	5-B	29	TRP	CE3-CZ3	9.72	1.54	1.38
1	5-B	229	CYS	CB-SG	-9.72	1.65	1.82
1	8-A	83	VAL	CB-CG2	9.72	1.73	1.52
1	7-A	205	VAL	CB-CG1	9.68	1.73	1.52
1	7-B	277	TYR	CD2-CE2	9.68	1.53	1.39
1	7-A	198	GLU	CB-CG	9.61	1.70	1.52
1	8-A	60	VAL	CB-CG2	8.99	1.71	1.52
1	7-B	9	ALA	CA-CB	8.99	1.71	1.52
1	7-A	198	GLU	CD-OE2	8.98	1.35	1.25
1	8-B	142	VAL	CB-CG2	8.89	1.71	1.52
1	5-B	14	TYR	CD2-CE2	8.73	1.52	1.39
1	6-A	175	LEU	CG-CD2	-8.71	1.19	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	29	TRP	CE3-CZ3	8.66	1.53	1.38
1	1-B	29	TRP	CE3-CZ3	8.65	1.53	1.38
1	5-A	229	CYS	CB-SG	-8.64	1.67	1.82
1	5-A	315	TYR	CD2-CE2	8.63	1.52	1.39
1	4-A	62	VAL	CB-CG2	8.62	1.71	1.52
1	8-A	154	ARG	CG-CD	8.58	1.73	1.51
1	6-B	150	GLU	CD-OE1	-8.51	1.16	1.25
1	3-A	366	CYS	CA-CB	8.42	1.72	1.53
1	8-B	230	CYS	CA-CB	8.39	1.72	1.53
1	6-A	174	CYS	CB-SG	-8.32	1.68	1.82
1	2-B	180	CYS	CB-SG	-8.23	1.68	1.82
1	2-A	148	ALA	CA-CB	8.21	1.69	1.52
1	6-A	193	GLU	CG-CD	8.16	1.64	1.51
1	2-B	82	VAL	CA-CB	8.13	1.71	1.54
1	2-B	40	ALA	CA-CB	8.11	1.69	1.52
1	7-A	168	VAL	CB-CG2	8.05	1.69	1.52
1	8-B	23	ALA	CA-CB	8.04	1.69	1.52
1	6-A	150	GLU	CB-CG	-8.03	1.36	1.52
1	7-B	29	TRP	CE3-CZ3	8.03	1.52	1.38
1	6-A	168	VAL	CB-CG2	8.02	1.69	1.52
1	6-B	314	PHE	CE1-CZ	7.97	1.52	1.37
1	6-B	197	GLU	CG-CD	7.89	1.63	1.51
1	8-A	198	GLU	CD-OE2	7.85	1.34	1.25
1	4-A	286	GLU	CG-CD	7.77	1.63	1.51
1	6-B	314	PHE	CD1-CE1	7.70	1.54	1.39
1	2-B	338	VAL	CB-CG2	7.70	1.69	1.52
1	4-B	40	ALA	CA-CB	7.67	1.68	1.52
1	6-A	148	ALA	CA-CB	7.66	1.68	1.52
1	8-B	40	ALA	CA-CB	7.63	1.68	1.52
1	3-B	40	ALA	CA-CB	7.61	1.68	1.52
1	6-A	280	GLU	CG-CD	7.59	1.63	1.51
1	1-B	150	GLU	CB-CG	7.57	1.66	1.52
1	6-B	93	ARG	CG-CD	7.56	1.70	1.51
1	7-A	358	VAL	CB-CG2	-7.56	1.36	1.52
1	7-B	70	GLU	CG-CD	7.55	1.63	1.51
1	5-A	360	ALA	CA-CB	7.53	1.68	1.52
1	8-B	78	GLU	CD-OE2	7.51	1.33	1.25
1	8-A	135	ASP	CB-CG	-7.46	1.36	1.51
1	6-B	277	TYR	CD2-CE2	7.45	1.50	1.39
1	8-B	314	PHE	CG-CD2	7.44	1.50	1.38
1	8-A	85	MSE	CG-SE	-7.41	1.70	1.95
1	2-A	44	GLN	CG-CD	7.41	1.68	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	221	THR	CB-CG2	-7.40	1.27	1.52
1	4-B	198	GLU	CB-CG	7.34	1.66	1.52
1	6-A	231	PHE	CE2-CZ	7.34	1.51	1.37
1	3-B	78	GLU	CD-OE1	-7.33	1.17	1.25
1	5-A	14	TYR	CZ-OH	7.33	1.50	1.37
1	2-A	180	CYS	CB-SG	-7.28	1.69	1.82
1	2-B	188	PRO	CG-CD	7.27	1.74	1.50
1	7-B	137	SER	CA-CB	7.26	1.63	1.52
1	3-B	335	ALA	N-CA	7.23	1.60	1.46
1	6-B	144	ARG	CZ-NH2	7.23	1.42	1.33
1	3-A	315	TYR	CD1-CE1	7.21	1.50	1.39
1	8-A	148	ALA	CA-CB	7.21	1.67	1.52
1	5-A	280	GLU	CG-CD	7.19	1.62	1.51
1	5-A	93	ARG	CG-CD	7.17	1.69	1.51
1	2-A	310	SER	CB-OG	-7.17	1.32	1.42
1	2-A	168	VAL	CB-CG1	7.16	1.67	1.52
1	4-A	230	CYS	CB-SG	-7.16	1.70	1.82
1	5-B	252	ARG	CZ-NH1	7.14	1.42	1.33
1	7-B	50	VAL	CB-CG1	7.12	1.67	1.52
1	7-B	73	ARG	C-O	-7.08	1.09	1.23
1	8-A	59	PRO	CB-CG	7.07	1.85	1.50
1	5-A	92	PHE	CG-CD1	7.07	1.49	1.38
1	5-B	150	GLU	CG-CD	7.07	1.62	1.51
1	6-B	218	ASP	CB-CG	7.07	1.66	1.51
1	2-B	78	GLU	CD-OE1	7.07	1.33	1.25
1	6-B	334	GLU	CG-CD	7.06	1.62	1.51
1	4-A	256	ALA	CA-CB	7.03	1.67	1.52
1	6-B	29	TRP	CE3-CZ3	7.03	1.50	1.38
1	8-B	275	LYS	CE-NZ	7.02	1.66	1.49
1	5-A	198	GLU	CD-OE2	7.02	1.33	1.25
1	8-B	150	GLU	CB-CG	-7.00	1.38	1.52
1	7-B	145	LYS	CB-CG	7.00	1.71	1.52
1	5-B	261	SER	CB-OG	6.99	1.51	1.42
1	6-A	136	TRP	CE3-CZ3	6.97	1.50	1.38
1	8-B	20	ASP	CB-CG	-6.97	1.37	1.51
1	7-B	334	GLU	CG-CD	6.96	1.62	1.51
1	8-A	280	GLU	CG-CD	6.96	1.62	1.51
1	7-A	356	GLU	CD-OE1	6.95	1.33	1.25
1	7-B	14	TYR	CD2-CE2	6.92	1.49	1.39
1	7-B	62	VAL	CA-CB	6.90	1.69	1.54
1	3-B	280	GLU	CG-CD	6.88	1.62	1.51
1	4-B	231	PHE	CD2-CE2	6.86	1.52	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	142	VAL	CB-CG2	6.86	1.67	1.52
1	6-A	75	GLN	CD-OE1	6.85	1.39	1.24
1	7-A	354	ALA	CA-CB	6.84	1.66	1.52
1	7-A	258	SER	CB-OG	6.79	1.51	1.42
1	3-B	29	TRP	CE3-CZ3	6.78	1.50	1.38
1	6-A	14	TYR	CZ-OH	6.78	1.49	1.37
1	1-B	280	GLU	CG-CD	6.78	1.62	1.51
1	4-A	366	CYS	CB-SG	-6.77	1.70	1.82
1	8-A	352	GLU	CG-CD	6.76	1.62	1.51
1	2-A	83	VAL	CB-CG2	6.75	1.67	1.52
1	2-B	230	CYS	CA-CB	6.74	1.68	1.53
1	8-A	190	MSE	CG-SE	6.74	2.18	1.95
1	8-A	205	VAL	CB-CG1	6.73	1.67	1.52
1	8-A	70	GLU	CG-CD	6.72	1.62	1.51
1	7-A	286	GLU	CG-CD	6.72	1.62	1.51
1	2-B	277	TYR	CD2-CE2	6.70	1.49	1.39
1	5-B	198	GLU	CD-OE1	6.69	1.33	1.25
1	8-A	21	SER	CA-CB	6.68	1.62	1.52
1	8-A	69	TRP	CB-CG	6.66	1.62	1.50
1	1-B	40	ALA	CA-CB	6.65	1.66	1.52
1	4-B	255	GLU	CD-OE1	6.62	1.32	1.25
1	8-B	266	ALA	CA-CB	6.62	1.66	1.52
1	5-A	92	PHE	CE1-CZ	6.62	1.50	1.37
1	6-B	31	GLU	CB-CG	-6.61	1.39	1.52
1	4-A	288	GLU	CG-CD	6.59	1.61	1.51
1	2-A	315	TYR	CE1-CZ	6.58	1.47	1.38
1	8-A	254	VAL	CB-CG1	6.58	1.66	1.52
1	4-B	17	ALA	CA-CB	6.58	1.66	1.52
1	7-B	210	TRP	C-O	6.57	1.35	1.23
1	6-A	231	PHE	CD1-CE1	6.56	1.52	1.39
1	3-B	92	PHE	C-O	6.55	1.35	1.23
1	7-B	18	GLU	CD-OE2	6.54	1.32	1.25
1	5-A	216	TYR	CD2-CE2	6.52	1.49	1.39
1	6-A	311	TYR	CE1-CZ	6.52	1.47	1.38
1	7-B	150	GLU	CB-CG	6.52	1.64	1.52
1	6-B	280	GLU	CG-CD	6.49	1.61	1.51
1	8-B	82	VAL	CB-CG1	6.49	1.66	1.52
1	3-A	70	GLU	CG-CD	6.48	1.61	1.51
1	7-B	323	ALA	CA-CB	6.48	1.66	1.52
1	7-B	252	ARG	CZ-NH1	6.47	1.41	1.33
1	8-A	354	ALA	CA-CB	6.41	1.66	1.52
1	4-B	150	GLU	CD-OE1	-6.41	1.18	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-B	142	VAL	CB-CG1	6.41	1.66	1.52
1	3-A	18	GLU	CD-OE1	6.40	1.32	1.25
1	7-B	176	VAL	CB-CG2	6.39	1.66	1.52
1	3-B	18	GLU	CD-OE2	6.38	1.32	1.25
1	5-A	361	GLY	C-O	6.36	1.33	1.23
1	2-A	258	SER	CB-OG	6.35	1.50	1.42
1	5-A	171	GLU	CG-CD	6.34	1.61	1.51
1	8-A	252	ARG	CZ-NH2	6.34	1.41	1.33
1	6-A	75	GLN	CG-CD	6.33	1.65	1.51
1	6-A	258	SER	CB-OG	6.33	1.50	1.42
1	7-A	216	TYR	CE2-CZ	6.33	1.46	1.38
1	5-A	70	GLU	CG-CD	6.31	1.61	1.51
1	6-A	70	GLU	CG-CD	6.30	1.61	1.51
1	4-A	48	ALA	CA-CB	6.30	1.65	1.52
1	4-B	374	GLU	CD-OE2	6.27	1.32	1.25
1	4-B	144	ARG	CZ-NH1	6.26	1.41	1.33
1	6-A	329	PRO	CG-CD	6.26	1.71	1.50
1	5-A	148	ALA	CA-CB	6.25	1.65	1.52
1	7-B	323	ALA	C-O	6.24	1.35	1.23
1	7-A	113	ARG	CB-CG	6.23	1.69	1.52
1	5-A	120	TRP	CG-CD1	6.22	1.45	1.36
1	4-B	97	PRO	CB-CG	6.21	1.81	1.50
1	8-B	29	TRP	CE3-CZ3	6.21	1.49	1.38
1	5-A	176	VAL	CA-CB	6.21	1.67	1.54
1	2-B	51	ALA	CA-CB	6.20	1.65	1.52
1	7-A	19	TRP	CB-CG	6.20	1.61	1.50
1	8-A	208	PHE	CG-CD2	6.19	1.48	1.38
1	6-A	75	GLN	CB-CG	6.18	1.69	1.52
1	2-A	69	TRP	CB-CG	6.18	1.61	1.50
1	1-A	366	CYS	CB-SG	6.17	1.92	1.82
1	8-B	210	TRP	C-O	6.15	1.35	1.23
1	7-A	366	CYS	CB-SG	6.15	1.92	1.82
1	8-A	253	SER	CB-OG	6.15	1.50	1.42
1	3-B	86	SER	CA-CB	6.14	1.62	1.52
1	8-B	162	GLU	CB-CG	6.12	1.63	1.52
1	7-A	144	ARG	CG-CD	-6.11	1.36	1.51
1	1-B	261	SER	CB-OG	6.10	1.50	1.42
1	2-A	286	GLU	CG-CD	6.10	1.61	1.51
1	5-B	176	VAL	CA-CB	6.10	1.67	1.54
1	7-A	116	ALA	CA-CB	6.10	1.65	1.52
1	2-B	7	SER	CA-CB	6.09	1.62	1.52
1	8-A	286	GLU	CG-CD	6.09	1.61	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	69	TRP	CG-CD1	6.09	1.45	1.36
1	6-A	159	MSE	CG-SE	6.09	2.16	1.95
1	4-B	29	TRP	CE3-CZ3	6.08	1.48	1.38
1	4-B	186	ARG	CB-CG	6.07	1.69	1.52
1	8-B	82	VAL	CA-CB	6.06	1.67	1.54
1	1-A	273	VAL	CB-CG1	6.05	1.65	1.52
1	4-B	200	LYS	CD-CE	-6.05	1.36	1.51
1	4-B	18	GLU	CD-OE2	6.04	1.32	1.25
1	7-B	177	THR	CA-CB	6.03	1.69	1.53
1	4-A	198	GLU	CD-OE2	6.03	1.32	1.25
1	6-B	150	GLU	CG-CD	-6.03	1.43	1.51
1	5-A	314	PHE	CG-CD2	6.02	1.47	1.38
1	6-A	178	GLU	CG-CD	6.00	1.60	1.51
1	8-A	14	TYR	CB-CG	6.00	1.60	1.51
1	4-B	196	GLU	CB-CG	5.99	1.63	1.52
1	8-A	216	TYR	CB-CG	5.99	1.60	1.51
1	6-A	83	VAL	CB-CG2	-5.99	1.40	1.52
1	7-A	210	TRP	CG-CD1	5.99	1.45	1.36
1	4-B	255	GLU	CG-CD	5.99	1.60	1.51
1	4-A	252	ARG	CZ-NH2	5.98	1.40	1.33
1	4-B	142	VAL	CB-CG1	5.97	1.65	1.52
1	6-B	184	LYS	CG-CD	5.97	1.72	1.52
1	6-B	335	ALA	N-CA	5.96	1.58	1.46
1	6-B	323	ALA	CA-CB	5.95	1.65	1.52
1	6-B	125	TRP	CB-CG	5.95	1.60	1.50
1	4-A	171	GLU	CD-OE2	5.94	1.32	1.25
1	1-A	23	ALA	CA-CB	5.93	1.65	1.52
1	6-B	40	ALA	CA-CB	5.93	1.65	1.52
1	3-A	158	SER	CB-OG	-5.92	1.34	1.42
1	6-B	197	GLU	CB-CG	5.92	1.63	1.52
1	5-B	334	GLU	CG-CD	5.92	1.60	1.51
1	7-B	265	ASP	CB-CG	5.92	1.64	1.51
1	6-A	348	VAL	C-O	5.91	1.34	1.23
1	1-A	91	TRP	CE3-CZ3	5.90	1.48	1.38
1	5-A	18	GLU	CD-OE1	5.89	1.32	1.25
1	1-A	207	SER	CB-OG	-5.89	1.34	1.42
1	5-B	162	GLU	CD-OE2	5.88	1.32	1.25
1	5-A	231	PHE	CE1-CZ	5.87	1.48	1.37
1	7-A	86	SER	CA-CB	5.87	1.61	1.52
1	4-B	150	GLU	CD-OE2	5.86	1.32	1.25
1	6-A	171	GLU	CG-CD	5.86	1.60	1.51
1	2-A	168	VAL	CB-CG2	5.86	1.65	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	81	ARG	CZ-NH2	5.85	1.40	1.33
1	4-A	338	VAL	CB-CG1	5.85	1.65	1.52
1	7-A	205	VAL	CB-CG2	5.84	1.65	1.52
1	7-A	14	TYR	CZ-OH	5.83	1.47	1.37
1	3-B	98	THR	CB-CG2	5.81	1.71	1.52
1	7-B	335	ALA	N-CA	5.81	1.57	1.46
1	7-B	52	LYS	CE-NZ	5.81	1.63	1.49
1	2-B	7	SER	CB-OG	5.80	1.49	1.42
1	8-B	208	PHE	CE2-CZ	5.80	1.48	1.37
1	1-B	317	ALA	CA-CB	5.80	1.64	1.52
1	5-A	231	PHE	CG-CD2	5.80	1.47	1.38
1	6-B	78	GLU	CG-CD	5.79	1.60	1.51
1	5-A	171	GLU	CD-OE1	5.79	1.32	1.25
1	8-B	168	VAL	CA-CB	5.78	1.66	1.54
1	6-B	132	CYS	CB-SG	5.77	1.92	1.82
1	8-B	347	SER	CA-CB	5.77	1.61	1.52
1	2-B	18	GLU	CD-OE2	5.77	1.31	1.25
1	1-A	334	GLU	CB-CG	5.76	1.63	1.52
1	6-B	84	GLU	CG-CD	5.76	1.60	1.51
1	3-A	301	ARG	CB-CG	5.76	1.68	1.52
1	6-B	162	GLU	CD-OE1	5.75	1.31	1.25
1	7-A	373	ALA	CA-CB	5.75	1.64	1.52
1	7-B	349	VAL	CB-CG1	5.75	1.65	1.52
1	6-A	62	VAL	CB-CG2	5.74	1.65	1.52
1	6-B	162	GLU	CD-OE2	5.74	1.31	1.25
1	3-A	162	GLU	CB-CG	5.73	1.63	1.52
1	3-A	190	MSE	CG-SE	5.73	2.15	1.95
1	7-B	263	SER	CB-OG	5.73	1.49	1.42
1	8-A	350	GLY	C-O	5.73	1.32	1.23
1	8-B	18	GLU	CB-CG	5.73	1.63	1.52
1	7-B	205	VAL	CB-CG1	5.73	1.64	1.52
1	2-B	369	GLN	CD-OE1	5.71	1.36	1.24
1	8-B	347	SER	CB-OG	-5.71	1.34	1.42
1	5-A	194	GLN	CB-CG	5.71	1.68	1.52
1	8-A	151	ARG	CZ-NH1	5.70	1.40	1.33
1	4-A	148	ALA	CA-CB	5.70	1.64	1.52
1	5-A	133	TYR	CE1-CZ	5.69	1.46	1.38
1	3-B	270	LYS	CE-NZ	5.69	1.63	1.49
1	8-B	18	GLU	CD-OE1	5.68	1.31	1.25
1	4-A	151	ARG	N-CA	5.67	1.57	1.46
1	3-A	216	TYR	CD1-CE1	5.67	1.47	1.39
1	5-B	208	PHE	CE1-CZ	5.67	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	84	GLU	CG-CD	5.67	1.60	1.51
1	5-B	150	GLU	CB-CG	5.67	1.62	1.52
1	5-B	214	GLY	N-CA	5.66	1.54	1.46
1	7-B	194	GLN	CD-OE1	5.66	1.36	1.24
1	4-A	312	VAL	CB-CG1	5.65	1.64	1.52
1	4-B	220	ASP	CB-CG	5.65	1.63	1.51
1	8-A	144	ARG	CG-CD	5.63	1.66	1.51
1	5-B	18	GLU	CD-OE2	5.63	1.31	1.25
1	7-B	266	ALA	CA-CB	5.62	1.64	1.52
1	8-B	258	SER	CB-OG	-5.62	1.34	1.42
1	4-B	51	ALA	CA-CB	5.62	1.64	1.52
1	7-A	31	GLU	CD-OE1	5.62	1.31	1.25
1	2-B	150	GLU	CG-CD	-5.61	1.43	1.51
1	7-A	139	ASP	CB-CG	5.61	1.63	1.51
1	1-A	48	ALA	CA-CB	5.61	1.64	1.52
1	6-B	274	ILE	C-O	5.61	1.34	1.23
1	8-B	231	PHE	CE1-CZ	5.61	1.48	1.37
1	6-B	58	GLU	CB-CG	5.60	1.62	1.52
1	6-B	88	ASN	C-O	5.60	1.33	1.23
1	8-A	258	SER	CB-OG	-5.59	1.34	1.42
1	7-A	142	VAL	CB-CG1	5.59	1.64	1.52
1	8-B	162	GLU	CD-OE2	5.58	1.31	1.25
1	5-A	158	SER	CA-CB	5.58	1.61	1.52
1	8-B	155	PHE	CD2-CE2	-5.58	1.28	1.39
1	3-B	91	TRP	CE3-CZ3	5.57	1.48	1.38
1	8-B	26	TRP	CE3-CZ3	5.55	1.47	1.38
1	1-B	175	LEU	CG-CD2	5.55	1.72	1.51
1	4-B	14	TYR	CD2-CE2	5.54	1.47	1.39
1	6-A	216	TYR	CD2-CE2	5.54	1.47	1.39
1	7-A	309	ALA	CA-CB	5.54	1.64	1.52
1	4-B	197	GLU	CG-CD	-5.53	1.43	1.51
1	8-B	334	GLU	CG-CD	5.53	1.60	1.51
1	1-A	343	PHE	CD2-CE2	5.51	1.50	1.39
1	5-B	231	PHE	CE1-CZ	5.51	1.47	1.37
1	7-B	162	GLU	CB-CG	5.51	1.62	1.52
1	5-A	69	TRP	CB-CG	5.51	1.60	1.50
1	5-A	14	TYR	CE2-CZ	5.50	1.45	1.38
1	5-B	69	TRP	CB-CG	-5.50	1.40	1.50
1	4-B	339	LEU	CG-CD2	5.50	1.72	1.51
1	7-A	259	VAL	CB-CG2	5.50	1.64	1.52
1	7-B	198	GLU	CD-OE1	5.49	1.31	1.25
1	2-A	145	LYS	CE-NZ	5.48	1.62	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-B	255	GLU	CG-CD	5.48	1.60	1.51
1	6-B	155	PHE	CD2-CE2	-5.47	1.28	1.39
1	6-B	151	ARG	CD-NE	5.47	1.55	1.46
1	6-A	125	TRP	CB-CG	5.46	1.60	1.50
1	4-A	196	GLU	CD-OE1	5.46	1.31	1.25
1	6-A	31	GLU	CG-CD	5.46	1.60	1.51
1	2-A	205	VAL	CB-CG1	5.45	1.64	1.52
1	3-A	158	SER	CA-CB	5.45	1.61	1.52
1	3-B	231	PHE	CE1-CZ	5.45	1.47	1.37
1	7-A	194	GLN	CB-CG	5.45	1.67	1.52
1	6-B	159	MSE	CG-SE	5.44	2.13	1.95
1	8-B	227	ASN	C-O	5.44	1.33	1.23
1	6-A	233	ARG	CZ-NH1	5.44	1.40	1.33
1	7-B	231	PHE	CE1-CZ	5.44	1.47	1.37
1	8-B	255	GLU	CD-OE1	5.43	1.31	1.25
1	2-A	40	ALA	CA-CB	5.43	1.63	1.52
1	3-A	148	ALA	CA-CB	5.42	1.63	1.52
1	4-B	238	LEU	CG-CD1	5.42	1.72	1.51
1	1-A	194	GLN	CB-CG	5.42	1.67	1.52
1	5-A	83	VAL	CB-CG2	-5.42	1.41	1.52
1	2-A	171	GLU	C-O	5.42	1.33	1.23
1	6-B	124	ALA	CA-CB	5.41	1.63	1.52
1	8-A	242	THR	C-O	-5.40	1.13	1.23
1	8-A	55	SER	CB-OG	5.40	1.49	1.42
1	6-A	36	TRP	CG-CD1	5.40	1.44	1.36
1	4-B	334	GLU	CG-CD	5.39	1.60	1.51
1	5-A	193	GLU	CG-CD	5.39	1.60	1.51
1	5-A	205	VAL	CB-CG1	5.39	1.64	1.52
1	6-B	208	PHE	CE2-CZ	5.39	1.47	1.37
1	3-B	374	GLU	CB-CG	5.39	1.62	1.52
1	5-B	40	ALA	CA-CB	5.39	1.63	1.52
1	1-B	124	ALA	CA-CB	5.38	1.63	1.52
1	6-A	18	GLU	CD-OE1	5.38	1.31	1.25
1	7-B	141	LEU	C-O	5.38	1.33	1.23
1	4-A	275	LYS	CE-NZ	5.38	1.62	1.49
1	5-B	270	LYS	CE-NZ	5.38	1.62	1.49
1	6-A	253	SER	CB-OG	5.36	1.49	1.42
1	8-A	216	TYR	CD2-CE2	5.36	1.47	1.39
1	5-A	187	ASN	CG-OD1	5.36	1.35	1.24
1	6-A	176	VAL	CB-CG2	5.36	1.64	1.52
1	7-B	26	TRP	CE3-CZ3	5.36	1.47	1.38
1	1-A	334	GLU	CD-OE1	5.35	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-B	275	LYS	CE-NZ	5.35	1.62	1.49
1	6-A	366	CYS	CB-SG	5.33	1.91	1.82
1	2-A	158	SER	CA-CB	5.33	1.60	1.52
1	7-B	187	ASN	CG-OD1	5.32	1.35	1.24
1	7-B	61	THR	CA-CB	5.32	1.67	1.53
1	5-A	256	ALA	CA-CB	5.32	1.63	1.52
1	2-B	332	ASP	C-O	5.32	1.33	1.23
1	1-A	231	PHE	CD2-CE2	5.31	1.49	1.39
1	4-B	31	GLU	CB-CG	-5.31	1.42	1.52
1	8-B	23	ALA	C-O	5.30	1.33	1.23
1	6-A	94	ASP	CB-CG	-5.30	1.40	1.51
1	1-A	91	TRP	CZ3-CH2	5.30	1.48	1.40
1	6-B	136	TRP	CE3-CZ3	5.29	1.47	1.38
1	1-A	14	TYR	CB-CG	5.28	1.59	1.51
1	6-A	205	VAL	CB-CG2	5.28	1.64	1.52
1	8-B	186	ARG	CD-NE	5.28	1.55	1.46
1	8-A	87	MSE	CG-SE	5.27	2.13	1.95
1	4-A	231	PHE	CE2-CZ	5.27	1.47	1.37
1	5-A	277	TYR	CD2-CE2	5.27	1.47	1.39
1	6-B	58	GLU	CD-OE1	5.27	1.31	1.25
1	3-A	84	GLU	CG-CD	5.26	1.59	1.51
1	3-A	198	GLU	CD-OE2	5.25	1.31	1.25
1	8-B	14	TYR	CD2-CE2	5.25	1.47	1.39
1	2-A	218	ASP	CB-CG	5.25	1.62	1.51
1	7-B	180	CYS	CB-SG	-5.24	1.73	1.81
1	2-A	288	GLU	CG-CD	5.24	1.59	1.51
1	3-B	83	VAL	CB-CG2	-5.24	1.41	1.52
1	6-B	241	TRP	CB-CG	5.24	1.59	1.50
1	8-A	200	LYS	CE-NZ	5.23	1.62	1.49
1	6-A	347	SER	CB-OG	5.22	1.49	1.42
1	8-A	155	PHE	CE1-CZ	5.22	1.47	1.37
1	8-A	311	TYR	CD2-CE2	5.22	1.47	1.39
1	3-B	101	VAL	CA-CB	5.21	1.65	1.54
1	4-B	178	GLU	CB-CG	-5.20	1.42	1.52
1	6-A	136	TRP	CB-CG	5.20	1.59	1.50
1	8-A	338	VAL	CB-CG1	5.20	1.63	1.52
1	6-B	369	GLN	CB-CG	5.20	1.66	1.52
1	3-A	240	SER	CB-OG	-5.19	1.35	1.42
1	8-A	234	PRO	CA-CB	5.19	1.64	1.53
1	2-A	311	TYR	CB-CG	-5.19	1.43	1.51
1	1-B	269	ARG	CG-CD	-5.19	1.39	1.51
1	3-A	324	PRO	CG-CD	5.19	1.67	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	84	GLU	CD-OE1	5.19	1.31	1.25
1	3-A	207	SER	CB-OG	-5.18	1.35	1.42
1	8-A	216	TYR	CG-CD1	5.18	1.45	1.39
1	1-B	84	GLU	CG-CD	5.18	1.59	1.51
1	8-B	352	GLU	CD-OE2	5.18	1.31	1.25
1	6-B	325	GLN	CD-OE1	5.17	1.35	1.24
1	6-A	186	ARG	CB-CG	5.17	1.66	1.52
1	7-A	155	PHE	CE1-CZ	5.17	1.47	1.37
1	6-B	241	TRP	CE3-CZ3	5.17	1.47	1.38
1	2-A	155	PHE	CE1-CZ	5.17	1.47	1.37
1	2-A	350	GLY	C-O	5.16	1.31	1.23
1	4-A	61	THR	C-O	5.16	1.33	1.23
1	1-B	14	TYR	CD2-CE2	5.16	1.47	1.39
1	5-A	370	GLN	CB-CG	5.16	1.66	1.52
1	4-A	231	PHE	CD2-CE2	5.16	1.49	1.39
1	5-A	366	CYS	CB-SG	-5.16	1.73	1.81
1	2-A	182	LEU	C-O	5.16	1.33	1.23
1	4-A	314	PHE	CE1-CZ	5.16	1.47	1.37
1	6-A	288	GLU	CB-CG	5.16	1.61	1.52
1	8-A	256	ALA	CA-CB	5.16	1.63	1.52
1	2-B	338	VAL	CA-CB	5.15	1.65	1.54
1	6-A	52	LYS	C-O	5.15	1.33	1.23
1	4-B	197	GLU	CD-OE2	5.15	1.31	1.25
1	8-A	154	ARG	CB-CG	5.15	1.66	1.52
1	4-A	193	GLU	CG-CD	5.15	1.59	1.51
1	7-B	84	GLU	CD-OE1	5.15	1.31	1.25
1	4-B	124	ALA	CA-CB	5.15	1.63	1.52
1	5-A	315	TYR	CE1-CZ	-5.14	1.31	1.38
1	1-A	198	GLU	CD-OE2	5.14	1.31	1.25
1	7-B	60	VAL	CB-CG2	5.14	1.63	1.52
1	8-A	242	THR	CB-CG2	-5.14	1.35	1.52
1	1-A	222	ASN	CB-CG	5.13	1.62	1.51
1	7-B	205	VAL	CB-CG2	5.13	1.63	1.52
1	8-A	222	ASN	CB-CG	5.13	1.62	1.51
1	4-A	125	TRP	CB-CG	5.13	1.59	1.50
1	6-A	256	ALA	CA-CB	5.13	1.63	1.52
1	4-B	366	CYS	CB-SG	5.13	1.91	1.82
1	6-A	165	SER	CB-OG	5.13	1.49	1.42
1	7-A	158	SER	CA-CB	5.13	1.60	1.52
1	8-B	232	ALA	CA-CB	5.12	1.63	1.52
1	2-B	369	GLN	CG-CD	5.12	1.62	1.51
1	6-A	205	VAL	CB-CG1	5.12	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-B	24	GLN	CG-CD	5.12	1.62	1.51
1	7-A	216	TYR	CD2-CE2	5.12	1.47	1.39
1	3-B	334	GLU	CD-OE1	5.11	1.31	1.25
1	4-B	311	TYR	CD2-CE2	5.11	1.47	1.39
1	2-B	150	GLU	CD-OE1	-5.11	1.20	1.25
1	1-A	348	VAL	C-O	5.10	1.33	1.23
1	5-A	151	ARG	N-CA	5.10	1.56	1.46
1	7-B	102	ARG	CG-CD	5.10	1.64	1.51
1	6-A	229	CYS	CA-CB	-5.09	1.42	1.53
1	2-A	42	PRO	CB-CG	5.09	1.75	1.50
1	7-A	144	ARG	CZ-NH1	-5.09	1.26	1.33
1	7-B	162	GLU	CD-OE2	5.09	1.31	1.25
1	4-A	338	VAL	CB-CG2	5.09	1.63	1.52
1	7-A	19	TRP	CG-CD1	5.09	1.43	1.36
1	1-A	251	GLU	CG-CD	5.08	1.59	1.51
1	5-B	198	GLU	CG-CD	5.08	1.59	1.51
1	7-A	311	TYR	CD2-CE2	5.08	1.47	1.39
1	8-A	236	VAL	CB-CG2	5.08	1.63	1.52
1	4-B	317	ALA	CA-CB	5.07	1.63	1.52
1	7-B	174	CYS	CB-SG	5.07	1.90	1.82
1	4-A	46	VAL	CB-CG2	5.07	1.63	1.52
1	1-A	287	GLU	CG-CD	5.07	1.59	1.51
1	3-A	241	TRP	CE3-CZ3	5.07	1.47	1.38
1	3-B	169	ASP	CB-CG	5.06	1.62	1.51
1	8-A	102	ARG	CG-CD	5.06	1.64	1.51
1	4-B	171	GLU	CD-OE2	-5.06	1.20	1.25
1	4-A	120	TRP	CG-CD1	5.05	1.43	1.36
1	8-B	78	GLU	CD-OE1	5.05	1.31	1.25
1	5-A	316	ILE	CA-CB	5.05	1.66	1.54
1	4-B	197	GLU	CB-CG	5.05	1.61	1.52
1	7-B	73	ARG	CZ-NH2	5.05	1.39	1.33
1	7-A	249	GLN	CA-CB	5.04	1.65	1.53
1	6-A	159	MSE	CB-CG	5.04	1.67	1.52
1	5-A	250	TYR	CZ-OH	5.03	1.46	1.37
1	3-B	316	ILE	CA-CB	5.03	1.66	1.54
1	4-B	273	VAL	CB-CG1	5.03	1.63	1.52
1	1-B	7	SER	CB-OG	5.02	1.48	1.42
1	1-A	268	GLY	C-O	5.02	1.31	1.23
1	6-A	354	ALA	CA-CB	5.02	1.62	1.52
1	6-B	251	GLU	CG-CD	5.02	1.59	1.51
1	4-A	133	TYR	CD1-CE1	5.01	1.46	1.39
1	1-B	136	TRP	CE3-CZ3	5.01	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-B	150	GLU	CD-OE1	-5.00	1.20	1.25

All (375) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	306	ARG	NE-CZ-NH1	15.13	127.87	120.30
1	5-B	174	CYS	CA-CB-SG	-13.16	90.31	114.00
1	4-B	151	ARG	NE-CZ-NH2	-13.04	113.78	120.30
1	2-A	265	ASP	CB-CG-OD1	12.68	129.71	118.30
1	5-A	331	ARG	NE-CZ-NH2	-12.39	114.10	120.30
1	7-A	331	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	7-A	119	ASP	CB-CG-OD1	12.10	129.19	118.30
1	6-A	331	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	7-B	73	ARG	NE-CZ-NH2	-11.79	114.40	120.30
1	6-A	331	ARG	NE-CZ-NH1	11.75	126.17	120.30
1	7-B	252	ARG	NE-CZ-NH2	-11.59	114.50	120.30
1	8-A	252	ARG	NE-CZ-NH1	-11.57	114.51	120.30
1	6-A	269	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	6-A	306	ARG	NE-CZ-NH2	-11.47	114.57	120.30
1	6-A	151	ARG	NE-CZ-NH1	11.33	125.96	120.30
1	8-A	267	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	6-B	218	ASP	CB-CG-OD1	11.25	128.42	118.30
1	7-A	247	ASP	CB-CG-OD2	-11.24	108.19	118.30
1	5-A	269	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	1-A	331	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	6-B	226	ASP	CB-CG-OD1	-11.21	108.21	118.30
1	5-B	252	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	7-A	331	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	5-B	144	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	4-A	89	ASP	CB-CG-OD2	10.57	127.81	118.30
1	8-A	331	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	1-B	73	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	5-A	331	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	1-A	267	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	6-A	186	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	5-B	331	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	1-A	331	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	4-A	252	ARG	NE-CZ-NH1	-10.07	115.27	120.30
1	7-B	252	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	7-A	151	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	2-B	94	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	3-A	355	ARG	NE-CZ-NH2	-9.64	115.48	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	226	ASP	CB-CG-OD2	9.63	126.97	118.30
1	8-A	154	ARG	NE-CZ-NH1	-9.59	115.50	120.30
1	1-B	331	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	3-A	301	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	4-A	113	ARG	NE-CZ-NH2	9.43	125.02	120.30
1	8-A	135	ASP	CB-CG-OD1	-9.38	109.86	118.30
1	7-A	145	LYS	CD-CE-NZ	-9.36	90.18	111.70
1	6-A	15	MSE	CB-CG-SE	-9.32	84.73	112.70
1	5-A	154	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	8-A	144	ARG	CG-CD-NE	-9.21	92.45	111.80
1	2-A	301	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	7-B	331	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	5-A	89	ASP	CB-CG-OD1	-9.17	110.05	118.30
1	2-A	144	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	1-B	144	ARG	CD-NE-CZ	8.96	136.14	123.60
1	6-A	193	GLU	OE1-CD-OE2	-8.93	112.59	123.30
1	4-B	252	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	5-B	252	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	7-B	265	ASP	CB-CG-OD2	8.87	126.29	118.30
1	7-B	331	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	3-A	81	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	6-A	151	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	7-A	151	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	2-A	331	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	6-A	269	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	7-B	144	ARG	NE-CZ-NH2	8.53	124.57	120.30
1	7-B	151	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	6-A	94	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	2-A	244	ASP	CB-CG-OD1	-8.46	110.69	118.30
1	7-B	244	ASP	CB-CG-OD1	-8.44	110.71	118.30
1	6-A	186	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	6-B	233	ARG	NE-CZ-NH1	-8.42	116.09	120.30
1	4-A	199	LEU	CA-CB-CG	-8.42	95.94	115.30
1	2-A	144	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	2-A	218	ASP	CB-CG-OD2	8.36	125.82	118.30
1	5-A	243	ASP	CB-CG-OD1	8.35	125.82	118.30
1	6-B	331	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	1-B	144	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	1-A	267	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	5-B	331	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	2-B	331	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	8-B	15	MSE	CG-SE-CE	8.21	116.96	98.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	144	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	6-A	154	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	6-B	119	ASP	CB-CG-OD1	8.04	125.53	118.30
1	7-A	154	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	8-B	27	ILE	CG1-CB-CG2	7.91	128.80	111.40
1	4-A	147	LEU	CA-CB-CG	-7.89	97.16	115.30
1	1-A	226	ASP	CB-CG-OD1	-7.88	111.21	118.30
1	1-A	113	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	5-B	119	ASP	CB-CG-OD1	7.81	125.33	118.30
1	7-B	328	ASP	CB-CG-OD1	7.79	125.31	118.30
1	8-A	331	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	5-A	93	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	3-A	132	CYS	CA-CB-SG	-7.72	100.10	114.00
1	6-B	174	CYS	CA-CB-SG	-7.71	100.12	114.00
1	3-A	141	LEU	CB-CG-CD1	-7.66	97.97	111.00
1	2-A	244	ASP	CB-CG-OD2	7.63	125.17	118.30
1	1-B	151	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	2-A	331	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	3-A	244	ASP	CB-CG-OD1	-7.57	111.49	118.30
1	5-A	213	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	4-A	331	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	6-A	213	ARG	NE-CZ-NH1	-7.47	116.57	120.30
1	1-B	218	ASP	CB-CG-OD1	7.45	125.00	118.30
1	3-B	98	THR	CA-CB-CG2	-7.44	101.98	112.40
1	6-B	274	ILE	N-CA-C	-7.44	90.92	111.00
1	8-A	243	ASP	CB-CG-OD1	-7.42	111.63	118.30
1	8-B	93	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	1-A	154	ARG	NE-CZ-NH1	-7.39	116.60	120.30
1	1-B	331	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	4-A	20	ASP	CB-CG-OD1	7.36	124.92	118.30
1	8-B	151	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	4-A	186	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	5-A	186	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	2-A	213	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	6-B	265	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	3-A	186	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	7-A	155	PHE	CB-CG-CD2	-7.16	115.79	120.80
1	8-A	113	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	4-A	154	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	6-B	15	MSE	CG-SE-CE	7.11	114.55	98.90
1	4-A	46	VAL	CG1-CB-CG2	-7.11	99.53	110.90
1	3-A	244	ASP	CB-CG-OD2	7.10	124.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	89	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	6-B	244	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	5-B	239	LEU	CB-CG-CD2	-7.07	98.98	111.00
1	5-B	93	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	5-B	269	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	3-A	218	ASP	CB-CG-OD1	6.98	124.59	118.30
1	7-A	73	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	7-A	175	LEU	CB-CG-CD2	-6.97	99.15	111.00
1	1-A	284	MSE	CG-SE-CE	6.94	114.16	98.90
1	6-B	252	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	5-B	144	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	8-A	151	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	4-B	203	LEU	CB-CG-CD2	-6.92	99.23	111.00
1	5-A	90	SER	N-CA-CB	-6.89	100.16	110.50
1	6-A	37	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	1-B	151	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	3-A	154	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	8-A	144	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	4-A	151	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	2-A	265	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	5-B	73	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	8-A	216	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	1-B	144	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	7-A	230	CYS	CA-CB-SG	-6.78	101.79	114.00
1	8-A	151	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	2-A	267	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	4-B	140	LEU	CB-CG-CD2	-6.77	99.48	111.00
1	3-A	193	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	2-B	247	ASP	CB-CG-OD2	6.75	124.37	118.30
1	2-B	331	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	5-A	94	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	1-A	332	ASP	CB-CG-OD1	6.71	124.34	118.30
1	3-B	337	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	3-A	331	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	8-B	228	MSE	CB-CG-SE	-6.68	92.66	112.70
1	6-B	331	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	5-A	151	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	8-A	220	ASP	CB-CG-OD1	6.62	124.26	118.30
1	5-A	93	ARG	CG-CD-NE	-6.61	97.92	111.80
1	7-A	142	VAL	CG1-CB-CG2	-6.61	100.33	110.90
1	3-A	144	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	2-A	310	SER	CA-CB-OG	-6.60	93.38	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-B	274	ILE	N-CA-C	-6.57	93.27	111.00
1	2-A	154	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	5-A	34	ASP	CB-CG-OD1	-6.52	112.44	118.30
1	6-B	89	ASP	CB-CG-OD1	6.52	124.17	118.30
1	7-A	149	LEU	CB-CG-CD2	6.51	122.06	111.00
1	7-A	301	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	7-A	373	ALA	N-CA-C	-6.47	93.52	111.00
1	1-B	130	ASP	CB-CA-C	-6.46	97.47	110.40
1	3-A	144	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	4-A	332	ASP	CB-CG-OD1	6.43	124.09	118.30
1	8-A	155	PHE	CB-CG-CD2	-6.39	116.33	120.80
1	7-B	186	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	4-B	252	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	5-B	151	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	7-A	89	ASP	CB-CG-OD2	6.28	123.95	118.30
1	3-A	331	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	6-B	239	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	6-B	93	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	5-A	89	ASP	CB-CG-OD2	6.25	123.93	118.30
1	4-B	247	ASP	CB-CG-OD2	6.21	123.89	118.30
1	1-A	186	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	3-B	97	PRO	C-N-CA	-6.20	106.21	121.70
1	7-A	181	LEU	CA-CB-CG	6.16	129.46	115.30
1	5-A	175	LEU	CB-CG-CD2	-6.13	100.57	111.00
1	2-B	93	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	3-A	240	SER	CA-CB-OG	-6.13	94.65	111.20
1	4-A	368	THR	CA-CB-CG2	6.12	120.97	112.40
1	6-B	73	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	8-A	352	GLU	OE1-CD-OE2	-6.11	115.97	123.30
1	6-A	154	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	8-B	27	ILE	CB-CA-C	-6.08	99.44	111.60
1	2-A	169	ASP	CB-CG-OD1	6.07	123.77	118.30
1	5-A	144	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	5-A	203	LEU	CB-CG-CD1	-6.07	100.69	111.00
1	1-A	224	HIS	CB-CA-C	-6.06	98.29	110.40
1	1-A	282	LEU	CB-CG-CD1	-6.04	100.73	111.00
1	6-B	144	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	5-B	226	ASP	CB-CG-OD2	6.03	123.73	118.30
1	8-A	144	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	8-A	228	MSE	CA-CB-CG	-6.02	103.07	113.30
1	6-B	113	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	7-B	174	CYS	CA-CB-SG	-6.00	103.20	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	149	LEU	CB-CG-CD2	5.98	121.16	111.00
1	4-B	220	ASP	CB-CG-OD1	5.96	123.66	118.30
1	2-A	155	PHE	CB-CG-CD2	-5.95	116.64	120.80
1	7-A	218	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	3-A	113	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	3-B	258	SER	N-CA-CB	-5.91	101.64	110.50
1	4-B	15	MSE	CG-SE-CE	-5.89	85.94	98.90
1	3-A	32	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	1-A	70	GLU	OE1-CD-OE2	5.87	130.35	123.30
1	1-A	60	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	6-A	306	ARG	CD-NE-CZ	5.86	131.80	123.60
1	5-A	370	GLN	CB-CA-C	-5.85	98.70	110.40
1	7-A	175	LEU	CB-CG-CD1	5.85	120.94	111.00
1	4-A	223	GLY	C-N-CA	-5.84	107.09	121.70
1	4-A	301	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	6-B	366	CYS	CB-CA-C	-5.83	98.74	110.40
1	3-A	139	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	1-B	21	SER	N-CA-C	5.82	126.71	111.00
1	3-B	310	SER	CA-CB-OG	-5.81	95.52	111.20
1	4-A	118	ILE	N-CA-C	-5.80	95.33	111.00
1	3-B	93	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	3-A	328	ASP	N-CA-C	-5.80	95.35	111.00
1	6-B	79	ASP	CB-CG-OD2	5.79	123.51	118.30
1	6-B	252	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	3-A	239	LEU	CA-CB-CG	-5.78	102.02	115.30
1	3-A	155	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	1-B	71	ASN	C-N-CA	-5.75	107.32	121.70
1	6-A	328	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	8-A	186	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	8-A	139	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	1-B	93	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	2-B	229	CYS	CA-CB-SG	-5.73	103.69	114.00
1	6-A	247	ASP	CB-CG-OD1	5.73	123.46	118.30
1	5-A	355	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	2-B	94	ASP	CB-CG-OD2	5.71	123.44	118.30
1	7-B	301	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	2-A	332	ASP	CB-CG-OD1	5.70	123.43	118.30
1	8-A	175	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	7-A	149	LEU	CB-CG-CD1	-5.70	101.32	111.00
1	5-A	216	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	8-A	211	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	4-B	242	THR	N-CA-CB	-5.67	99.53	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	50	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	4-A	213	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	2-A	87	MSE	CG-SE-CE	-5.66	86.44	98.90
1	1-A	76	LEU	CA-CB-CG	-5.66	102.28	115.30
1	6-B	243	ASP	CB-CG-OD1	5.66	123.39	118.30
1	7-B	325	GLN	N-CA-C	-5.65	95.75	111.00
1	1-B	230	CYS	CB-CA-C	-5.63	99.14	110.40
1	5-B	44	GLN	CB-CA-C	-5.62	99.15	110.40
1	2-A	37	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	2-B	104	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	4-A	155	PHE	CB-CG-CD2	-5.61	116.87	120.80
1	3-B	169	ASP	CB-CG-OD2	5.60	123.34	118.30
1	1-A	284	MSE	CA-CB-CG	5.57	122.77	113.30
1	4-A	328	ASP	N-CA-C	-5.54	96.06	111.00
1	7-A	144	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	2-B	29	TRP	N-CA-CB	-5.53	100.64	110.60
1	4-A	199	LEU	CB-CG-CD1	-5.53	101.59	111.00
1	4-B	150	GLU	CG-CD-OE2	5.53	129.36	118.30
1	4-B	331	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	4-A	218	ASP	CB-CG-OD2	5.51	123.26	118.30
1	2-B	332	ASP	CB-CG-OD2	5.50	123.25	118.30
1	4-B	178	GLU	OE1-CD-OE2	5.49	129.89	123.30
1	1-A	175	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	1-A	252	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	4-B	238	LEU	CB-CG-CD1	5.47	120.30	111.00
1	7-A	70	GLU	OE1-CD-OE2	5.47	129.86	123.30
1	6-B	87	MSE	CG-SE-CE	-5.46	86.88	98.90
1	1-A	265	ASP	CB-CG-OD1	5.46	123.21	118.30
1	4-B	73	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	5-B	225	ILE	CG1-CB-CG2	-5.44	99.43	111.40
1	5-A	207	SER	N-CA-CB	5.44	118.66	110.50
1	8-B	150	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	1-A	216	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	5-A	315	TYR	CZ-CE2-CD2	-5.42	114.93	119.80
1	5-A	301	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	5-B	14	TYR	CG-CD2-CE2	-5.41	116.97	121.30
1	6-B	154	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	8-A	89	ASP	CB-CG-OD2	5.41	123.17	118.30
1	6-A	93	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	7-B	144	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	1-A	58	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	7-A	139	ASP	CB-CG-OD2	5.37	123.13	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	180	CYS	CA-CB-SG	-5.36	104.36	114.00
1	6-B	155	PHE	CG-CD2-CE2	5.35	126.69	120.80
1	1-B	230	CYS	N-CA-CB	5.35	120.23	110.60
1	3-A	154	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	8-A	87	MSE	CG-SE-CE	5.34	110.64	98.90
1	3-B	101	VAL	CB-CA-C	-5.34	101.26	111.40
1	7-A	126	GLY	C-N-CA	-5.33	111.10	122.30
1	4-A	62	VAL	CA-CB-CG2	5.33	118.89	110.90
1	4-B	239	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	5-B	87	MSE	CG-SE-CE	-5.32	87.19	98.90
1	1-A	117	GLY	N-CA-C	-5.32	99.81	113.10
1	5-A	139	ASP	CB-CG-OD1	-5.32	113.52	118.30
1	2-A	373	ALA	N-CA-C	-5.31	96.66	111.00
1	5-B	79	ASP	CB-CG-OD1	5.30	123.07	118.30
1	6-B	15	MSE	CB-CG-SE	-5.30	96.81	112.70
1	7-A	182	LEU	CB-CG-CD1	-5.30	102.00	111.00
1	7-B	326	PHE	C-N-CA	-5.29	111.19	122.30
1	1-A	230	CYS	CB-CA-C	-5.29	99.82	110.40
1	3-A	141	LEU	CB-CG-CD2	5.28	119.97	111.00
1	7-B	151	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	5-A	244	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	5-A	21	SER	N-CA-C	5.27	125.22	111.00
1	8-A	154	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	1-B	341	ASP	CB-CG-OD1	5.26	123.04	118.30
1	1-A	143	SER	N-CA-CB	5.26	118.39	110.50
1	5-B	149	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	7-A	216	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	2-B	104	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	6-A	52	LYS	CD-CE-NZ	5.24	123.76	111.70
1	1-B	208	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	7-B	261	SER	CA-CB-OG	-5.24	97.06	111.20
1	7-A	22	HIS	CB-CA-C	-5.24	99.93	110.40
1	4-B	150	GLU	CG-CD-OE1	-5.22	107.85	118.30
1	5-B	140	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	4-A	155	PHE	CB-CG-CD1	5.22	124.45	120.80
1	8-A	83	VAL	CA-CB-CG1	-5.21	103.09	110.90
1	8-A	202	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	1-A	216	TYR	CG-CD1-CE1	-5.20	117.14	121.30
1	6-B	144	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	2-B	230	CYS	CB-CA-C	-5.20	100.00	110.40
1	4-B	233	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	6-A	231	PHE	CB-CG-CD1	-5.18	117.17	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-B	80	ILE	N-CA-C	-5.18	97.01	111.00
1	7-A	205	VAL	CA-CB-CG1	-5.18	103.14	110.90
1	5-B	7	SER	N-CA-C	-5.17	97.03	111.00
1	6-A	282	LEU	CB-CG-CD1	5.17	119.79	111.00
1	1-A	22	HIS	CB-CA-C	-5.17	100.06	110.40
1	5-B	278	ILE	CB-CA-C	-5.16	101.28	111.60
1	5-B	132	CYS	CA-CB-SG	-5.14	104.75	114.00
1	7-B	113	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	5-B	260	LEU	CA-CB-CG	-5.13	103.50	115.30
1	3-B	140	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	6-A	282	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	6-B	306	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	1-A	143	SER	CA-CB-OG	-5.11	97.40	111.20
1	2-A	113	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	6-B	144	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	4-B	250	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	4-A	142	VAL	CA-CB-CG2	-5.09	103.26	110.90
1	3-B	233	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	5-B	233	ARG	N-CA-C	-5.09	97.26	111.00
1	4-A	331	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	7-A	127	GLY	O-C-N	5.08	130.83	122.70
1	5-B	180	CYS	CA-CB-SG	-5.08	104.86	114.00
1	3-B	311	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	8-B	122	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	7-A	65	SER	N-CA-CB	-5.07	102.90	110.50
1	3-A	130	ASP	CB-CG-OD1	5.07	122.86	118.30
1	8-A	316	ILE	CG1-CB-CG2	5.07	122.54	111.40
1	7-A	202	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	7-A	119	ASP	OD1-CG-OD2	-5.05	113.70	123.30
1	1-B	113	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	4-B	238	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	3-A	141	LEU	CA-CB-CG	-5.03	103.72	115.30
1	1-A	225	ILE	CB-CA-C	-5.03	101.54	111.60
1	3-B	269	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	1-B	209	ILE	N-CA-C	-5.03	97.43	111.00
1	3-A	228	MSE	CB-CG-SE	-5.02	97.64	112.70
1	2-B	127	GLY	N-CA-C	5.01	125.63	113.10
1	6-A	326	PHE	C-N-CA	-5.01	111.77	122.30
1	8-A	83	VAL	CB-CA-C	-5.01	101.88	111.40
1	7-A	182	LEU	CB-CG-CD2	5.01	119.51	111.00
1	8-A	64	ALA	N-CA-CB	-5.01	103.09	110.10
1	5-B	113	ARG	NE-CZ-NH1	-5.00	117.80	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	8-A	149	LEU	CB-CG-CD1	-5.00	102.50	111.00
1	8-B	155	PHE	CG-CD2-CE2	5.00	126.30	120.80

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	216	TYR	Sidechain
1	1-B	13	TYR	Sidechain
1	1-B	202	TYR	Sidechain
1	2-A	311	TYR	Sidechain
1	3-B	315	TYR	Sidechain
1	4-A	122	PHE	Sidechain
1	4-A	133	TYR	Sidechain
1	5-A	155	PHE	Sidechain
1	5-A	315	TYR	Sidechain
1	5-B	133	TYR	Sidechain
1	5-B	250	TYR	Sidechain
1	6-B	202	TYR	Sidechain
1	7-A	277	TYR	Sidechain
1	7-A	283	TYR	Sidechain
1	7-B	13	TYR	Sidechain
1	7-B	138	HIS	Sidechain
1	8-A	202	TYR	Sidechain
1	8-A	277	TYR	Sidechain
1	8-B	202	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2902	0	2786	172	0
1	1-B	2882	0	2767	130	0
1	2-A	2902	0	2786	168	0
1	2-B	2882	0	2767	166	0
1	3-A	2902	0	2786	153	0
1	3-B	2882	0	2767	141	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-A	2902	0	2786	166	0
1	4-B	2882	0	2767	193	0
1	5-A	2902	0	2786	141	0
1	5-B	2882	0	2767	184	0
1	6-A	2902	0	2786	185	0
1	6-B	2882	0	2767	211	0
1	7-A	2902	0	2786	131	0
1	7-B	2882	0	2767	193	0
1	8-A	2902	0	2786	167	0
1	8-B	2882	0	2767	151	0
2	1-A	1	0	0	0	0
2	1-B	1	0	0	0	0
2	2-A	1	0	0	0	0
2	2-B	1	0	0	0	0
2	3-A	1	0	0	0	0
2	3-B	1	0	0	0	0
2	4-A	1	0	0	0	0
2	4-B	1	0	0	0	0
2	5-A	1	0	0	0	0
2	5-B	1	0	0	0	0
2	6-A	1	0	0	1	0
2	6-B	1	0	0	0	0
2	7-A	1	0	0	0	0
2	7-B	1	0	0	0	0
2	8-A	1	0	0	0	0
2	8-B	1	0	0	0	0
3	1-A	28	0	42	4	0
3	1-B	24	0	36	7	0
3	2-A	28	0	42	8	0
3	2-B	24	0	36	10	0
3	3-A	28	0	42	11	0
3	3-B	24	0	36	10	0
3	4-A	28	0	42	2	0
3	4-B	24	0	36	7	0
3	5-A	28	0	42	8	0
3	5-B	24	0	36	10	0
3	6-A	28	0	42	7	0
3	6-B	24	0	36	13	0
3	7-A	28	0	42	9	0
3	7-B	24	0	36	12	0
3	8-A	28	0	42	18	0
3	8-B	24	0	36	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1-A	13	0	15	0	0
4	2-A	13	0	15	0	0
4	3-A	13	0	15	0	0
4	4-A	13	0	15	0	0
4	5-A	13	0	15	1	0
4	6-A	13	0	15	1	0
4	7-A	13	0	15	0	0
4	8-A	13	0	15	1	0
5	1-A	404	0	0	17	0
5	1-B	375	0	0	23	0
5	2-A	409	0	0	25	0
5	2-B	370	0	0	18	0
5	3-A	404	0	0	27	0
5	3-B	375	0	0	24	0
5	4-A	410	0	0	30	0
5	4-B	369	0	0	22	0
5	5-A	407	0	0	20	0
5	5-B	372	0	0	27	0
5	6-A	403	0	0	31	0
5	6-B	376	0	0	25	0
5	7-A	405	0	0	23	0
5	7-B	374	0	0	28	0
5	8-A	409	0	0	19	0
5	8-B	370	0	0	22	0
All	All	53040	0	45168	2624	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (2624) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:CD1	1:B:166:ILE:CG1	1.77	1.55
1:B:100:ILE:CD1	1:B:100:ILE:CG1	1.79	1.55
1:B:195:ILE:CG1	1:B:195:ILE:CD1	1.81	1.55
1:B:188:PRO:CD	1:B:188:PRO:CG	1.74	1.55
1:B:225:ILE:CG1	1:B:225:ILE:CD1	1.82	1.53
1:B:168:VAL:HG12	1:B:174:CYS:SG	1.49	1.52
1:A:59:PRO:CB	1:A:59:PRO:CG	1.85	1.52
1:A:42:PRO:CG	1:A:42:PRO:CB	1.75	1.49
1:B:97:PRO:CG	1:B:97:PRO:CB	1.81	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:MSE:SE	1:A:190:MSE:CG	2.14	1.43
1:A:87:MSE:SE	1:A:87:MSE:CE	2.16	1.43
1:A:190:MSE:CG	1:A:190:MSE:SE	2.18	1.42
1:A:159:MSE:CG	1:A:159:MSE:SE	2.16	1.42
1:B:15:MSE:SE	1:B:15:MSE:CE	2.17	1.42
1:B:15:MSE:CE	1:B:15:MSE:SE	2.18	1.41
1:B:230:CYS:SG	1:B:230:CYS:CB	2.07	1.40
1:A:15:MSE:SE	1:A:15:MSE:CE	2.20	1.39
1:B:174:CYS:SG	1:B:205:VAL:HG11	1.63	1.38
1:B:230:CYS:CB	1:B:230:CYS:SG	2.12	1.37
1:B:7:SER:OG	1:B:8:PRO:HD3	1.28	1.30
1:A:362:GLY:HA2	5:A:1169:HOH:O	1.31	1.27
1:B:150:GLU:OE1	5:B:1154:HOH:O	1.53	1.26
1:B:70:GLU:OE1	5:B:1103:HOH:O	1.53	1.25
1:B:168:VAL:CG1	1:B:174:CYS:SG	2.24	1.25
1:A:221:THR:OG1	5:A:1200:HOH:O	1.53	1.20
1:B:56:LYS:HD2	5:B:1070:HOH:O	1.44	1.17
1:B:103:LYS:H	1:B:103:LYS:HD2	1.06	1.15
1:A:230:CYS:SG	1:A:231:PHE:N	2.19	1.14
1:B:9:ALA:CA	5:B:1263:HOH:O	1.96	1.14
1:B:20:ASP:OD2	5:B:1045:HOH:O	1.66	1.13
1:B:230:CYS:SG	1:B:312:VAL:HG13	1.88	1.12
1:A:159:MSE:HE1	1:A:195:ILE:HG12	1.31	1.12
1:B:104:ARG:HB2	1:B:114:ASN:HD21	1.05	1.12
1:A:85:MSE:HE2	5:A:1217:HOH:O	1.48	1.11
1:B:282:LEU:HB3	1:B:307:LEU:HD22	1.30	1.10
1:A:78:GLU:HG2	5:A:1331:HOH:O	1.52	1.09
1:A:185:ASN:ND2	1:A:222:ASN:HD21	1.52	1.07
1:A:149:LEU:HD11	1:B:149:LEU:HD11	1.34	1.07
1:B:9:ALA:HB2	5:B:1263:HOH:O	1.54	1.06
1:B:7:SER:HB3	1:B:8:PRO:HD3	1.36	1.06
1:A:85:MSE:HG3	5:B:1117:HOH:O	1.55	1.06
1:A:189:HIS:HB2	5:A:1242:HOH:O	1.56	1.05
1:B:9:ALA:CB	5:B:1263:HOH:O	2.04	1.05
1:B:9:ALA:HA	5:B:1263:HOH:O	1.55	1.04
1:B:284:MSE:HE1	1:B:301:ARG:NH1	1.73	1.03
1:A:68:GLN:HE22	1:A:71:ASN:HD22	1.05	1.02
1:A:68:GLN:HE22	1:A:71:ASN:HD22	1.03	1.02
1:A:174:CYS:HB2	1:A:205:VAL:HG11	1.43	1.00
1:B:190:MSE:HE3	5:B:1198:HOH:O	1.60	1.00
1:B:160:ILE:HD12	1:B:186:ARG:O	1.62	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MSE:SE	1:A:203:LEU:HD22	2.11	1.00
1:A:104:ARG:HH21	1:A:104:ARG:HB3	1.25	1.00
1:A:104:ARG:HH21	1:A:104:ARG:HB3	1.23	1.00
1:A:149:LEU:HD22	1:B:149:LEU:HD11	1.42	0.99
1:A:89:ASP:OD2	5:A:1044:HOH:O	1.81	0.99
1:A:218:ASP:OD1	5:A:1204:HOH:O	1.79	0.99
1:A:328:ASP:O	1:A:332:ASP:HB2	1.63	0.98
1:A:26:TRP:HE1	1:A:371:GLN:HE21	1.02	0.98
1:B:191:SER:H	1:B:194:GLN:HE21	1.00	0.98
1:A:149:LEU:CD2	1:B:149:LEU:HD11	1.94	0.97
1:A:216:TYR:H	1:A:249:GLN:NE2	1.61	0.97
1:B:70:GLU:OE1	5:B:1107:HOH:O	1.83	0.97
1:B:150:GLU:OE1	1:B:150:GLU:HA	1.61	0.96
1:A:191:SER:CB	1:A:194:GLN:HE21	1.79	0.96
1:B:355:ARG:NH1	5:B:1051:HOH:O	1.97	0.96
1:A:160:ILE:H	1:A:187:ASN:ND2	1.64	0.96
1:B:174:CYS:SG	1:B:205:VAL:CG1	2.54	0.96
1:B:15:MSE:CE	1:B:203:LEU:HD22	1.95	0.96
1:B:23:ALA:HB2	1:B:373:ALA:HA	1.45	0.96
1:A:15:MSE:SE	1:A:203:LEU:HD22	2.16	0.96
1:B:61:THR:O	1:B:61:THR:HG22	1.66	0.95
1:A:35:ASN:ND2	1:A:301:ARG:HH21	1.64	0.95
1:B:33:GLN:HE21	1:B:39:ASN:HA	1.31	0.95
1:A:192:LYS:O	1:A:196:GLU:HB2	1.67	0.95
1:B:93:ARG:HH12	1:B:370:GLN:HE22	0.97	0.95
1:B:22:HIS:H	1:B:318:ASN:HD21	1.00	0.94
1:B:222:ASN:HD21	3:B:911:EDO:C1	1.80	0.94
1:A:362:GLY:HA3	1:A:366:CYS:SG	2.06	0.94
1:B:292:ILE:HG21	1:B:301:ARG:HG3	1.49	0.94
1:A:225:ILE:HG13	1:A:225:ILE:O	1.65	0.94
1:B:366:CYS:SG	1:B:367:ILE:HG23	2.07	0.94
1:A:364:ILE:N	1:A:366:CYS:SG	2.40	0.94
1:A:134:ASN:HD21	1:A:297:GLU:HA	1.30	0.94
1:A:98:THR:HG22	5:A:1031:HOH:O	1.67	0.94
1:A:97:PRO:HD3	1:A:143:SER:HA	1.49	0.94
1:A:160:ILE:H	1:A:187:ASN:HD21	1.00	0.94
1:A:191:SER:H	1:A:194:GLN:NE2	1.63	0.94
1:A:185:ASN:HD21	1:A:222:ASN:HD21	0.98	0.94
1:A:191:SER:H	1:A:194:GLN:HE21	1.16	0.93
1:B:63:CYS:HB2	1:B:87:MSE:HE1	1.47	0.93
1:B:50:VAL:HG11	1:B:367:ILE:HD11	1.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:MSE:HE2	5:A:1144:HOH:O	1.65	0.93
1:A:185:ASN:HD21	1:A:222:ASN:ND2	1.66	0.93
1:B:7:SER:OG	1:B:8:PRO:CD	2.17	0.93
1:A:284:MSE:CE	5:A:1144:HOH:O	2.13	0.93
1:A:270:LYS:HE2	5:A:1386:HOH:O	1.68	0.93
1:A:160:ILE:N	1:A:187:ASN:HD21	1.66	0.93
1:B:7:SER:HB2	1:B:155:PHE:CE1	2.03	0.93
1:A:27:ILE:HG23	1:A:367:ILE:O	1.68	0.93
1:B:220:ASP:CG	5:B:1230:HOH:O	2.05	0.93
1:B:144:ARG:NH2	5:B:1136:HOH:O	2.00	0.92
1:B:144:ARG:NH1	1:B:156:GLN:HE21	1.66	0.92
1:B:302:LEU:O	1:B:305:THR:HG23	1.70	0.92
1:B:104:ARG:HB2	1:B:114:ASN:HD21	1.34	0.92
1:A:191:SER:HB3	1:A:194:GLN:NE2	1.84	0.92
1:B:247:ASP:OD1	5:B:1029:HOH:O	1.86	0.92
1:B:77:PRO:HD2	1:B:80:ILE:HD12	1.50	0.92
5:A:1152:HOH:O	1:B:85:MSE:HG3	1.66	0.92
1:B:78:GLU:HB3	5:B:1062:HOH:O	1.70	0.92
1:B:186:ARG:HH12	1:B:222:ASN:HD22	1.17	0.92
1:B:302:LEU:O	1:B:305:THR:HG23	1.70	0.91
1:B:79:ASP:OD2	5:B:1200:HOH:O	1.89	0.91
1:A:191:SER:H	1:A:194:GLN:HE21	1.07	0.91
1:A:190:MSE:HE2	1:A:195:ILE:HG13	1.53	0.91
1:B:230:CYS:SG	1:B:312:VAL:CG1	2.58	0.91
1:B:160:ILE:H	1:B:187:ASN:HD21	1.11	0.91
1:A:104:ARG:HH21	1:A:104:ARG:HB3	1.32	0.90
1:A:160:ILE:H	1:A:187:ASN:HD21	1.08	0.90
1:B:22:HIS:H	1:B:318:ASN:HD21	0.95	0.90
1:B:191:SER:H	1:B:194:GLN:HE21	1.13	0.90
1:B:97:PRO:HD3	1:B:143:SER:HA	1.52	0.90
1:B:22:HIS:H	1:B:318:ASN:HD21	1.13	0.90
1:A:160:ILE:HD12	1:A:160:ILE:N	1.85	0.90
1:A:191:SER:H	1:A:194:GLN:NE2	1.70	0.90
1:B:186:ARG:HH12	1:B:222:ASN:HD22	1.11	0.90
1:B:104:ARG:HB2	1:B:114:ASN:ND2	1.87	0.90
1:B:186:ARG:HH12	1:B:222:ASN:HD22	1.17	0.90
1:A:66:PRO:HD2	5:A:1154:HOH:O	1.72	0.90
1:A:15:MSE:HE1	1:A:203:LEU:HD13	1.52	0.90
1:A:159:MSE:HE1	1:A:195:ILE:HG23	1.52	0.89
1:A:372:PRO:HB3	5:A:1110:HOH:O	1.71	0.89
1:B:9:ALA:CA	5:B:1263:HOH:O	2.13	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:HIS:H	1:B:318:ASN:HD21	1.20	0.89
1:A:184:LYS:HE3	5:A:1377:HOH:O	1.73	0.89
1:B:90:SER:O	5:B:916:HOH:O	1.88	0.89
1:A:293:THR:HG22	1:A:295:ASP:H	1.37	0.89
1:A:20:ASP:OD1	5:A:1034:HOH:O	1.91	0.89
1:B:88:ASN:OD1	1:B:136:TRP:HA	1.73	0.89
1:A:166:ILE:HG22	1:A:176:VAL:HG12	1.53	0.89
1:A:59:PRO:HD3	5:A:1209:HOH:O	1.73	0.89
1:B:282:LEU:HB3	1:B:307:LEU:HD22	1.54	0.89
1:A:218:ASP:OD1	5:A:1203:HOH:O	1.91	0.89
1:B:29:TRP:CZ2	1:B:44:GLN:HG2	2.08	0.89
1:A:218:ASP:CG	5:A:1204:HOH:O	2.11	0.88
1:B:7:SER:HB3	1:B:8:PRO:HD3	1.55	0.88
1:A:104:ARG:HB3	1:A:104:ARG:NH2	1.88	0.88
1:B:89:ASP:OD1	1:B:133:TYR:HE1	1.56	0.88
1:B:44:GLN:OE1	1:B:75:GLN:OE1	1.91	0.88
1:A:159:MSE:CE	1:A:195:ILE:HG12	2.02	0.88
1:B:37:ARG:HE	1:B:359:LEU:HD13	1.38	0.88
1:A:185:ASN:HA	3:A:906:EDO:H12	1.55	0.88
1:A:144:ARG:CZ	1:A:154:ARG:HH11	1.86	0.88
1:B:103:LYS:N	1:B:103:LYS:HD2	1.88	0.88
1:A:191:SER:CB	1:A:194:GLN:NE2	2.37	0.88
1:B:159:MSE:HE3	1:B:187:ASN:OD1	1.73	0.88
1:B:168:VAL:HG12	1:B:174:CYS:SG	2.14	0.88
1:A:84:GLU:OE1	1:B:145:LYS:NZ	2.07	0.88
1:A:190:MSE:HE1	1:A:195:ILE:HA	1.55	0.88
1:A:206:GLN:HG3	5:A:1393:HOH:O	1.73	0.88
1:B:138:HIS:CD2	5:B:1082:HOH:O	2.25	0.88
1:B:186:ARG:HH12	1:B:222:ASN:HD22	1.17	0.88
1:B:330:ILE:HG23	5:B:1103:HOH:O	1.73	0.88
1:A:218:ASP:CG	5:A:1203:HOH:O	2.12	0.87
1:A:113:ARG:NH2	1:A:151:ARG:O	2.07	0.87
1:B:282:LEU:HD12	1:B:282:LEU:N	1.89	0.87
1:A:352:GLU:OE2	5:A:1271:HOH:O	1.91	0.87
1:B:357:ILE:HG22	1:B:362:GLY:O	1.74	0.87
1:B:230:CYS:SG	5:B:930:HOH:O	2.30	0.87
1:A:362:GLY:HA2	5:A:1166:HOH:O	1.73	0.87
1:B:150:GLU:OE1	5:B:1152:HOH:O	1.91	0.87
1:A:24:GLN:HE22	1:B:151:ARG:HH22	1.21	0.86
1:A:33:GLN:OE1	1:A:39:ASN:ND2	2.09	0.86
1:B:150:GLU:OE1	5:B:1152:HOH:O	1.92	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:HG21	3:A:903:EDO:H22	1.54	0.86
1:B:191:SER:H	1:B:194:GLN:HE21	1.22	0.86
1:A:151:ARG:HG3	5:A:1148:HOH:O	1.74	0.86
1:A:363:ASN:N	1:A:366:CYS:SG	2.48	0.86
1:A:283:TYR:HA	1:A:305:THR:O	1.75	0.86
1:A:68:GLN:HE22	1:A:71:ASN:HD22	1.22	0.86
1:A:352:GLU:OE2	5:A:1271:HOH:O	1.93	0.86
1:B:91:TRP:CZ3	1:B:362:GLY:HA3	2.11	0.85
1:A:20:ASP:OD2	5:A:1229:HOH:O	1.93	0.85
1:A:243:ASP:OD2	5:A:1385:HOH:O	1.94	0.85
1:A:272:GLN:NE2	5:A:1296:HOH:O	1.84	0.85
1:B:68:GLN:HE22	1:B:71:ASN:HD22	1.17	0.85
1:B:115:ILE:HG23	1:B:152:ILE:HG23	1.59	0.85
1:B:284:MSE:HE1	1:B:301:ARG:HH11	1.41	0.85
1:A:185:ASN:HD21	1:A:222:ASN:HD21	1.24	0.85
1:B:219:GLU:OE1	5:B:1023:HOH:O	1.94	0.84
1:B:162:GLU:OE2	1:B:224:HIS:HE1	1.60	0.84
1:A:15:MSE:HE3	1:A:168:VAL:HG11	1.58	0.84
1:A:219:GLU:OE2	5:A:1381:HOH:O	1.94	0.84
1:B:263:SER:HB3	5:B:1061:HOH:O	1.77	0.84
1:B:186:ARG:HH12	1:B:222:ASN:HD22	1.23	0.84
3:A:908:EDO:O1	1:B:149:LEU:HD13	1.77	0.84
1:A:299:ILE:HD12	1:A:299:ILE:O	1.77	0.84
1:B:125:TRP:O	3:B:911:EDO:H12	1.75	0.84
1:A:154:ARG:NH1	1:A:156:GLN:OE1	2.10	0.84
1:B:69:TRP:NE1	1:B:82:VAL:HG12	1.92	0.84
1:A:229:CYS:HA	1:A:312:VAL:HG21	1.60	0.84
1:A:166:ILE:HG22	1:A:176:VAL:CG1	2.08	0.84
1:A:18:GLU:HG2	1:A:316:ILE:HB	1.60	0.84
1:B:191:SER:H	1:B:194:GLN:NE2	1.74	0.84
1:B:243:ASP:OD1	5:B:1130:HOH:O	1.95	0.84
1:A:119:ASP:OD2	1:A:154:ARG:HD2	1.77	0.83
1:B:77:PRO:HD2	1:B:80:ILE:HD12	1.58	0.83
1:A:104:ARG:HB3	1:A:104:ARG:NH2	1.92	0.83
1:A:226:ASP:OD2	1:A:365:HIS:HD2	1.61	0.83
1:B:89:ASP:OD1	1:B:133:TYR:CE1	2.32	0.83
1:A:41:LEU:CD1	5:A:1225:HOH:O	2.26	0.83
1:B:330:ILE:HG23	5:B:1103:HOH:O	1.79	0.83
1:A:35:ASN:HD21	1:A:301:ARG:HH21	1.27	0.83
1:B:103:LYS:H	1:B:103:LYS:HZ2	1.25	0.83
1:B:230:CYS:HG	1:B:312:VAL:HG13	1.42	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:HH12	1:B:156:GLN:HE21	1.21	0.83
1:A:157:HIS:ND1	1:A:159:MSE:HG2	1.91	0.83
1:A:352:GLU:OE2	5:A:1269:HOH:O	1.95	0.83
1:B:160:ILE:H	1:B:187:ASN:HD21	1.25	0.83
1:A:249:GLN:HG2	1:A:278:ILE:HD13	1.59	0.83
1:A:191:SER:H	1:A:194:GLN:HE21	1.27	0.83
5:A:1154:HOH:O	1:B:85:MSE:HE2	1.79	0.83
1:B:262:ASN:OD1	5:B:1247:HOH:O	1.97	0.82
1:A:112:ASN:HD22	1:A:112:ASN:N	1.75	0.82
1:A:24:GLN:HE22	1:B:151:ARG:NH2	1.78	0.82
1:A:313:ASN:HD22	1:A:365:HIS:H	1.27	0.82
1:B:222:ASN:HD21	3:B:911:EDO:H11	1.45	0.82
1:B:175:LEU:HD11	1:B:211:LEU:HD21	1.62	0.82
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.44	0.82
1:B:164:GLY:O	1:B:226:ASP:OD1	1.98	0.82
1:B:160:ILE:HD12	5:B:1163:HOH:O	1.78	0.82
1:A:299:ILE:HD12	1:A:299:ILE:C	2.00	0.82
1:B:15:MSE:N	1:B:203:LEU:O	2.12	0.82
1:A:302:LEU:O	1:A:305:THR:OG1	1.96	0.81
1:B:22:HIS:N	1:B:318:ASN:HD21	1.74	0.81
1:A:196:GLU:O	1:A:200:LYS:HG3	1.80	0.81
1:A:230:CYS:SG	1:A:231:PHE:O	2.39	0.81
1:B:138:HIS:HD2	5:B:1081:HOH:O	1.64	0.81
1:B:88:ASN:ND2	1:B:138:HIS:HB2	1.95	0.81
1:A:363:ASN:CG	1:A:364:ILE:H	1.84	0.81
1:A:18:GLU:OE1	1:A:365:HIS:HE1	1.64	0.81
1:B:103:LYS:CD	1:B:103:LYS:H	1.92	0.81
1:A:284:MSE:HE1	5:A:1143:HOH:O	1.80	0.81
1:A:160:ILE:H	1:A:187:ASN:HD21	0.85	0.81
1:A:35:ASN:ND2	1:A:301:ARG:NH2	2.28	0.81
1:B:138:HIS:HD2	5:B:1084:HOH:O	1.63	0.81
1:B:77:PRO:HD2	1:B:80:ILE:HD12	1.61	0.80
1:B:104:ARG:HB2	1:B:114:ASN:ND2	1.95	0.80
1:A:160:ILE:HD12	1:A:160:ILE:H	1.45	0.80
1:A:341:ASP:O	1:A:344:PRO:HD3	1.80	0.80
1:A:160:ILE:H	1:A:187:ASN:HD21	1.28	0.80
1:B:34:ASP:HB2	1:B:295:ASP:OD1	1.81	0.80
1:B:186:ARG:HH12	1:B:222:ASN:HD22	1.25	0.80
1:A:263:SER:OG	5:A:1095:HOH:O	1.97	0.80
1:B:222:ASN:HD21	3:B:911:EDO:C1	1.95	0.80
1:A:26:TRP:HE1	1:A:371:GLN:NE2	1.76	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:HG3	5:A:1119:HOH:O	1.81	0.80
1:B:238:LEU:HD22	1:B:276:LEU:HD22	1.62	0.80
1:A:68:GLN:HE22	1:A:71:ASN:HD22	1.28	0.80
1:A:18:GLU:OE1	1:A:365:HIS:HE1	1.64	0.80
1:A:363:ASN:C	1:A:366:CYS:SG	2.59	0.80
1:B:267:ARG:O	5:B:984:HOH:O	2.00	0.80
1:A:52:LYS:NZ	5:A:1395:HOH:O	2.15	0.80
1:A:216:TYR:H	1:A:249:GLN:NE2	1.78	0.80
1:A:31:GLU:HG2	5:A:1335:HOH:O	1.80	0.80
1:A:283:TYR:OH	5:A:1178:HOH:O	1.99	0.80
1:A:149:LEU:CD1	1:B:149:LEU:HD11	2.11	0.80
1:A:227:ASN:ND2	5:A:1383:HOH:O	2.15	0.80
1:B:22:HIS:N	1:B:318:ASN:HD21	1.78	0.80
1:A:207:SER:OG	5:A:1210:HOH:O	1.98	0.80
1:B:222:ASN:ND2	3:B:911:EDO:H11	1.97	0.80
1:A:12:GLY:O	1:A:103:LYS:NZ	2.15	0.79
1:B:261:SER:HA	5:B:1194:HOH:O	1.82	0.79
1:B:324:PRO:HB3	1:B:363:ASN:HD21	1.47	0.79
1:B:217:GLY:N	5:B:1023:HOH:O	2.14	0.79
1:B:11:HIS:HB3	1:B:102:ARG:NH2	1.96	0.79
1:A:68:GLN:HE22	1:A:71:ASN:HD22	1.29	0.79
1:B:7:SER:N	1:B:8:PRO:HD3	1.98	0.79
1:B:68:GLN:HE22	1:B:71:ASN:HD22	1.28	0.79
1:B:282:LEU:O	1:B:307:LEU:HD13	1.81	0.79
1:B:229:CYS:HB3	1:B:239:LEU:HD12	1.63	0.79
1:B:11:HIS:HB3	1:B:102:ARG:NH2	1.97	0.79
1:A:216:TYR:H	1:A:249:GLN:HE22	1.31	0.79
1:B:192:LYS:O	1:B:196:GLU:HG3	1.83	0.79
1:A:221:THR:HG22	1:A:221:THR:O	1.80	0.79
1:A:61:THR:HG21	1:A:81:ARG:HH11	1.47	0.79
1:B:98:THR:HB	1:B:118:ILE:HB	1.65	0.79
1:A:185:ASN:HA	3:A:906:EDO:H12	1.63	0.79
1:B:282:LEU:HD12	1:B:282:LEU:N	1.97	0.79
1:B:103:LYS:H	1:B:103:LYS:NZ	1.80	0.79
1:B:112:ASN:ND2	5:B:1255:HOH:O	2.16	0.79
1:A:370:GLN:OE1	1:A:370:GLN:N	2.14	0.79
1:A:66:PRO:HB3	1:A:84:GLU:OE2	1.83	0.79
1:A:50:VAL:HG11	1:A:367:ILE:HD11	1.62	0.78
1:A:313:ASN:HD22	1:A:363:ASN:HB3	1.47	0.78
1:A:372:PRO:HB3	5:A:1113:HOH:O	1.83	0.78
1:B:326:PHE:O	1:B:332:ASP:OD1	2.01	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:HIS:N	1:B:318:ASN:HD21	1.82	0.78
1:A:104:ARG:NH2	1:A:104:ARG:HB3	1.97	0.78
1:A:191:SER:N	1:A:194:GLN:HE21	1.81	0.78
1:B:31:GLU:OE2	5:B:1059:HOH:O	2.02	0.78
1:A:247:ASP:OD2	5:A:1039:HOH:O	2.01	0.78
1:A:77:PRO:HB2	1:A:79:ASP:OD2	1.84	0.78
1:A:241:TRP:O	1:A:277:TYR:HA	1.84	0.78
1:B:357:ILE:HD12	1:B:367:ILE:HD13	1.64	0.78
1:A:35:ASN:ND2	1:A:301:ARG:HE	1.81	0.78
1:B:238:LEU:HD11	1:B:342:THR:HG21	1.64	0.77
1:A:15:MSE:CE	1:A:203:LEU:HD13	2.14	0.77
1:B:93:ARG:HH12	1:B:370:GLN:NE2	1.79	0.77
1:A:113:ARG:HB3	1:A:374:GLU:OE2	1.83	0.77
1:B:280:GLU:O	1:B:282:LEU:HD12	1.84	0.77
1:A:160:ILE:H	1:A:187:ASN:ND2	1.82	0.77
1:A:68:GLN:NE2	1:A:71:ASN:HD22	1.82	0.77
1:B:91:TRP:CH2	1:B:362:GLY:HA3	2.19	0.77
1:B:104:ARG:HB2	1:B:114:ASN:HD21	1.49	0.77
1:B:222:ASN:ND2	3:B:911:EDO:H11	1.98	0.77
1:A:64:ALA:HA	1:A:87:MSE:HE1	1.65	0.77
1:A:134:ASN:HD21	1:A:297:GLU:CA	1.96	0.77
1:B:7:SER:HG	1:B:8:PRO:HD3	1.49	0.77
1:A:313:ASN:ND2	1:A:363:ASN:HB3	2.00	0.77
1:B:282:LEU:O	1:B:307:LEU:HD13	1.85	0.77
1:B:92:PHE:O	1:B:96:GLY:N	2.17	0.77
1:A:288:GLU:OE2	5:A:1265:HOH:O	2.03	0.77
1:B:123:ASN:O	1:B:127:GLY:N	2.17	0.77
1:A:228:MSE:O	1:A:239:LEU:HD12	1.85	0.77
1:B:156:GLN:H	3:B:912:EDO:H21	1.48	0.77
1:B:15:MSE:HE2	1:B:203:LEU:HD22	1.66	0.77
1:B:93:ARG:NH1	1:B:370:GLN:HE22	1.78	0.77
1:A:313:ASN:HD22	1:A:363:ASN:HB3	1.50	0.77
1:B:31:GLU:OE2	5:B:1205:HOH:O	2.03	0.77
1:A:216:TYR:H	1:A:249:GLN:HE22	1.29	0.76
1:A:94:ASP:OD2	3:A:903:EDO:H12	1.85	0.76
1:B:255:GLU:O	1:B:259:VAL:HG23	1.85	0.76
1:B:18:GLU:OE2	1:B:365:HIS:HE1	1.68	0.76
1:A:41:LEU:HD12	5:A:1225:HOH:O	1.82	0.76
1:A:104:ARG:NH2	1:A:104:ARG:HB3	2.01	0.76
1:B:41:LEU:HB3	1:B:45:ARG:NH2	2.00	0.76
1:B:57:PHE:O	5:B:964:HOH:O	2.04	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:SER:N	1:B:8:PRO:CD	2.47	0.76
1:A:102:ARG:O	1:A:375:PRO:HG2	1.84	0.76
1:A:367:ILE:O	5:A:1001:HOH:O	2.03	0.75
1:B:140:LEU:CD2	5:B:1252:HOH:O	2.34	0.75
1:B:7:SER:HB3	1:B:8:PRO:CD	2.14	0.75
1:A:117:GLY:HA3	1:A:147:LEU:HD11	1.67	0.75
1:A:136:TRP:O	1:A:140:LEU:HG	1.85	0.75
1:A:198:GLU:O	1:A:199:LEU:C	2.22	0.75
1:A:8:PRO:HD2	1:A:202:TYR:CD2	2.21	0.75
1:B:322:ILE:HG22	1:B:364:ILE:HD13	1.67	0.75
1:A:313:ASN:ND2	1:A:365:HIS:HB3	2.01	0.75
1:A:235:GLY:N	5:A:1009:HOH:O	2.12	0.75
1:A:11:HIS:HB2	1:A:13:TYR:CE2	2.22	0.75
1:A:94:ASP:OD2	3:A:903:EDO:H12	1.85	0.75
1:A:226:ASP:OD2	1:A:365:HIS:HD2	1.70	0.75
1:A:247:ASP:OD1	1:A:306:ARG:NH1	2.18	0.75
1:A:29:TRP:HE1	1:A:68:GLN:HE21	1.32	0.75
1:A:68:GLN:NE2	1:A:71:ASN:HD22	1.83	0.75
1:A:8:PRO:HG3	1:A:155:PHE:CE1	2.21	0.75
1:B:98:THR:O	1:B:118:ILE:N	2.17	0.75
1:A:219:GLU:OE2	5:A:1376:HOH:O	2.04	0.75
1:A:26:TRP:HE1	1:A:371:GLN:HE21	1.35	0.75
1:A:162:GLU:OE2	5:A:1007:HOH:O	2.04	0.75
1:B:294:GLN:HE22	1:B:301:ARG:H	1.34	0.74
1:A:26:TRP:HE1	1:A:371:GLN:HE21	1.36	0.74
1:B:272:GLN:NE2	5:B:1196:HOH:O	2.20	0.74
1:B:227:ASN:OD1	1:B:313:ASN:ND2	2.16	0.74
1:A:144:ARG:NH2	5:A:1213:HOH:O	2.19	0.74
1:A:279:PRO:HD3	1:A:311:TYR:CE2	2.22	0.74
1:B:9:ALA:HA	5:B:1263:HOH:O	1.69	0.74
1:B:286:GLU:O	1:B:290:SER:HB3	1.87	0.74
1:B:87:MSE:SE	1:B:90:SER:HB3	2.37	0.74
1:A:221:THR:HG21	3:A:903:EDO:H22	1.69	0.74
1:B:77:PRO:HB2	1:B:79:ASP:OD1	1.87	0.74
1:A:65:SER:HA	1:A:85:MSE:O	1.87	0.74
1:A:355:ARG:HA	1:A:358:VAL:HG12	1.69	0.74
1:A:18:GLU:OE1	1:A:365:HIS:HE1	1.70	0.74
1:B:282:LEU:HB3	1:B:307:LEU:CD2	2.14	0.74
1:A:183:ASN:O	5:A:1043:HOH:O	2.05	0.74
1:B:102:ARG:HA	1:B:103:LYS:HZ2	1.52	0.74
1:B:328:ASP:HB2	5:B:1061:HOH:O	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:THR:HA	1:A:211:LEU:O	1.87	0.74
1:B:101:VAL:HG21	3:B:913:EDO:H11	1.70	0.74
1:B:63:CYS:CB	1:B:87:MSE:HE1	2.16	0.73
1:A:112:ASN:ND2	1:A:112:ASN:N	2.33	0.73
1:A:144:ARG:HG2	1:A:154:ARG:HD2	1.70	0.73
1:B:321:ILE:O	1:B:322:ILE:C	2.23	0.73
3:A:908:EDO:H11	1:B:83:VAL:HB	1.70	0.73
1:B:241:TRP:O	1:B:278:ILE:HG12	1.88	0.73
1:B:154:ARG:HG2	1:B:154:ARG:NH1	2.02	0.73
1:B:37:ARG:HH11	1:B:37:ARG:HG3	1.52	0.73
1:B:160:ILE:H	1:B:187:ASN:HD21	1.34	0.73
1:A:31:GLU:O	5:A:1333:HOH:O	2.05	0.73
1:A:230:CYS:SG	1:A:312:VAL:HG22	2.28	0.73
1:A:261:SER:O	5:A:1315:HOH:O	2.05	0.73
1:B:230:CYS:SG	5:B:931:HOH:O	2.46	0.73
1:B:186:ARG:HH12	1:B:222:ASN:ND2	1.86	0.73
1:A:94:ASP:OD2	3:A:903:EDO:H12	1.89	0.73
1:A:5:ARG:HH12	1:A:158:SER:H	1.35	0.73
1:B:218:ASP:OD1	5:B:1129:HOH:O	2.05	0.73
1:B:61:THR:CG2	1:B:61:THR:O	2.28	0.73
1:B:7:SER:N	1:B:8:PRO:HD3	2.04	0.73
1:A:18:GLU:OE1	1:A:365:HIS:HE1	1.71	0.73
1:A:144:ARG:CZ	1:A:154:ARG:NH1	2.50	0.73
1:A:61:THR:CG2	1:A:81:ARG:HE	2.02	0.73
1:A:61:THR:HG22	1:A:81:ARG:HE	1.52	0.73
1:A:18:GLU:OE1	1:A:365:HIS:HE1	1.70	0.73
1:A:160:ILE:HD12	1:A:186:ARG:O	1.89	0.73
1:B:191:SER:H	1:B:194:GLN:NE2	1.86	0.73
1:B:191:SER:H	1:B:194:GLN:HE21	1.34	0.73
1:B:118:ILE:HA	1:B:155:PHE:O	1.87	0.73
1:A:113:ARG:HB3	1:A:374:GLU:OE2	1.89	0.73
1:B:104:ARG:HB2	1:B:114:ASN:HD21	1.53	0.72
1:B:174:CYS:SG	1:B:205:VAL:HG11	2.28	0.72
1:A:239:LEU:HD12	1:A:240:SER:N	2.04	0.72
1:B:22:HIS:H	1:B:318:ASN:ND2	1.78	0.72
1:B:22:HIS:H	1:B:318:ASN:ND2	1.83	0.72
1:B:178:GLU:HB2	1:B:212:PRO:HA	1.72	0.72
1:A:32:ARG:HD2	1:A:88:ASN:O	1.89	0.72
1:A:24:GLN:NE2	1:A:61:THR:HG23	2.03	0.72
1:B:57:PHE:HB3	1:B:318:ASN:O	1.90	0.72
1:A:329:PRO:HD2	5:A:1327:HOH:O	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:HIS:ND1	1:B:159:MSE:HG2	2.04	0.72
1:B:226:ASP:OD2	1:B:365:HIS:HD2	1.73	0.72
1:B:166:ILE:HG22	1:B:176:VAL:CG1	2.20	0.72
1:B:307:LEU:HD21	1:B:359:LEU:HD23	1.71	0.72
1:A:68:GLN:HE22	1:A:71:ASN:HD22	1.36	0.72
1:A:160:ILE:CD1	1:A:160:ILE:N	2.51	0.72
1:B:197:GLU:OE1	5:B:1207:HOH:O	2.06	0.72
1:B:200:LYS:HE3	1:B:208:PHE:HE1	1.55	0.72
1:B:154:ARG:HG2	1:B:154:ARG:HH11	1.54	0.72
1:A:21:SER:HA	1:A:318:ASN:OD1	1.89	0.72
1:A:160:ILE:H	1:A:187:ASN:HD21	1.35	0.72
1:B:222:ASN:HD21	3:B:911:EDO:C1	2.03	0.72
1:A:190:MSE:HE2	1:A:195:ILE:CG1	2.19	0.72
1:B:229:CYS:HA	1:B:312:VAL:HG21	1.70	0.72
1:B:7:SER:O	1:B:10:GLU:HB2	1.90	0.72
1:A:144:ARG:NH2	5:A:1244:HOH:O	2.16	0.72
1:B:226:ASP:OD2	1:B:365:HIS:HD2	1.71	0.71
1:A:236:VAL:HG22	1:A:272:GLN:HB3	1.72	0.71
1:B:185:ASN:HD21	1:B:222:ASN:ND2	1.87	0.71
1:B:22:HIS:H	1:B:318:ASN:HD21	1.39	0.71
1:B:23:ALA:HB2	1:B:373:ALA:HA	1.72	0.71
1:B:150:GLU:OE1	5:B:1240:HOH:O	2.08	0.71
1:B:275:LYS:NZ	5:B:1171:HOH:O	2.19	0.71
1:B:324:PRO:HB3	1:B:363:ASN:ND2	2.05	0.71
1:B:29:TRP:HE1	1:B:68:GLN:HE21	1.39	0.71
1:B:22:HIS:H	1:B:318:ASN:HD21	1.37	0.71
1:A:297:GLU:OE1	1:A:297:GLU:HA	1.91	0.71
1:B:132:CYS:SG	1:B:133:TYR:N	2.63	0.71
1:A:190:MSE:HE3	1:A:194:GLN:C	2.11	0.71
1:A:190:MSE:CE	1:A:195:ILE:HA	2.20	0.71
2:A:802:MG:MG	5:A:1040:HOH:O	1.34	0.71
1:A:29:TRP:CZ2	1:A:44:GLN:HG2	2.25	0.71
1:A:284:MSE:HB2	1:A:305:THR:HB	1.71	0.71
1:A:218:ASP:OD2	5:A:1292:HOH:O	2.08	0.71
1:A:171:GLU:OE2	1:A:269:ARG:NH2	2.22	0.71
1:A:246:THR:OG1	3:A:910:EDO:H21	1.91	0.71
1:B:67:ALA:HB3	5:B:1058:HOH:O	1.89	0.71
1:A:356:GLU:OE1	5:A:1070:HOH:O	2.07	0.71
1:B:100:ILE:HD13	1:B:118:ILE:HD11	1.73	0.71
1:B:22:HIS:H	1:B:318:ASN:ND2	1.88	0.71
1:B:91:TRP:CZ3	1:B:362:GLY:HA3	2.26	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLY:O	1:A:47:PHE:CE2	2.44	0.71
1:B:162:GLU:OE2	1:B:224:HIS:HE1	1.74	0.71
1:A:68:GLN:NE2	1:A:71:ASN:HD22	1.89	0.71
1:A:160:ILE:H	1:A:160:ILE:CD1	2.04	0.71
1:B:71:ASN:N	5:B:953:HOH:O	2.04	0.71
1:B:22:HIS:N	1:B:318:ASN:HD21	1.89	0.71
1:B:66:PRO:HB3	1:B:84:GLU:OE1	1.90	0.71
1:B:334:GLU:O	1:B:338:VAL:HG23	1.91	0.71
1:A:121:ASN:HB3	1:A:160:ILE:HA	1.72	0.70
1:B:26:TRP:HH2	1:B:149:LEU:HD23	1.55	0.70
1:B:68:GLN:NE2	1:B:71:ASN:HD22	1.87	0.70
1:B:55:SER:HB3	1:B:80:ILE:HD11	1.72	0.70
1:A:226:ASP:OD2	1:A:365:HIS:HD2	1.73	0.70
1:B:91:TRP:CE3	1:B:367:ILE:HG22	2.27	0.70
1:B:150:GLU:HG2	1:B:371:GLN:HE22	1.57	0.70
1:B:103:LYS:O	1:B:104:ARG:O	2.09	0.70
1:B:141:LEU:HA	1:B:144:ARG:HD2	1.73	0.70
1:B:215:LEU:HB3	1:B:218:ASP:OD1	1.92	0.70
1:B:132:CYS:SG	1:B:133:TYR:CD1	2.81	0.70
1:B:50:VAL:HG11	1:B:367:ILE:HD11	1.73	0.70
1:B:113:ARG:NH1	5:B:1101:HOH:O	2.14	0.70
1:A:37:ARG:HH11	1:A:38:HIS:HD2	1.39	0.70
1:B:168:VAL:HG13	1:B:174:CYS:SG	2.27	0.70
1:B:29:TRP:HE1	1:B:68:GLN:HE21	1.38	0.70
1:A:35:ASN:HD21	1:A:301:ARG:HH21	1.39	0.70
1:B:211:LEU:HD22	1:B:211:LEU:N	2.05	0.70
1:B:104:ARG:CB	1:B:114:ASN:HD21	2.05	0.70
1:A:190:MSE:CE	1:A:195:ILE:N	2.55	0.70
1:A:144:ARG:NE	1:A:154:ARG:NE	2.39	0.70
1:A:294:GLN:HG2	5:A:1264:HOH:O	1.90	0.70
1:A:311:TYR:CD1	1:A:324:PRO:HG2	2.27	0.70
1:B:220:ASP:O	3:B:911:EDO:C1	2.40	0.70
1:B:197:GLU:HG3	1:B:201:LYS:HE2	1.73	0.70
1:B:18:GLU:OE2	1:B:365:HIS:HE1	1.74	0.70
1:A:183:ASN:HB3	1:A:185:ASN:OD1	1.92	0.69
1:A:24:GLN:NE2	1:B:151:ARG:HH22	1.91	0.69
1:B:140:LEU:HD23	5:B:1252:HOH:O	1.92	0.69
1:B:229:CYS:HB2	1:B:238:LEU:O	1.92	0.69
1:B:31:GLU:OE2	5:B:1058:HOH:O	2.10	0.69
1:B:120:TRP:CZ3	1:B:159:MSE:HE2	2.28	0.69
1:A:178:GLU:HG2	1:A:182:LEU:CD1	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:CYS:HA	1:B:222:ASN:HB3	1.73	0.69
1:B:235:GLY:N	5:B:925:HOH:O	2.20	0.69
1:A:191:SER:H	1:A:194:GLN:HE21	1.38	0.69
1:B:145:LYS:NZ	5:B:958:HOH:O	2.18	0.69
1:B:230:CYS:SG	5:B:930:HOH:O	2.50	0.69
1:B:103:LYS:HD3	1:B:103:LYS:H	1.56	0.69
1:B:222:ASN:HD21	3:B:911:EDO:H11	1.53	0.69
1:B:138:HIS:HD2	5:B:1082:HOH:O	1.74	0.69
1:B:7:SER:N	1:B:8:PRO:CD	2.55	0.69
1:B:244:ASP:OD2	5:B:1066:HOH:O	2.10	0.69
1:B:179:GLU:OE2	5:B:1001:HOH:O	2.09	0.69
1:B:68:GLN:HE22	1:B:71:ASN:HD22	1.41	0.69
1:A:94:ASP:OD2	3:A:903:EDO:H12	1.92	0.69
1:B:33:GLN:HE21	1:B:39:ASN:HA	1.58	0.69
1:A:261:SER:O	5:A:1311:HOH:O	2.10	0.69
1:A:34:ASP:HA	1:A:293:THR:HB	1.75	0.69
1:A:190:MSE:HA	1:A:194:GLN:NE2	2.07	0.69
1:B:58:GLU:HB3	1:B:318:ASN:OD1	1.92	0.69
1:A:44:GLN:HE22	1:A:71:ASN:HD21	1.41	0.69
1:A:162:GLU:OE1	5:A:1023:HOH:O	2.08	0.69
1:A:144:ARG:HG2	1:A:154:ARG:CD	2.23	0.69
1:B:103:LYS:H	1:B:103:LYS:NZ	1.90	0.69
1:B:332:ASP:O	1:B:336:ILE:HG12	1.91	0.69
3:A:908:EDO:H21	1:B:84:GLU:O	1.93	0.69
1:B:162:GLU:OE2	1:B:224:HIS:CE1	2.46	0.69
1:B:186:ARG:NH1	1:B:222:ASN:ND2	2.40	0.69
1:A:100:ILE:HG13	1:A:116:ALA:HB3	1.75	0.69
1:A:127:GLY:HA2	1:A:136:TRP:CH2	2.29	0.68
1:B:238:LEU:HD21	1:B:342:THR:HG21	1.75	0.68
1:B:68:GLN:HE22	1:B:71:ASN:HD22	1.41	0.68
1:A:24:GLN:NE2	1:B:151:ARG:NH2	2.41	0.68
1:A:284:MSE:CE	5:A:1143:HOH:O	2.39	0.68
1:A:160:ILE:N	1:A:160:ILE:HD12	2.08	0.68
1:B:282:LEU:C	1:B:307:LEU:HD13	2.14	0.68
1:B:138:HIS:HD2	5:B:1085:HOH:O	1.74	0.68
1:A:35:ASN:HD21	1:A:301:ARG:NH2	1.90	0.68
1:A:59:PRO:HB3	5:A:1409:HOH:O	1.92	0.68
1:A:224:HIS:HB2	5:A:1200:HOH:O	1.92	0.68
1:B:60:VAL:O	1:B:80:ILE:HG23	1.93	0.68
1:A:151:ARG:HH22	1:B:24:GLN:NE2	1.91	0.68
1:B:144:ARG:HE	1:B:154:ARG:NE	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HD13	5:A:1207:HOH:O	1.93	0.68
1:A:37:ARG:HD2	5:A:1124:HOH:O	1.93	0.68
1:B:251:GLU:CD	5:B:1256:HOH:O	2.32	0.68
1:A:366:CYS:SG	1:A:367:ILE:HG23	2.34	0.68
1:A:249:GLN:HG2	1:A:278:ILE:HD13	1.74	0.68
1:A:216:TYR:HB2	1:A:252:ARG:HD2	1.73	0.68
1:B:88:ASN:ND2	1:B:139:ASP:H	1.92	0.68
1:B:219:GLU:O	3:B:911:EDO:H22	1.92	0.68
1:B:31:GLU:OE1	5:B:1079:HOH:O	2.11	0.68
1:B:169:ASP:OD1	5:B:999:HOH:O	2.12	0.68
1:A:33:GLN:HG2	1:A:39:ASN:HA	1.75	0.68
1:B:220:ASP:OD2	5:B:1230:HOH:O	2.06	0.68
1:A:121:ASN:HD22	1:A:122:PHE:H	1.42	0.68
1:B:160:ILE:H	1:B:187:ASN:HD21	1.39	0.68
1:A:248:PRO:O	1:A:249:GLN:C	2.31	0.68
1:B:18:GLU:OE2	1:B:365:HIS:HE1	1.76	0.68
1:A:280:GLU:HG2	1:A:328:ASP:OD1	1.93	0.68
1:A:24:GLN:NE2	1:B:151:ARG:HH22	1.90	0.68
1:A:258:SER:HB3	5:A:1327:HOH:O	1.94	0.68
1:A:311:TYR:HA	1:A:324:PRO:HG3	1.76	0.68
1:B:196:GLU:OE1	5:B:1110:HOH:O	2.12	0.68
1:A:94:ASP:OD2	3:A:903:EDO:H12	1.94	0.68
1:B:273:VAL:O	5:B:958:HOH:O	2.11	0.68
1:A:248:PRO:O	5:A:1105:HOH:O	2.11	0.68
1:A:285:THR:HG22	5:A:1302:HOH:O	1.93	0.68
1:A:85:MSE:HG3	5:A:1212:HOH:O	1.94	0.67
1:B:226:ASP:OD2	1:B:365:HIS:CD2	2.47	0.67
1:B:219:GLU:OE1	5:B:1023:HOH:O	2.12	0.67
1:A:145:LYS:NZ	1:B:84:GLU:OE2	2.23	0.67
1:B:103:LYS:NZ	1:B:103:LYS:H	1.92	0.67
1:B:162:GLU:OE2	1:B:224:HIS:HE1	1.77	0.67
1:B:125:TRP:O	3:B:911:EDO:H12	1.94	0.67
1:B:22:HIS:H	1:B:318:ASN:HD21	1.42	0.67
1:B:33:GLN:HE21	1:B:39:ASN:CA	2.05	0.67
1:A:18:GLU:OE1	1:A:365:HIS:HE1	1.76	0.67
1:A:211:LEU:HD13	1:A:256:ALA:HB1	1.75	0.67
1:A:191:SER:HB2	1:A:193:GLU:OE1	1.94	0.67
1:A:219:GLU:OE2	5:A:1380:HOH:O	2.12	0.67
1:B:88:ASN:HD21	1:B:138:HIS:H	1.41	0.67
1:B:120:TRP:CZ2	1:B:203:LEU:HD21	2.30	0.67
1:B:220:ASP:OD2	5:B:1226:HOH:O	2.12	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:TYR:CE1	1:B:317:ALA:HB2	2.30	0.67
1:A:100:ILE:HG12	1:A:116:ALA:O	1.95	0.67
1:B:103:LYS:H	1:B:103:LYS:CD	2.06	0.67
1:A:242:THR:CG2	1:A:250:TYR:HA	2.24	0.67
1:A:279:PRO:HA	1:A:331:ARG:CB	2.24	0.67
1:B:18:GLU:OE2	1:B:365:HIS:HE1	1.77	0.67
1:A:190:MSE:CE	1:A:195:ILE:CA	2.72	0.67
1:B:282:LEU:HB3	1:B:307:LEU:HD22	1.77	0.67
1:B:97:PRO:HB3	1:B:143:SER:HB3	1.77	0.67
1:B:226:ASP:OD2	1:B:365:HIS:HD2	1.77	0.67
1:B:231:PHE:HB2	5:B:920:HOH:O	1.94	0.67
1:A:366:CYS:HB2	3:A:903:EDO:H11	1.75	0.67
1:B:222:ASN:ND2	3:B:911:EDO:H11	2.09	0.67
1:A:366:CYS:SG	1:A:367:ILE:HG23	2.33	0.67
1:A:15:MSE:HE2	1:A:203:LEU:HB3	1.75	0.67
1:B:324:PRO:HB2	1:B:326:PHE:CE2	2.29	0.67
1:B:363:ASN:ND2	1:B:364:ILE:H	1.92	0.67
1:B:279:PRO:HA	1:B:331:ARG:HG3	1.77	0.67
1:B:131:GLY:HA2	3:B:911:EDO:O1	1.95	0.67
1:B:279:PRO:HA	1:B:331:ARG:HG3	1.75	0.67
1:B:352:GLU:OE1	5:B:1121:HOH:O	2.12	0.67
1:A:190:MSE:CE	1:A:194:GLN:C	2.63	0.67
1:B:226:ASP:OD2	1:B:365:HIS:HD2	1.77	0.67
1:B:354:ALA:O	1:B:358:VAL:HG23	1.95	0.66
1:A:311:TYR:HD1	1:A:324:PRO:HG2	1.58	0.66
1:B:156:GLN:H	3:B:912:EDO:H21	1.60	0.66
1:A:120:TRP:CD2	1:A:161:LEU:HB3	2.31	0.66
1:B:102:ARG:HA	1:B:103:LYS:HZ2	1.61	0.66
1:B:150:GLU:OE1	5:B:1240:HOH:O	2.12	0.66
1:B:160:ILE:N	1:B:187:ASN:HD21	1.91	0.66
1:B:7:SER:HA	1:B:10:GLU:OE1	1.94	0.66
1:A:227:ASN:OD1	1:A:310:SER:HB2	1.95	0.66
1:B:186:ARG:HH12	1:B:222:ASN:ND2	1.91	0.66
1:B:18:GLU:OE2	1:B:365:HIS:HE1	1.78	0.66
1:B:19:TRP:CD1	3:B:905:EDO:H21	2.30	0.66
1:A:216:TYR:H	1:A:249:GLN:NE2	1.92	0.66
1:A:225:ILE:HD11	1:A:229:CYS:SG	2.36	0.66
1:A:185:ASN:HA	3:A:906:EDO:H12	1.78	0.66
1:A:91:TRP:CZ3	1:A:362:GLY:HA3	2.31	0.66
1:A:351:ILE:HB	1:A:364:ILE:HD11	1.76	0.66
1:B:363:ASN:ND2	1:B:364:ILE:H	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:OD2	5:A:1203:HOH:O	2.11	0.66
1:A:59:PRO:HA	5:A:1078:HOH:O	1.96	0.66
1:B:289:SER:OG	1:B:302:LEU:HA	1.95	0.66
1:B:88:ASN:HD22	1:B:139:ASP:H	1.42	0.66
1:B:329:PRO:HD2	5:B:1048:HOH:O	1.96	0.66
1:B:50:VAL:CG1	1:B:367:ILE:HD11	2.25	0.66
1:B:88:ASN:HD21	1:B:138:HIS:HB2	1.61	0.66
1:A:363:ASN:CG	1:A:364:ILE:N	2.49	0.66
1:B:228:MSE:HE3	1:B:228:MSE:O	1.96	0.66
1:B:320:GLY:HA2	1:B:347:SER:O	1.95	0.66
1:A:88:ASN:N	1:A:139:ASP:OD2	2.18	0.66
1:A:57:PHE:HB3	1:A:318:ASN:O	1.95	0.66
1:A:94:ASP:HB3	1:A:162:GLU:HB3	1.76	0.66
1:B:278:ILE:O	1:B:278:ILE:HG13	1.95	0.66
1:A:217:GLY:N	3:A:907:EDO:O2	2.25	0.66
1:B:120:TRP:CH2	1:B:203:LEU:HD21	2.30	0.66
1:B:234:PRO:HD2	5:B:1055:HOH:O	1.96	0.66
1:A:9:ALA:CA	5:A:1310:HOH:O	2.43	0.66
1:B:138:HIS:HD2	5:B:1081:HOH:O	1.78	0.66
1:A:46:VAL:HG21	1:A:356:GLU:HB2	1.76	0.66
1:A:78:GLU:OE1	5:A:1156:HOH:O	2.14	0.66
1:A:44:GLN:NE2	1:A:75:GLN:OE1	2.29	0.66
1:A:77:PRO:HD2	1:A:80:ILE:HD12	1.77	0.66
1:B:329:PRO:HG2	5:B:1048:HOH:O	1.95	0.65
1:A:191:SER:HB3	1:A:194:GLN:HE21	1.46	0.65
1:A:226:ASP:OD2	1:A:365:HIS:HD2	1.79	0.65
1:A:49:GLY:HA2	1:A:52:LYS:HE3	1.78	0.65
1:A:83:VAL:HB	3:A:908:EDO:O1	1.97	0.65
1:B:160:ILE:H	1:B:187:ASN:HD21	1.42	0.65
1:B:37:ARG:HH11	1:B:38:HIS:CE1	2.15	0.65
1:A:35:ASN:HD22	1:A:301:ARG:NE	1.95	0.65
1:B:160:ILE:H	1:B:187:ASN:HD21	1.43	0.65
1:A:160:ILE:HD12	1:A:186:ARG:O	1.97	0.65
1:B:26:TRP:CH2	1:B:149:LEU:HD23	2.30	0.65
1:B:12:GLY:HA3	5:B:1270:HOH:O	1.97	0.65
1:B:88:ASN:N	1:B:88:ASN:HD22	1.95	0.65
1:A:35:ASN:ND2	1:A:301:ARG:NE	2.44	0.65
1:A:29:TRP:HE1	1:A:68:GLN:NE2	1.94	0.65
1:B:156:GLN:H	3:B:912:EDO:H21	1.62	0.65
1:A:230:CYS:SG	5:A:1014:HOH:O	2.55	0.65
1:B:87:MSE:HE1	1:B:92:PHE:CZ	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLN:NE2	1:B:71:ASN:HD22	1.93	0.65
1:B:88:ASN:ND2	1:B:139:ASP:H	1.93	0.65
1:B:355:ARG:HA	1:B:358:VAL:HB	1.78	0.65
1:B:166:ILE:HG22	1:B:176:VAL:HG12	1.78	0.65
1:A:218:ASP:OD2	5:A:1204:HOH:O	2.15	0.65
1:B:70:GLU:OE1	5:B:1104:HOH:O	2.14	0.65
1:B:313:ASN:HB3	1:B:363:ASN:HB3	1.79	0.65
1:B:226:ASP:OD2	1:B:365:HIS:HD2	1.80	0.65
1:B:373:ALA:O	1:B:375:PRO:HD3	1.97	0.65
1:B:33:GLN:HE21	1:B:39:ASN:ND2	1.95	0.64
3:A:908:EDO:O1	1:B:149:LEU:HD13	1.96	0.64
1:A:191:SER:N	1:A:194:GLN:NE2	2.41	0.64
1:A:286:GLU:HA	1:A:303:ALA:HB2	1.80	0.64
1:A:190:MSE:HE1	1:A:195:ILE:CA	2.27	0.64
1:A:242:THR:O	1:A:242:THR:HG23	1.98	0.64
1:B:162:GLU:OE2	1:B:224:HIS:HE1	1.81	0.64
1:A:24:GLN:HE22	1:A:61:THR:HG23	1.61	0.64
1:A:219:GLU:OE2	5:A:1375:HOH:O	2.13	0.64
1:B:363:ASN:ND2	1:B:364:ILE:H	1.94	0.64
1:A:38:HIS:CD2	5:A:1124:HOH:O	2.50	0.64
1:B:282:LEU:CD1	1:B:282:LEU:N	2.58	0.64
1:B:7:SER:N	1:B:8:PRO:CD	2.61	0.64
1:A:24:GLN:HE22	1:B:151:ARG:HH22	1.45	0.64
1:A:157:HIS:CG	1:A:159:MSE:HG2	2.32	0.64
1:B:211:LEU:HD11	1:B:229:CYS:SG	2.38	0.64
1:B:307:LEU:N	1:B:307:LEU:HD12	2.12	0.64
1:A:134:ASN:ND2	1:A:297:GLU:CA	2.61	0.64
1:A:26:TRP:HE1	1:A:371:GLN:HE21	1.46	0.64
1:A:221:THR:HB	5:A:1204:HOH:O	1.96	0.64
1:A:299:ILE:HG13	1:A:301:ARG:HH12	1.62	0.64
1:A:30:PRO:HD3	1:A:47:PHE:CD2	2.32	0.64
1:B:19:TRP:CD1	3:B:905:EDO:H21	2.33	0.64
1:B:225:ILE:CD1	1:B:225:ILE:CB	2.70	0.64
1:B:212:PRO:HD3	1:B:259:VAL:HG21	1.78	0.63
1:B:121:ASN:HD22	1:B:160:ILE:HG12	1.63	0.63
1:A:133:TYR:HD1	1:A:134:ASN:O	1.81	0.63
1:A:234:PRO:HB3	1:A:269:ARG:NH2	2.13	0.63
1:A:32:ARG:HG2	5:A:1044:HOH:O	1.98	0.63
1:B:160:ILE:H	1:B:187:ASN:HD21	1.46	0.63
1:B:131:GLY:O	1:B:299:ILE:HD13	1.98	0.63
1:B:191:SER:H	1:B:194:GLN:HE21	1.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:NH1	5:A:1358:HOH:O	2.28	0.63
1:B:133:TYR:HA	1:B:297:GLU:O	1.98	0.63
1:B:25:THR:OG1	1:B:58:GLU:OE1	2.16	0.63
1:B:267:ARG:HB2	1:B:269:ARG:NE	2.13	0.63
1:B:46:VAL:CG1	1:B:357:ILE:HD11	2.28	0.63
1:A:41:LEU:HD11	5:A:1225:HOH:O	1.92	0.63
1:B:99:PHE:HA	1:B:117:GLY:HA2	1.79	0.63
1:B:166:ILE:HA	1:B:176:VAL:HG12	1.79	0.63
1:A:149:LEU:CD2	1:B:149:LEU:CD1	2.73	0.63
1:B:144:ARG:NH1	1:B:156:GLN:NE2	2.42	0.63
1:B:280:GLU:O	1:B:282:LEU:CD1	2.47	0.63
1:B:7:SER:HB2	1:B:155:PHE:CD1	2.32	0.63
1:B:123:ASN:OD1	1:B:160:ILE:HD13	1.99	0.63
1:B:112:ASN:OD1	1:B:112:ASN:N	2.31	0.63
1:B:29:TRP:HE1	1:B:68:GLN:HE21	1.46	0.63
1:B:200:LYS:HG2	1:B:205:VAL:O	1.98	0.63
1:A:144:ARG:HD3	1:B:69:TRP:HZ3	1.62	0.63
1:A:178:GLU:HG2	1:A:182:LEU:HD11	1.79	0.63
1:A:50:VAL:HG22	1:A:351:ILE:HG13	1.80	0.63
1:B:281:PRO:C	1:B:282:LEU:HD12	2.18	0.63
1:B:33:GLN:HE21	1:B:39:ASN:HA	1.63	0.63
1:A:91:TRP:CZ3	1:A:362:GLY:HA3	2.34	0.63
1:A:119:ASP:CG	1:A:143:SER:HB3	2.19	0.63
1:B:7:SER:N	1:B:8:PRO:CD	2.61	0.63
1:A:329:PRO:HD2	5:A:1328:HOH:O	1.97	0.63
1:A:117:GLY:HA3	1:A:147:LEU:HD21	1.79	0.63
1:A:113:ARG:HB2	1:A:374:GLU:OE2	1.98	0.63
1:A:144:ARG:NE	1:A:154:ARG:HE	1.96	0.63
1:A:130:ASP:CB	1:A:185:ASN:HD22	2.12	0.63
1:A:26:TRP:HE1	1:A:371:GLN:HE21	1.46	0.63
1:B:222:ASN:HD21	3:B:911:EDO:H12	1.61	0.63
1:B:124:ALA:O	1:B:132:CYS:SG	2.57	0.63
1:B:279:PRO:HB2	1:B:282:LEU:HD11	1.81	0.63
1:B:219:GLU:O	3:B:911:EDO:H22	1.99	0.62
1:B:282:LEU:HB3	1:B:307:LEU:CD2	2.28	0.62
1:A:185:ASN:HD21	1:A:222:ASN:ND2	1.96	0.62
1:A:314:PHE:O	1:A:365:HIS:HB2	1.99	0.62
1:A:176:VAL:C	1:A:225:ILE:HD13	2.20	0.62
1:A:190:MSE:HE1	1:A:198:GLU:HG2	1.80	0.62
1:A:278:ILE:HB	1:A:279:PRO:HD2	1.81	0.62
1:B:88:ASN:HD21	1:B:138:HIS:H	1.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:HG3	1:A:201:LYS:HE2	1.80	0.62
1:A:44:GLN:NE2	1:A:71:ASN:HD21	1.97	0.62
1:A:52:LYS:HD3	1:A:77:PRO:HD3	1.80	0.62
1:B:269:ARG:NH2	5:B:998:HOH:O	2.29	0.62
1:A:114:ASN:N	1:A:374:GLU:OE2	2.25	0.62
1:B:112:ASN:ND2	5:B:1249:HOH:O	2.31	0.62
1:A:215:LEU:HD22	1:A:227:ASN:ND2	2.13	0.62
1:A:190:MSE:HE1	1:A:198:GLU:CG	2.30	0.62
1:B:220:ASP:O	3:B:911:EDO:O1	2.17	0.62
1:B:219:GLU:O	3:B:911:EDO:H22	2.00	0.62
1:B:123:ASN:ND2	1:B:126:GLY:H	1.97	0.62
1:A:104:ARG:HB3	1:A:104:ARG:NH2	2.15	0.62
1:A:229:CYS:CA	1:A:312:VAL:HG21	2.29	0.62
1:B:226:ASP:OD2	1:B:365:HIS:HD2	1.81	0.62
3:A:908:EDO:H21	1:B:84:GLU:O	2.00	0.62
1:B:331:ARG:HH11	1:B:331:ARG:HG3	1.64	0.62
1:A:68:GLN:HE22	1:A:71:ASN:HD22	1.46	0.62
1:A:5:ARG:HH12	1:A:158:SER:H	1.46	0.62
1:A:226:ASP:OD2	1:A:365:HIS:CD2	2.49	0.62
1:A:149:LEU:HD23	1:B:83:VAL:HG12	1.82	0.62
1:A:132:CYS:SG	1:A:220:ASP:HB3	2.39	0.62
1:A:5:ARG:HH12	1:A:158:SER:H	1.47	0.62
1:A:41:LEU:HD12	1:A:44:GLN:OE1	1.99	0.62
1:B:123:ASN:ND2	1:B:126:GLY:H	1.97	0.62
1:B:103:LYS:HD2	5:B:1266:HOH:O	1.99	0.62
1:A:226:ASP:OD2	1:A:365:HIS:HD2	1.82	0.62
1:A:39:ASN:O	1:A:41:LEU:HD13	2.00	0.62
1:A:118:ILE:HG21	1:A:120:TRP:CH2	2.34	0.62
1:B:113:ARG:NE	1:B:374:GLU:OE1	2.30	0.62
1:B:7:SER:HB2	1:B:155:PHE:HE1	1.59	0.62
1:B:219:GLU:O	3:B:911:EDO:H22	2.00	0.62
1:B:103:LYS:CD	5:B:1266:HOH:O	2.47	0.62
1:B:136:TRP:O	1:B:140:LEU:HG	1.99	0.62
1:B:219:GLU:O	3:B:911:EDO:H22	2.00	0.61
1:A:70:GLU:HG3	5:A:1117:HOH:O	2.00	0.61
1:A:284:MSE:HE2	1:A:359:LEU:CD2	2.30	0.61
1:B:125:TRP:O	3:B:911:EDO:C1	2.48	0.61
1:A:160:ILE:H	1:A:187:ASN:HD21	1.47	0.61
1:B:32:ARG:HG3	1:B:35:ASN:HB3	1.80	0.61
1:B:55:SER:HB3	1:B:80:ILE:HD11	1.81	0.61
1:A:363:ASN:H	1:A:366:CYS:HG	1.46	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLU:O	1:B:282:LEU:HD13	2.01	0.61
1:B:37:ARG:NH1	1:B:38:HIS:CE1	2.68	0.61
1:A:175:LEU:HD23	1:A:231:PHE:CE2	2.34	0.61
1:A:151:ARG:HH22	1:B:24:GLN:NE2	1.97	0.61
1:B:250:TYR:CZ	1:B:254:VAL:HG21	2.34	0.61
1:A:178:GLU:HB2	1:A:212:PRO:HA	1.81	0.61
1:B:156:GLN:H	3:B:912:EDO:C2	2.12	0.61
1:B:284:MSE:CE	1:B:359:LEU:HD22	2.30	0.61
1:B:185:ASN:OD1	1:B:222:ASN:ND2	2.32	0.61
1:B:138:HIS:O	1:B:139:ASP:C	2.36	0.61
1:A:327:GLY:N	1:A:332:ASP:OD2	2.29	0.61
1:A:313:ASN:ND2	1:A:365:HIS:H	1.96	0.61
1:B:23:ALA:CB	1:B:373:ALA:HA	2.27	0.61
1:A:11:HIS:CD2	1:A:13:TYR:HE2	2.17	0.61
1:B:32:ARG:HH21	1:B:297:GLU:HB3	1.65	0.61
1:A:363:ASN:CA	1:A:366:CYS:SG	2.88	0.61
1:A:284:MSE:CG	1:A:302:LEU:O	2.49	0.61
1:B:230:CYS:SG	1:B:314:PHE:CE2	2.93	0.61
1:B:186:ARG:HH12	1:B:222:ASN:ND2	1.93	0.61
1:A:7:SER:HB2	1:A:201:LYS:HB3	1.82	0.61
1:A:226:ASP:OD2	1:A:365:HIS:HD2	1.84	0.61
1:B:324:PRO:HB3	1:B:363:ASN:HD21	1.66	0.61
1:A:352:GLU:OE2	5:A:1274:HOH:O	2.16	0.61
1:A:120:TRP:CG	1:A:161:LEU:HB3	2.35	0.61
1:B:186:ARG:HH12	1:B:222:ASN:HD22	1.48	0.61
1:B:186:ARG:HH12	1:B:222:ASN:ND2	1.95	0.61
1:B:186:ARG:NH1	1:B:222:ASN:HD22	1.92	0.61
1:B:68:GLN:HE22	1:B:71:ASN:HD22	1.49	0.61
1:B:280:GLU:O	1:B:282:LEU:HD12	2.00	0.61
1:A:102:ARG:NE	1:A:113:ARG:O	2.33	0.61
1:B:280:GLU:O	1:B:282:LEU:HD13	2.01	0.61
1:B:76:LEU:HD22	1:B:80:ILE:HG21	1.82	0.61
1:B:88:ASN:HD21	1:B:138:HIS:H	1.47	0.61
1:A:181:LEU:O	1:A:182:LEU:HD23	2.01	0.61
1:A:44:GLN:HE22	1:A:71:ASN:HD21	1.49	0.61
1:A:284:MSE:O	1:A:304:GLY:N	2.27	0.61
1:A:104:ARG:CB	1:A:104:ARG:NH2	2.64	0.61
1:B:125:TRP:HB2	1:B:132:CYS:HG	1.66	0.61
1:A:26:TRP:HE1	1:A:371:GLN:HE21	1.49	0.60
1:B:222:ASN:HD21	3:B:911:EDO:H11	1.66	0.60
1:B:284:MSE:CE	1:B:301:ARG:HH11	2.13	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:CB	1:B:114:ASN:HD21	1.97	0.60
1:A:138:HIS:CD2	5:A:1218:HOH:O	2.53	0.60
1:A:35:ASN:HD21	1:A:301:ARG:NH2	1.98	0.60
1:A:133:TYR:HE1	1:A:136:TRP:HB3	1.66	0.60
1:B:31:GLU:HG2	5:B:1142:HOH:O	2.01	0.60
1:B:11:HIS:HB3	1:B:102:ARG:HH21	1.64	0.60
1:A:133:TYR:OH	1:A:139:ASP:OD1	2.13	0.60
1:A:91:TRP:CZ3	1:A:366:CYS:SG	2.94	0.60
1:A:91:TRP:CZ3	1:A:367:ILE:HG23	2.36	0.60
1:B:41:LEU:HB3	1:B:45:ARG:HH22	1.66	0.60
1:B:261:SER:HB3	5:B:1191:HOH:O	2.01	0.60
1:A:160:ILE:CD1	5:A:1207:HOH:O	2.47	0.60
1:A:363:ASN:ND2	1:A:364:ILE:H	1.99	0.60
1:A:324:PRO:HD3	1:A:364:ILE:HD12	1.82	0.60
1:A:355:ARG:O	1:A:359:LEU:HG	2.01	0.60
1:A:187:ASN:HB3	1:A:190:MSE:SE	2.51	0.60
1:B:222:ASN:HD21	3:B:911:EDO:C1	2.15	0.60
1:B:333:LYS:O	1:B:336:ILE:HB	2.01	0.60
1:A:44:GLN:NE2	1:A:71:ASN:HD21	2.00	0.60
1:A:8:PRO:HB3	1:A:100:ILE:HD12	1.84	0.60
1:B:112:ASN:HD22	1:B:113:ARG:H	1.49	0.60
1:A:214:GLY:HA3	1:A:223:GLY:O	2.01	0.60
1:B:41:LEU:O	1:B:45:ARG:HG3	2.02	0.60
1:B:103:LYS:N	1:B:103:LYS:HZ2	1.98	0.60
1:A:97:PRO:HD2	1:A:369:GLN:HG2	1.83	0.60
1:B:15:MSE:HG2	1:B:168:VAL:HG21	1.82	0.60
1:A:123:ASN:ND2	1:A:126:GLY:H	2.00	0.60
1:A:229:CYS:HA	1:A:238:LEU:O	2.01	0.60
1:A:246:THR:OG1	3:A:910:EDO:H21	2.02	0.60
1:A:124:ALA:O	1:A:131:GLY:HA2	2.02	0.60
1:A:104:ARG:HA	1:A:114:ASN:HD21	1.66	0.60
1:A:284:MSE:HE2	1:A:359:LEU:HD22	1.83	0.60
1:B:86:SER:HB2	1:B:145:LYS:NZ	2.17	0.60
1:A:369:GLN:HE21	1:A:370:GLN:NE2	2.00	0.60
1:A:104:ARG:CB	1:A:104:ARG:HH21	2.09	0.60
1:B:179:GLU:HG2	1:B:222:ASN:O	2.01	0.60
1:B:156:GLN:H	3:B:912:EDO:H21	1.67	0.60
1:A:247:ASP:OD1	1:A:306:ARG:NH1	2.33	0.60
1:A:35:ASN:ND2	1:A:301:ARG:HE	1.99	0.60
1:A:216:TYR:H	1:A:249:GLN:HE22	1.50	0.59
1:B:369:GLN:NE2	5:B:932:HOH:O	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASN:OD1	1:B:365:HIS:HB3	2.02	0.59
1:B:125:TRP:HB2	1:B:132:CYS:SG	2.41	0.59
1:A:248:PRO:O	1:A:250:TYR:N	2.35	0.59
1:B:261:SER:O	5:B:997:HOH:O	2.16	0.59
1:A:112:ASN:HD22	1:A:112:ASN:N	2.00	0.59
1:B:7:SER:N	1:B:8:PRO:HD3	2.16	0.59
1:B:91:TRP:CZ3	1:B:362:GLY:HA3	2.37	0.59
1:A:150:GLU:HG3	1:A:371:GLN:HE22	1.67	0.59
1:B:171:GLU:HG2	1:B:267:ARG:HG3	1.84	0.59
1:A:216:TYR:H	1:A:249:GLN:HE22	1.49	0.59
1:A:328:ASP:C	1:A:328:ASP:OD2	2.41	0.59
3:A:908:EDO:H11	1:B:83:VAL:HB	1.84	0.59
1:A:185:ASN:HA	3:A:906:EDO:H12	1.85	0.59
1:B:27:ILE:HG22	1:B:28:GLY:O	2.03	0.59
1:B:270:LYS:HG2	5:B:995:HOH:O	2.02	0.59
1:B:144:ARG:HH11	1:B:154:ARG:CZ	2.16	0.59
1:B:219:GLU:O	3:B:911:EDO:H22	2.03	0.59
1:A:30:PRO:HD3	1:A:47:PHE:CD2	2.38	0.59
1:B:27:ILE:HG22	1:B:28:GLY:O	2.02	0.59
1:A:160:ILE:H	1:A:160:ILE:HD12	1.57	0.59
1:A:216:TYR:HB2	1:A:252:ARG:HD2	1.83	0.59
1:B:190:MSE:HA	1:B:194:GLN:HE21	1.67	0.59
1:B:104:ARG:HB2	1:B:114:ASN:ND2	2.15	0.59
1:B:33:GLN:HE21	1:B:39:ASN:HD21	1.50	0.59
1:A:253:SER:O	1:A:256:ALA:HB3	2.03	0.59
1:B:180:CYS:SG	1:B:181:LEU:HD12	2.43	0.59
1:A:177:THR:OG1	1:A:180:CYS:HB3	2.01	0.59
1:B:357:ILE:N	1:B:357:ILE:HD13	2.16	0.59
1:B:282:LEU:CB	1:B:307:LEU:HD22	2.33	0.59
1:A:9:ALA:HA	5:A:1310:HOH:O	2.00	0.59
1:B:171:GLU:CD	1:B:269:ARG:HH22	2.06	0.59
1:B:77:PRO:HD2	1:B:80:ILE:HD12	1.85	0.59
1:A:94:ASP:OD2	3:A:903:EDO:H12	2.02	0.59
1:A:191:SER:H	1:A:194:GLN:NE2	1.94	0.59
1:B:11:HIS:HB3	1:B:102:ARG:HH21	1.66	0.59
1:A:241:TRP:O	1:A:278:ILE:HG12	2.03	0.59
1:B:88:ASN:HD22	1:B:139:ASP:H	1.50	0.59
1:B:175:LEU:CD1	1:B:211:LEU:HD21	2.31	0.59
1:A:291:GLY:HA3	5:A:1124:HOH:O	2.02	0.59
1:B:179:GLU:HB2	1:B:213:ARG:HA	1.84	0.59
1:A:38:HIS:O	1:A:41:LEU:HD13	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:HE21	1:B:39:ASN:ND2	2.01	0.59
1:B:183:ASN:OD1	1:B:185:ASN:OD1	2.21	0.59
1:A:151:ARG:HD3	5:A:1064:HOH:O	2.01	0.59
1:A:198:GLU:OE2	1:A:201:LYS:NZ	2.33	0.59
1:B:112:ASN:ND2	5:B:1282:HOH:O	2.35	0.59
1:A:137:SER:HB2	5:A:1215:HOH:O	2.03	0.59
1:B:162:GLU:OE2	1:B:224:HIS:CE1	2.49	0.59
1:A:296:GLY:O	1:A:297:GLU:OE1	2.21	0.59
1:B:88:ASN:HD22	1:B:138:HIS:HB2	1.68	0.59
1:B:88:ASN:ND2	1:B:138:HIS:HB2	2.18	0.59
1:B:88:ASN:HD21	1:B:138:HIS:CB	2.15	0.58
1:A:19:TRP:HB3	1:A:316:ILE:HG21	1.84	0.58
1:B:156:GLN:H	3:B:912:EDO:C2	2.16	0.58
1:B:175:LEU:HD11	1:B:211:LEU:CD2	2.31	0.58
1:B:168:VAL:HG12	1:B:174:CYS:HG	1.66	0.58
1:B:280:GLU:O	1:B:282:LEU:HD13	2.03	0.58
1:B:65:SER:HA	1:B:85:MSE:O	2.03	0.58
1:B:94:ASP:CB	1:B:162:GLU:HB3	2.33	0.58
1:A:142:VAL:O	1:A:146:ILE:HG13	2.03	0.58
5:A:1181:HOH:O	1:B:138:HIS:HD2	1.85	0.58
1:B:114:ASN:HB3	1:B:375:PRO:HD2	1.83	0.58
1:A:149:LEU:HD11	1:B:149:LEU:CD1	2.22	0.58
1:A:35:ASN:HD21	1:A:301:ARG:HH21	1.50	0.58
1:A:18:GLU:O	1:A:22:HIS:NE2	2.29	0.58
1:B:213:ARG:HD2	1:B:252:ARG:CZ	2.33	0.58
1:A:221:THR:HG21	1:A:224:HIS:CD2	2.38	0.58
1:A:216:TYR:H	1:A:249:GLN:HE21	1.48	0.58
1:A:97:PRO:HB3	1:A:143:SER:HB3	1.84	0.58
1:B:168:VAL:HB	5:B:960:HOH:O	2.02	0.58
1:A:23:ALA:HB2	1:A:373:ALA:HA	1.84	0.58
1:B:284:MSE:CE	1:B:301:ARG:NH1	2.56	0.58
1:A:122:PHE:CE2	1:A:133:TYR:OH	2.56	0.58
1:A:191:SER:H	1:A:194:GLN:NE2	2.02	0.58
1:A:85:MSE:HG3	5:B:1115:HOH:O	2.03	0.58
1:A:191:SER:N	1:A:194:GLN:NE2	2.44	0.58
1:A:370:GLN:HG2	1:A:370:GLN:O	2.03	0.58
1:B:284:MSE:CE	1:B:359:LEU:HD22	2.33	0.58
1:B:121:ASN:HD22	1:B:122:PHE:H	1.49	0.58
1:B:191:SER:H	1:B:194:GLN:HE21	1.51	0.58
1:B:299:ILE:HD12	1:B:299:ILE:O	2.04	0.58
1:B:12:GLY:O	1:B:102:ARG:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:HB3	1:A:374:GLU:OE1	2.04	0.58
1:A:189:HIS:HB2	5:A:1315:HOH:O	2.03	0.58
1:B:156:GLN:H	3:B:912:EDO:C2	2.16	0.58
1:A:113:ARG:HB2	1:A:153:PRO:HG2	1.84	0.58
1:A:138:HIS:O	1:A:139:ASP:C	2.41	0.58
1:B:27:ILE:HD11	1:B:54:ILE:CD1	2.33	0.58
1:B:27:ILE:HD11	1:B:54:ILE:HD12	1.86	0.58
1:A:38:HIS:CD2	5:A:1122:HOH:O	2.57	0.58
1:A:22:HIS:HE1	1:A:316:ILE:O	1.87	0.58
1:A:216:TYR:HA	1:A:252:ARG:CZ	2.33	0.58
1:B:88:ASN:HD21	1:B:138:HIS:H	1.51	0.58
1:B:88:ASN:HD21	1:B:138:HIS:H	1.52	0.58
1:B:104:ARG:HB2	1:B:114:ASN:HD21	1.69	0.58
1:B:29:TRP:HE1	1:B:68:GLN:HE21	1.52	0.58
1:A:229:CYS:CB	1:A:238:LEU:O	2.51	0.58
1:B:222:ASN:HD21	3:B:911:EDO:C1	2.17	0.58
3:A:908:EDO:H11	1:B:83:VAL:HB	1.86	0.58
1:A:215:LEU:HD23	1:A:308:ALA:HB1	1.85	0.58
1:A:325:GLN:O	1:A:354:ALA:HB3	2.04	0.58
1:A:29:TRP:HE1	1:A:68:GLN:HE21	1.52	0.58
1:B:112:ASN:ND2	1:B:113:ARG:H	2.01	0.58
1:A:36:TRP:CZ3	1:A:360:ALA:HB3	2.38	0.58
1:A:221:THR:CG2	5:A:1203:HOH:O	2.52	0.58
1:A:207:SER:HB2	5:A:1211:HOH:O	2.03	0.58
1:A:321:ILE:HD11	1:A:343:PHE:CG	2.39	0.58
1:A:41:LEU:HD12	1:A:41:LEU:N	2.19	0.58
1:A:29:TRP:HE1	1:A:68:GLN:HE21	1.52	0.58
1:A:186:ARG:O	1:A:187:ASN:OD1	2.22	0.58
1:A:174:CYS:HB2	1:A:205:VAL:CG1	2.28	0.57
1:B:229:CYS:HA	1:B:238:LEU:O	2.04	0.57
1:B:179:GLU:O	1:B:183:ASN:HB2	2.04	0.57
1:B:69:TRP:CD1	1:B:82:VAL:HG12	2.39	0.57
1:B:97:PRO:HG2	1:B:99:PHE:CE1	2.39	0.57
1:A:179:GLU:O	1:A:183:ASN:HB2	2.04	0.57
1:A:104:ARG:CB	1:A:104:ARG:HH21	2.17	0.57
3:A:908:EDO:O1	5:B:942:HOH:O	2.03	0.57
1:A:119:ASP:CB	1:A:154:ARG:HD2	2.34	0.57
1:B:88:ASN:HD21	1:B:138:HIS:N	2.01	0.57
1:B:121:ASN:HD22	1:B:122:PHE:H	1.50	0.57
1:A:38:HIS:CD2	5:A:1124:HOH:O	2.58	0.57
1:A:171:GLU:OE2	1:A:267:ARG:HD2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:SER:HA	1:A:58:GLU:O	2.04	0.57
1:B:321:ILE:O	1:B:323:ALA:N	2.37	0.57
1:A:144:ARG:HG3	1:A:154:ARG:NE	2.19	0.57
1:B:101:VAL:HG21	3:B:913:EDO:H11	1.85	0.57
1:B:140:LEU:HD21	5:B:1252:HOH:O	2.02	0.57
1:A:211:LEU:HD22	1:A:256:ALA:HB1	1.86	0.57
1:B:313:ASN:OD1	1:B:363:ASN:HB3	2.05	0.57
1:A:34:ASP:HB2	1:A:295:ASP:OD1	2.04	0.57
1:B:67:ALA:CB	5:B:1058:HOH:O	2.50	0.57
1:A:31:GLU:OE2	5:A:1224:HOH:O	2.17	0.57
1:A:157:HIS:ND1	1:A:159:MSE:HG2	2.20	0.57
1:B:12:GLY:HA3	5:B:1270:HOH:O	2.02	0.57
1:B:85:MSE:O	1:B:87:MSE:HE2	2.04	0.57
1:A:284:MSE:HE1	1:A:292:ILE:CD1	2.34	0.57
1:B:15:MSE:HG3	1:B:203:LEU:HD22	1.86	0.57
1:A:94:ASP:OD1	1:A:224:HIS:HE1	1.88	0.57
1:A:15:MSE:HG3	1:A:203:LEU:HA	1.85	0.57
1:B:103:LYS:H	1:B:103:LYS:HZ3	1.50	0.57
1:A:307:LEU:HB3	1:A:358:VAL:HG12	1.87	0.57
1:A:35:ASN:ND2	1:A:301:ARG:HE	2.03	0.57
1:A:214:GLY:O	1:A:252:ARG:HD3	2.04	0.57
1:B:307:LEU:CD1	1:B:307:LEU:N	2.67	0.57
1:B:179:GLU:O	1:B:183:ASN:HB2	2.05	0.57
1:A:226:ASP:OD2	1:A:365:HIS:CD2	2.56	0.57
1:A:52:LYS:HD3	1:A:77:PRO:CD	2.34	0.57
1:B:287:GLU:O	1:B:290:SER:OG	2.22	0.57
1:A:103:LYS:CE	1:A:103:LYS:H	2.18	0.57
1:B:324:PRO:HB3	1:B:363:ASN:HD21	1.70	0.57
1:A:301:ARG:HG2	1:A:301:ARG:NH1	2.15	0.57
1:A:185:ASN:HA	3:A:906:EDO:H12	1.86	0.57
1:A:26:TRP:HB2	1:A:369:GLN:HB3	1.86	0.57
1:B:150:GLU:OE1	5:B:1157:HOH:O	2.17	0.57
1:B:125:TRP:O	3:B:911:EDO:O1	2.23	0.57
1:B:160:ILE:CD1	1:B:186:ARG:O	2.43	0.57
1:A:34:ASP:OD2	1:A:297:GLU:HB2	2.04	0.57
1:A:48:ALA:O	1:A:52:LYS:HG3	2.05	0.57
1:B:301:ARG:O	1:B:302:LEU:HD23	2.04	0.57
1:A:218:ASP:OD1	1:A:227:ASN:ND2	2.28	0.57
1:B:68:GLN:NE2	1:B:71:ASN:HD22	2.03	0.57
1:A:26:TRP:HE1	1:A:371:GLN:NE2	2.00	0.57
1:A:123:ASN:HA	1:A:136:TRP:NE1	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ASN:ND2	1:B:364:ILE:HG13	2.20	0.57
1:B:88:ASN:ND2	1:B:139:ASP:H	2.03	0.57
1:B:86:SER:HB3	1:B:138:HIS:ND1	2.20	0.57
1:B:177:THR:HA	1:B:211:LEU:O	2.04	0.57
1:B:8:PRO:HG3	1:B:155:PHE:CD2	2.39	0.57
1:B:372:PRO:HB3	5:B:969:HOH:O	2.04	0.57
1:B:192:LYS:HE3	1:B:210:TRP:CD2	2.40	0.57
1:A:219:GLU:O	1:A:219:GLU:HG3	2.03	0.57
1:A:91:TRP:CZ3	1:A:367:ILE:CG2	2.87	0.57
1:B:113:ARG:NE	1:B:374:GLU:OE2	2.35	0.57
1:B:99:PHE:CB	1:B:372:PRO:HD2	2.35	0.57
1:A:280:GLU:HG2	1:A:328:ASP:OD1	2.05	0.57
1:A:149:LEU:HD21	1:B:149:LEU:CD1	2.35	0.57
1:A:5:ARG:NH1	1:A:158:SER:H	2.03	0.57
1:B:95:SER:O	1:B:143:SER:OG	2.23	0.57
1:B:141:LEU:HA	1:B:144:ARG:CD	2.34	0.56
1:B:15:MSE:HE1	1:B:203:LEU:HD22	1.81	0.56
1:B:104:ARG:HG2	1:B:104:ARG:O	2.05	0.56
1:A:134:ASN:ND2	1:A:297:GLU:HA	2.10	0.56
1:A:273:VAL:O	5:A:1116:HOH:O	2.17	0.56
1:A:7:SER:CB	1:A:201:LYS:HB3	2.35	0.56
1:A:161:LEU:HD11	1:A:181:LEU:HD11	1.86	0.56
1:A:26:TRP:HE1	1:A:371:GLN:NE2	2.01	0.56
1:B:284:MSE:HE2	1:B:359:LEU:HD22	1.87	0.56
1:A:334:GLU:CD	1:A:337:ARG:HE	2.09	0.56
1:A:150:GLU:HG3	1:A:371:GLN:NE2	2.20	0.56
1:A:123:ASN:ND2	1:A:126:GLY:H	2.02	0.56
1:B:138:HIS:CD2	5:B:1081:HOH:O	2.48	0.56
1:B:189:HIS:CD2	1:B:190:MSE:HG3	2.39	0.56
1:A:54:ILE:HG12	1:A:322:ILE:HG13	1.87	0.56
1:B:103:LYS:O	1:B:103:LYS:HG2	2.04	0.56
1:B:200:LYS:HA	1:B:205:VAL:HG22	1.88	0.56
1:A:36:TRP:CZ3	1:A:360:ALA:HB3	2.41	0.56
1:B:37:ARG:NH1	1:B:37:ARG:HG3	2.17	0.56
1:A:11:HIS:HD2	1:A:13:TYR:HE2	1.53	0.56
1:A:306:ARG:O	5:A:1099:HOH:O	2.18	0.56
1:A:160:ILE:H	1:A:187:ASN:HD21	1.53	0.56
1:B:351:ILE:HB	1:B:364:ILE:HD11	1.87	0.56
1:A:18:GLU:OE1	1:A:365:HIS:CE1	2.57	0.56
1:A:320:GLY:N	1:A:346:HIS:HD2	2.02	0.56
1:B:316:ILE:HG12	1:B:321:ILE:HD12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD12	5:B:914:HOH:O	2.04	0.56
1:A:362:GLY:CA	1:A:366:CYS:SG	2.87	0.56
1:B:282:LEU:CD1	1:B:282:LEU:N	2.66	0.56
1:B:193:GLU:HG3	5:B:948:HOH:O	2.06	0.56
1:A:282:LEU:HB2	1:A:307:LEU:HB2	1.88	0.56
1:B:39:ASN:N	5:B:1035:HOH:O	2.07	0.56
1:A:241:TRP:CE2	1:A:275:LYS:HD3	2.41	0.56
1:B:125:TRP:O	3:B:911:EDO:C1	2.54	0.56
1:B:88:ASN:HD21	1:B:138:HIS:N	2.04	0.56
1:B:186:ARG:NH1	1:B:222:ASN:HD22	1.97	0.56
1:A:286:GLU:HA	1:A:303:ALA:HB2	1.86	0.56
1:A:292:ILE:CD1	1:A:292:ILE:N	2.68	0.56
1:A:174:CYS:HB2	1:A:205:VAL:HG11	1.87	0.56
1:B:351:ILE:HB	1:B:364:ILE:HD11	1.87	0.56
1:A:366:CYS:HB3	5:A:1109:HOH:O	2.05	0.56
1:B:226:ASP:HB2	5:B:924:HOH:O	2.06	0.56
1:A:313:ASN:ND2	1:A:365:HIS:CB	2.68	0.56
1:A:83:VAL:HG11	1:B:149:LEU:CD1	2.36	0.56
1:A:189:HIS:HB3	5:A:1248:HOH:O	2.05	0.56
1:B:60:VAL:O	1:B:80:ILE:HG23	2.06	0.56
1:A:357:ILE:HD13	1:A:367:ILE:HD13	1.88	0.56
1:A:211:LEU:HD13	1:A:228:MSE:SE	2.56	0.56
1:B:280:GLU:O	1:B:282:LEU:CD1	2.52	0.56
1:B:46:VAL:HG12	1:B:357:ILE:HD11	1.87	0.56
1:A:361:GLY:O	3:A:903:EDO:O2	2.19	0.56
1:B:103:LYS:N	1:B:103:LYS:CD	2.68	0.56
1:B:195:ILE:CB	1:B:195:ILE:CD1	2.81	0.56
1:B:222:ASN:HD21	3:B:911:EDO:C1	2.19	0.56
1:B:31:GLU:HA	1:B:40:ALA:HB3	1.87	0.56
1:B:351:ILE:HB	1:B:364:ILE:HD11	1.87	0.56
1:A:179:GLU:OE2	5:A:1058:HOH:O	2.18	0.56
1:A:89:ASP:HB2	1:A:133:TYR:CE2	2.41	0.56
1:A:241:TRP:CE3	1:A:253:SER:HB3	2.41	0.56
1:B:22:HIS:H	1:B:318:ASN:ND2	1.96	0.56
1:B:7:SER:HB3	1:B:8:PRO:CD	2.33	0.56
1:A:147:LEU:HD22	1:A:152:ILE:HG22	1.88	0.56
1:B:244:ASP:O	1:B:250:TYR:HB2	2.06	0.56
1:B:191:SER:H	1:B:194:GLN:NE2	1.99	0.56
1:A:154:ARG:CZ	1:A:156:GLN:OE1	2.54	0.56
1:B:88:ASN:HD22	1:B:139:ASP:H	1.53	0.56
1:B:87:MSE:HE2	1:B:92:PHE:CZ	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HA	1:B:82:VAL:HG21	1.88	0.56
1:A:118:ILE:HG21	1:A:120:TRP:CZ3	2.40	0.56
1:A:68:GLN:NE2	1:A:71:ASN:HD22	2.01	0.55
1:A:88:ASN:OD1	1:A:136:TRP:HA	2.06	0.55
1:B:177:THR:O	1:B:181:LEU:HD13	2.06	0.55
1:A:24:GLN:NE2	1:A:61:THR:OG1	2.39	0.55
1:B:302:LEU:O	1:B:305:THR:HG23	2.06	0.55
1:A:281:PRO:O	1:A:282:LEU:HD23	2.06	0.55
1:B:102:ARG:CA	1:B:103:LYS:HZ2	2.19	0.55
1:A:11:HIS:HB2	1:A:13:TYR:CD2	2.40	0.55
1:A:313:ASN:ND2	1:A:363:ASN:H	2.04	0.55
1:A:160:ILE:HD13	5:A:1207:HOH:O	2.05	0.55
1:B:87:MSE:HE2	1:B:92:PHE:CE1	2.41	0.55
1:A:29:TRP:HE1	1:A:68:GLN:HE21	1.52	0.55
1:A:233:ARG:HB2	1:A:234:PRO:CD	2.37	0.55
1:A:149:LEU:HD22	1:B:149:LEU:HD11	1.87	0.55
1:A:103:LYS:O	1:A:104:ARG:HB3	2.06	0.55
1:A:326:PHE:HE2	1:A:363:ASN:HD21	1.55	0.55
1:B:121:ASN:HD22	1:B:122:PHE:H	1.55	0.55
1:A:94:ASP:CB	1:A:162:GLU:HB3	2.37	0.55
1:B:134:ASN:N	1:B:134:ASN:HD22	2.04	0.55
1:B:255:GLU:O	1:B:259:VAL:HG23	2.07	0.55
1:A:313:ASN:HB3	1:A:363:ASN:HB3	1.89	0.55
1:B:69:TRP:NE1	1:B:82:VAL:HG12	2.21	0.55
1:B:141:LEU:HD22	1:B:144:ARG:HD2	1.87	0.55
1:B:280:GLU:HG3	1:B:328:ASP:OD2	2.06	0.55
1:B:32:ARG:NH2	1:B:297:GLU:HB3	2.20	0.55
1:B:363:ASN:HD22	1:B:364:ILE:H	1.54	0.55
1:B:162:GLU:OE2	1:B:224:HIS:HE1	1.88	0.55
1:A:44:GLN:HE22	1:A:71:ASN:HD21	1.54	0.55
1:A:89:ASP:OD1	1:A:133:TYR:CE2	2.60	0.55
1:B:185:ASN:HD21	1:B:222:ASN:HD21	1.50	0.55
1:B:192:LYS:HE2	1:B:210:TRP:CE2	2.42	0.55
1:A:34:ASP:HB3	1:A:295:ASP:OD2	2.06	0.55
1:A:15:MSE:SE	1:A:166:ILE:HD12	2.56	0.55
1:B:251:GLU:OE2	5:B:1256:HOH:O	2.18	0.55
1:A:225:ILE:HD11	1:A:229:CYS:HB3	1.89	0.55
3:A:908:EDO:H12	5:B:1053:HOH:O	2.05	0.55
3:A:908:EDO:O1	5:B:942:HOH:O	2.18	0.55
1:B:100:ILE:HD11	1:B:155:PHE:CD2	2.42	0.55
1:B:9:ALA:CB	5:B:1263:HOH:O	2.48	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:HG22	1:A:295:ASP:N	2.14	0.55
1:A:41:LEU:N	1:A:41:LEU:CD1	2.70	0.55
1:A:25:THR:HG22	1:A:26:TRP:N	2.21	0.55
1:A:319:GLY:HA2	1:A:346:HIS:CD2	2.41	0.55
1:B:160:ILE:HB	1:B:187:ASN:OD1	2.07	0.55
1:A:144:ARG:HG2	1:B:69:TRP:HH2	1.71	0.55
1:B:103:LYS:H	1:B:103:LYS:HZ2	1.54	0.55
1:B:86:SER:C	1:B:87:MSE:HG3	2.26	0.55
1:A:197:GLU:O	1:A:201:LYS:HG3	2.07	0.55
1:B:41:LEU:O	1:B:45:ARG:HG3	2.06	0.55
1:A:334:GLU:OE2	1:A:337:ARG:NH2	2.40	0.55
1:A:24:GLN:HB2	1:A:59:PRO:HB2	1.88	0.55
1:B:363:ASN:HD22	1:B:364:ILE:H	1.55	0.55
1:B:36:TRP:HB2	1:B:40:ALA:HB2	1.88	0.55
1:A:33:GLN:OE1	1:A:39:ASN:ND2	2.39	0.55
1:B:190:MSE:HA	1:B:194:GLN:NE2	2.22	0.55
1:A:79:ASP:OD1	5:A:1340:HOH:O	2.18	0.55
1:B:177:THR:HG23	1:B:225:ILE:HB	1.88	0.55
1:B:112:ASN:HD22	1:B:112:ASN:N	2.04	0.55
1:A:280:GLU:HG2	1:A:328:ASP:HB2	1.89	0.55
1:A:272:GLN:NE2	5:A:1294:HOH:O	2.13	0.55
1:A:313:ASN:HD22	1:A:363:ASN:C	2.10	0.55
1:B:160:ILE:HG21	1:B:186:ARG:HD2	1.89	0.55
1:B:150:GLU:OE1	5:B:1151:HOH:O	2.18	0.55
1:B:185:ASN:HD21	1:B:222:ASN:ND2	2.04	0.55
1:A:160:ILE:N	1:A:187:ASN:HD21	2.02	0.55
1:B:133:TYR:CE2	1:B:135:ASP:O	2.59	0.55
1:B:282:LEU:HB3	1:B:307:LEU:HD22	1.88	0.55
1:B:16:PRO:HG3	1:B:101:VAL:HG22	1.87	0.55
1:A:194:GLN:NE2	5:A:1253:HOH:O	2.40	0.54
1:B:264:ILE:HA	1:B:269:ARG:O	2.06	0.54
1:A:84:GLU:O	3:A:908:EDO:H22	2.06	0.54
1:A:119:ASP:O	1:A:156:GLN:HA	2.07	0.54
1:A:50:VAL:CG2	1:A:351:ILE:HG13	2.37	0.54
1:B:103:LYS:H	1:B:103:LYS:HZ2	1.56	0.54
1:B:156:GLN:H	3:B:912:EDO:C2	2.20	0.54
1:A:186:ARG:HH12	1:A:222:ASN:HD22	1.53	0.54
1:A:144:ARG:HG3	5:A:1088:HOH:O	2.07	0.54
1:B:355:ARG:O	1:B:359:LEU:HG	2.06	0.54
1:A:211:LEU:HD22	1:A:256:ALA:CB	2.37	0.54
1:B:293:THR:HG22	1:B:295:ASP:OD1	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:THR:HG23	1:A:225:ILE:HD12	1.87	0.54
1:A:211:LEU:CD1	1:A:228:MSE:SE	3.05	0.54
1:A:37:ARG:NH1	1:A:38:HIS:HD2	2.05	0.54
1:B:330:ILE:CG2	5:B:1103:HOH:O	2.45	0.54
1:A:197:GLU:OE1	1:A:201:LYS:HD3	2.08	0.54
1:B:7:SER:O	1:B:10:GLU:N	2.39	0.54
1:B:220:ASP:O	3:B:911:EDO:O1	2.19	0.54
1:A:28:GLY:O	1:A:47:PHE:HE2	1.89	0.54
1:A:284:MSE:HE1	1:A:292:ILE:HD11	1.89	0.54
1:B:104:ARG:NH1	5:B:1285:HOH:O	2.41	0.54
1:A:159:MSE:HE3	1:A:187:ASN:OD1	2.08	0.54
1:A:151:ARG:HH22	1:B:24:GLN:HE22	1.55	0.54
1:A:225:ILE:CG1	1:A:229:CYS:O	2.55	0.54
1:A:20:ASP:CB	5:A:1110:HOH:O	2.56	0.54
1:B:7:SER:HB2	5:B:1277:HOH:O	2.06	0.54
1:A:366:CYS:SG	3:A:903:EDO:H21	2.47	0.54
1:A:41:LEU:CD1	1:A:41:LEU:N	2.70	0.54
1:A:229:CYS:HB3	1:A:239:LEU:HA	1.90	0.54
1:A:228:MSE:HE3	1:A:228:MSE:HA	1.89	0.54
1:A:35:ASN:ND2	1:A:301:ARG:CZ	2.70	0.54
3:A:908:EDO:O1	5:A:1038:HOH:O	2.18	0.54
1:B:103:LYS:H	1:B:103:LYS:HZ2	1.53	0.54
1:A:119:ASP:OD2	1:A:154:ARG:HD2	2.07	0.54
1:B:276:LEU:HG	1:B:311:TYR:HB2	1.88	0.54
1:A:281:PRO:HB3	1:A:306:ARG:CZ	2.38	0.54
1:A:121:ASN:HB3	1:A:160:ILE:CG1	2.38	0.54
1:B:229:CYS:CB	1:B:239:LEU:HA	2.38	0.54
1:A:207:SER:HB2	5:A:1107:HOH:O	2.08	0.54
3:A:908:EDO:H11	1:B:83:VAL:HB	1.89	0.54
1:B:91:TRP:HE3	1:B:367:ILE:HG22	1.73	0.54
1:A:50:VAL:HG21	1:A:364:ILE:HG12	1.88	0.54
1:A:176:VAL:HG23	1:A:210:TRP:CE3	2.43	0.54
1:A:366:CYS:HB3	3:A:903:EDO:H11	1.89	0.54
1:A:91:TRP:HD1	1:A:125:TRP:HH2	1.56	0.54
1:A:168:VAL:HA	1:A:174:CYS:HA	1.90	0.54
1:A:361:GLY:O	3:A:903:EDO:O2	2.25	0.54
1:B:220:ASP:CG	5:B:1226:HOH:O	2.45	0.53
1:B:121:ASN:HB3	1:B:160:ILE:HA	1.90	0.53
1:B:87:MSE:HE1	1:B:92:PHE:CE1	2.43	0.53
1:A:149:LEU:HD21	1:B:149:LEU:HD11	1.85	0.53
1:A:46:VAL:HG11	1:A:357:ILE:CG1	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:H	1:B:187:ASN:HD21	1.56	0.53
1:B:22:HIS:HA	1:B:372:PRO:HA	1.90	0.53
1:A:103:LYS:H	1:A:103:LYS:HZ2	1.57	0.53
1:A:127:GLY:O	1:A:131:GLY:N	2.41	0.53
1:B:59:PRO:HG2	5:B:1128:HOH:O	2.08	0.53
1:A:85:MSE:SE	1:A:146:ILE:HG13	2.58	0.53
1:B:136:TRP:HD1	1:B:140:LEU:HG	1.73	0.53
1:A:159:MSE:HE2	1:A:161:LEU:HD12	1.90	0.53
1:A:159:MSE:CE	1:A:187:ASN:OD1	2.57	0.53
1:B:7:SER:HA	1:B:10:GLU:OE1	2.09	0.53
1:B:31:GLU:HG3	1:B:68:GLN:OE1	2.08	0.53
1:A:123:ASN:ND2	1:A:126:GLY:H	2.05	0.53
1:A:35:ASN:HD22	1:A:301:ARG:HE	1.48	0.53
1:B:88:ASN:CG	1:B:136:TRP:HA	2.28	0.53
1:B:102:ARG:CA	1:B:103:LYS:HZ2	2.20	0.53
1:B:100:ILE:HG21	1:B:202:TYR:O	2.08	0.53
1:B:354:ALA:O	1:B:358:VAL:HG23	2.08	0.53
1:B:217:GLY:C	1:B:308:ALA:HB2	2.29	0.53
1:A:134:ASN:ND2	1:A:297:GLU:O	2.42	0.53
1:A:85:MSE:HG3	5:A:1216:HOH:O	2.08	0.53
1:A:366:CYS:HB3	3:A:903:EDO:H11	1.91	0.53
1:A:327:GLY:O	1:A:329:PRO:HD3	2.09	0.53
1:B:166:ILE:CD1	1:B:166:ILE:CB	2.81	0.53
1:B:125:TRP:HA	1:B:186:ARG:CZ	2.38	0.53
1:B:125:TRP:O	3:B:911:EDO:C1	2.52	0.53
1:B:31:GLU:HA	1:B:40:ALA:CB	2.39	0.53
1:B:133:TYR:HA	1:B:298:ALA:HA	1.89	0.53
1:B:313:ASN:OD1	1:B:363:ASN:HB3	2.08	0.53
1:A:159:MSE:HE1	1:A:195:ILE:HG23	1.91	0.53
1:A:38:HIS:CD2	5:A:1122:HOH:O	2.61	0.53
1:B:125:TRP:O	3:B:911:EDO:C1	2.56	0.53
1:A:185:ASN:HA	3:A:906:EDO:H12	1.91	0.53
1:A:121:ASN:HD22	1:A:122:PHE:H	1.56	0.53
1:A:117:GLY:CA	1:A:147:LEU:HD11	2.37	0.53
1:B:33:GLN:HE21	1:B:39:ASN:ND2	2.06	0.53
1:A:83:VAL:HG11	1:B:149:LEU:HD12	1.91	0.53
1:A:357:ILE:HG22	1:A:362:GLY:C	2.29	0.53
1:B:280:GLU:O	1:B:282:LEU:HD13	2.09	0.53
1:B:157:HIS:ND1	1:B:159:MSE:HG2	2.23	0.53
1:A:52:LYS:HE2	5:A:1164:HOH:O	2.08	0.53
1:A:248:PRO:O	5:A:1105:HOH:O	2.19	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLU:HA	1:B:219:GLU:OE2	2.08	0.53
1:B:7:SER:N	1:B:8:PRO:HD3	2.24	0.53
1:B:125:TRP:O	3:B:911:EDO:C1	2.57	0.53
1:A:313:ASN:OD1	1:A:365:HIS:HB3	2.09	0.53
1:A:324:PRO:HB3	1:A:363:ASN:OD1	2.08	0.53
1:A:68:GLN:NE2	1:A:71:ASN:HD22	2.04	0.53
1:B:21:SER:HA	1:B:318:ASN:ND2	2.24	0.53
1:B:29:TRP:HE1	1:B:68:GLN:NE2	2.06	0.53
1:B:220:ASP:OD1	1:B:299:ILE:HD11	2.09	0.53
1:A:216:TYR:H	1:A:249:GLN:NE2	2.07	0.53
1:B:121:ASN:ND2	1:B:122:PHE:H	2.06	0.53
1:A:369:GLN:NE2	1:A:370:GLN:NE2	2.56	0.53
1:B:27:ILE:O	1:B:62:VAL:HA	2.09	0.53
1:A:29:TRP:HE1	1:A:68:GLN:HE21	1.57	0.53
1:A:100:ILE:O	1:A:115:ILE:HG13	2.09	0.53
1:B:213:ARG:NH1	5:B:1105:HOH:O	2.38	0.53
1:A:160:ILE:CD1	5:A:1207:HOH:O	2.56	0.53
1:B:14:TYR:CB	1:B:204:GLY:HA3	2.39	0.52
1:A:284:MSE:HB2	1:A:305:THR:CB	2.38	0.52
1:B:134:ASN:HB2	1:B:297:GLU:OE2	2.09	0.52
1:A:26:TRP:HE1	1:A:371:GLN:CD	2.12	0.52
3:A:908:EDO:H11	1:B:83:VAL:HB	1.90	0.52
1:A:266:ALA:C	1:A:268:GLY:H	2.12	0.52
1:A:149:LEU:CD2	5:A:1314:HOH:O	2.57	0.52
1:B:353:ASN:HA	5:B:1217:HOH:O	2.09	0.52
1:B:213:ARG:HH22	1:B:251:GLU:HG3	1.73	0.52
1:B:9:ALA:N	5:B:1263:HOH:O	2.28	0.52
1:A:173:THR:OG1	1:A:265:ASP:HB2	2.10	0.52
1:B:144:ARG:O	1:B:148:ALA:N	2.41	0.52
1:A:144:ARG:HD3	1:B:69:TRP:CZ3	2.43	0.52
1:A:376:THR:HG22	5:A:1355:HOH:O	2.09	0.52
1:A:216:TYR:H	1:A:249:GLN:NE2	2.06	0.52
1:B:30:PRO:HD3	1:B:47:PHE:CD2	2.44	0.52
3:B:913:EDO:H22	5:B:969:HOH:O	2.09	0.52
1:A:199:LEU:O	1:A:205:VAL:HG22	2.10	0.52
1:B:174:CYS:SG	1:B:205:VAL:HG21	2.49	0.52
1:B:178:GLU:HB3	1:B:182:LEU:HD12	1.91	0.52
1:B:141:LEU:HD13	1:B:145:LYS:HE3	1.92	0.52
1:A:159:MSE:SE	1:A:190:MSE:HE1	2.59	0.52
1:A:112:ASN:N	5:A:1389:HOH:O	2.41	0.52
1:A:154:ARG:HH22	1:A:156:GLN:HB2	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:TYR:HA	1:B:204:GLY:HA3	1.90	0.52
1:B:174:CYS:SG	1:B:205:VAL:HG21	2.50	0.52
1:A:121:ASN:HB3	1:A:160:ILE:HG12	1.91	0.52
1:B:200:LYS:HA	1:B:205:VAL:CG2	2.39	0.52
1:A:9:ALA:HB2	5:A:1310:HOH:O	2.09	0.52
1:A:112:ASN:HD22	1:A:112:ASN:N	2.07	0.52
1:B:24:GLN:NE2	1:B:61:THR:OG1	2.42	0.52
1:B:98:THR:N	1:B:118:ILE:O	2.41	0.52
1:B:51:ALA:HB1	1:B:80:ILE:HD13	1.92	0.52
1:B:265:ASP:CG	1:B:269:ARG:HE	2.13	0.52
1:A:41:LEU:N	1:A:41:LEU:HD12	2.24	0.52
1:B:101:VAL:HG21	3:B:913:EDO:H11	1.91	0.52
1:B:222:ASN:ND2	3:B:911:EDO:H11	2.25	0.52
1:A:102:ARG:HG2	1:A:114:ASN:HA	1.90	0.52
1:A:104:ARG:HB3	1:A:104:ARG:CZ	2.39	0.52
1:A:239:LEU:HD12	1:A:240:SER:H	1.73	0.52
1:A:157:HIS:ND1	1:A:158:SER:N	2.58	0.52
1:A:283:TYR:OH	5:A:1181:HOH:O	2.18	0.52
1:A:186:ARG:NH1	1:A:222:ASN:OD1	2.41	0.52
1:B:93:ARG:HG3	1:B:164:GLY:N	2.25	0.52
1:B:88:ASN:OD1	1:B:135:ASP:O	2.27	0.52
1:A:24:GLN:HE22	1:B:151:ARG:HH22	1.57	0.52
1:A:225:ILE:HG12	1:A:229:CYS:O	2.10	0.52
1:A:313:ASN:ND2	1:A:365:HIS:N	2.57	0.52
1:B:91:TRP:CZ3	1:B:362:GLY:HA3	2.44	0.52
1:A:97:PRO:HG2	1:A:99:PHE:CE1	2.45	0.52
1:B:191:SER:H	1:B:194:GLN:HE21	1.57	0.52
1:B:255:GLU:OE1	5:B:1099:HOH:O	2.18	0.52
1:B:363:ASN:HD22	1:B:364:ILE:H	1.55	0.52
1:B:248:PRO:HA	5:B:987:HOH:O	2.10	0.52
1:A:77:PRO:HG2	5:A:1140:HOH:O	2.10	0.52
1:A:6:GLU:HB3	1:A:10:GLU:OE2	2.09	0.52
1:B:134:ASN:OD1	1:B:297:GLU:HA	2.10	0.52
1:B:226:ASP:OD2	1:B:365:HIS:HD2	1.93	0.52
1:A:102:ARG:O	1:A:114:ASN:HB3	2.10	0.52
1:B:213:ARG:HB3	1:B:252:ARG:NH1	2.26	0.52
1:B:88:ASN:HD21	1:B:138:HIS:N	2.08	0.51
1:B:101:VAL:HG21	3:B:913:EDO:H11	1.91	0.51
1:A:196:GLU:HG2	1:A:208:PHE:CE1	2.44	0.51
1:A:35:ASN:OD1	1:A:360:ALA:HB1	2.11	0.51
1:A:197:GLU:OE1	5:A:1204:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLN:CD	1:A:370:GLN:H	2.14	0.51
1:A:125:TRP:HZ3	1:A:133:TYR:HE2	1.56	0.51
1:B:132:CYS:SG	1:B:220:ASP:HB3	2.49	0.51
1:A:160:ILE:N	1:A:187:ASN:HD21	1.85	0.51
1:A:85:MSE:CE	5:A:1217:HOH:O	2.26	0.51
1:B:225:ILE:HD12	1:B:228:MSE:HB3	1.91	0.51
1:B:24:GLN:NE2	1:B:61:THR:OG1	2.43	0.51
1:B:363:ASN:HD22	1:B:364:ILE:H	1.55	0.51
1:B:211:LEU:HD23	1:B:211:LEU:N	2.24	0.51
1:B:11:HIS:HB2	1:B:13:TYR:CE1	2.46	0.51
1:B:46:VAL:HG21	1:B:356:GLU:HB2	1.92	0.51
1:A:69:TRP:CZ3	1:B:144:ARG:HG3	2.45	0.51
1:B:217:GLY:HA3	1:B:308:ALA:HB2	1.93	0.51
1:B:238:LEU:HA	1:B:274:ILE:O	2.11	0.51
1:B:161:LEU:HG	1:B:162:GLU:H	1.74	0.51
1:B:15:MSE:HG2	1:B:168:VAL:HG21	1.92	0.51
1:B:134:ASN:N	1:B:134:ASN:HD22	2.07	0.51
1:A:5:ARG:HG3	1:A:5:ARG:HH21	1.75	0.51
1:A:13:TYR:HA	1:A:101:VAL:O	2.11	0.51
1:A:216:TYR:H	1:A:249:GLN:NE2	2.09	0.51
1:A:8:PRO:HD2	1:A:202:TYR:CG	2.44	0.51
1:B:94:ASP:OD1	1:B:125:TRP:NE1	2.34	0.51
1:B:121:ASN:ND2	1:B:122:PHE:H	2.08	0.51
1:A:149:LEU:HD23	5:A:1314:HOH:O	2.10	0.51
1:A:331:ARG:NH1	5:A:1382:HOH:O	2.12	0.51
1:B:14:TYR:OH	1:B:103:LYS:CE	2.59	0.51
1:B:218:ASP:OD2	1:B:227:ASN:ND2	2.42	0.51
1:A:196:GLU:HB3	1:A:208:PHE:CE1	2.46	0.51
1:A:50:VAL:HG23	1:A:351:ILE:HG21	1.91	0.51
1:B:229:CYS:SG	1:B:239:LEU:CD1	2.99	0.51
1:B:132:CYS:O	1:B:298:ALA:HA	2.11	0.51
1:B:15:MSE:HG2	1:B:168:VAL:HG21	1.92	0.51
1:A:185:ASN:HD21	1:A:222:ASN:CG	2.13	0.51
1:A:221:THR:HG21	5:A:1203:HOH:O	2.10	0.51
1:B:307:LEU:HD12	1:B:307:LEU:N	2.24	0.51
1:B:192:LYS:HE2	1:B:210:TRP:CD2	2.46	0.51
1:A:29:TRP:HE1	1:A:68:GLN:NE2	2.08	0.51
1:B:168:VAL:HG12	1:B:174:CYS:SG	2.51	0.51
1:A:51:ALA:HB1	1:A:60:VAL:HG11	1.92	0.51
1:A:37:ARG:O	1:A:42:PRO:HD2	2.11	0.51
1:B:36:TRP:HB2	1:B:40:ALA:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:MSE:O	1:B:168:VAL:HG21	2.11	0.51
1:A:226:ASP:O	1:A:313:ASN:ND2	2.44	0.51
1:A:22:HIS:CE1	1:A:315:TYR:OH	2.64	0.51
1:B:117:GLY:HA3	1:B:147:LEU:HD21	1.93	0.51
1:B:284:MSE:HE2	1:B:359:LEU:HD22	1.93	0.51
1:B:103:LYS:CD	1:B:103:LYS:N	2.60	0.51
1:B:138:HIS:CE1	5:B:1192:HOH:O	2.63	0.51
1:B:123:ASN:ND2	1:B:126:GLY:H	2.09	0.51
1:A:66:PRO:HG3	1:A:84:GLU:OE2	2.10	0.51
1:A:175:LEU:HD21	1:A:229:CYS:SG	2.51	0.51
1:A:100:ILE:HD11	1:A:116:ALA:HB3	1.92	0.51
1:A:68:GLN:NE2	1:A:71:ASN:HD22	2.00	0.51
1:A:91:TRP:CZ3	1:A:366:CYS:SG	3.04	0.51
1:A:190:MSE:HE1	1:A:198:GLU:HG2	1.93	0.51
1:A:281:PRO:O	5:A:1212:HOH:O	2.20	0.51
1:B:15:MSE:HE3	1:B:203:LEU:HB3	1.93	0.51
1:B:357:ILE:HD12	1:B:367:ILE:CD1	2.38	0.51
1:A:167:HIS:CD2	1:A:230:CYS:HB2	2.45	0.51
1:A:36:TRP:HZ3	1:A:357:ILE:HA	1.76	0.50
1:B:218:ASP:CB	1:B:223:GLY:HA2	2.40	0.50
1:A:85:MSE:HE1	1:A:146:ILE:HG13	1.93	0.50
1:A:175:LEU:HG	1:A:225:ILE:HD11	1.92	0.50
1:B:141:LEU:HD23	1:B:144:ARG:HD2	1.92	0.50
1:B:255:GLU:OE1	5:B:1095:HOH:O	2.18	0.50
1:A:122:PHE:HE2	1:A:133:TYR:OH	1.94	0.50
1:A:320:GLY:HA2	1:A:346:HIS:HB3	1.92	0.50
1:A:85:MSE:HG3	5:A:1216:HOH:O	2.09	0.50
1:B:311:TYR:HA	1:B:324:PRO:CG	2.42	0.50
1:A:284:MSE:HB3	1:A:305:THR:H	1.76	0.50
1:B:297:GLU:O	1:B:297:GLU:OE2	2.28	0.50
1:B:113:ARG:HB3	1:B:374:GLU:OE2	2.11	0.50
1:A:115:ILE:O	1:A:153:PRO:HD2	2.11	0.50
1:A:87:MSE:SE	1:A:90:SER:HB3	2.61	0.50
1:B:282:LEU:HG	1:B:355:ARG:NH1	2.26	0.50
1:A:282:LEU:HB3	1:A:307:LEU:HD12	1.94	0.50
1:A:325:GLN:HB2	1:A:351:ILE:O	2.11	0.50
1:A:175:LEU:HD21	1:A:229:CYS:SG	2.51	0.50
1:B:102:ARG:O	1:B:114:ASN:HB3	2.11	0.50
1:A:295:ASP:OD1	1:A:296:GLY:N	2.45	0.50
1:B:125:TRP:HD1	1:B:224:HIS:CE1	2.28	0.50
1:A:26:TRP:HE1	1:A:371:GLN:NE2	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HG2	1:B:69:TRP:CH2	2.46	0.50
1:A:12:GLY:O	1:A:103:LYS:NZ	2.44	0.50
1:B:366:CYS:SG	1:B:367:ILE:N	2.84	0.50
1:A:26:TRP:HE1	1:A:371:GLN:NE2	2.09	0.50
1:A:182:LEU:O	1:A:183:ASN:C	2.47	0.50
1:A:15:MSE:O	1:A:168:VAL:HG21	2.11	0.50
1:A:366:CYS:HB3	3:A:903:EDO:H11	1.93	0.50
1:A:102:ARG:CG	1:A:114:ASN:HA	2.42	0.50
1:B:175:LEU:O	1:B:225:ILE:HG21	2.11	0.50
1:B:150:GLU:HG3	1:B:371:GLN:HE22	1.76	0.50
3:A:908:EDO:H21	1:B:84:GLU:O	2.12	0.50
1:B:287:GLU:HB3	5:B:1176:HOH:O	2.11	0.50
1:B:363:ASN:O	1:B:366:CYS:SG	2.69	0.50
1:A:64:ALA:O	1:A:84:GLU:HA	2.11	0.50
1:A:297:GLU:OE1	1:A:297:GLU:HA	2.12	0.50
1:B:280:GLU:HG2	5:B:1243:HOH:O	2.12	0.50
1:A:193:GLU:H	1:A:193:GLU:CD	2.15	0.50
1:A:250:TYR:HB3	5:A:1077:HOH:O	2.12	0.50
1:B:123:ASN:ND2	5:B:937:HOH:O	2.43	0.50
1:A:103:LYS:H	1:A:103:LYS:HE3	1.76	0.50
1:B:191:SER:N	1:B:194:GLN:HE21	1.86	0.50
1:A:5:ARG:HH12	1:A:158:SER:N	2.08	0.50
1:A:366:CYS:HB3	3:A:903:EDO:H11	1.93	0.50
1:B:265:ASP:C	1:B:265:ASP:OD2	2.50	0.50
1:A:210:TRP:O	1:A:259:VAL:HG11	2.11	0.50
1:A:102:ARG:N	1:A:114:ASN:O	2.44	0.50
1:B:125:TRP:O	3:B:911:EDO:H12	2.10	0.50
1:B:281:PRO:HB3	1:B:283:TYR:CE1	2.46	0.50
1:B:310:SER:O	1:B:310:SER:OG	2.29	0.50
1:A:149:LEU:CD2	1:B:83:VAL:HG12	2.41	0.50
1:B:197:GLU:HB3	5:B:934:HOH:O	2.10	0.50
1:B:11:HIS:HB3	1:B:102:ARG:NH2	2.26	0.50
1:B:141:LEU:CA	1:B:144:ARG:HD2	2.41	0.50
1:A:207:SER:HB2	5:A:1209:HOH:O	2.11	0.50
1:B:241:TRP:CE3	1:B:253:SER:HB3	2.47	0.50
1:A:307:LEU:HB3	1:A:358:VAL:HG13	1.93	0.50
1:B:102:ARG:O	1:B:375:PRO:HG2	2.11	0.50
1:B:214:GLY:O	1:B:228:MSE:HE2	2.12	0.50
1:A:15:MSE:HG2	1:A:99:PHE:O	2.12	0.50
1:A:190:MSE:CE	1:A:198:GLU:HG2	2.42	0.50
1:A:188:PRO:CD	3:A:906:EDO:H22	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:NH1	5:B:1289:HOH:O	2.44	0.50
1:B:29:TRP:HE1	1:B:68:GLN:NE2	2.09	0.50
1:A:157:HIS:NE2	1:A:198:GLU:OE1	2.42	0.50
1:B:324:PRO:HB3	1:B:363:ASN:ND2	2.21	0.50
1:A:190:MSE:CG	1:A:190:MSE:CE	2.86	0.50
1:B:101:VAL:HA	1:B:115:ILE:HA	1.93	0.50
1:A:151:ARG:CD	5:A:1064:HOH:O	2.57	0.50
1:A:221:THR:HG21	1:A:224:HIS:CG	2.47	0.50
1:B:329:PRO:HG2	5:B:1048:HOH:O	2.10	0.50
1:A:118:ILE:HD13	1:A:120:TRP:CH2	2.47	0.50
1:B:229:CYS:SG	1:B:239:LEU:HD12	2.52	0.50
1:A:102:ARG:O	1:A:375:PRO:HG2	2.12	0.50
1:B:167:HIS:O	1:B:174:CYS:HA	2.12	0.49
1:B:29:TRP:CD1	1:B:68:GLN:HB3	2.47	0.49
1:B:212:PRO:HG2	1:B:255:GLU:CD	2.32	0.49
1:A:313:ASN:HD22	1:A:363:ASN:HB3	1.77	0.49
1:A:226:ASP:HB2	5:A:1019:HOH:O	2.11	0.49
1:B:125:TRP:O	3:B:911:EDO:H12	2.12	0.49
1:B:370:GLN:O	1:B:370:GLN:HG2	2.11	0.49
1:A:175:LEU:CD2	1:A:231:PHE:CE2	2.94	0.49
1:B:125:TRP:O	3:B:911:EDO:C1	2.60	0.49
1:B:85:MSE:SE	1:B:142:VAL:HG13	2.62	0.49
1:B:264:ILE:CD1	1:B:270:LYS:HG2	2.41	0.49
1:B:71:ASN:C	1:B:71:ASN:OD1	2.50	0.49
1:B:167:HIS:CD2	1:B:230:CYS:HB3	2.46	0.49
1:A:299:ILE:C	1:A:299:ILE:CD1	2.71	0.49
1:A:242:THR:O	1:A:242:THR:CG2	2.60	0.49
1:A:192:LYS:O	1:A:196:GLU:HG3	2.11	0.49
1:B:242:THR:HG21	1:B:249:GLN:HG3	1.93	0.49
1:B:25:THR:OG1	1:B:58:GLU:OE1	2.23	0.49
1:A:30:PRO:HG2	1:A:44:GLN:HG3	1.94	0.49
1:B:19:TRP:NE1	3:B:905:EDO:H21	2.28	0.49
1:B:64:ALA:O	1:B:84:GLU:HA	2.12	0.49
1:A:183:ASN:C	1:A:185:ASN:N	2.65	0.49
1:B:44:GLN:O	1:B:48:ALA:N	2.25	0.49
1:B:228:MSE:HE2	1:B:239:LEU:CD1	2.41	0.49
1:A:159:MSE:HB2	1:A:187:ASN:ND2	2.27	0.49
1:A:119:ASP:CG	1:A:154:ARG:HD2	2.33	0.49
1:A:230:CYS:SG	1:A:312:VAL:CG2	3.00	0.49
1:B:102:ARG:HA	1:B:103:LYS:HZ2	1.76	0.49
1:B:186:ARG:HH12	1:B:222:ASN:ND2	1.99	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLU:OE1	1:A:365:HIS:CE1	2.55	0.49
1:A:167:HIS:O	1:A:168:VAL:HG13	2.12	0.49
1:A:182:LEU:CD2	1:A:195:ILE:HD12	2.42	0.49
1:B:284:MSE:HE2	1:B:359:LEU:HD22	1.94	0.49
1:A:219:GLU:CD	5:A:1375:HOH:O	2.49	0.49
1:B:162:GLU:OE2	1:B:224:HIS:HE1	1.95	0.49
1:A:30:PRO:HD3	1:A:47:PHE:CD2	2.47	0.49
1:B:33:GLN:HE21	1:B:39:ASN:ND2	2.10	0.49
1:B:19:TRP:CZ2	1:B:234:PRO:HD3	2.47	0.49
1:B:88:ASN:HD21	1:B:138:HIS:N	2.10	0.49
1:A:104:ARG:HA	1:A:114:ASN:OD1	2.13	0.49
1:B:179:GLU:HB2	1:B:213:ARG:HA	1.93	0.49
1:A:40:ALA:O	1:A:44:GLN:HG3	2.13	0.49
1:A:232:ALA:HB3	1:A:233:ARG:HD3	1.94	0.49
1:B:73:ARG:NH1	1:B:80:ILE:O	2.45	0.49
1:B:87:MSE:O	1:B:88:ASN:C	2.49	0.49
1:B:230:CYS:SG	1:B:314:PHE:CZ	3.06	0.49
1:B:33:GLN:NE2	1:B:39:ASN:HA	2.14	0.49
1:A:144:ARG:NH1	1:A:154:ARG:HH11	2.10	0.49
1:A:203:LEU:N	1:A:203:LEU:HD23	2.27	0.49
1:A:24:GLN:NE2	1:B:151:ARG:HH22	2.10	0.49
1:A:55:SER:O	1:A:56:LYS:C	2.50	0.49
1:A:63:CYS:O	1:A:87:MSE:HE1	2.12	0.49
1:B:222:ASN:ND2	3:B:911:EDO:C1	2.58	0.49
1:B:94:ASP:OD1	3:B:904:EDO:H22	2.13	0.49
1:B:186:ARG:NH1	1:B:222:ASN:HD22	2.03	0.49
1:A:78:GLU:HG2	5:A:1328:HOH:O	2.12	0.49
1:B:19:TRP:HB3	1:B:316:ILE:HG21	1.93	0.49
1:B:279:PRO:HG3	1:B:326:PHE:CD1	2.47	0.49
1:B:125:TRP:O	3:B:911:EDO:C1	2.61	0.49
1:B:59:PRO:HB3	5:B:1101:HOH:O	2.11	0.49
1:A:255:GLU:O	1:A:258:SER:HB2	2.12	0.49
1:A:52:LYS:CE	5:A:1167:HOH:O	2.60	0.49
1:B:233:ARG:NH1	5:B:1119:HOH:O	2.34	0.49
1:A:121:ASN:ND2	1:A:122:PHE:H	2.10	0.49
1:B:363:ASN:HD22	1:B:364:ILE:N	2.11	0.49
1:A:61:THR:HG21	1:A:81:ARG:NH1	2.24	0.49
1:A:125:TRP:CG	1:A:221:THR:HG22	2.48	0.49
1:B:156:GLN:H	3:B:912:EDO:H21	1.77	0.49
1:B:37:ARG:HB3	1:B:292:ILE:CG1	2.43	0.49
1:B:263:SER:CB	5:B:1061:HOH:O	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ALA:O	1:B:131:GLY:HA2	2.12	0.49
1:A:200:LYS:HG2	1:A:205:VAL:O	2.13	0.49
1:B:282:LEU:HD11	5:B:1061:HOH:O	2.12	0.49
1:A:190:MSE:CE	1:A:195:ILE:HA	2.42	0.49
1:B:250:TYR:HB3	5:B:987:HOH:O	2.13	0.49
1:B:40:ALA:O	1:B:44:GLN:HG3	2.12	0.49
1:B:61:THR:HA	1:B:81:ARG:O	2.12	0.49
1:A:284:MSE:HE1	5:A:1144:HOH:O	1.98	0.49
1:A:84:GLU:CD	1:B:145:LYS:NZ	2.66	0.49
1:A:211:LEU:HD11	1:A:229:CYS:SG	2.53	0.49
1:A:84:GLU:O	3:A:908:EDO:H22	2.13	0.49
1:B:25:THR:OG1	1:B:58:GLU:OE1	2.30	0.49
1:B:88:ASN:HD21	1:B:138:HIS:H	1.59	0.49
1:B:112:ASN:HB2	5:B:1260:HOH:O	2.12	0.49
1:B:73:ARG:NH2	1:B:77:PRO:O	2.46	0.49
1:B:124:ALA:O	1:B:131:GLY:CA	2.61	0.49
1:B:215:LEU:HD23	1:B:308:ALA:HB1	1.95	0.49
1:A:163:GLY:O	1:A:166:ILE:HD12	2.13	0.49
1:A:260:LEU:HD22	1:A:271:ILE:HG21	1.95	0.49
1:A:276:LEU:HD13	1:A:338:VAL:HG11	1.95	0.49
1:A:313:ASN:HD22	1:A:363:ASN:CA	2.26	0.49
1:B:23:ALA:HB2	1:B:373:ALA:CA	2.32	0.49
1:A:313:ASN:ND2	1:A:365:HIS:H	2.11	0.49
1:A:357:ILE:HG22	1:A:362:GLY:O	2.12	0.49
1:B:20:ASP:OD1	5:B:1126:HOH:O	2.20	0.49
1:A:160:ILE:HD12	1:A:186:ARG:O	2.13	0.49
1:A:55:SER:HA	1:A:58:GLU:O	2.13	0.49
1:A:102:ARG:HG3	1:A:114:ASN:OD1	2.13	0.48
1:A:366:CYS:HG	1:A:367:ILE:HG23	1.78	0.48
1:A:188:PRO:HD2	5:A:1247:HOH:O	2.13	0.48
1:B:216:TYR:HB2	1:B:252:ARG:HD2	1.94	0.48
1:B:330:ILE:HG13	5:B:1051:HOH:O	2.12	0.48
1:A:123:ASN:HA	1:A:136:TRP:NE1	2.28	0.48
1:B:103:LYS:HD3	5:B:1266:HOH:O	2.12	0.48
1:B:190:MSE:HE1	1:B:198:GLU:HG2	1.95	0.48
3:A:908:EDO:H21	1:B:84:GLU:O	2.13	0.48
1:A:59:PRO:HG2	5:A:1161:HOH:O	2.12	0.48
1:B:159:MSE:HE1	1:B:195:ILE:HG12	1.94	0.48
1:A:35:ASN:HD21	1:A:301:ARG:HH21	1.61	0.48
1:A:78:GLU:HG2	5:A:1325:HOH:O	2.13	0.48
1:B:37:ARG:HH21	1:B:359:LEU:CD1	2.26	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASP:O	3:B:911:EDO:C1	2.61	0.48
1:A:216:TYR:HB2	1:A:252:ARG:CD	2.43	0.48
1:A:357:ILE:HG22	1:A:362:GLY:O	2.13	0.48
1:B:213:ARG:HB2	5:B:1098:HOH:O	2.12	0.48
1:B:145:LYS:O	1:B:146:ILE:C	2.50	0.48
1:A:52:LYS:HE2	5:A:1167:HOH:O	2.12	0.48
1:B:40:ALA:O	1:B:44:GLN:HG3	2.13	0.48
1:B:9:ALA:HB2	5:B:1263:HOH:O	2.12	0.48
1:B:190:MSE:CE	1:B:194:GLN:O	2.61	0.48
1:A:34:ASP:OD2	1:A:298:ALA:HB2	2.14	0.48
1:B:156:GLN:H	3:B:912:EDO:C2	2.25	0.48
1:A:85:MSE:HE2	5:B:1114:HOH:O	2.12	0.48
1:B:123:ASN:ND2	1:B:126:GLY:H	2.12	0.48
1:A:178:GLU:HG2	1:A:182:LEU:HD12	1.94	0.48
1:A:144:ARG:NH2	1:B:73:ARG:HG3	2.28	0.48
1:B:7:SER:N	1:B:8:PRO:CD	2.75	0.48
1:B:228:MSE:HE1	1:B:249:GLN:HE22	1.77	0.48
1:B:332:ASP:O	1:B:336:ILE:HG12	2.13	0.48
1:B:18:GLU:OE2	1:B:365:HIS:HE1	1.96	0.48
1:A:228:MSE:HE1	1:A:252:ARG:HB3	1.96	0.48
1:B:372:PRO:HB3	5:B:969:HOH:O	2.13	0.48
1:B:141:LEU:CD2	1:B:144:ARG:HD2	2.44	0.48
1:A:185:ASN:HA	3:A:906:EDO:H12	1.96	0.48
1:B:120:TRP:CE2	1:B:161:LEU:HD23	2.48	0.48
1:A:41:LEU:CD1	1:A:41:LEU:N	2.76	0.48
1:B:338:VAL:HG21	5:B:946:HOH:O	2.13	0.48
1:A:19:TRP:CB	1:A:316:ILE:HG21	2.44	0.48
1:B:219:GLU:HG2	5:B:1024:HOH:O	2.13	0.48
1:A:325:GLN:OE1	1:A:332:ASP:HB3	2.14	0.48
1:A:93:ARG:HH22	1:A:370:GLN:HE22	1.61	0.48
1:B:229:CYS:HB3	1:B:239:LEU:HA	1.94	0.48
1:B:174:CYS:SG	1:B:205:VAL:HG11	2.53	0.48
1:A:133:TYR:HA	1:A:298:ALA:HA	1.96	0.48
1:A:34:ASP:HB3	1:A:295:ASP:OD2	2.13	0.48
1:A:102:ARG:NH2	1:A:113:ARG:O	2.46	0.48
1:B:265:ASP:OD2	1:B:267:ARG:N	2.43	0.48
1:B:171:GLU:CD	1:B:234:PRO:HG2	2.33	0.48
1:B:219:GLU:CA	1:B:219:GLU:OE2	2.61	0.48
1:A:166:ILE:HD12	1:A:166:ILE:O	2.13	0.48
3:A:908:EDO:O1	1:B:149:LEU:HD13	2.14	0.48
1:A:63:CYS:O	1:A:87:MSE:HE1	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:HA	5:B:972:HOH:O	2.13	0.48
1:B:94:ASP:HB3	1:B:162:GLU:HB3	1.95	0.48
1:A:279:PRO:O	1:A:280:GLU:C	2.52	0.48
1:A:17:ALA:HB2	1:A:169:ASP:C	2.33	0.48
1:B:29:TRP:HE1	1:B:68:GLN:NE2	2.07	0.48
1:B:141:LEU:O	1:B:144:ARG:CG	2.62	0.48
1:B:241:TRP:O	1:B:278:ILE:HG12	2.12	0.48
1:A:363:ASN:OD1	1:A:364:ILE:HG13	2.14	0.48
1:A:325:GLN:O	1:A:354:ALA:CB	2.61	0.48
1:A:362:GLY:CA	5:A:1166:HOH:O	2.44	0.48
1:A:225:ILE:HG13	1:A:225:ILE:O	2.13	0.48
1:A:178:GLU:HB2	1:A:212:PRO:HA	1.95	0.48
1:B:190:MSE:HE2	1:B:195:ILE:HA	1.95	0.48
1:B:254:VAL:O	5:B:989:HOH:O	2.19	0.48
1:A:15:MSE:SE	1:A:98:THR:HG21	2.64	0.48
3:A:908:EDO:O1	1:B:149:LEU:HD13	2.14	0.48
1:B:16:PRO:HG3	1:B:101:VAL:CG2	2.44	0.48
1:B:71:ASN:O	1:B:71:ASN:OD1	2.31	0.48
1:A:91:TRP:CZ3	1:A:362:GLY:HA3	2.48	0.48
1:A:85:MSE:HE1	1:A:146:ILE:CG1	2.44	0.48
1:A:37:ARG:NH1	1:A:38:HIS:HD2	2.10	0.48
1:A:91:TRP:CE3	1:A:367:ILE:CG2	2.97	0.48
1:A:20:ASP:HB3	5:A:1110:HOH:O	2.13	0.48
1:A:147:LEU:HD22	1:A:152:ILE:CG2	2.43	0.48
1:B:165:SER:C	1:B:225:ILE:HG22	2.34	0.48
1:B:99:PHE:HB3	1:B:372:PRO:HD2	1.95	0.48
1:B:190:MSE:HA	1:B:194:GLN:NE2	2.29	0.48
1:B:214:GLY:O	1:B:252:ARG:HD3	2.13	0.48
1:A:347:SER:O	1:A:348:VAL:C	2.50	0.48
1:A:8:PRO:HB2	1:A:202:TYR:HA	1.96	0.48
1:B:65:SER:HA	1:B:85:MSE:O	2.14	0.48
1:B:18:GLU:HG2	1:B:316:ILE:HB	1.95	0.48
1:A:99:PHE:HB2	1:A:372:PRO:CD	2.43	0.48
1:A:307:LEU:HB3	1:A:358:VAL:CG1	2.43	0.48
1:B:165:SER:HB2	1:B:181:LEU:HD11	1.95	0.48
1:A:33:GLN:HG2	1:A:39:ASN:HA	1.94	0.48
1:A:241:TRP:CE3	1:A:253:SER:HB3	2.48	0.48
1:B:59:PRO:HB3	5:B:1102:HOH:O	2.12	0.48
1:A:134:ASN:HB3	5:A:1176:HOH:O	2.13	0.48
1:A:190:MSE:CE	1:A:194:GLN:O	2.61	0.48
1:B:159:MSE:HA	1:B:187:ASN:HD21	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:HB2	1:A:153:PRO:CD	2.42	0.48
1:A:193:GLU:CD	1:A:193:GLU:H	2.17	0.48
1:A:215:LEU:O	1:A:218:ASP:HB2	2.14	0.48
3:B:913:EDO:H22	5:B:972:HOH:O	2.13	0.48
1:B:199:LEU:O	1:B:200:LYS:C	2.51	0.48
1:A:85:MSE:HG3	1:A:86:SER:O	2.13	0.48
1:B:302:LEU:O	1:B:305:THR:HG23	2.13	0.48
1:B:15:MSE:HE1	1:B:203:LEU:HD13	1.96	0.48
1:B:11:HIS:HB3	1:B:102:ARG:HH21	1.78	0.48
1:A:44:GLN:NE2	1:A:71:ASN:HD21	2.10	0.48
1:B:88:ASN:OD1	1:B:136:TRP:CA	2.55	0.48
1:B:370:GLN:H	1:B:370:GLN:NE2	2.12	0.48
1:B:141:LEU:O	1:B:144:ARG:HG2	2.14	0.48
1:B:37:ARG:CA	1:B:292:ILE:HG12	2.43	0.48
1:B:99:PHE:HB2	1:B:372:PRO:CD	2.43	0.48
1:A:313:ASN:HD22	1:A:365:HIS:N	2.02	0.48
1:B:37:ARG:HH11	1:B:38:HIS:CE1	2.31	0.48
1:A:113:ARG:HB3	1:A:374:GLU:OE2	2.14	0.48
1:B:313:ASN:OD1	1:B:365:HIS:CB	2.62	0.48
1:B:37:ARG:HE	1:B:359:LEU:CD1	2.19	0.48
1:B:186:ARG:NH1	1:B:222:ASN:HD22	1.98	0.48
1:A:19:TRP:CZ2	1:A:234:PRO:HD3	2.49	0.48
1:B:248:PRO:O	1:B:251:GLU:HG2	2.14	0.47
1:B:22:HIS:HB2	1:B:318:ASN:ND2	2.29	0.47
3:B:913:EDO:H22	5:B:968:HOH:O	2.13	0.47
1:A:192:LYS:HE2	1:A:192:LYS:HB2	1.61	0.47
1:A:327:GLY:O	1:A:329:PRO:HD3	2.14	0.47
1:B:39:ASN:N	1:B:39:ASN:HD22	2.12	0.47
1:B:295:ASP:OD2	1:B:297:GLU:HB2	2.14	0.47
1:A:213:ARG:NH1	5:A:1303:HOH:O	2.25	0.47
1:A:5:ARG:HG2	1:A:5:ARG:HH21	1.78	0.47
1:B:99:PHE:HB2	1:B:372:PRO:HD3	1.96	0.47
1:A:159:MSE:HE2	1:A:161:LEU:CD1	2.43	0.47
1:A:242:THR:HG21	1:A:250:TYR:N	2.29	0.47
1:A:103:LYS:HG3	1:A:104:ARG:H	1.79	0.47
1:A:89:ASP:CB	5:A:1095:HOH:O	2.62	0.47
1:A:104:ARG:HA	1:A:114:ASN:ND2	2.29	0.47
1:A:120:TRP:HB2	1:A:161:LEU:O	2.14	0.47
1:B:188:PRO:HG2	1:B:189:HIS:N	2.29	0.47
1:A:213:ARG:O	1:A:228:MSE:HE2	2.13	0.47
1:A:6:GLU:HB3	1:A:11:HIS:HE1	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASN:ND2	1:A:222:ASN:HD22	2.11	0.47
1:B:22:HIS:HE1	1:B:316:ILE:O	1.97	0.47
1:B:185:ASN:HD21	1:B:222:ASN:HD21	1.62	0.47
1:B:302:LEU:O	1:B:305:THR:HG23	2.14	0.47
1:A:58:GLU:HB2	1:A:59:PRO:CD	2.44	0.47
1:B:68:GLN:NE2	1:B:71:ASN:HD22	2.11	0.47
1:A:113:ARG:HB2	1:A:153:PRO:CG	2.43	0.47
1:A:190:MSE:HE2	1:A:195:ILE:HA	1.95	0.47
1:B:88:ASN:HD21	1:B:138:HIS:N	2.12	0.47
1:A:52:LYS:CE	5:A:1164:HOH:O	2.62	0.47
1:B:191:SER:H	1:B:194:GLN:NE2	2.11	0.47
1:B:160:ILE:CG2	1:B:186:ARG:HD2	2.44	0.47
1:A:236:VAL:HA	1:A:272:GLN:O	2.14	0.47
1:A:15:MSE:HG2	1:A:16:PRO:O	2.15	0.47
1:A:77:PRO:HG2	5:A:1140:HOH:O	2.15	0.47
1:A:320:GLY:N	1:A:346:HIS:CD2	2.82	0.47
1:B:156:GLN:H	3:B:912:EDO:C2	2.27	0.47
1:A:288:GLU:O	1:A:289:SER:C	2.53	0.47
1:A:66:PRO:HD2	1:A:67:ALA:H	1.80	0.47
1:A:312:VAL:C	1:A:314:PHE:H	2.17	0.47
1:B:159:MSE:HE2	1:B:161:LEU:HB2	1.97	0.47
1:B:19:TRP:HB3	1:B:316:ILE:HG21	1.96	0.47
1:A:176:VAL:HB	1:A:181:LEU:CD2	2.44	0.47
1:A:112:ASN:N	1:A:112:ASN:ND2	2.63	0.47
1:A:5:ARG:NH2	1:A:158:SER:H	2.12	0.47
1:A:275:LYS:NZ	5:A:1158:HOH:O	2.47	0.47
1:A:8:PRO:HB3	1:A:100:ILE:HD12	1.95	0.47
1:B:21:SER:HA	1:B:318:ASN:HD21	1.78	0.47
1:A:291:GLY:HA3	5:A:1124:HOH:O	2.14	0.47
1:A:260:LEU:HD13	1:A:273:VAL:HG22	1.97	0.47
1:A:157:HIS:ND1	1:A:159:MSE:HG2	2.29	0.47
1:A:22:HIS:HE1	1:A:316:ILE:O	1.97	0.47
1:B:186:ARG:HH12	1:B:222:ASN:ND2	2.02	0.47
1:A:123:ASN:HA	1:A:136:TRP:CE2	2.50	0.47
1:A:236:VAL:HG13	1:A:272:GLN:HB3	1.95	0.47
1:A:228:MSE:CE	1:A:240:SER:HB2	2.45	0.47
1:A:144:ARG:HE	1:A:154:ARG:HE	1.63	0.47
1:B:164:GLY:O	1:B:224:HIS:HB3	2.15	0.47
1:B:222:ASN:HD21	3:B:911:EDO:H12	1.77	0.47
1:A:79:ASP:HB3	5:A:1345:HOH:O	2.14	0.47
1:B:8:PRO:HB3	1:B:13:TYR:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:O	3:A:908:EDO:H22	2.15	0.47
1:B:203:LEU:HB2	1:B:205:VAL:HG13	1.96	0.47
1:B:132:CYS:HB2	5:B:1274:HOH:O	2.14	0.47
1:A:225:ILE:CD1	1:A:229:CYS:SG	3.02	0.47
1:A:369:GLN:NE2	1:A:370:GLN:HE22	2.11	0.47
1:A:180:CYS:SG	1:A:181:LEU:N	2.87	0.47
1:B:328:ASP:HB2	5:B:1059:HOH:O	2.14	0.47
1:A:185:ASN:HA	3:A:906:EDO:C1	2.39	0.47
3:A:908:EDO:H11	1:B:83:VAL:HB	1.96	0.47
1:A:113:ARG:NH2	1:A:151:ARG:O	2.47	0.47
1:A:219:GLU:HB2	3:A:907:EDO:O1	2.15	0.47
1:A:183:ASN:O	5:A:1043:HOH:O	2.19	0.47
1:B:156:GLN:H	3:B:912:EDO:C2	2.28	0.47
1:A:159:MSE:HE3	1:A:187:ASN:CG	2.35	0.47
1:A:187:ASN:O	1:A:190:MSE:N	2.44	0.47
1:B:211:LEU:N	1:B:211:LEU:CD2	2.76	0.47
1:A:84:GLU:O	3:A:908:EDO:H22	2.15	0.47
1:B:133:TYR:HE2	1:B:135:ASP:O	1.96	0.47
1:A:174:CYS:SG	1:A:208:PHE:CD2	3.08	0.47
1:A:55:SER:HA	1:A:58:GLU:O	2.15	0.47
1:A:265:ASP:OD1	1:A:265:ASP:C	2.53	0.47
1:B:8:PRO:O	1:B:13:TYR:HD1	1.98	0.47
1:A:24:GLN:NE2	1:B:151:ARG:HH22	2.12	0.47
1:A:85:MSE:HG3	1:A:86:SER:N	2.27	0.47
1:B:22:HIS:ND1	1:B:58:GLU:OE2	2.42	0.47
1:A:35:ASN:HD21	1:A:301:ARG:HH21	1.62	0.47
1:A:324:PRO:CD	1:A:364:ILE:HD12	2.45	0.47
1:A:178:GLU:HG3	1:A:212:PRO:HA	1.95	0.47
1:B:225:ILE:HG23	1:B:226:ASP:N	2.29	0.47
1:A:313:ASN:HD22	1:A:363:ASN:HB3	1.80	0.47
1:A:177:THR:HA	1:A:211:LEU:O	2.15	0.47
1:B:337:ARG:NH1	1:B:338:VAL:HG22	2.29	0.47
1:B:87:MSE:CE	1:B:92:PHE:CE1	2.97	0.47
1:B:103:LYS:HZ2	1:B:103:LYS:N	2.13	0.47
1:A:178:GLU:HB2	1:A:212:PRO:HA	1.96	0.47
1:B:138:HIS:CD2	5:B:1084:HOH:O	2.50	0.47
1:B:112:ASN:HD22	1:B:113:ARG:N	2.13	0.47
3:A:908:EDO:O1	1:B:149:LEU:HD22	2.14	0.47
1:B:313:ASN:HB3	1:B:363:ASN:CB	2.43	0.47
1:B:220:ASP:O	3:B:911:EDO:C2	2.63	0.47
1:A:123:ASN:HA	1:A:136:TRP:CD1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLU:O	1:B:20:ASP:N	2.48	0.47
1:B:36:TRP:HB2	1:B:40:ALA:HB2	1.96	0.47
1:B:33:GLN:HE21	1:B:39:ASN:CA	2.27	0.47
1:A:91:TRP:HD1	1:A:125:TRP:CH2	2.33	0.47
1:B:228:MSE:HE1	1:B:252:ARG:HB3	1.96	0.47
1:B:191:SER:N	1:B:194:GLN:HE21	1.94	0.47
1:B:8:PRO:HG2	1:B:202:TYR:CD2	2.50	0.47
1:B:222:ASN:HD21	3:B:911:EDO:H12	1.80	0.47
1:A:282:LEU:HB3	1:A:307:LEU:HD12	1.97	0.47
1:A:144:ARG:HG2	1:B:69:TRP:HH2	1.79	0.47
1:B:19:TRP:CD1	3:B:905:EDO:H21	2.50	0.47
1:B:55:SER:CB	1:B:80:ILE:HD11	2.43	0.46
1:B:147:LEU:HD22	1:B:152:ILE:CG2	2.46	0.46
1:B:13:TYR:HB3	1:B:100:ILE:HD12	1.96	0.46
1:B:352:GLU:HG2	5:B:1038:HOH:O	2.14	0.46
1:A:34:ASP:CB	1:A:295:ASP:OD1	2.64	0.46
1:A:184:LYS:HE2	5:A:1149:HOH:O	2.14	0.46
1:B:211:LEU:HD21	1:B:260:LEU:CD2	2.45	0.46
1:B:26:TRP:CE3	1:B:63:CYS:SG	3.08	0.46
1:A:91:TRP:CE3	1:A:366:CYS:SG	3.08	0.46
1:B:7:SER:O	1:B:10:GLU:HB2	2.16	0.46
1:B:75:GLN:NE2	5:B:1040:HOH:O	2.49	0.46
1:A:172:GLY:O	1:A:206:GLN:N	2.44	0.46
1:B:37:ARG:HB3	1:B:292:ILE:HG13	1.97	0.46
1:A:5:ARG:NH1	1:A:158:SER:OG	2.47	0.46
1:A:221:THR:HG22	1:A:221:THR:O	2.16	0.46
1:B:54:ILE:HG12	1:B:322:ILE:HG13	1.97	0.46
1:A:35:ASN:HD21	1:A:301:ARG:NH2	2.01	0.46
1:A:177:THR:CA	1:A:211:LEU:O	2.62	0.46
1:A:185:ASN:ND2	1:A:222:ASN:ND2	2.34	0.46
1:B:220:ASP:HB2	5:B:1133:HOH:O	2.15	0.46
1:B:180:CYS:SG	1:B:223:GLY:C	2.93	0.46
1:B:157:HIS:CE1	1:B:159:MSE:HG2	2.50	0.46
1:A:28:GLY:O	1:A:47:PHE:CD2	2.68	0.46
1:B:141:LEU:CD2	1:B:144:ARG:HD2	2.45	0.46
1:A:216:TYR:H	1:A:249:GLN:HE22	1.64	0.46
1:B:197:GLU:HG3	1:B:201:LYS:HE2	1.97	0.46
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.76	0.46
1:A:5:ARG:HG2	1:A:5:ARG:HH21	1.80	0.46
1:B:47:PHE:CE1	1:B:357:ILE:HD12	2.50	0.46
1:A:200:LYS:NZ	5:A:1252:HOH:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLU:OE1	1:A:365:HIS:CE1	2.55	0.46
1:A:321:ILE:HD11	1:A:343:PHE:CD2	2.50	0.46
1:A:183:ASN:CG	1:A:222:ASN:HD22	2.19	0.46
1:A:190:MSE:HE2	1:A:195:ILE:N	2.31	0.46
1:A:20:ASP:HB2	5:A:1110:HOH:O	2.14	0.46
1:B:115:ILE:HG21	1:B:152:ILE:HG12	1.96	0.46
1:A:180:CYS:HB2	1:A:222:ASN:O	2.16	0.46
1:A:35:ASN:ND2	1:A:301:ARG:HE	2.13	0.46
1:A:160:ILE:HD13	1:A:187:ASN:OD1	2.16	0.46
1:A:84:GLU:HG2	1:B:84:GLU:OE1	2.15	0.46
1:A:319:GLY:N	5:A:1368:HOH:O	2.48	0.46
1:B:143:SER:O	1:B:147:LEU:HG	2.16	0.46
1:A:11:HIS:HB2	1:A:13:TYR:CD2	2.49	0.46
1:B:159:MSE:HE2	1:B:161:LEU:HD13	1.97	0.46
1:A:313:ASN:ND2	1:A:363:ASN:HB3	2.25	0.46
1:A:102:ARG:CG	1:A:114:ASN:HA	2.46	0.46
1:B:325:GLN:CG	1:B:350:GLY:HA3	2.45	0.46
1:B:115:ILE:O	1:B:153:PRO:HD2	2.15	0.46
1:B:64:ALA:O	1:B:84:GLU:HA	2.15	0.46
1:B:279:PRO:HA	1:B:331:ARG:CG	2.44	0.46
1:B:313:ASN:ND2	1:B:365:HIS:HB3	2.30	0.46
1:B:282:LEU:C	1:B:307:LEU:HD13	2.35	0.46
1:A:84:GLU:O	3:A:908:EDO:C2	2.64	0.46
1:A:52:LYS:HG2	1:A:77:PRO:HG2	1.98	0.46
1:B:315:TYR:O	1:B:322:ILE:HG12	2.15	0.46
1:B:26:TRP:O	1:B:369:GLN:N	2.40	0.46
1:B:160:ILE:H	1:B:187:ASN:ND2	2.12	0.46
1:B:194:GLN:O	1:B:197:GLU:HB3	2.16	0.46
1:A:46:VAL:HG21	1:A:356:GLU:HB2	1.96	0.46
1:A:176:VAL:O	1:A:225:ILE:HD13	2.16	0.46
1:B:325:GLN:NE2	1:B:332:ASP:HB3	2.30	0.46
1:A:76:LEU:HA	1:A:77:PRO:HD3	1.83	0.46
1:A:58:GLU:O	1:A:59:PRO:C	2.47	0.46
1:A:84:GLU:O	3:A:908:EDO:H22	2.16	0.46
1:B:93:ARG:HB2	1:B:366:CYS:HA	1.98	0.46
1:B:113:ARG:NH2	5:B:1101:HOH:O	2.47	0.46
1:B:249:GLN:CD	1:B:249:GLN:O	2.54	0.46
1:B:220:ASP:O	3:B:911:EDO:H11	2.15	0.46
1:B:91:TRP:CZ3	1:B:367:ILE:CG2	2.99	0.46
1:A:266:ALA:C	1:A:268:GLY:N	2.69	0.46
1:B:280:GLU:O	1:B:282:LEU:HD11	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:MSE:HE1	1:A:195:ILE:HG12	1.97	0.46
1:A:325:GLN:H	1:A:354:ALA:HB2	1.80	0.46
1:B:144:ARG:HH11	1:B:154:ARG:NH1	2.14	0.46
1:B:91:TRP:CH2	1:B:362:GLY:HA3	2.50	0.46
1:B:33:GLN:NE2	1:B:39:ASN:HA	2.31	0.46
1:A:336:ILE:HG23	1:A:348:VAL:CG1	2.45	0.46
1:A:191:SER:HB3	1:A:194:GLN:HE22	1.75	0.46
1:B:160:ILE:O	1:B:161:LEU:HB2	2.16	0.46
1:A:84:GLU:O	3:A:908:EDO:C2	2.64	0.46
1:B:134:ASN:CG	1:B:297:GLU:HA	2.36	0.46
1:A:307:LEU:HB3	1:A:358:VAL:CG1	2.45	0.46
1:B:222:ASN:ND2	3:B:911:EDO:C1	2.78	0.46
1:B:283:TYR:HA	1:B:307:LEU:CD1	2.46	0.46
1:B:19:TRP:CZ2	1:B:234:PRO:HD3	2.50	0.46
1:A:114:ASN:HB2	1:A:374:GLU:HG2	1.98	0.46
1:A:164:GLY:O	1:A:224:HIS:HB3	2.15	0.46
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.16	0.46
1:A:366:CYS:HB2	3:A:903:EDO:H11	1.96	0.46
1:B:200:LYS:HG2	1:B:205:VAL:O	2.16	0.46
1:B:76:LEU:O	1:B:77:PRO:C	2.53	0.46
1:A:144:ARG:NH1	1:A:154:ARG:NH1	2.63	0.46
1:B:103:LYS:H	1:B:103:LYS:CD	2.27	0.46
1:B:88:ASN:ND2	1:B:139:ASP:H	2.14	0.46
1:A:160:ILE:N	1:A:187:ASN:HD21	1.92	0.46
1:A:317:ALA:O	1:A:319:GLY:N	2.49	0.46
1:B:11:HIS:HB3	1:B:102:ARG:HH22	1.78	0.46
1:B:22:HIS:H	1:B:318:ASN:HD21	1.64	0.46
1:A:159:MSE:HE3	1:A:159:MSE:HB2	1.78	0.46
1:B:26:TRP:HB3	1:B:92:PHE:HD2	1.81	0.46
1:A:29:TRP:CD1	1:A:68:GLN:HB3	2.51	0.46
1:B:42:PRO:HA	1:B:45:ARG:HG3	1.97	0.46
1:B:102:ARG:HA	1:B:103:LYS:NZ	2.27	0.46
1:B:152:ILE:HG23	1:B:153:PRO:HD2	1.98	0.46
1:A:17:ALA:HB1	1:A:19:TRP:CE2	2.51	0.46
1:A:68:GLN:HE22	1:A:71:ASN:ND2	1.88	0.46
1:B:29:TRP:HE1	1:B:68:GLN:NE2	2.12	0.46
1:B:125:TRP:O	3:B:911:EDO:H12	2.16	0.46
1:A:160:ILE:H	1:A:160:ILE:CD1	2.21	0.46
1:B:238:LEU:HD22	1:B:276:LEU:HD22	1.97	0.46
1:A:14:TYR:CZ	4:A:9000:MPO:H72	2.51	0.46
1:B:242:THR:O	1:B:242:THR:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:HG2	5:A:1330:HOH:O	2.16	0.46
1:A:190:MSE:HA	1:A:194:GLN:HE21	1.81	0.46
1:B:359:LEU:HA	1:B:359:LEU:HD23	1.72	0.46
1:B:99:PHE:CD1	1:B:371:GLN:HA	2.51	0.46
5:A:1314:HOH:O	1:B:148:ALA:HB1	2.15	0.46
1:B:242:THR:HB	1:B:278:ILE:HD11	1.98	0.45
1:A:373:ALA:O	1:A:375:PRO:HD3	2.16	0.45
1:B:325:GLN:NE2	1:B:332:ASP:HB3	2.31	0.45
1:B:190:MSE:HE2	1:B:195:ILE:HG13	1.98	0.45
1:B:93:ARG:NH1	1:B:370:GLN:OE1	2.48	0.45
1:B:103:LYS:H	1:B:103:LYS:NZ	2.14	0.45
1:A:189:HIS:HB2	5:A:1314:HOH:O	2.15	0.45
1:B:260:LEU:HD13	1:B:273:VAL:HG22	1.98	0.45
1:B:74:LYS:HD2	5:B:1150:HOH:O	2.15	0.45
1:B:88:ASN:HD22	1:B:139:ASP:H	1.63	0.45
1:B:29:TRP:CH2	1:B:44:GLN:HB3	2.51	0.45
1:B:229:CYS:O	1:B:230:CYS:HB2	2.15	0.45
1:A:149:LEU:C	1:A:149:LEU:HD23	2.37	0.45
1:A:221:THR:CG2	1:A:224:HIS:CD2	2.99	0.45
1:A:125:TRP:O	1:A:131:GLY:HA2	2.17	0.45
1:A:96:GLY:HA3	1:A:369:GLN:OE1	2.16	0.45
1:B:83:VAL:HG11	1:B:149:LEU:HD21	1.98	0.45
1:B:161:LEU:HG	1:B:162:GLU:N	2.30	0.45
1:B:156:GLN:H	3:B:912:EDO:H21	1.82	0.45
1:A:159:MSE:CB	1:A:187:ASN:ND2	2.79	0.45
1:A:93:ARG:HH22	1:A:370:GLN:NE2	2.14	0.45
1:B:254:VAL:HG12	5:B:1169:HOH:O	2.17	0.45
1:A:282:LEU:HB3	1:A:307:LEU:HD12	1.97	0.45
1:A:149:LEU:HD23	1:B:83:VAL:HG12	1.98	0.45
1:B:363:ASN:ND2	1:B:364:ILE:H	2.15	0.45
1:A:149:LEU:HD23	1:B:83:VAL:HG12	1.96	0.45
1:A:5:ARG:HG2	1:A:202:TYR:OH	2.16	0.45
1:B:13:TYR:CE2	1:B:102:ARG:HG2	2.51	0.45
1:A:125:TRP:CZ3	1:A:133:TYR:HE2	2.35	0.45
1:A:89:ASP:HB3	5:A:1095:HOH:O	2.16	0.45
1:B:225:ILE:HD11	1:B:229:CYS:SG	2.56	0.45
1:A:187:ASN:HB3	1:A:190:MSE:SE	2.67	0.45
1:B:103:LYS:HD3	1:B:103:LYS:N	2.32	0.45
1:B:191:SER:H	1:B:194:GLN:NE2	2.08	0.45
1:B:24:GLN:HA	1:B:59:PRO:O	2.16	0.45
1:B:192:LYS:O	1:B:196:GLU:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLY:O	5:A:1169:HOH:O	2.21	0.45
1:B:124:ALA:HB2	1:B:136:TRP:HB3	1.99	0.45
1:B:40:ALA:O	1:B:44:GLN:HG3	2.16	0.45
1:B:129:ASN:OD1	1:B:129:ASN:N	2.49	0.45
1:A:327:GLY:H	1:A:332:ASP:CG	2.20	0.45
1:A:180:CYS:SG	1:A:181:LEU:HD22	2.56	0.45
1:A:325:GLN:OE1	1:A:332:ASP:HB3	2.17	0.45
1:A:99:PHE:HA	1:A:117:GLY:HA2	1.98	0.45
1:A:249:GLN:HG2	1:A:278:ILE:CD1	2.40	0.45
1:B:165:SER:HB2	1:B:181:LEU:CD1	2.46	0.45
1:B:220:ASP:CB	5:B:1230:HOH:O	2.57	0.45
1:B:7:SER:CB	1:B:8:PRO:HD3	2.38	0.45
1:A:125:TRP:CD1	1:A:162:GLU:HG2	2.51	0.45
1:A:185:ASN:C	1:A:185:ASN:OD1	2.55	0.45
1:B:44:GLN:HE22	1:B:68:GLN:NE2	2.14	0.45
1:B:285:THR:HB	5:B:1216:HOH:O	2.16	0.45
1:B:264:ILE:HA	1:B:269:ARG:O	2.16	0.45
1:B:212:PRO:CD	1:B:259:VAL:HG21	2.44	0.45
1:B:76:LEU:HD22	1:B:80:ILE:CD1	2.47	0.45
1:A:245:GLU:HG2	1:A:250:TYR:CE1	2.51	0.45
1:B:216:TYR:HB2	1:B:252:ARG:HD2	1.98	0.45
1:A:226:ASP:HB2	1:A:365:HIS:CD2	2.51	0.45
1:A:190:MSE:HA	1:A:194:GLN:NE2	2.31	0.45
1:B:11:HIS:CD2	5:B:1084:HOH:O	2.69	0.45
1:A:221:THR:O	1:A:222:ASN:HB2	2.17	0.45
1:B:241:TRP:CE3	1:B:253:SER:HB3	2.52	0.45
1:A:20:ASP:CB	5:A:1113:HOH:O	2.65	0.45
1:A:186:ARG:HH12	1:A:222:ASN:CG	2.20	0.45
1:A:35:ASN:ND2	1:A:301:ARG:HE	2.14	0.45
1:A:74:LYS:HE3	5:A:1216:HOH:O	2.16	0.45
1:A:173:THR:CG2	1:A:174:CYS:N	2.80	0.45
1:A:180:CYS:HB2	1:A:223:GLY:O	2.16	0.45
1:B:249:GLN:CG	1:B:249:GLN:O	2.64	0.45
1:B:167:HIS:O	1:B:174:CYS:HA	2.16	0.45
1:B:282:LEU:HB3	1:B:307:LEU:HD22	1.99	0.45
1:B:325:GLN:HB2	1:B:352:GLU:OE2	2.17	0.45
1:A:284:MSE:HB3	1:A:304:GLY:N	2.32	0.45
1:A:30:PRO:HD3	1:A:47:PHE:CE2	2.52	0.45
1:B:154:ARG:CG	1:B:154:ARG:HH11	2.23	0.45
1:B:167:HIS:CE1	1:B:230:CYS:HG	2.35	0.45
1:B:151:ARG:NH2	5:B:957:HOH:O	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:PRO:HB3	3:B:913:EDO:H22	1.99	0.45
1:B:62:VAL:O	1:B:82:VAL:HA	2.17	0.45
1:B:32:ARG:HH22	1:B:297:GLU:HB3	1.81	0.45
1:A:56:LYS:NZ	5:A:1154:HOH:O	2.40	0.45
1:A:52:LYS:HD3	1:A:77:PRO:CD	2.46	0.45
1:B:55:SER:HA	1:B:58:GLU:O	2.17	0.45
1:B:145:LYS:HA	1:B:148:ALA:HB3	1.99	0.45
1:B:93:ARG:NH2	1:B:365:HIS:CE1	2.85	0.45
1:A:165:SER:C	1:A:225:ILE:HG22	2.37	0.45
1:B:85:MSE:HB3	1:B:87:MSE:HE3	1.99	0.45
1:B:126:GLY:HA2	1:B:185:ASN:HB2	1.99	0.45
1:B:307:LEU:N	1:B:307:LEU:CD1	2.80	0.45
1:A:279:PRO:HD3	1:A:311:TYR:HE2	1.77	0.45
1:B:329:PRO:CG	5:B:1048:HOH:O	2.64	0.45
1:B:255:GLU:O	1:B:258:SER:HB3	2.16	0.45
1:B:60:VAL:HB	1:B:80:ILE:HG23	1.98	0.44
1:B:14:TYR:HB2	1:B:204:GLY:HA3	1.99	0.44
1:B:18:GLU:HG2	1:B:316:ILE:HB	1.98	0.44
1:A:258:SER:HA	5:A:1200:HOH:O	2.16	0.44
1:A:121:ASN:HD22	1:A:122:PHE:H	1.65	0.44
1:B:123:ASN:ND2	1:B:126:GLY:H	2.15	0.44
1:A:221:THR:CG2	3:A:903:EDO:H22	2.37	0.44
1:A:123:ASN:O	1:A:127:GLY:N	2.45	0.44
1:A:233:ARG:HG2	1:A:236:VAL:HB	1.99	0.44
1:B:229:CYS:HB2	1:B:239:LEU:HA	2.00	0.44
1:B:7:SER:CA	1:B:10:GLU:OE1	2.63	0.44
1:B:313:ASN:HB3	1:B:363:ASN:HB3	1.99	0.44
1:B:85:MSE:HE3	1:B:85:MSE:HB2	1.92	0.44
1:A:181:LEU:N	1:A:181:LEU:HD22	2.31	0.44
1:B:320:GLY:O	1:B:346:HIS:HD2	2.00	0.44
1:B:144:ARG:HH21	1:B:144:ARG:HG2	1.81	0.44
1:B:369:GLN:NE2	5:B:932:HOH:O	2.45	0.44
1:A:5:ARG:HG2	1:A:5:ARG:HH21	1.82	0.44
1:A:25:THR:CG2	1:A:368:THR:HB	2.47	0.44
1:A:160:ILE:N	1:A:187:ASN:HD21	2.15	0.44
1:A:149:LEU:HD23	1:A:149:LEU:O	2.18	0.44
1:A:327:GLY:O	1:A:329:PRO:HD3	2.18	0.44
1:B:141:LEU:C	1:B:144:ARG:HG2	2.37	0.44
1:B:153:PRO:HG2	5:B:1029:HOH:O	2.18	0.44
1:A:123:ASN:ND2	1:A:126:GLY:H	2.15	0.44
1:A:196:GLU:O	1:A:200:LYS:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:MSE:HE3	1:B:359:LEU:HD22	1.99	0.44
1:A:292:ILE:N	1:A:292:ILE:HD12	2.32	0.44
1:B:275:LYS:NZ	5:B:1134:HOH:O	2.50	0.44
1:B:313:ASN:OD1	1:B:363:ASN:HB3	2.17	0.44
1:B:103:LYS:H	1:B:103:LYS:HG2	1.59	0.44
1:B:14:TYR:OH	1:B:103:LYS:HE2	2.16	0.44
1:A:146:ILE:O	1:A:149:LEU:HB2	2.17	0.44
1:A:190:MSE:HE1	1:A:194:GLN:O	2.17	0.44
1:A:18:GLU:OE1	1:A:365:HIS:CE1	2.60	0.44
1:B:177:THR:HG21	1:B:223:GLY:O	2.18	0.44
1:A:218:ASP:OD2	1:A:221:THR:OG1	2.35	0.44
1:A:58:GLU:HB2	1:A:59:PRO:HD2	1.98	0.44
1:A:282:LEU:HB2	1:A:307:LEU:HB2	1.98	0.44
1:B:325:GLN:NE2	1:B:332:ASP:HB3	2.33	0.44
1:A:35:ASN:ND2	5:A:1277:HOH:O	2.50	0.44
1:B:264:ILE:N	5:B:1010:HOH:O	2.22	0.44
1:B:225:ILE:HD11	1:B:229:CYS:HB2	1.98	0.44
1:A:276:LEU:HD13	1:A:338:VAL:HG11	1.98	0.44
1:A:91:TRP:CH2	1:A:362:GLY:HA3	2.52	0.44
1:B:190:MSE:CE	1:B:195:ILE:HA	2.48	0.44
1:A:312:VAL:O	1:A:312:VAL:HG22	2.17	0.44
1:B:355:ARG:HB2	5:B:959:HOH:O	2.18	0.44
1:B:37:ARG:HG2	5:B:1198:HOH:O	2.17	0.44
1:A:216:TYR:N	1:A:249:GLN:HE22	2.06	0.44
1:A:30:PRO:HD3	1:A:47:PHE:CD2	2.52	0.44
1:B:241:TRP:O	1:B:277:TYR:HA	2.16	0.44
1:A:264:ILE:HA	1:A:269:ARG:O	2.17	0.44
1:B:29:TRP:CE2	1:B:72:ALA:HB2	2.53	0.44
1:A:363:ASN:ND2	1:A:364:ILE:N	2.65	0.44
1:B:316:ILE:HG12	1:B:321:ILE:HD13	2.00	0.44
1:A:276:LEU:HD13	1:A:338:VAL:CG1	2.47	0.44
1:A:104:ARG:HH21	1:A:104:ARG:CB	2.11	0.44
1:A:66:PRO:O	5:A:1119:HOH:O	2.20	0.44
1:B:179:GLU:CD	1:B:222:ASN:O	2.56	0.44
1:A:292:ILE:HB	5:A:1205:HOH:O	2.17	0.44
1:A:37:ARG:NH1	1:A:38:HIS:CD2	2.86	0.44
1:A:157:HIS:CG	1:A:159:MSE:HG2	2.53	0.44
1:A:55:SER:HA	1:A:58:GLU:O	2.18	0.44
1:A:313:ASN:ND2	1:A:363:ASN:HB3	2.32	0.44
1:A:170:GLY:O	4:A:9000:MPO:O1	2.35	0.44
1:A:337:ARG:HG2	1:A:337:ARG:NH1	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:MSE:HE1	1:B:198:GLU:CG	2.47	0.44
1:A:211:LEU:HD11	1:A:229:CYS:SG	2.57	0.44
1:A:241:TRP:CE3	1:A:253:SER:HB3	2.51	0.44
1:B:344:PRO:HD2	5:B:941:HOH:O	2.17	0.44
1:B:47:PHE:CE1	1:B:357:ILE:HD12	2.53	0.44
1:A:38:HIS:O	1:A:41:LEU:HD13	2.18	0.44
1:A:5:ARG:NH1	1:A:158:SER:H	2.15	0.44
1:A:195:ILE:O	1:A:196:GLU:C	2.54	0.44
1:B:260:LEU:O	1:B:263:SER:HB2	2.17	0.44
1:B:101:VAL:HG21	3:B:913:EDO:H11	1.99	0.44
1:B:119:ASP:OD2	1:B:154:ARG:HD2	2.18	0.44
1:A:313:ASN:HD21	1:A:366:CYS:H	1.65	0.44
1:B:315:TYR:HE1	1:B:317:ALA:HB2	1.78	0.44
1:A:175:LEU:HG	1:A:225:ILE:CD1	2.48	0.44
1:A:9:ALA:CB	5:A:1310:HOH:O	2.64	0.44
1:B:37:ARG:HE	1:B:356:GLU:CD	2.21	0.44
1:B:63:CYS:HB3	1:B:85:MSE:HB3	2.00	0.44
1:B:11:HIS:HD2	5:B:1084:HOH:O	2.00	0.44
1:B:102:ARG:HA	1:B:103:LYS:HZ2	1.82	0.44
1:A:20:ASP:HB3	5:A:1113:HOH:O	2.18	0.44
1:B:335:ALA:O	1:B:339:LEU:HG	2.18	0.44
1:B:264:ILE:HG22	1:B:265:ASP:O	2.17	0.44
1:A:55:SER:HA	1:A:58:GLU:O	2.18	0.44
1:B:151:ARG:CD	5:B:1046:HOH:O	2.66	0.44
1:A:41:LEU:N	1:A:41:LEU:HD12	2.33	0.44
1:A:313:ASN:HB3	1:A:363:ASN:OD1	2.17	0.44
1:B:36:TRP:CZ3	1:B:360:ALA:CB	3.01	0.44
1:B:243:ASP:OD1	5:B:1171:HOH:O	2.21	0.44
1:A:66:PRO:HG3	1:A:84:GLU:OE2	2.17	0.44
1:A:35:ASN:HD21	1:A:301:ARG:CZ	2.31	0.44
1:B:144:ARG:HE	1:B:154:ARG:CZ	2.31	0.44
1:B:192:LYS:HE2	1:B:210:TRP:CE2	2.53	0.44
1:A:229:CYS:C	1:A:230:CYS:SG	2.96	0.44
1:B:264:ILE:CG2	1:B:268:GLY:HA2	2.48	0.44
1:B:173:THR:HA	1:B:207:SER:O	2.18	0.44
1:A:33:GLN:HG2	1:A:39:ASN:HD22	1.82	0.43
1:A:363:ASN:N	1:A:366:CYS:HG	2.10	0.43
1:A:287:GLU:HB3	5:A:1161:HOH:O	2.16	0.43
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.64	0.43
1:A:190:MSE:HE2	1:A:195:ILE:CA	2.46	0.43
1:A:216:TYR:HB2	1:A:252:ARG:NE	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:CYS:HB3	1:B:208:PHE:CD2	2.53	0.43
1:A:159:MSE:HG3	1:A:190:MSE:SE	2.67	0.43
1:B:366:CYS:SG	1:B:367:ILE:CG2	2.95	0.43
1:B:25:THR:HG23	1:B:315:TYR:OH	2.18	0.43
1:B:142:VAL:O	1:B:146:ILE:HG13	2.17	0.43
1:B:40:ALA:O	1:B:44:GLN:HG3	2.18	0.43
1:B:8:PRO:HG2	1:B:202:TYR:CD2	2.53	0.43
1:B:55:SER:CB	1:B:80:ILE:HD11	2.44	0.43
1:A:29:TRP:HE1	1:A:68:GLN:NE2	2.13	0.43
1:B:145:LYS:O	1:B:148:ALA:HB3	2.18	0.43
1:A:179:GLU:HB2	1:A:213:ARG:HA	2.00	0.43
1:B:267:ARG:HB2	1:B:269:ARG:CZ	2.47	0.43
3:A:908:EDO:C1	5:B:942:HOH:O	2.65	0.43
1:B:46:VAL:HG11	1:B:357:ILE:HD11	1.99	0.43
1:A:123:ASN:ND2	1:A:126:GLY:H	2.16	0.43
1:B:11:HIS:HB2	1:B:13:TYR:CE1	2.53	0.43
1:B:36:TRP:CB	1:B:40:ALA:HB2	2.49	0.43
1:B:173:THR:OG1	1:B:265:ASP:HB2	2.18	0.43
1:A:194:GLN:HB3	5:A:1073:HOH:O	2.18	0.43
1:B:180:CYS:CB	1:B:222:ASN:O	2.66	0.43
1:B:11:HIS:HB3	1:B:102:ARG:HH22	1.80	0.43
1:B:363:ASN:HD22	1:B:364:ILE:N	2.15	0.43
1:A:334:GLU:OE2	1:A:337:ARG:NE	2.49	0.43
1:A:103:LYS:H	1:A:103:LYS:CE	2.31	0.43
1:A:79:ASP:OD1	5:A:1337:HOH:O	2.21	0.43
1:A:198:GLU:O	1:A:200:LYS:N	2.51	0.43
1:A:351:ILE:HG13	1:A:364:ILE:HD13	1.99	0.43
1:B:363:ASN:HD22	1:B:364:ILE:N	2.15	0.43
1:A:159:MSE:HE2	5:A:1103:HOH:O	2.17	0.43
1:B:32:ARG:HG3	1:B:35:ASN:CB	2.48	0.43
1:A:61:THR:CG2	1:A:81:ARG:HH11	2.26	0.43
1:A:343:PHE:HB3	1:A:346:HIS:HB2	2.01	0.43
1:A:117:GLY:HA3	1:A:147:LEU:CD1	2.41	0.43
1:A:14:TYR:CZ	4:A:9000:MPO:H72	2.52	0.43
1:B:274:ILE:HD13	1:B:342:THR:HG23	2.00	0.43
1:A:17:ALA:CB	1:A:19:TRP:CZ2	3.01	0.43
1:B:27:ILE:HG22	1:B:28:GLY:O	2.19	0.43
1:B:239:LEU:HD22	1:B:260:LEU:HD12	2.01	0.43
1:B:162:GLU:CD	1:B:186:ARG:HH21	2.21	0.43
1:B:26:TRP:HB3	1:B:92:PHE:CD2	2.54	0.43
1:B:28:GLY:HA2	1:B:63:CYS:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:MSE:HE2	1:A:161:LEU:HD13	2.00	0.43
1:B:86:SER:O	1:B:138:HIS:HB3	2.19	0.43
1:B:334:GLU:O	1:B:338:VAL:HG23	2.19	0.43
1:B:132:CYS:O	1:B:298:ALA:HB1	2.19	0.43
1:A:46:VAL:HG11	1:A:357:ILE:HG13	1.99	0.43
1:B:279:PRO:CB	1:B:282:LEU:HD11	2.49	0.43
1:A:255:GLU:O	1:A:259:VAL:HG23	2.18	0.43
1:B:216:TYR:HB2	1:B:252:ARG:HD2	1.99	0.43
1:A:211:LEU:HD13	1:A:256:ALA:CB	2.45	0.43
1:B:325:GLN:HG2	1:B:350:GLY:CA	2.49	0.43
1:A:121:ASN:HD22	1:A:122:PHE:H	1.67	0.43
1:B:220:ASP:OD1	1:B:299:ILE:HD12	2.18	0.43
1:A:54:ILE:CG1	1:A:322:ILE:HG13	2.48	0.43
1:A:70:GLU:HG3	5:A:1117:HOH:O	2.19	0.43
1:A:144:ARG:HG3	5:A:1085:HOH:O	2.19	0.43
1:B:120:TRP:HZ3	1:B:159:MSE:HE2	1.80	0.43
1:B:307:LEU:O	1:B:309:ALA:N	2.52	0.43
1:B:91:TRP:HD1	1:B:125:TRP:HH2	1.67	0.43
1:B:148:ALA:HB1	5:B:1204:HOH:O	2.19	0.43
1:A:212:PRO:HG2	1:A:255:GLU:CG	2.48	0.43
1:A:301:ARG:CG	1:A:301:ARG:NH1	2.81	0.43
1:A:156:GLN:HG2	1:A:157:HIS:N	2.32	0.43
1:A:84:GLU:O	3:A:908:EDO:C2	2.67	0.43
1:A:362:GLY:O	1:A:363:ASN:HB2	2.19	0.43
1:A:52:LYS:HD3	1:A:77:PRO:HD3	2.00	0.43
1:A:181:LEU:N	1:A:181:LEU:HD23	2.33	0.43
1:B:284:MSE:HE3	1:B:359:LEU:HD22	1.99	0.43
1:B:65:SER:OG	1:B:68:GLN:HB2	2.18	0.43
1:B:282:LEU:H	1:B:282:LEU:HD12	1.83	0.43
1:B:345:HIS:N	5:B:941:HOH:O	2.42	0.43
1:A:213:ARG:CB	1:A:252:ARG:HG2	2.48	0.43
1:B:329:PRO:CD	5:B:1048:HOH:O	2.61	0.43
1:B:32:ARG:HE	1:B:34:ASP:CG	2.22	0.43
1:B:353:ASN:CG	5:B:1217:HOH:O	2.57	0.43
1:B:233:ARG:HB2	1:B:234:PRO:CD	2.49	0.43
1:B:37:ARG:NH1	1:B:38:HIS:CE1	2.87	0.43
1:B:221:THR:O	1:B:222:ASN:HB2	2.18	0.43
1:B:199:LEU:HD22	1:B:203:LEU:HD11	2.01	0.43
1:A:93:ARG:NH1	1:A:365:HIS:CE1	2.87	0.43
1:A:321:ILE:HB	1:A:348:VAL:HG22	2.01	0.43
1:A:154:ARG:NH2	1:A:154:ARG:HG2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:H	1:B:103:LYS:CD	2.32	0.43
1:A:26:TRP:HE1	1:A:371:GLN:NE2	2.15	0.43
1:B:102:ARG:HA	1:B:103:LYS:NZ	2.32	0.43
1:A:91:TRP:HZ3	1:A:366:CYS:SG	2.41	0.43
1:B:86:SER:HB2	1:B:145:LYS:HZ2	1.83	0.43
1:B:74:LYS:HD2	5:B:1052:HOH:O	2.18	0.43
1:A:121:ASN:HB3	1:A:160:ILE:CA	2.43	0.43
1:A:103:LYS:O	1:A:104:ARG:HB3	2.19	0.43
1:B:68:GLN:HE22	1:B:71:ASN:HD22	1.66	0.43
1:A:241:TRP:O	1:A:277:TYR:HA	2.19	0.43
1:A:371:GLN:OE1	5:A:1036:HOH:O	2.21	0.43
1:A:84:GLU:O	3:A:908:EDO:H22	2.19	0.43
1:B:284:MSE:N	1:B:307:LEU:HD11	2.33	0.43
1:A:211:LEU:O	1:A:212:PRO:C	2.56	0.43
1:B:211:LEU:HD21	1:B:260:LEU:HD21	1.99	0.42
1:A:174:CYS:HB2	1:A:205:VAL:HG21	2.01	0.42
1:A:123:ASN:HD21	1:A:126:GLY:H	1.66	0.42
1:B:88:ASN:ND2	1:B:136:TRP:HA	2.34	0.42
1:A:233:ARG:HE	1:A:236:VAL:HB	1.83	0.42
1:A:35:ASN:ND2	1:A:301:ARG:HH21	2.17	0.42
1:A:326:PHE:HZ	1:A:363:ASN:HD21	1.66	0.42
1:A:196:GLU:O	1:A:197:GLU:C	2.57	0.42
1:A:187:ASN:OD1	5:A:1103:HOH:O	2.21	0.42
1:A:144:ARG:HE	1:A:154:ARG:NE	2.17	0.42
1:B:121:ASN:HB3	1:B:160:ILE:CA	2.49	0.42
1:A:226:ASP:OD2	1:A:365:HIS:HD2	2.02	0.42
1:A:279:PRO:HG3	1:A:326:PHE:CD1	2.54	0.42
1:B:125:TRP:O	3:B:911:EDO:C1	2.66	0.42
1:B:99:PHE:CB	1:B:372:PRO:CD	2.97	0.42
1:A:188:PRO:HD3	3:A:906:EDO:H22	2.01	0.42
1:B:228:MSE:O	1:B:229:CYS:HB2	2.19	0.42
1:A:229:CYS:HA	1:A:238:LEU:O	2.19	0.42
1:B:184:LYS:NZ	5:B:1159:HOH:O	2.41	0.42
1:A:198:GLU:OE1	5:A:1291:HOH:O	2.22	0.42
1:A:279:PRO:HD3	1:A:311:TYR:CD2	2.54	0.42
1:B:7:SER:N	1:B:202:TYR:HH	2.17	0.42
1:B:279:PRO:HD3	1:B:311:TYR:CE2	2.54	0.42
1:B:117:GLY:HA3	1:B:147:LEU:HD11	2.01	0.42
1:A:264:ILE:HA	1:A:269:ARG:O	2.18	0.42
1:A:159:MSE:HE1	1:A:195:ILE:HG23	2.00	0.42
1:B:139:ASP:HA	1:B:142:VAL:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:N	1:B:187:ASN:HD21	2.12	0.42
1:B:159:MSE:HE3	1:B:190:MSE:SE	2.69	0.42
1:B:102:ARG:HA	1:B:103:LYS:NZ	2.33	0.42
1:A:30:PRO:HD3	1:A:47:PHE:CG	2.54	0.42
1:A:147:LEU:HA	1:A:147:LEU:HD23	1.66	0.42
1:A:121:ASN:O	1:A:160:ILE:HA	2.19	0.42
1:A:230:CYS:SG	1:A:231:PHE:CA	3.07	0.42
1:A:101:VAL:HG12	1:A:115:ILE:HG13	2.01	0.42
1:B:233:ARG:HD3	5:B:994:HOH:O	2.19	0.42
1:A:288:GLU:O	1:A:292:ILE:HD13	2.19	0.42
1:B:321:ILE:HG22	1:B:321:ILE:O	2.18	0.42
1:A:317:ALA:O	1:A:318:ASN:C	2.57	0.42
1:B:355:ARG:O	1:B:359:LEU:HG	2.19	0.42
1:B:228:MSE:HE1	1:B:252:ARG:HB3	2.01	0.42
1:A:6:GLU:HA	1:A:10:GLU:OE2	2.19	0.42
1:A:241:TRP:CD1	1:A:242:THR:N	2.87	0.42
1:B:88:ASN:HD21	1:B:138:HIS:H	1.68	0.42
1:B:87:MSE:CE	1:B:92:PHE:CZ	3.01	0.42
1:A:31:GLU:HA	1:A:40:ALA:HB3	2.01	0.42
1:B:22:HIS:HE1	1:B:316:ILE:O	2.02	0.42
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.83	0.42
1:B:164:GLY:O	1:B:224:HIS:HB3	2.19	0.42
3:B:913:EDO:H22	5:B:970:HOH:O	2.19	0.42
1:B:85:MSE:HG3	5:B:1050:HOH:O	2.19	0.42
1:A:169:ASP:O	1:A:234:PRO:HG3	2.18	0.42
1:B:284:MSE:HE3	1:B:307:LEU:HD11	2.01	0.42
1:A:180:CYS:HB2	1:A:222:ASN:O	2.19	0.42
1:A:348:VAL:N	5:A:1097:HOH:O	2.50	0.42
1:B:226:ASP:OD1	1:B:226:ASP:N	2.48	0.42
1:A:39:ASN:O	1:A:40:ALA:HB3	2.19	0.42
1:A:175:LEU:HD11	1:A:229:CYS:SG	2.59	0.42
1:A:281:PRO:HB3	1:A:306:ARG:HD2	2.01	0.42
1:B:32:ARG:NH2	1:B:297:GLU:OE2	2.45	0.42
1:A:276:LEU:HA	1:A:276:LEU:HD12	1.73	0.42
1:B:156:GLN:H	3:B:912:EDO:C2	2.32	0.42
1:B:133:TYR:HA	1:B:298:ALA:HA	2.01	0.42
1:A:120:TRP:CG	1:A:161:LEU:HB3	2.54	0.42
1:A:100:ILE:O	1:A:115:ILE:HA	2.20	0.42
1:A:313:ASN:HD21	1:A:366:CYS:H	1.67	0.42
1:B:91:TRP:CE3	3:B:904:EDO:H21	2.55	0.42
1:B:15:MSE:CA	1:B:100:ILE:HG22	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:MSE:HE2	1:B:195:ILE:CA	2.50	0.42
1:B:42:PRO:HB2	1:B:356:GLU:OE1	2.19	0.42
1:B:87:MSE:CE	1:B:92:PHE:CZ	3.02	0.42
1:A:229:CYS:HB3	1:A:238:LEU:O	2.20	0.42
1:B:102:ARG:O	1:B:375:PRO:HG2	2.19	0.42
1:A:17:ALA:CB	1:A:19:TRP:CE2	3.02	0.42
1:A:84:GLU:O	3:A:908:EDO:H22	2.20	0.42
1:B:58:GLU:HA	3:B:909:EDO:H22	2.02	0.42
1:A:24:GLN:OE1	1:A:371:GLN:NE2	2.52	0.42
1:B:22:HIS:HB2	1:B:318:ASN:HD21	1.85	0.42
1:A:148:ALA:O	1:B:81:ARG:HG3	2.20	0.42
1:A:216:TYR:N	1:A:249:GLN:HE22	2.05	0.42
1:B:331:ARG:NH1	1:B:331:ARG:HG3	2.31	0.42
1:A:211:LEU:CD1	1:A:229:CYS:SG	3.08	0.42
1:B:274:ILE:HD13	1:B:342:THR:CG2	2.49	0.42
1:B:160:ILE:H	1:B:187:ASN:ND2	1.95	0.42
1:B:217:GLY:CA	1:B:308:ALA:HB2	2.49	0.42
1:A:286:GLU:HA	1:A:303:ALA:HB2	2.01	0.42
1:A:212:PRO:HG2	1:A:255:GLU:HG2	2.02	0.42
1:A:27:ILE:O	1:A:63:CYS:N	2.40	0.42
1:A:250:TYR:HB3	5:A:1076:HOH:O	2.18	0.42
1:B:134:ASN:N	1:B:297:GLU:O	2.44	0.42
1:B:218:ASP:OD1	5:B:1131:HOH:O	2.22	0.42
1:A:357:ILE:HD12	1:A:363:ASN:O	2.19	0.42
3:A:908:EDO:H12	5:B:1053:HOH:O	2.19	0.42
1:A:311:TYR:CG	1:A:335:ALA:HB1	2.55	0.42
1:A:183:ASN:C	1:A:185:ASN:H	2.22	0.42
1:A:219:GLU:HG3	1:A:219:GLU:O	2.19	0.42
1:A:39:ASN:O	1:A:40:ALA:HB3	2.20	0.42
1:B:125:TRP:HE3	1:B:132:CYS:SG	2.43	0.42
1:A:63:CYS:O	1:A:87:MSE:HE1	2.20	0.42
1:B:179:GLU:HG2	1:B:222:ASN:C	2.40	0.42
1:B:26:TRP:HB2	1:B:369:GLN:HB3	2.01	0.42
1:A:226:ASP:OD2	1:A:365:HIS:CD2	2.64	0.42
1:B:156:GLN:H	3:B:912:EDO:H21	1.84	0.42
1:B:184:LYS:O	1:B:188:PRO:HD3	2.19	0.42
1:A:15:MSE:HE3	1:A:168:VAL:CG1	2.41	0.42
1:B:125:TRP:O	3:B:911:EDO:H12	2.19	0.42
1:B:185:ASN:HD21	1:B:222:ASN:ND2	2.18	0.42
1:A:279:PRO:HA	1:A:331:ARG:HB2	1.98	0.42
1:A:310:SER:OG	1:A:312:VAL:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:O	1:B:98:THR:HG22	2.14	0.42
1:B:141:LEU:O	1:B:145:LYS:HG3	2.20	0.42
1:A:190:MSE:HE2	1:A:195:ILE:N	2.35	0.42
1:B:137:SER:HA	1:B:140:LEU:HD12	2.02	0.42
1:A:17:ALA:HB2	1:A:169:ASP:C	2.40	0.42
1:B:85:MSE:O	1:B:87:MSE:HE2	2.19	0.42
1:B:357:ILE:HG22	1:B:362:GLY:O	2.19	0.42
1:A:36:TRP:HB3	1:A:40:ALA:HA	2.01	0.42
1:B:88:ASN:ND2	1:B:136:TRP:C	2.74	0.42
1:B:314:PHE:O	1:B:365:HIS:HB2	2.18	0.42
1:A:48:ALA:CB	1:A:76:LEU:HD21	2.50	0.42
1:B:326:PHE:HE2	1:B:358:VAL:HG21	1.84	0.42
1:A:84:GLU:O	3:A:908:EDO:C2	2.68	0.42
1:A:313:ASN:ND2	1:A:365:HIS:N	2.67	0.42
1:B:179:GLU:HB2	1:B:213:ARG:HA	2.01	0.42
1:A:189:HIS:HB2	5:A:1245:HOH:O	2.20	0.42
1:A:136:TRP:HD1	1:A:140:LEU:HG	1.85	0.42
1:A:163:GLY:O	1:A:166:ILE:CD1	2.68	0.42
1:B:363:ASN:ND2	1:B:364:ILE:N	2.64	0.41
1:B:112:ASN:HB2	5:B:1265:HOH:O	2.19	0.41
1:A:284:MSE:HB2	1:A:284:MSE:HE3	1.79	0.41
1:B:276:LEU:HD13	1:B:338:VAL:HG11	2.02	0.41
1:A:26:TRP:NE1	1:A:371:GLN:NE2	2.57	0.41
1:B:313:ASN:CB	1:B:363:ASN:HB3	2.49	0.41
1:A:137:SER:HB2	5:A:1216:HOH:O	2.20	0.41
1:A:146:ILE:O	1:A:149:LEU:HB2	2.20	0.41
1:B:30:PRO:HG3	1:B:47:PHE:CD1	2.55	0.41
1:B:159:MSE:HB2	1:B:159:MSE:HE3	1.84	0.41
1:B:187:ASN:HB3	1:B:189:HIS:CE1	2.54	0.41
1:A:98:THR:CB	1:A:120:TRP:HE1	2.33	0.41
1:B:12:GLY:O	1:B:103:LYS:NZ	2.44	0.41
1:B:177:THR:HG21	1:B:223:GLY:O	2.19	0.41
1:A:161:LEU:CD1	1:A:181:LEU:HD11	2.50	0.41
1:B:89:ASP:HB3	1:B:91:TRP:CD1	2.55	0.41
1:B:220:ASP:O	3:B:911:EDO:H11	2.20	0.41
1:B:67:ALA:N	5:B:1005:HOH:O	2.34	0.41
1:B:343:PHE:HB3	1:B:346:HIS:HB2	2.01	0.41
1:A:322:ILE:HG22	1:A:364:ILE:HD13	2.01	0.41
1:B:39:ASN:N	1:B:39:ASN:HD22	2.18	0.41
1:A:19:TRP:HA	1:A:316:ILE:HG21	2.02	0.41
1:B:176:VAL:C	1:B:225:ILE:HD13	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ASP:CG	1:B:365:HIS:HD2	2.23	0.41
1:B:181:LEU:HD12	1:B:181:LEU:N	2.33	0.41
1:B:120:TRP:CE2	1:B:161:LEU:HD23	2.54	0.41
1:A:15:MSE:CA	1:A:100:ILE:HG22	2.51	0.41
1:A:15:MSE:HA	1:A:100:ILE:HG22	2.02	0.41
1:B:97:PRO:HD3	1:B:143:SER:CA	2.37	0.41
1:B:30:PRO:HD3	1:B:47:PHE:CE2	2.55	0.41
1:B:201:LYS:NZ	5:B:1046:HOH:O	2.52	0.41
1:B:102:ARG:HB2	1:B:103:LYS:NZ	2.35	0.41
1:B:363:ASN:HD22	1:B:364:ILE:H	1.68	0.41
1:A:165:SER:C	1:A:225:ILE:HG22	2.40	0.41
1:A:269:ARG:NH1	5:A:1062:HOH:O	2.34	0.41
1:B:26:TRP:HE3	1:B:63:CYS:SG	2.43	0.41
1:B:196:GLU:O	1:B:200:LYS:HG3	2.20	0.41
1:A:279:PRO:HD2	1:A:309:ALA:O	2.20	0.41
1:A:275:LYS:NZ	5:A:1082:HOH:O	2.50	0.41
1:A:282:LEU:O	1:A:306:ARG:HD2	2.20	0.41
1:B:281:PRO:HB3	1:B:283:TYR:CE1	2.55	0.41
1:B:116:ALA:CB	1:B:155:PHE:CZ	3.03	0.41
1:A:176:VAL:HB	1:A:181:LEU:HD21	2.02	0.41
1:A:18:GLU:OE1	1:A:93:ARG:NH1	2.54	0.41
1:A:93:ARG:NH2	1:A:370:GLN:OE1	2.53	0.41
1:B:123:ASN:HA	1:B:136:TRP:CD1	2.55	0.41
1:B:99:PHE:CD2	1:B:115:ILE:HD11	2.55	0.41
1:A:8:PRO:HD2	1:A:202:TYR:CE2	2.54	0.41
1:A:9:ALA:HB2	1:A:201:LYS:HA	2.02	0.41
1:B:184:LYS:HA	1:B:188:PRO:HB3	2.02	0.41
1:A:65:SER:HB2	1:A:66:PRO:CD	2.51	0.41
1:B:94:ASP:OD2	1:B:162:GLU:HB3	2.20	0.41
1:A:279:PRO:HG3	1:A:309:ALA:HB3	2.02	0.41
1:A:113:ARG:CB	1:A:374:GLU:OE2	2.62	0.41
1:B:88:ASN:HD22	1:B:139:ASP:H	1.69	0.41
1:B:63:CYS:O	1:B:87:MSE:HE1	2.20	0.41
1:B:184:LYS:HE2	1:B:184:LYS:HB2	1.79	0.41
1:B:241:TRP:CE3	1:B:253:SER:HB3	2.54	0.41
1:A:190:MSE:HA	1:A:194:GLN:HE21	1.83	0.41
1:B:112:ASN:HD22	1:B:113:ARG:H	1.68	0.41
1:B:199:LEU:O	1:B:205:VAL:HG22	2.20	0.41
1:A:284:MSE:CE	1:A:292:ILE:HD11	2.50	0.41
1:A:65:SER:HA	1:A:85:MSE:O	2.20	0.41
1:B:75:GLN:HE21	1:B:75:GLN:HB3	1.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:CYS:HB3	1:B:208:PHE:CD2	2.55	0.41
1:B:102:ARG:HG3	1:B:114:ASN:HD22	1.85	0.41
1:B:175:LEU:CD1	1:B:211:LEU:CD2	2.96	0.41
1:A:5:ARG:CG	1:A:5:ARG:HH21	2.33	0.41
1:A:63:CYS:HB2	1:A:87:MSE:HE1	2.01	0.41
1:B:11:HIS:HB2	1:B:13:TYR:CE1	2.55	0.41
1:B:226:ASP:HB2	1:B:365:HIS:CD2	2.55	0.41
1:A:141:LEU:O	1:A:145:LYS:HG3	2.20	0.41
1:B:174:CYS:SG	1:B:205:VAL:CB	3.08	0.41
1:A:216:TYR:CD2	1:A:248:PRO:HB2	2.55	0.41
1:B:74:LYS:HG3	1:B:74:LYS:O	2.20	0.41
1:A:180:CYS:O	1:A:186:ARG:HG3	2.20	0.41
1:B:185:ASN:HD21	1:B:222:ASN:ND2	2.18	0.41
1:B:17:ALA:CB	1:B:19:TRP:CE2	3.04	0.41
1:B:55:SER:HA	1:B:58:GLU:O	2.20	0.41
1:B:166:ILE:CG2	1:B:176:VAL:HG12	2.48	0.41
1:B:278:ILE:O	1:B:278:ILE:CG1	2.64	0.41
1:A:185:ASN:C	1:A:185:ASN:OD1	2.58	0.41
1:A:119:ASP:HB3	1:A:154:ARG:HD2	2.01	0.41
1:A:258:SER:HB2	5:A:1330:HOH:O	2.20	0.41
1:A:14:TYR:HA	1:A:203:LEU:O	2.19	0.41
1:B:132:CYS:HA	1:B:299:ILE:HG23	2.03	0.41
1:A:134:ASN:ND2	1:A:297:GLU:C	2.74	0.41
1:B:121:ASN:HD22	1:B:122:PHE:N	2.16	0.41
1:A:321:ILE:O	1:A:322:ILE:HD13	2.20	0.41
1:A:323:ALA:O	1:A:324:PRO:C	2.57	0.41
1:A:197:GLU:O	1:A:200:LYS:HB2	2.20	0.41
1:B:264:ILE:HD13	1:B:270:LYS:HG2	2.03	0.41
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.90	0.41
1:A:93:ARG:CB	1:A:366:CYS:HA	2.50	0.41
1:B:26:TRP:HH2	1:B:149:LEU:HD23	1.85	0.41
1:A:37:ARG:HB3	1:A:292:ILE:HD11	2.03	0.41
1:B:94:ASP:CB	1:B:162:GLU:HB3	2.50	0.41
1:A:99:PHE:CE2	1:A:371:GLN:HG3	2.56	0.41
1:A:282:LEU:HD22	1:A:355:ARG:NH1	2.36	0.41
1:A:184:LYS:HA	5:A:1286:HOH:O	2.20	0.41
1:A:121:ASN:CB	1:A:160:ILE:HA	2.46	0.41
1:B:79:ASP:CG	5:B:1200:HOH:O	2.45	0.41
1:B:60:VAL:O	1:B:80:ILE:CG2	2.65	0.41
1:A:55:SER:HA	1:A:58:GLU:O	2.20	0.41
1:A:241:TRP:HE1	1:A:243:ASP:CG	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:CYS:O	1:B:208:PHE:HA	2.20	0.41
1:B:307:LEU:HD12	1:B:307:LEU:HA	1.71	0.41
1:B:180:CYS:O	1:B:186:ARG:HG2	2.21	0.41
1:B:91:TRP:CZ3	1:B:367:ILE:HG22	2.55	0.41
1:A:33:GLN:O	1:A:292:ILE:HG23	2.21	0.41
1:A:15:MSE:HE2	1:A:15:MSE:HB3	1.49	0.41
3:A:908:EDO:C1	1:B:83:VAL:HB	2.51	0.41
1:A:102:ARG:NH2	1:A:113:ARG:O	2.53	0.41
1:A:179:GLU:HB2	1:A:213:ARG:HA	2.02	0.41
1:B:133:TYR:HA	1:B:298:ALA:HA	2.02	0.41
1:B:214:GLY:C	1:B:228:MSE:HG3	2.40	0.41
1:B:62:VAL:O	1:B:82:VAL:HA	2.21	0.41
1:B:22:HIS:HE1	1:B:316:ILE:O	2.03	0.41
1:A:321:ILE:HB	1:A:348:VAL:HG22	2.03	0.41
1:B:222:ASN:ND2	3:B:911:EDO:H11	2.35	0.41
1:B:64:ALA:O	1:B:84:GLU:HA	2.20	0.41
1:A:321:ILE:HG13	1:A:343:PHE:CD1	2.55	0.41
1:B:37:ARG:HH11	1:B:38:HIS:CE1	2.39	0.41
1:A:61:THR:HA	1:A:81:ARG:O	2.20	0.41
1:B:37:ARG:HA	1:B:292:ILE:HG12	2.02	0.41
1:A:141:LEU:O	1:A:142:VAL:C	2.59	0.41
1:A:190:MSE:HE2	1:A:195:ILE:CA	2.50	0.41
1:A:279:PRO:HD3	1:A:311:TYR:CE2	2.56	0.41
1:A:211:LEU:HD12	1:A:228:MSE:SE	2.70	0.41
1:B:230:CYS:HB3	5:B:920:HOH:O	2.20	0.41
1:B:100:ILE:CG2	1:B:118:ILE:HD11	2.50	0.41
1:B:57:PHE:HB3	1:B:318:ASN:O	2.20	0.41
1:B:88:ASN:ND2	1:B:139:ASP:H	2.18	0.41
1:A:103:LYS:O	1:A:104:ARG:HB3	2.20	0.41
1:B:199:LEU:HA	1:B:199:LEU:HD23	1.93	0.41
1:A:216:TYR:H	1:A:249:GLN:HE22	1.68	0.41
1:A:255:GLU:HG2	1:A:255:GLU:O	2.21	0.41
1:A:8:PRO:HB3	1:A:100:ILE:HD12	2.03	0.41
1:B:281:PRO:O	1:B:283:TYR:CE1	2.74	0.41
1:A:230:CYS:SG	1:A:231:PHE:C	2.98	0.41
1:B:32:ARG:HH12	1:B:133:TYR:CB	2.33	0.41
1:B:16:PRO:HD3	1:B:101:VAL:HG22	2.02	0.41
1:B:122:PHE:O	1:B:140:LEU:HD21	2.21	0.41
1:A:238:LEU:HD11	1:A:342:THR:HG21	2.02	0.41
1:B:301:ARG:O	1:B:302:LEU:HD23	2.20	0.41
1:A:31:GLU:HG3	1:A:68:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLU:O	1:B:353:ASN:HB2	2.20	0.41
1:B:132:CYS:HA	1:B:299:ILE:HG23	2.03	0.41
1:A:279:PRO:HA	1:A:331:ARG:HG3	2.01	0.41
1:A:36:TRP:CZ2	1:A:91:TRP:CZ2	3.08	0.41
3:B:913:EDO:H22	5:B:971:HOH:O	2.20	0.41
1:A:147:LEU:HD23	1:A:147:LEU:HA	1.90	0.41
1:A:115:ILE:O	1:A:153:PRO:HD2	2.21	0.41
1:B:119:ASP:OD2	1:B:144:ARG:HB3	2.21	0.41
1:B:36:TRP:CZ3	1:B:360:ALA:HB3	2.55	0.41
1:A:190:MSE:HE1	1:A:198:GLU:CG	2.50	0.41
1:B:12:GLY:O	1:B:102:ARG:HB3	2.21	0.41
1:A:372:PRO:HB3	5:A:1112:HOH:O	2.21	0.41
1:A:233:ARG:HD2	5:A:1042:HOH:O	2.20	0.41
1:A:242:THR:HG21	1:A:250:TYR:HA	1.99	0.41
1:B:112:ASN:HD22	1:B:113:ARG:N	2.19	0.41
1:B:282:LEU:HD11	5:B:1058:HOH:O	2.21	0.41
1:A:152:ILE:HG22	1:A:153:PRO:O	2.21	0.41
1:B:233:ARG:O	1:B:234:PRO:C	2.59	0.41
1:B:359:LEU:HA	1:B:359:LEU:HD23	1.90	0.41
1:B:162:GLU:OE2	1:B:224:HIS:HE1	2.04	0.41
1:A:349:VAL:HG12	1:A:350:GLY:N	2.36	0.41
1:B:222:ASN:ND2	3:B:911:EDO:C1	2.83	0.41
1:A:185:ASN:C	1:A:185:ASN:OD1	2.59	0.41
1:B:46:VAL:HG21	1:B:356:GLU:HB2	2.03	0.41
1:A:301:ARG:CZ	5:A:1279:HOH:O	2.68	0.41
1:B:88:ASN:N	1:B:88:ASN:ND2	2.67	0.41
1:A:306:ARG:HG3	1:A:307:LEU:N	2.36	0.41
1:B:327:GLY:O	1:B:328:ASP:C	2.59	0.41
1:B:114:ASN:HB2	1:B:374:GLU:HG2	2.03	0.41
1:A:115:ILE:HG23	1:A:115:ILE:O	2.21	0.41
1:B:302:LEU:O	1:B:305:THR:HG23	2.20	0.41
1:A:196:GLU:O	1:A:200:LYS:HG3	2.21	0.41
1:B:29:TRP:CZ2	1:B:44:GLN:CG	2.92	0.41
1:A:36:TRP:CH2	1:A:360:ALA:HB3	2.55	0.41
1:B:264:ILE:HA	1:B:269:ARG:O	2.21	0.41
1:B:55:SER:HA	1:B:58:GLU:O	2.21	0.41
1:A:121:ASN:HD22	1:A:122:PHE:H	1.68	0.41
1:B:171:GLU:O	1:B:267:ARG:CZ	2.69	0.41
1:B:126:GLY:HA3	1:B:130:ASP:HB2	2.02	0.41
1:A:15:MSE:SE	1:A:168:VAL:HG21	2.71	0.41
1:B:326:PHE:CE2	1:B:358:VAL:HG21	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASN:HD22	1:A:301:ARG:HE	1.69	0.40
1:A:289:SER:OG	1:A:301:ARG:O	2.34	0.40
1:A:51:ALA:O	1:A:60:VAL:HG21	2.20	0.40
1:A:337:ARG:HG2	1:A:337:ARG:HH11	1.86	0.40
1:B:357:ILE:HG22	1:B:362:GLY:O	2.21	0.40
1:B:173:THR:HG23	1:B:207:SER:O	2.21	0.40
1:B:191:SER:H	1:B:194:GLN:NE2	2.17	0.40
1:B:88:ASN:ND2	1:B:136:TRP:HA	2.36	0.40
1:B:280:GLU:O	1:B:282:LEU:CD1	2.69	0.40
1:A:233:ARG:NE	1:A:236:VAL:HG21	2.36	0.40
1:B:123:ASN:OD1	5:B:1134:HOH:O	2.22	0.40
1:B:311:TYR:HA	1:B:324:PRO:HG2	2.02	0.40
1:A:11:HIS:HB2	1:A:13:TYR:CD2	2.56	0.40
1:B:103:LYS:CD	1:B:103:LYS:H	2.33	0.40
1:B:264:ILE:CG2	1:B:268:GLY:HA2	2.51	0.40
1:B:23:ALA:O	1:B:59:PRO:HG2	2.21	0.40
1:B:104:ARG:HB2	1:B:114:ASN:ND2	2.36	0.40
1:B:278:ILE:O	1:B:331:ARG:NH1	2.54	0.40
1:A:120:TRP:CE2	1:A:161:LEU:HD23	2.56	0.40
1:A:98:THR:HG23	5:A:1110:HOH:O	2.21	0.40
1:A:311:TYR:HA	1:A:324:PRO:HG2	2.04	0.40
1:A:144:ARG:HG3	1:A:154:ARG:CD	2.52	0.40
1:A:179:GLU:N	1:A:212:PRO:O	2.53	0.40
1:B:64:ALA:HB1	1:B:69:TRP:HA	2.02	0.40
1:A:175:LEU:HG	1:A:225:ILE:HG12	2.04	0.40
1:A:216:TYR:H	1:A:249:GLN:HE22	1.68	0.40
1:B:37:ARG:N	1:B:292:ILE:HG12	2.37	0.40
1:B:264:ILE:HA	1:B:264:ILE:HD13	1.75	0.40
1:B:102:ARG:NH1	1:B:112:ASN:OD1	2.55	0.40
1:B:322:ILE:H	1:B:322:ILE:HG12	1.60	0.40
3:A:908:EDO:C2	1:B:84:GLU:O	2.69	0.40
1:A:15:MSE:HG2	1:A:100:ILE:HG22	2.03	0.40
1:B:260:LEU:HA	1:B:260:LEU:HD23	1.91	0.40
1:B:191:SER:N	1:B:194:GLN:HE21	2.03	0.40
1:A:351:ILE:HB	1:A:364:ILE:CD1	2.46	0.40
1:B:30:PRO:HG2	1:B:44:GLN:HG2	2.03	0.40
1:A:241:TRP:CZ2	1:A:275:LYS:HE2	2.56	0.40
1:A:144:ARG:HD3	1:B:69:TRP:CH2	2.57	0.40
1:A:226:ASP:O	1:A:312:VAL:HG12	2.21	0.40
1:A:121:ASN:HD22	1:A:122:PHE:H	1.69	0.40
1:A:316:ILE:HG12	1:A:321:ILE:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:HG22	1:B:167:HIS:N	2.37	0.40
1:B:93:ARG:O	1:B:163:GLY:HA3	2.22	0.40
1:A:102:ARG:HG2	1:A:114:ASN:CA	2.50	0.40
1:B:353:ASN:ND2	5:B:1217:HOH:O	2.53	0.40
1:B:38:HIS:N	1:B:291:GLY:O	2.37	0.40
1:A:283:TYR:CD2	1:A:304:GLY:O	2.75	0.40
1:B:241:TRP:O	1:B:277:TYR:HA	2.21	0.40
1:A:183:ASN:O	1:A:185:ASN:N	2.54	0.40
1:B:73:ARG:HA	1:B:82:VAL:HG21	2.03	0.40
1:A:327:GLY:N	1:A:332:ASP:OD2	2.49	0.40
1:A:178:GLU:HB3	1:A:182:LEU:HD12	2.04	0.40
1:B:85:MSE:HE1	1:B:146:ILE:HG12	2.03	0.40
1:A:5:ARG:HG2	1:A:5:ARG:HH21	1.86	0.40
1:A:316:ILE:HG12	1:A:321:ILE:CD1	2.51	0.40
1:B:93:ARG:CG	1:B:164:GLY:N	2.84	0.40
1:B:314:PHE:HE1	1:B:316:ILE:CG1	2.35	0.40
1:B:86:SER:HB3	1:B:138:HIS:CD2	2.56	0.40
1:A:130:ASP:CG	1:A:185:ASN:HD22	2.25	0.40
1:A:343:PHE:HB3	1:A:346:HIS:HB2	2.02	0.40
1:A:193:GLU:CD	1:A:193:GLU:N	2.75	0.40
1:B:38:HIS:ND1	1:B:291:GLY:HA3	2.35	0.40
1:B:255:GLU:O	1:B:258:SER:HB3	2.21	0.40
1:A:102:ARG:O	1:A:375:PRO:HG2	2.21	0.40
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.82	0.40
1:B:60:VAL:HB	1:B:80:ILE:HG23	2.03	0.40
1:B:186:ARG:NH1	1:B:222:ASN:CG	2.75	0.40
1:A:9:ALA:N	5:A:1310:HOH:O	2.54	0.40
1:B:17:ALA:O	1:B:18:GLU:C	2.59	0.40
1:A:343:PHE:N	1:A:344:PRO:CD	2.84	0.40
1:B:99:PHE:HA	1:B:117:GLY:HA2	2.03	0.40
1:B:282:LEU:CB	1:B:307:LEU:HD22	2.51	0.40
1:B:316:ILE:HG12	1:B:321:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	361/383 (94%)	342 (95%)	17 (5%)	2 (1%)	30	7
1	1-B	359/383 (94%)	336 (94%)	22 (6%)	1 (0%)	46	19
1	2-A	361/383 (94%)	346 (96%)	15 (4%)	0	100	100
1	2-B	359/383 (94%)	336 (94%)	21 (6%)	2 (1%)	30	7
1	3-A	361/383 (94%)	342 (95%)	16 (4%)	3 (1%)	24	4
1	3-B	359/383 (94%)	337 (94%)	20 (6%)	2 (1%)	30	7
1	4-A	361/383 (94%)	342 (95%)	18 (5%)	1 (0%)	46	19
1	4-B	359/383 (94%)	335 (93%)	18 (5%)	6 (2%)	11	1
1	5-A	361/383 (94%)	349 (97%)	11 (3%)	1 (0%)	46	19
1	5-B	359/383 (94%)	337 (94%)	20 (6%)	2 (1%)	30	7
1	6-A	361/383 (94%)	329 (91%)	30 (8%)	2 (1%)	30	7
1	6-B	359/383 (94%)	330 (92%)	26 (7%)	3 (1%)	24	4
1	7-A	361/383 (94%)	340 (94%)	17 (5%)	4 (1%)	17	2
1	7-B	359/383 (94%)	332 (92%)	24 (7%)	3 (1%)	24	4
1	8-A	361/383 (94%)	339 (94%)	20 (6%)	2 (1%)	30	7
1	8-B	359/383 (94%)	336 (94%)	22 (6%)	1 (0%)	46	19
All	All	5760/6128 (94%)	5408 (94%)	317 (6%)	35 (1%)	30	7

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3-A	318	ASN
1	8-A	318	ASN
1	2-B	318	ASN
1	3-B	322	ILE
1	4-B	292	ILE
1	5-A	318	ASN
1	5-B	128	ALA
1	6-B	31	GLU
1	8-B	19	TRP
1	1-A	363	ASN
1	4-B	128	ALA
1	4-B	303	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-B	222	ASN
1	6-A	135	ASP
1	6-B	123	ASN
1	7-A	37	ARG
1	7-A	295	ASP
1	7-A	318	ASN
1	7-B	11	HIS
1	7-B	318	ASN
1	8-A	369	GLN
1	3-A	313	ASN
1	4-B	281	PRO
1	7-A	31	GLU
1	7-B	10	GLU
1	1-A	233	ARG
1	1-B	233	ARG
1	2-B	31	GLU
1	3-A	31	GLU
1	3-B	328	ASP
1	4-A	31	GLU
1	4-B	31	GLU
1	6-A	249	GLN
1	6-B	77	PRO
1	4-B	131	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1-A	310/318 (98%)	297 (96%)	13 (4%)	36 7
1	1-B	308/318 (97%)	294 (96%)	14 (4%)	34 5
1	2-A	310/318 (98%)	298 (96%)	12 (4%)	39 8
1	2-B	308/318 (97%)	299 (97%)	9 (3%)	50 16
1	3-A	310/318 (98%)	295 (95%)	15 (5%)	31 5
1	3-B	308/318 (97%)	296 (96%)	12 (4%)	39 8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-A	310/318 (98%)	297 (96%)	13 (4%)	36	7
1	4-B	308/318 (97%)	294 (96%)	14 (4%)	34	5
1	5-A	310/318 (98%)	297 (96%)	13 (4%)	36	7
1	5-B	308/318 (97%)	297 (96%)	11 (4%)	42	10
1	6-A	310/318 (98%)	290 (94%)	20 (6%)	21	2
1	6-B	308/318 (97%)	290 (94%)	18 (6%)	25	3
1	7-A	310/318 (98%)	297 (96%)	13 (4%)	36	7
1	7-B	308/318 (97%)	286 (93%)	22 (7%)	18	1
1	8-A	310/318 (98%)	300 (97%)	10 (3%)	46	13
1	8-B	308/318 (97%)	295 (96%)	13 (4%)	36	7
All	All	4944/5088 (97%)	4722 (96%)	222 (4%)	34	5

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	5	ARG
1	1-A	8	PRO
1	1-A	41	LEU
1	1-A	61	THR
1	1-A	104	ARG
1	1-A	121	ASN
1	1-A	123	ASN
1	1-A	181	LEU
1	1-A	219	GLU
1	1-A	225	ILE
1	1-A	228	MSE
1	1-A	284	MSE
1	1-A	292	ILE
1	1-B	103	LYS
1	1-B	121	ASN
1	1-B	123	ASN
1	1-B	134	ASN
1	1-B	143	SER
1	1-B	144	ARG
1	1-B	150	GLU
1	1-B	207	SER
1	1-B	230	CYS
1	1-B	281	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-B	282	LEU
1	1-B	307	LEU
1	1-B	312	VAL
1	1-B	363	ASN
1	2-A	5	ARG
1	2-A	8	PRO
1	2-A	39	ASN
1	2-A	41	LEU
1	2-A	103	LYS
1	2-A	121	ASN
1	2-A	123	ASN
1	2-A	166	ILE
1	2-A	180	CYS
1	2-A	301	ARG
1	2-A	313	ASN
1	2-A	328	ASP
1	2-B	88	ASN
1	2-B	103	LYS
1	2-B	121	ASN
1	2-B	123	ASN
1	2-B	130	ASP
1	2-B	180	CYS
1	2-B	188	PRO
1	2-B	307	LEU
1	2-B	363	ASN
1	3-A	5	ARG
1	3-A	8	PRO
1	3-A	30	PRO
1	3-A	35	ASN
1	3-A	47	PHE
1	3-A	121	ASN
1	3-A	123	ASN
1	3-A	133	TYR
1	3-A	158	SER
1	3-A	181	LEU
1	3-A	240	SER
1	3-A	313	ASN
1	3-A	324	PRO
1	3-A	358	VAL
1	3-A	366	CYS
1	3-B	86	SER
1	3-B	112	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-B	121	ASN
1	3-B	123	ASN
1	3-B	130	ASP
1	3-B	224	HIS
1	3-B	226	ASP
1	3-B	228	MSE
1	3-B	281	PRO
1	3-B	282	LEU
1	3-B	307	LEU
1	3-B	363	ASN
1	4-A	5	ARG
1	4-A	8	PRO
1	4-A	31	GLU
1	4-A	41	LEU
1	4-A	89	ASP
1	4-A	103	LYS
1	4-A	104	ARG
1	4-A	112	ASN
1	4-A	121	ASN
1	4-A	123	ASN
1	4-A	137	SER
1	4-A	226	ASP
1	4-A	230	CYS
1	4-B	10	GLU
1	4-B	30	PRO
1	4-B	102	ARG
1	4-B	103	LYS
1	4-B	112	ASN
1	4-B	123	ASN
1	4-B	134	ASN
1	4-B	135	ASP
1	4-B	167	HIS
1	4-B	203	LEU
1	4-B	228	MSE
1	4-B	305	THR
1	4-B	307	LEU
1	4-B	363	ASN
1	5-A	8	PRO
1	5-A	15	MSE
1	5-A	31	GLU
1	5-A	35	ASN
1	5-A	38	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-A	90	SER
1	5-A	92	PHE
1	5-A	103	LYS
1	5-A	121	ASN
1	5-A	123	ASN
1	5-A	180	CYS
1	5-A	181	LEU
1	5-A	363	ASN
1	5-B	102	ARG
1	5-B	103	LYS
1	5-B	121	ASN
1	5-B	123	ASN
1	5-B	150	GLU
1	5-B	198	GLU
1	5-B	218	ASP
1	5-B	227	ASN
1	5-B	230	CYS
1	5-B	307	LEU
1	5-B	363	ASN
1	6-A	5	ARG
1	6-A	8	PRO
1	6-A	15	MSE
1	6-A	30	PRO
1	6-A	104	ARG
1	6-A	121	ASN
1	6-A	123	ASN
1	6-A	135	ASP
1	6-A	149	LEU
1	6-A	161	LEU
1	6-A	167	HIS
1	6-A	175	LEU
1	6-A	176	VAL
1	6-A	184	LYS
1	6-A	206	GLN
1	6-A	227	ASN
1	6-A	229	CYS
1	6-A	230	CYS
1	6-A	265	ASP
1	6-A	332	ASP
1	6-B	15	MSE
1	6-B	31	GLU
1	6-B	77	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-B	87	MSE
1	6-B	103	LYS
1	6-B	121	ASN
1	6-B	123	ASN
1	6-B	130	ASP
1	6-B	139	ASP
1	6-B	174	CYS
1	6-B	224	HIS
1	6-B	248	PRO
1	6-B	262	ASN
1	6-B	263	SER
1	6-B	307	LEU
1	6-B	363	ASN
1	6-B	370	GLN
1	6-B	375	PRO
1	7-A	8	PRO
1	7-A	16	PRO
1	7-A	20	ASP
1	7-A	30	PRO
1	7-A	31	GLU
1	7-A	103	LYS
1	7-A	104	ARG
1	7-A	112	ASN
1	7-A	121	ASN
1	7-A	123	ASN
1	7-A	144	ARG
1	7-A	167	HIS
1	7-A	181	LEU
1	7-B	42	PRO
1	7-B	74	LYS
1	7-B	89	ASP
1	7-B	102	ARG
1	7-B	103	LYS
1	7-B	104	ARG
1	7-B	112	ASN
1	7-B	121	ASN
1	7-B	123	ASN
1	7-B	130	ASP
1	7-B	134	ASN
1	7-B	161	LEU
1	7-B	177	THR
1	7-B	224	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-B	226	ASP
1	7-B	265	ASP
1	7-B	282	LEU
1	7-B	307	LEU
1	7-B	328	ASP
1	7-B	357	ILE
1	7-B	363	ASN
1	7-B	370	GLN
1	8-A	24	GLN
1	8-A	102	ARG
1	8-A	121	ASN
1	8-A	123	ASN
1	8-A	130	ASP
1	8-A	161	LEU
1	8-A	192	LYS
1	8-A	226	ASP
1	8-A	228	MSE
1	8-A	233	ARG
1	8-B	20	ASP
1	8-B	31	GLU
1	8-B	103	LYS
1	8-B	112	ASN
1	8-B	121	ASN
1	8-B	123	ASN
1	8-B	129	ASN
1	8-B	130	ASP
1	8-B	226	ASP
1	8-B	230	CYS
1	8-B	261	SER
1	8-B	307	LEU
1	8-B	363	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (292) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	22	HIS
1	1-A	24	GLN
1	1-A	35	ASN
1	1-A	38	HIS
1	1-A	39	ASN
1	1-A	44	GLN
1	1-A	68	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	75	GLN
1	1-A	112	ASN
1	1-A	121	ASN
1	1-A	123	ASN
1	1-A	187	ASN
1	1-A	194	GLN
1	1-A	222	ASN
1	1-A	224	HIS
1	1-A	249	GLN
1	1-A	313	ASN
1	1-A	346	HIS
1	1-A	353	ASN
1	1-A	365	HIS
1	1-A	371	GLN
1	1-B	39	ASN
1	1-B	68	GLN
1	1-B	75	GLN
1	1-B	88	ASN
1	1-B	114	ASN
1	1-B	121	ASN
1	1-B	123	ASN
1	1-B	134	ASN
1	1-B	156	GLN
1	1-B	187	ASN
1	1-B	194	GLN
1	1-B	222	ASN
1	1-B	224	HIS
1	1-B	272	GLN
1	1-B	318	ASN
1	1-B	325	GLN
1	1-B	363	ASN
1	1-B	365	HIS
1	2-A	24	GLN
1	2-A	35	ASN
1	2-A	39	ASN
1	2-A	44	GLN
1	2-A	68	GLN
1	2-A	75	GLN
1	2-A	112	ASN
1	2-A	121	ASN
1	2-A	123	ASN
1	2-A	187	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	194	GLN
1	2-A	249	GLN
1	2-A	353	ASN
1	2-A	365	HIS
1	2-A	369	GLN
1	2-A	371	GLN
1	2-B	11	HIS
1	2-B	24	GLN
1	2-B	33	GLN
1	2-B	39	ASN
1	2-B	68	GLN
1	2-B	88	ASN
1	2-B	112	ASN
1	2-B	121	ASN
1	2-B	123	ASN
1	2-B	134	ASN
1	2-B	138	HIS
1	2-B	187	ASN
1	2-B	194	GLN
1	2-B	222	ASN
1	2-B	272	GLN
1	2-B	318	ASN
1	2-B	325	GLN
1	2-B	346	HIS
1	2-B	363	ASN
1	2-B	365	HIS
1	3-A	24	GLN
1	3-A	33	GLN
1	3-A	35	ASN
1	3-A	38	HIS
1	3-A	39	ASN
1	3-A	44	GLN
1	3-A	68	GLN
1	3-A	75	GLN
1	3-A	112	ASN
1	3-A	121	ASN
1	3-A	123	ASN
1	3-A	187	ASN
1	3-A	194	GLN
1	3-A	249	GLN
1	3-A	313	ASN
1	3-A	353	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-A	365	HIS
1	3-A	371	GLN
1	3-B	24	GLN
1	3-B	33	GLN
1	3-B	39	ASN
1	3-B	68	GLN
1	3-B	75	GLN
1	3-B	88	ASN
1	3-B	112	ASN
1	3-B	114	ASN
1	3-B	121	ASN
1	3-B	123	ASN
1	3-B	134	ASN
1	3-B	156	GLN
1	3-B	187	ASN
1	3-B	194	GLN
1	3-B	222	ASN
1	3-B	224	HIS
1	3-B	318	ASN
1	3-B	325	GLN
1	3-B	363	ASN
1	3-B	365	HIS
1	4-A	24	GLN
1	4-A	35	ASN
1	4-A	38	HIS
1	4-A	39	ASN
1	4-A	44	GLN
1	4-A	68	GLN
1	4-A	75	GLN
1	4-A	121	ASN
1	4-A	123	ASN
1	4-A	187	ASN
1	4-A	194	GLN
1	4-A	206	GLN
1	4-A	249	GLN
1	4-A	346	HIS
1	4-A	353	ASN
1	4-A	365	HIS
1	4-A	371	GLN
1	4-B	24	GLN
1	4-B	33	GLN
1	4-B	39	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	68	GLN
1	4-B	75	GLN
1	4-B	88	ASN
1	4-B	112	ASN
1	4-B	114	ASN
1	4-B	121	ASN
1	4-B	123	ASN
1	4-B	129	ASN
1	4-B	134	ASN
1	4-B	156	GLN
1	4-B	189	HIS
1	4-B	194	GLN
1	4-B	222	ASN
1	4-B	224	HIS
1	4-B	272	GLN
1	4-B	294	GLN
1	4-B	318	ASN
1	4-B	325	GLN
1	4-B	363	ASN
1	4-B	365	HIS
1	5-A	24	GLN
1	5-A	35	ASN
1	5-A	39	ASN
1	5-A	44	GLN
1	5-A	68	GLN
1	5-A	121	ASN
1	5-A	123	ASN
1	5-A	187	ASN
1	5-A	194	GLN
1	5-A	249	GLN
1	5-A	313	ASN
1	5-A	369	GLN
1	5-A	371	GLN
1	5-B	24	GLN
1	5-B	39	ASN
1	5-B	44	GLN
1	5-B	71	ASN
1	5-B	88	ASN
1	5-B	112	ASN
1	5-B	121	ASN
1	5-B	123	ASN
1	5-B	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-B	167	HIS
1	5-B	187	ASN
1	5-B	194	GLN
1	5-B	227	ASN
1	5-B	272	GLN
1	5-B	318	ASN
1	5-B	325	GLN
1	5-B	363	ASN
1	5-B	365	HIS
1	6-A	11	HIS
1	6-A	24	GLN
1	6-A	35	ASN
1	6-A	44	GLN
1	6-A	68	GLN
1	6-A	112	ASN
1	6-A	121	ASN
1	6-A	123	ASN
1	6-A	134	ASN
1	6-A	187	ASN
1	6-A	194	GLN
1	6-A	206	GLN
1	6-A	224	HIS
1	6-A	249	GLN
1	6-A	313	ASN
1	6-A	365	HIS
1	6-A	371	GLN
1	6-B	24	GLN
1	6-B	39	ASN
1	6-B	68	GLN
1	6-B	75	GLN
1	6-B	88	ASN
1	6-B	112	ASN
1	6-B	114	ASN
1	6-B	121	ASN
1	6-B	123	ASN
1	6-B	156	GLN
1	6-B	194	GLN
1	6-B	222	ASN
1	6-B	224	HIS
1	6-B	272	GLN
1	6-B	318	ASN
1	6-B	325	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-B	363	ASN
1	6-B	365	HIS
1	6-B	369	GLN
1	7-A	24	GLN
1	7-A	35	ASN
1	7-A	39	ASN
1	7-A	44	GLN
1	7-A	68	GLN
1	7-A	75	GLN
1	7-A	121	ASN
1	7-A	123	ASN
1	7-A	187	ASN
1	7-A	194	GLN
1	7-A	224	HIS
1	7-A	249	GLN
1	7-A	313	ASN
1	7-A	365	HIS
1	7-A	369	GLN
1	7-A	371	GLN
1	7-B	11	HIS
1	7-B	24	GLN
1	7-B	39	ASN
1	7-B	68	GLN
1	7-B	71	ASN
1	7-B	88	ASN
1	7-B	114	ASN
1	7-B	121	ASN
1	7-B	123	ASN
1	7-B	134	ASN
1	7-B	156	GLN
1	7-B	187	ASN
1	7-B	194	GLN
1	7-B	222	ASN
1	7-B	224	HIS
1	7-B	272	GLN
1	7-B	318	ASN
1	7-B	363	ASN
1	7-B	365	HIS
1	7-B	370	GLN
1	8-A	24	GLN
1	8-A	35	ASN
1	8-A	39	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-A	44	GLN
1	8-A	68	GLN
1	8-A	121	ASN
1	8-A	123	ASN
1	8-A	134	ASN
1	8-A	194	GLN
1	8-A	222	ASN
1	8-A	249	GLN
1	8-A	313	ASN
1	8-A	346	HIS
1	8-A	365	HIS
1	8-B	11	HIS
1	8-B	24	GLN
1	8-B	39	ASN
1	8-B	68	GLN
1	8-B	75	GLN
1	8-B	88	ASN
1	8-B	112	ASN
1	8-B	114	ASN
1	8-B	121	ASN
1	8-B	123	ASN
1	8-B	134	ASN
1	8-B	156	GLN
1	8-B	187	ASN
1	8-B	194	GLN
1	8-B	222	ASN
1	8-B	224	HIS
1	8-B	272	GLN
1	8-B	318	ASN
1	8-B	325	GLN
1	8-B	346	HIS
1	8-B	363	ASN
1	8-B	365	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 128 ligands modelled in this entry, 16 are monoatomic - leaving 112 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	MPO	1-A	9000	-	12,13,13	2.29	5 (41%)	15,17,17	5.73	4 (26%)
3	EDO	1-A	901	-	3,3,3	0.62	0	2,2,2	0.38	0
3	EDO	1-A	902	-	3,3,3	0.91	0	2,2,2	0.33	0
3	EDO	1-A	903	-	3,3,3	0.63	0	2,2,2	0.91	0
3	EDO	1-A	906	-	3,3,3	0.65	0	2,2,2	0.34	0
3	EDO	1-A	907	-	3,3,3	0.96	0	2,2,2	0.66	0
3	EDO	1-A	908	-	3,3,3	0.90	0	2,2,2	0.49	0
3	EDO	1-A	910	-	3,3,3	0.60	0	2,2,2	0.56	0
3	EDO	1-B	904	-	3,3,3	0.42	0	2,2,2	0.51	0
3	EDO	1-B	905	-	3,3,3	0.22	0	2,2,2	0.66	0
3	EDO	1-B	909	-	3,3,3	0.42	0	2,2,2	0.75	0
3	EDO	1-B	911	-	3,3,3	0.87	0	2,2,2	0.49	0
3	EDO	1-B	912	-	3,3,3	0.94	0	2,2,2	0.63	0
3	EDO	1-B	913	-	3,3,3	0.73	0	2,2,2	0.56	0
4	MPO	2-A	9000	-	12,13,13	1.98	2 (16%)	15,17,17	5.94	7 (46%)
3	EDO	2-A	901	-	3,3,3	0.64	0	2,2,2	0.37	0
3	EDO	2-A	902	-	3,3,3	0.91	0	2,2,2	0.33	0
3	EDO	2-A	903	-	3,3,3	0.50	0	2,2,2	0.99	0
3	EDO	2-A	906	-	3,3,3	0.66	0	2,2,2	0.32	0
3	EDO	2-A	907	-	3,3,3	0.87	0	2,2,2	0.87	0
3	EDO	2-A	908	-	3,3,3	0.69	0	2,2,2	0.47	0
3	EDO	2-A	910	-	3,3,3	0.61	0	2,2,2	0.57	0
3	EDO	2-B	904	-	3,3,3	0.45	0	2,2,2	0.50	0
3	EDO	2-B	905	-	3,3,3	0.22	0	2,2,2	0.63	0
3	EDO	2-B	909	-	3,3,3	0.43	0	2,2,2	0.74	0
3	EDO	2-B	911	-	3,3,3	1.49	1 (33%)	2,2,2	0.58	0
3	EDO	2-B	912	-	3,3,3	0.94	0	2,2,2	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	2-B	913	-	3,3,3	0.73	0	2,2,2	0.59	0
4	MPO	3-A	9000	-	12,13,13	1.90	2 (16%)	15,17,17	6.08	5 (33%)
3	EDO	3-A	901	-	3,3,3	0.62	0	2,2,2	0.43	0
3	EDO	3-A	902	-	3,3,3	0.91	0	2,2,2	0.33	0
3	EDO	3-A	903	-	3,3,3	0.63	0	2,2,2	0.90	0
3	EDO	3-A	906	-	3,3,3	0.66	0	2,2,2	0.32	0
3	EDO	3-A	907	-	3,3,3	1.00	0	2,2,2	0.65	0
3	EDO	3-A	908	-	3,3,3	0.72	0	2,2,2	0.57	0
3	EDO	3-A	910	-	3,3,3	0.60	0	2,2,2	0.56	0
3	EDO	3-B	904	-	3,3,3	0.40	0	2,2,2	0.53	0
3	EDO	3-B	905	-	3,3,3	0.23	0	2,2,2	0.61	0
3	EDO	3-B	909	-	3,3,3	0.43	0	2,2,2	0.74	0
3	EDO	3-B	911	-	3,3,3	1.49	0	2,2,2	0.50	0
3	EDO	3-B	912	-	3,3,3	0.99	0	2,2,2	0.61	0
3	EDO	3-B	913	-	3,3,3	0.76	0	2,2,2	0.61	0
4	MPO	4-A	9000	-	12,13,13	2.38	4 (33%)	15,17,17	5.35	5 (33%)
3	EDO	4-A	901	-	3,3,3	0.58	0	2,2,2	0.36	0
3	EDO	4-A	902	-	3,3,3	0.91	0	2,2,2	0.33	0
3	EDO	4-A	903	-	3,3,3	0.63	0	2,2,2	0.82	0
3	EDO	4-A	906	-	3,3,3	0.66	0	2,2,2	0.32	0
3	EDO	4-A	907	-	3,3,3	0.87	0	2,2,2	0.98	0
3	EDO	4-A	908	-	3,3,3	1.12	0	2,2,2	0.30	0
3	EDO	4-A	910	-	3,3,3	0.60	0	2,2,2	0.56	0
3	EDO	4-B	904	-	3,3,3	0.43	0	2,2,2	0.53	0
3	EDO	4-B	905	-	3,3,3	0.22	0	2,2,2	0.61	0
3	EDO	4-B	909	-	3,3,3	0.42	0	2,2,2	0.75	0
3	EDO	4-B	911	-	3,3,3	1.57	1 (33%)	2,2,2	0.51	0
3	EDO	4-B	912	-	3,3,3	1.03	0	2,2,2	0.61	0
3	EDO	4-B	913	-	3,3,3	0.76	0	2,2,2	0.60	0
4	MPO	5-A	9000	-	12,13,13	2.40	3 (25%)	15,17,17	6.27	6 (40%)
3	EDO	5-A	901	-	3,3,3	0.68	0	2,2,2	0.33	0
3	EDO	5-A	902	-	3,3,3	1.18	0	2,2,2	0.47	0
3	EDO	5-A	903	-	3,3,3	0.63	0	2,2,2	0.85	0
3	EDO	5-A	906	-	3,3,3	0.66	0	2,2,2	0.32	0
3	EDO	5-A	907	-	3,3,3	0.93	0	2,2,2	0.81	0
3	EDO	5-A	908	-	3,3,3	1.12	0	2,2,2	0.37	0
3	EDO	5-A	910	-	3,3,3	0.60	0	2,2,2	0.60	0
3	EDO	5-B	904	-	3,3,3	0.43	0	2,2,2	0.61	0
3	EDO	5-B	905	-	3,3,3	0.22	0	2,2,2	0.66	0
3	EDO	5-B	909	-	3,3,3	0.42	0	2,2,2	0.78	0
3	EDO	5-B	911	-	3,3,3	1.43	1 (33%)	2,2,2	0.29	0
3	EDO	5-B	912	-	3,3,3	1.03	0	2,2,2	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	5-B	913	-	3,3,3	0.89	0	2,2,2	0.68	0
4	MPO	6-A	9000	-	12,13,13	2.16	3 (25%)	15,17,17	6.50	7 (46%)
3	EDO	6-A	901	-	3,3,3	0.68	0	2,2,2	0.35	0
3	EDO	6-A	902	-	3,3,3	1.19	0	2,2,2	0.47	0
3	EDO	6-A	903	-	3,3,3	0.54	0	2,2,2	1.10	0
3	EDO	6-A	906	-	3,3,3	0.67	0	2,2,2	0.26	0
3	EDO	6-A	907	-	3,3,3	0.92	0	2,2,2	0.78	0
3	EDO	6-A	908	-	3,3,3	1.22	0	2,2,2	0.36	0
3	EDO	6-A	910	-	3,3,3	0.53	0	2,2,2	0.62	0
3	EDO	6-B	904	-	3,3,3	0.50	0	2,2,2	0.58	0
3	EDO	6-B	905	-	3,3,3	0.21	0	2,2,2	0.66	0
3	EDO	6-B	909	-	3,3,3	0.42	0	2,2,2	0.78	0
3	EDO	6-B	911	-	3,3,3	1.67	1 (33%)	2,2,2	0.58	0
3	EDO	6-B	912	-	3,3,3	1.05	0	2,2,2	0.67	0
3	EDO	6-B	913	-	3,3,3	0.75	0	2,2,2	0.55	0
4	MPO	7-A	9000	-	12,13,13	1.65	2 (16%)	15,17,17	6.42	5 (33%)
3	EDO	7-A	901	-	3,3,3	0.60	0	2,2,2	0.55	0
3	EDO	7-A	902	-	3,3,3	1.33	0	2,2,2	0.60	0
3	EDO	7-A	903	-	3,3,3	0.59	0	2,2,2	0.97	0
3	EDO	7-A	906	-	3,3,3	0.67	0	2,2,2	0.31	0
3	EDO	7-A	907	-	3,3,3	0.93	0	2,2,2	0.94	0
3	EDO	7-A	908	-	3,3,3	1.25	0	2,2,2	0.35	0
3	EDO	7-A	910	-	3,3,3	0.62	0	2,2,2	0.60	0
3	EDO	7-B	904	-	3,3,3	0.42	0	2,2,2	0.52	0
3	EDO	7-B	905	-	3,3,3	0.22	0	2,2,2	0.65	0
3	EDO	7-B	909	-	3,3,3	0.42	0	2,2,2	0.77	0
3	EDO	7-B	911	-	3,3,3	2.00	1 (33%)	2,2,2	0.69	0
3	EDO	7-B	912	-	3,3,3	1.07	0	2,2,2	0.63	0
3	EDO	7-B	913	-	3,3,3	0.79	0	2,2,2	0.60	0
4	MPO	8-A	9000	-	12,13,13	2.75	6 (50%)	15,17,17	5.38	4 (26%)
3	EDO	8-A	901	-	3,3,3	0.69	0	2,2,2	0.33	0
3	EDO	8-A	902	-	3,3,3	1.18	0	2,2,2	0.47	0
3	EDO	8-A	903	-	3,3,3	0.50	0	2,2,2	1.09	0
3	EDO	8-A	906	-	3,3,3	0.67	0	2,2,2	0.26	0
3	EDO	8-A	907	-	3,3,3	0.91	0	2,2,2	0.79	0
3	EDO	8-A	908	-	3,3,3	0.93	0	2,2,2	0.52	0
3	EDO	8-A	910	-	3,3,3	0.59	0	2,2,2	0.60	0
3	EDO	8-B	904	-	3,3,3	0.51	0	2,2,2	0.52	0
3	EDO	8-B	905	-	3,3,3	0.22	0	2,2,2	0.64	0
3	EDO	8-B	909	-	3,3,3	0.43	0	2,2,2	0.78	0
3	EDO	8-B	911	-	3,3,3	1.82	1 (33%)	2,2,2	0.56	0
3	EDO	8-B	912	-	3,3,3	1.07	0	2,2,2	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	8-B	913	-	3,3,3	0.89	0	2,2,2	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPO	1-A	9000	-	-	0/7/15/15	0/1/1/1
3	EDO	1-A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	902	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	903	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	908	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	910	-	-	0/1/1/1	0/0/0/0
3	EDO	1-B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	1-B	905	-	-	0/1/1/1	0/0/0/0
3	EDO	1-B	909	-	-	0/1/1/1	0/0/0/0
3	EDO	1-B	911	-	-	0/1/1/1	0/0/0/0
3	EDO	1-B	912	-	-	0/1/1/1	0/0/0/0
3	EDO	1-B	913	-	-	0/1/1/1	0/0/0/0
4	MPO	2-A	9000	-	-	0/7/15/15	0/1/1/1
3	EDO	2-A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	902	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	903	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	908	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	910	-	-	0/1/1/1	0/0/0/0
3	EDO	2-B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	2-B	905	-	-	0/1/1/1	0/0/0/0
3	EDO	2-B	909	-	-	0/1/1/1	0/0/0/0
3	EDO	2-B	911	-	-	0/1/1/1	0/0/0/0
3	EDO	2-B	912	-	-	0/1/1/1	0/0/0/0
3	EDO	2-B	913	-	-	0/1/1/1	0/0/0/0
4	MPO	3-A	9000	-	-	0/7/15/15	0/1/1/1
3	EDO	3-A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	902	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	903	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	908	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	3-A	910	-	-	0/1/1/1	0/0/0/0
3	EDO	3-B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	3-B	905	-	-	0/1/1/1	0/0/0/0
3	EDO	3-B	909	-	-	0/1/1/1	0/0/0/0
3	EDO	3-B	911	-	-	0/1/1/1	0/0/0/0
3	EDO	3-B	912	-	-	0/1/1/1	0/0/0/0
3	EDO	3-B	913	-	-	0/1/1/1	0/0/0/0
4	MPO	4-A	9000	-	-	0/7/15/15	0/1/1/1
3	EDO	4-A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	902	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	903	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	908	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	910	-	-	0/1/1/1	0/0/0/0
3	EDO	4-B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	4-B	905	-	-	0/1/1/1	0/0/0/0
3	EDO	4-B	909	-	-	0/1/1/1	0/0/0/0
3	EDO	4-B	911	-	-	0/1/1/1	0/0/0/0
3	EDO	4-B	912	-	-	0/1/1/1	0/0/0/0
3	EDO	4-B	913	-	-	0/1/1/1	0/0/0/0
4	MPO	5-A	9000	-	-	0/7/15/15	0/1/1/1
3	EDO	5-A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	902	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	903	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	908	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	910	-	-	0/1/1/1	0/0/0/0
3	EDO	5-B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	5-B	905	-	-	0/1/1/1	0/0/0/0
3	EDO	5-B	909	-	-	0/1/1/1	0/0/0/0
3	EDO	5-B	911	-	-	0/1/1/1	0/0/0/0
3	EDO	5-B	912	-	-	0/1/1/1	0/0/0/0
3	EDO	5-B	913	-	-	0/1/1/1	0/0/0/0
4	MPO	6-A	9000	-	-	0/7/15/15	0/1/1/1
3	EDO	6-A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	902	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	903	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	908	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	6-A	910	-	-	0/1/1/1	0/0/0/0
3	EDO	6-B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	6-B	905	-	-	0/1/1/1	0/0/0/0
3	EDO	6-B	909	-	-	0/1/1/1	0/0/0/0
3	EDO	6-B	911	-	-	0/1/1/1	0/0/0/0
3	EDO	6-B	912	-	-	0/1/1/1	0/0/0/0
3	EDO	6-B	913	-	-	0/1/1/1	0/0/0/0
4	MPO	7-A	9000	-	-	0/7/15/15	0/1/1/1
3	EDO	7-A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	902	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	903	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	908	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	910	-	-	0/1/1/1	0/0/0/0
3	EDO	7-B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	7-B	905	-	-	0/1/1/1	0/0/0/0
3	EDO	7-B	909	-	-	0/1/1/1	0/0/0/0
3	EDO	7-B	911	-	-	0/1/1/1	0/0/0/0
3	EDO	7-B	912	-	-	0/1/1/1	0/0/0/0
3	EDO	7-B	913	-	-	0/1/1/1	0/0/0/0
4	MPO	8-A	9000	-	-	0/7/15/15	0/1/1/1
3	EDO	8-A	901	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	902	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	903	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	906	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	907	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	908	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	910	-	-	0/1/1/1	0/0/0/0
3	EDO	8-B	904	-	-	0/1/1/1	0/0/0/0
3	EDO	8-B	905	-	-	0/1/1/1	0/0/0/0
3	EDO	8-B	909	-	-	0/1/1/1	0/0/0/0
3	EDO	8-B	911	-	-	0/1/1/1	0/0/0/0
3	EDO	8-B	912	-	-	0/1/1/1	0/0/0/0
3	EDO	8-B	913	-	-	0/1/1/1	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	8-A	9000	MPO	C7-C6	2.00	1.58	1.50
4	4-A	9000	MPO	O2-S1	2.00	1.51	1.45
3	5-B	911	EDO	C2-C1	2.05	1.62	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-A	9000	MPO	C3-N1	2.08	1.52	1.47
3	4-B	911	EDO	O1-C1	2.10	1.53	1.42
4	4-A	9000	MPO	C2-C1	2.22	1.58	1.52
3	2-B	911	EDO	O1-C1	2.24	1.54	1.42
4	8-A	9000	MPO	C2-C3	2.27	1.61	1.51
4	1-A	9000	MPO	O1-S1	2.30	1.52	1.45
4	6-A	9000	MPO	O1-S1	2.45	1.52	1.45
3	8-B	911	EDO	O1-C1	2.46	1.55	1.42
4	1-A	9000	MPO	C2-C1	2.50	1.59	1.52
3	6-B	911	EDO	O1-C1	2.53	1.55	1.42
4	1-A	9000	MPO	O2-S1	2.54	1.53	1.45
4	7-A	9000	MPO	O2-S1	2.54	1.53	1.45
4	8-A	9000	MPO	C3-N1	2.58	1.53	1.47
4	2-A	9000	MPO	O2-S1	2.61	1.53	1.45
3	7-B	911	EDO	O1-C1	2.71	1.56	1.42
4	3-A	9000	MPO	O2-S1	2.90	1.54	1.45
4	6-A	9000	MPO	O2-S1	2.94	1.54	1.45
4	8-A	9000	MPO	C2-C1	3.24	1.62	1.52
4	5-A	9000	MPO	O1-S1	3.32	1.55	1.45
4	5-A	9000	MPO	O2-S1	3.50	1.56	1.45
4	7-A	9000	MPO	O3-S1	3.69	1.56	1.46
4	4-A	9000	MPO	O1-S1	4.02	1.57	1.45
4	8-A	9000	MPO	O1-S1	4.59	1.59	1.45
4	3-A	9000	MPO	O3-S1	4.69	1.58	1.46
4	1-A	9000	MPO	O3-S1	5.13	1.59	1.46
4	4-A	9000	MPO	O3-S1	5.15	1.59	1.46
4	2-A	9000	MPO	O3-S1	5.35	1.60	1.46
4	6-A	9000	MPO	O3-S1	5.78	1.61	1.46
4	8-A	9000	MPO	O3-S1	5.78	1.61	1.46
4	5-A	9000	MPO	O3-S1	6.11	1.62	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-A	9000	MPO	O3-S1-O1	-16.71	72.72	111.61
4	1-A	9000	MPO	O3-S1-O1	-15.15	76.36	111.61
4	3-A	9000	MPO	O3-S1-O1	-14.57	77.70	111.61
4	8-A	9000	MPO	O3-S1-O1	-13.89	79.28	111.61
4	4-A	9000	MPO	O3-S1-O1	-13.01	81.32	111.61
4	5-A	9000	MPO	O3-S1-O1	-12.04	83.60	111.61
4	2-A	9000	MPO	O3-S1-O1	-12.02	83.64	111.61
4	6-A	9000	MPO	O3-S1-O1	-11.85	84.02	111.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-A	9000	MPO	O3-S1-O2	-11.73	84.31	111.61
4	8-A	9000	MPO	O3-S1-O2	-11.17	85.61	111.61
4	4-A	9000	MPO	O3-S1-O2	-11.13	85.71	111.61
4	3-A	9000	MPO	O3-S1-O2	-10.28	87.67	111.61
4	2-A	9000	MPO	O3-S1-O2	-10.21	87.84	111.61
4	7-A	9000	MPO	O3-S1-O2	-9.49	89.53	111.61
4	6-A	9000	MPO	O3-S1-O2	-9.41	89.71	111.61
4	5-A	9000	MPO	O3-S1-O2	-9.19	90.23	111.61
4	2-A	9000	MPO	C3-C2-C1	-4.94	104.24	112.37
4	6-A	9000	MPO	C3-C2-C1	-3.98	105.82	112.37
4	7-A	9000	MPO	C2-C3-N1	-3.23	105.76	113.89
4	5-A	9000	MPO	C3-C2-C1	-2.49	108.27	112.37
4	3-A	9000	MPO	C2-C3-N1	-2.47	107.67	113.89
4	2-A	9000	MPO	C6-C7-N1	-2.41	106.48	110.12
4	5-A	9000	MPO	C2-C3-N1	-2.38	107.92	113.89
4	6-A	9000	MPO	O4-C6-C7	-2.22	106.75	111.84
4	2-A	9000	MPO	C3-N1-C4	-2.22	105.57	111.27
4	6-A	9000	MPO	C6-C7-N1	-2.07	106.98	110.12
4	4-A	9000	MPO	O2-S1-C1	2.14	108.73	106.91
4	5-A	9000	MPO	O2-S1-O1	3.53	126.33	113.48
4	6-A	9000	MPO	O2-S1-O1	3.84	127.47	113.48
4	7-A	9000	MPO	O2-S1-O1	4.51	129.90	113.48
4	3-A	9000	MPO	O2-S1-O1	4.53	129.96	113.48
4	2-A	9000	MPO	O2-S1-O1	4.63	130.32	113.48
4	4-A	9000	MPO	O2-S1-O1	5.03	131.79	113.48
4	8-A	9000	MPO	O2-S1-O1	5.49	133.47	113.48
4	1-A	9000	MPO	O2-S1-O1	5.51	133.55	113.48
4	8-A	9000	MPO	O1-S1-C1	8.89	114.49	106.91
4	1-A	9000	MPO	O1-S1-C1	9.27	114.81	106.91
4	4-A	9000	MPO	O1-S1-C1	9.82	115.29	106.91
4	3-A	9000	MPO	O1-S1-C1	14.08	118.92	106.91
4	7-A	9000	MPO	O1-S1-C1	14.33	119.13	106.91
4	2-A	9000	MPO	O1-S1-C1	14.69	119.44	106.91
4	5-A	9000	MPO	O1-S1-C1	18.09	122.34	106.91
4	6-A	9000	MPO	O1-S1-C1	18.84	122.98	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

58 monomers are involved in 152 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-A	903	EDO	1	0
3	1-A	906	EDO	1	0
3	1-A	908	EDO	2	0
3	1-B	905	EDO	2	0
3	1-B	911	EDO	2	0
3	1-B	912	EDO	1	0
3	1-B	913	EDO	2	0
3	2-A	903	EDO	3	0
3	2-A	906	EDO	1	0
3	2-A	908	EDO	4	0
3	2-B	911	EDO	7	0
3	2-B	912	EDO	2	0
3	2-B	913	EDO	1	0
3	3-A	903	EDO	2	0
3	3-A	906	EDO	2	0
3	3-A	908	EDO	7	0
3	3-B	911	EDO	7	0
3	3-B	912	EDO	2	0
3	3-B	913	EDO	1	0
3	4-A	903	EDO	1	0
3	4-A	908	EDO	1	0
3	4-B	911	EDO	5	0
3	4-B	912	EDO	2	0
4	5-A	9000	MPO	1	0
3	5-A	903	EDO	2	0
3	5-A	906	EDO	2	0
3	5-A	908	EDO	4	0
3	5-B	904	EDO	1	0
3	5-B	911	EDO	6	0
3	5-B	912	EDO	2	0
3	5-B	913	EDO	1	0
4	6-A	9000	MPO	1	0
3	6-A	903	EDO	1	0
3	6-A	906	EDO	1	0
3	6-A	908	EDO	4	0
3	6-A	910	EDO	1	0
3	6-B	904	EDO	1	0
3	6-B	905	EDO	1	0
3	6-B	911	EDO	6	0
3	6-B	912	EDO	2	0
3	6-B	913	EDO	3	0
3	7-A	903	EDO	2	0
3	7-A	906	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	7-A	908	EDO	6	0
3	7-B	909	EDO	1	0
3	7-B	911	EDO	8	0
3	7-B	912	EDO	2	0
3	7-B	913	EDO	1	0
4	8-A	9000	MPO	1	0
3	8-A	903	EDO	6	0
3	8-A	906	EDO	2	0
3	8-A	907	EDO	2	0
3	8-A	908	EDO	7	0
3	8-A	910	EDO	1	0
3	8-B	905	EDO	1	0
3	8-B	911	EDO	8	0
3	8-B	912	EDO	2	0
3	8-B	913	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1-A	358/383 (93%)	-0.16	15 (4%)	40	42	7, 14, 32, 56	358 (100%)
1	1-B	356/383 (92%)	-0.07	29 (8%)	15	15	8, 15, 46, 72	356 (100%)
1	2-A	358/383 (93%)	-0.16	15 (4%)	40	42	7, 14, 32, 56	358 (100%)
1	2-B	356/383 (92%)	-0.07	29 (8%)	15	15	8, 15, 46, 72	356 (100%)
1	3-A	358/383 (93%)	-0.16	15 (4%)	40	42	7, 14, 32, 56	358 (100%)
1	3-B	356/383 (92%)	-0.07	29 (8%)	15	15	8, 15, 46, 72	356 (100%)
1	4-A	358/383 (93%)	-0.16	15 (4%)	40	42	7, 14, 32, 56	358 (100%)
1	4-B	356/383 (92%)	-0.07	29 (8%)	15	15	8, 15, 46, 72	356 (100%)
1	5-A	358/383 (93%)	-0.16	15 (4%)	40	42	7, 14, 32, 56	358 (100%)
1	5-B	356/383 (92%)	-0.07	29 (8%)	15	15	8, 15, 46, 72	356 (100%)
1	6-A	358/383 (93%)	-0.16	15 (4%)	40	42	7, 14, 32, 56	358 (100%)
1	6-B	356/383 (92%)	-0.07	29 (8%)	15	15	8, 15, 46, 72	356 (100%)
1	7-A	358/383 (93%)	-0.16	15 (4%)	40	42	7, 14, 32, 56	358 (100%)
1	7-B	356/383 (92%)	-0.07	29 (8%)	15	15	8, 15, 46, 72	356 (100%)
1	8-A	358/383 (93%)	-0.16	15 (4%)	40	42	7, 14, 32, 56	358 (100%)
1	8-B	356/383 (92%)	-0.07	29 (8%)	15	15	8, 15, 46, 72	356 (100%)
All	All	5712/6128 (93%)	-0.12	352 (6%)	26	24	7, 14, 39, 72	5712 (100%)

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	295	ASP	10.5
1	2-B	295	ASP	10.5
1	3-B	295	ASP	10.5
1	4-B	295	ASP	10.5
1	5-B	295	ASP	10.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	6-B	295	ASP	10.5
1	7-B	295	ASP	10.5
1	8-B	295	ASP	10.5
1	1-B	298	ALA	7.2
1	2-B	298	ALA	7.2
1	3-B	298	ALA	7.2
1	4-B	298	ALA	7.2
1	5-B	298	ALA	7.2
1	6-B	298	ALA	7.2
1	7-B	298	ALA	7.2
1	8-B	298	ALA	7.2
1	1-B	297	GLU	5.7
1	2-B	297	GLU	5.7
1	3-B	297	GLU	5.7
1	4-B	297	GLU	5.7
1	5-B	297	GLU	5.7
1	6-B	297	GLU	5.7
1	7-B	297	GLU	5.7
1	8-B	297	GLU	5.7
1	1-A	295	ASP	5.6
1	2-A	295	ASP	5.6
1	3-A	295	ASP	5.6
1	4-A	295	ASP	5.6
1	5-A	295	ASP	5.6
1	6-A	295	ASP	5.6
1	7-A	295	ASP	5.6
1	8-A	295	ASP	5.6
1	1-A	296	GLY	5.3
1	2-A	296	GLY	5.3
1	3-A	296	GLY	5.3
1	4-A	296	GLY	5.3
1	5-A	296	GLY	5.3
1	6-A	296	GLY	5.3
1	7-A	296	GLY	5.3
1	8-A	296	GLY	5.3
1	1-A	112	ASN	5.2
1	2-A	112	ASN	5.2
1	3-A	112	ASN	5.2
1	4-A	112	ASN	5.2
1	5-A	112	ASN	5.2
1	6-A	112	ASN	5.2
1	7-A	112	ASN	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	8-A	112	ASN	5.2
1	1-B	290	SER	5.2
1	2-B	290	SER	5.2
1	3-B	290	SER	5.2
1	4-B	290	SER	5.2
1	5-B	290	SER	5.2
1	6-B	290	SER	5.2
1	7-B	290	SER	5.2
1	8-B	290	SER	5.2
1	1-B	296	GLY	4.9
1	2-B	296	GLY	4.9
1	3-B	296	GLY	4.9
1	4-B	296	GLY	4.9
1	5-B	296	GLY	4.9
1	6-B	296	GLY	4.9
1	7-B	296	GLY	4.9
1	8-B	296	GLY	4.9
1	1-A	376	THR	4.7
1	2-A	376	THR	4.7
1	3-A	376	THR	4.7
1	4-A	376	THR	4.7
1	5-A	376	THR	4.7
1	6-A	376	THR	4.7
1	7-A	376	THR	4.7
1	8-A	376	THR	4.7
1	1-B	299	ILE	4.6
1	2-B	299	ILE	4.6
1	3-B	299	ILE	4.6
1	4-B	299	ILE	4.6
1	5-B	299	ILE	4.6
1	6-B	299	ILE	4.6
1	7-B	299	ILE	4.6
1	8-B	299	ILE	4.6
1	1-B	376	THR	4.0
1	2-B	376	THR	4.0
1	3-B	376	THR	4.0
1	4-B	376	THR	4.0
1	5-B	376	THR	4.0
1	6-B	376	THR	4.0
1	7-B	376	THR	4.0
1	8-B	376	THR	4.0
1	1-A	103	LYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-A	103	LYS	4.0
1	3-A	103	LYS	4.0
1	4-A	103	LYS	4.0
1	5-A	103	LYS	4.0
1	6-A	103	LYS	4.0
1	7-A	103	LYS	4.0
1	8-A	103	LYS	4.0
1	1-A	128	ALA	4.0
1	2-A	128	ALA	4.0
1	3-A	128	ALA	4.0
1	4-A	128	ALA	4.0
1	5-A	128	ALA	4.0
1	6-A	128	ALA	4.0
1	7-A	128	ALA	4.0
1	8-A	128	ALA	4.0
1	1-A	294	GLN	3.9
1	2-A	294	GLN	3.9
1	3-A	294	GLN	3.9
1	4-A	294	GLN	3.9
1	5-A	294	GLN	3.9
1	6-A	294	GLN	3.9
1	7-A	294	GLN	3.9
1	8-A	294	GLN	3.9
1	1-A	297	GLU	3.6
1	2-A	297	GLU	3.6
1	3-A	297	GLU	3.6
1	4-A	297	GLU	3.6
1	5-A	297	GLU	3.6
1	6-A	297	GLU	3.6
1	7-A	297	GLU	3.6
1	8-A	297	GLU	3.6
1	1-A	129	ASN	3.4
1	2-A	129	ASN	3.4
1	3-A	129	ASN	3.4
1	4-A	129	ASN	3.4
1	5-A	129	ASN	3.4
1	6-A	129	ASN	3.4
1	7-A	129	ASN	3.4
1	8-A	129	ASN	3.4
1	1-A	104	ARG	3.3
1	2-A	104	ARG	3.3
1	3-A	104	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	4-A	104	ARG	3.3
1	5-A	104	ARG	3.3
1	6-A	104	ARG	3.3
1	7-A	104	ARG	3.3
1	8-A	104	ARG	3.3
1	1-B	300	PRO	3.3
1	2-B	300	PRO	3.3
1	3-B	300	PRO	3.3
1	4-B	300	PRO	3.3
1	5-B	300	PRO	3.3
1	6-B	300	PRO	3.3
1	7-B	300	PRO	3.3
1	8-B	300	PRO	3.3
1	1-A	10	GLU	3.3
1	2-A	10	GLU	3.3
1	3-A	10	GLU	3.3
1	4-A	10	GLU	3.3
1	5-A	10	GLU	3.3
1	6-A	10	GLU	3.3
1	7-A	10	GLU	3.3
1	8-A	10	GLU	3.3
1	1-B	10	GLU	3.2
1	2-B	10	GLU	3.2
1	3-B	10	GLU	3.2
1	4-B	10	GLU	3.2
1	5-B	10	GLU	3.2
1	6-B	10	GLU	3.2
1	7-B	10	GLU	3.2
1	8-B	10	GLU	3.2
1	1-B	129	ASN	3.2
1	2-B	129	ASN	3.2
1	3-B	129	ASN	3.2
1	4-B	129	ASN	3.2
1	5-B	129	ASN	3.2
1	6-B	129	ASN	3.2
1	7-B	129	ASN	3.2
1	8-B	129	ASN	3.2
1	1-A	5	ARG	3.2
1	2-A	5	ARG	3.2
1	3-A	5	ARG	3.2
1	4-A	5	ARG	3.2
1	5-A	5	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	6-A	5	ARG	3.2
1	7-A	5	ARG	3.2
1	8-A	5	ARG	3.2
1	1-B	292	ILE	3.1
1	2-B	292	ILE	3.1
1	3-B	292	ILE	3.1
1	4-B	292	ILE	3.1
1	5-B	292	ILE	3.1
1	6-B	292	ILE	3.1
1	7-B	292	ILE	3.1
1	8-B	292	ILE	3.1
1	1-B	294	GLN	3.1
1	2-B	294	GLN	3.1
1	3-B	294	GLN	3.1
1	4-B	294	GLN	3.1
1	5-B	294	GLN	3.1
1	6-B	294	GLN	3.1
1	7-B	294	GLN	3.1
1	8-B	294	GLN	3.1
1	1-B	112	ASN	3.0
1	2-B	112	ASN	3.0
1	3-B	112	ASN	3.0
1	4-B	112	ASN	3.0
1	5-B	112	ASN	3.0
1	6-B	112	ASN	3.0
1	7-B	112	ASN	3.0
1	8-B	112	ASN	3.0
1	1-A	130	ASP	3.0
1	2-A	130	ASP	3.0
1	3-A	130	ASP	3.0
1	4-A	130	ASP	3.0
1	5-A	130	ASP	3.0
1	6-A	130	ASP	3.0
1	7-A	130	ASP	3.0
1	8-A	130	ASP	3.0
1	1-B	301	ARG	2.9
1	2-B	301	ARG	2.9
1	3-B	301	ARG	2.9
1	4-B	301	ARG	2.9
1	5-B	301	ARG	2.9
1	6-B	301	ARG	2.9
1	7-B	301	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	8-B	301	ARG	2.9
1	1-B	303	ALA	2.8
1	2-B	303	ALA	2.8
1	3-B	303	ALA	2.8
1	4-B	303	ALA	2.8
1	5-B	303	ALA	2.8
1	6-B	303	ALA	2.8
1	7-B	303	ALA	2.8
1	8-B	303	ALA	2.8
1	1-B	134	ASN	2.8
1	2-B	134	ASN	2.8
1	3-B	134	ASN	2.8
1	4-B	134	ASN	2.8
1	5-B	134	ASN	2.8
1	6-B	134	ASN	2.8
1	7-B	134	ASN	2.8
1	8-B	134	ASN	2.8
1	1-B	291	GLY	2.7
1	2-B	291	GLY	2.7
1	3-B	291	GLY	2.7
1	4-B	291	GLY	2.7
1	5-B	291	GLY	2.7
1	6-B	291	GLY	2.7
1	7-B	291	GLY	2.7
1	8-B	291	GLY	2.7
1	1-B	286	GLU	2.6
1	2-B	286	GLU	2.6
1	3-B	286	GLU	2.6
1	4-B	286	GLU	2.6
1	5-B	286	GLU	2.6
1	6-B	286	GLU	2.6
1	7-B	286	GLU	2.6
1	8-B	286	GLU	2.6
1	1-B	302	LEU	2.5
1	2-B	302	LEU	2.5
1	3-B	302	LEU	2.5
1	4-B	302	LEU	2.5
1	5-B	302	LEU	2.5
1	6-B	302	LEU	2.5
1	7-B	302	LEU	2.5
1	8-B	302	LEU	2.5
1	1-A	300	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2-A	300	PRO	2.4
1	3-A	300	PRO	2.4
1	4-A	300	PRO	2.4
1	5-A	300	PRO	2.4
1	6-A	300	PRO	2.4
1	7-A	300	PRO	2.4
1	8-A	300	PRO	2.4
1	1-B	38	HIS	2.3
1	2-B	38	HIS	2.3
1	3-B	38	HIS	2.3
1	4-B	38	HIS	2.3
1	5-B	38	HIS	2.3
1	6-B	38	HIS	2.3
1	7-B	38	HIS	2.3
1	8-B	38	HIS	2.3
1	1-B	128	ALA	2.3
1	2-B	128	ALA	2.3
1	3-B	128	ALA	2.3
1	4-B	128	ALA	2.3
1	5-B	128	ALA	2.3
1	6-B	128	ALA	2.3
1	7-B	128	ALA	2.3
1	8-B	128	ALA	2.3
1	1-B	103	LYS	2.3
1	2-B	103	LYS	2.3
1	3-B	103	LYS	2.3
1	4-B	103	LYS	2.3
1	5-B	103	LYS	2.3
1	6-B	103	LYS	2.3
1	7-B	103	LYS	2.3
1	8-B	103	LYS	2.3
1	1-B	11	HIS	2.2
1	2-B	11	HIS	2.2
1	3-B	11	HIS	2.2
1	4-B	11	HIS	2.2
1	5-B	11	HIS	2.2
1	6-B	11	HIS	2.2
1	7-B	11	HIS	2.2
1	8-B	11	HIS	2.2
1	1-B	287	GLU	2.2
1	2-B	287	GLU	2.2
1	3-B	287	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	4-B	287	GLU	2.2
1	5-B	287	GLU	2.2
1	6-B	287	GLU	2.2
1	7-B	287	GLU	2.2
1	8-B	287	GLU	2.2
1	1-B	305	THR	2.2
1	2-B	305	THR	2.2
1	3-B	305	THR	2.2
1	4-B	305	THR	2.2
1	5-B	305	THR	2.2
1	6-B	305	THR	2.2
1	7-B	305	THR	2.2
1	8-B	305	THR	2.2
1	1-B	345	HIS	2.1
1	2-B	345	HIS	2.1
1	3-B	345	HIS	2.1
1	4-B	345	HIS	2.1
1	5-B	345	HIS	2.1
1	6-B	345	HIS	2.1
1	7-B	345	HIS	2.1
1	8-B	345	HIS	2.1
1	1-B	304	GLY	2.1
1	2-B	304	GLY	2.1
1	3-B	304	GLY	2.1
1	4-B	304	GLY	2.1
1	5-B	304	GLY	2.1
1	6-B	304	GLY	2.1
1	7-B	304	GLY	2.1
1	8-B	304	GLY	2.1
1	1-B	7	SER	2.1
1	2-B	7	SER	2.1
1	3-B	7	SER	2.1
1	4-B	7	SER	2.1
1	5-B	7	SER	2.1
1	6-B	7	SER	2.1
1	7-B	7	SER	2.1
1	8-B	7	SER	2.1
1	1-B	39	ASN	2.1
1	2-B	39	ASN	2.1
1	3-B	39	ASN	2.1
1	4-B	39	ASN	2.1
1	5-B	39	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	6-B	39	ASN	2.1
1	7-B	39	ASN	2.1
1	8-B	39	ASN	2.1
1	1-A	181	LEU	2.0
1	2-A	181	LEU	2.0
1	3-A	181	LEU	2.0
1	4-A	181	LEU	2.0
1	5-A	181	LEU	2.0
1	6-A	181	LEU	2.0
1	7-A	181	LEU	2.0
1	8-A	181	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MPO	3-A	9000	13/13	0.76	0.45	15.59	38,46,55,55	13
4	MPO	6-A	9000	13/13	0.76	0.45	15.20	38,46,55,55	13
4	MPO	2-A	9000	13/13	0.76	0.45	15.20	38,46,55,55	13
4	MPO	5-A	9000	13/13	0.76	0.45	13.86	38,46,55,55	13
4	MPO	4-A	9000	13/13	0.76	0.45	13.86	38,46,55,55	13
3	EDO	4-A	903	4/4	0.80	0.20	8.26	43,43,48,50	4
3	EDO	2-A	903	4/4	0.80	0.20	8.26	43,44,48,50	4
3	EDO	6-A	903	4/4	0.80	0.20	8.11	43,44,48,50	4
3	EDO	5-A	903	4/4	0.80	0.20	8.11	43,43,48,50	4
3	EDO	8-A	903	4/4	0.80	0.20	8.11	43,44,48,50	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	7-A	903	4/4	0.80	0.20	8.11	43,43,48,50	4
3	EDO	1-A	903	4/4	0.80	0.20	8.09	43,43,48,50	4
3	EDO	3-A	903	4/4	0.80	0.20	7.90	43,43,48,50	4
3	EDO	5-A	908	4/4	0.83	0.23	6.01	27,30,31,43	4
3	EDO	6-A	908	4/4	0.83	0.23	6.01	27,30,31,43	4
3	EDO	3-A	908	4/4	0.83	0.23	6.01	27,30,31,43	4
3	EDO	2-A	908	4/4	0.83	0.23	6.01	27,31,31,43	4
3	EDO	1-A	908	4/4	0.83	0.23	6.01	27,31,31,43	4
3	EDO	8-A	908	4/4	0.83	0.23	6.01	27,30,31,43	4
3	EDO	7-A	908	4/4	0.83	0.23	5.99	27,30,31,43	4
3	EDO	4-A	908	4/4	0.83	0.23	5.99	27,30,31,43	4
3	EDO	7-A	906	4/4	0.86	0.21	5.80	41,42,43,44	4
3	EDO	3-A	906	4/4	0.86	0.21	5.80	41,42,43,44	4
3	EDO	5-A	906	4/4	0.86	0.21	5.80	41,42,43,44	4
3	EDO	4-A	906	4/4	0.86	0.21	5.80	41,42,43,44	4
3	EDO	1-A	906	4/4	0.86	0.21	5.80	41,42,43,44	4
3	EDO	2-A	906	4/4	0.86	0.21	5.51	41,42,43,44	4
3	EDO	4-B	911	4/4	0.85	0.21	4.08	21,28,31,36	4
4	MPO	1-A	9000	13/13	0.76	0.45	3.98	38,46,55,55	13
4	MPO	7-A	9000	13/13	0.76	0.45	3.98	38,46,55,55	13
3	EDO	3-B	913	4/4	0.82	0.16	3.85	29,31,34,37	4
3	EDO	6-B	913	4/4	0.82	0.16	3.85	28,31,34,37	4
3	EDO	5-B	913	4/4	0.82	0.16	3.85	29,31,34,37	4
3	EDO	4-B	913	4/4	0.82	0.16	3.85	29,31,34,37	4
3	EDO	8-B	913	4/4	0.82	0.16	3.85	29,31,34,37	4
3	EDO	1-B	913	4/4	0.82	0.16	3.85	29,31,34,37	4
3	EDO	7-B	913	4/4	0.82	0.16	3.85	29,31,34,37	4
3	EDO	2-B	913	4/4	0.82	0.16	3.85	29,31,34,37	4
4	MPO	8-A	9000	13/13	0.76	0.45	3.83	37,46,55,55	13
3	EDO	3-B	911	4/4	0.85	0.21	3.50	22,28,31,36	4
3	EDO	8-B	911	4/4	0.85	0.21	3.50	21,28,31,36	4
3	EDO	1-B	911	4/4	0.85	0.21	3.46	21,28,31,36	4
3	EDO	6-B	911	4/4	0.85	0.21	3.46	21,28,30,36	4
3	EDO	5-B	911	4/4	0.85	0.21	3.46	20,28,31,36	4
3	EDO	7-B	911	4/4	0.85	0.21	3.46	22,28,30,36	4
3	EDO	2-B	911	4/4	0.85	0.21	3.46	21,28,30,36	4
3	EDO	6-A	902	4/4	0.95	0.12	3.39	27,28,29,33	4
3	EDO	3-A	902	4/4	0.95	0.12	3.37	27,27,29,33	4
3	EDO	8-A	902	4/4	0.95	0.12	3.13	27,28,29,33	4
3	EDO	1-A	902	4/4	0.95	0.12	3.13	27,27,29,33	4
3	EDO	5-A	902	4/4	0.95	0.12	3.13	27,28,29,33	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	2-A	902	4/4	0.95	0.12	3.13	27,27,29,33	4
3	EDO	6-B	904	4/4	0.95	0.08	2.20	35,37,38,41	4
3	EDO	8-B	904	4/4	0.95	0.08	2.16	35,37,38,41	4
3	EDO	4-B	904	4/4	0.95	0.08	2.16	35,37,38,41	4
3	EDO	1-B	904	4/4	0.95	0.08	2.16	35,37,38,41	4
3	EDO	5-B	904	4/4	0.95	0.08	2.16	35,37,38,41	4
3	EDO	2-B	904	4/4	0.95	0.08	2.16	35,37,38,41	4
3	EDO	7-B	904	4/4	0.95	0.08	2.16	35,37,38,41	4
3	EDO	3-B	904	4/4	0.95	0.08	2.16	35,37,38,41	4
3	EDO	8-A	901	4/4	0.94	0.11	2.15	32,33,33,35	4
3	EDO	2-A	901	4/4	0.94	0.11	2.15	32,33,33,35	4
3	EDO	3-A	901	4/4	0.94	0.11	2.14	32,33,33,35	4
3	EDO	4-A	901	4/4	0.94	0.11	2.12	32,33,33,35	4
3	EDO	7-A	901	4/4	0.94	0.11	2.12	32,33,33,35	4
3	EDO	1-A	901	4/4	0.94	0.11	2.12	32,33,33,35	4
3	EDO	6-A	901	4/4	0.94	0.11	2.12	32,33,33,35	4
3	EDO	5-A	901	4/4	0.94	0.11	2.08	32,33,33,35	4
3	EDO	8-A	906	4/4	0.86	0.21	2.06	41,42,43,44	4
3	EDO	6-A	906	4/4	0.86	0.21	1.78	41,42,43,44	4
3	EDO	5-A	907	4/4	0.97	0.11	1.69	27,31,32,32	4
3	EDO	2-A	907	4/4	0.97	0.11	1.69	27,31,32,32	4
3	EDO	7-A	907	4/4	0.97	0.11	1.69	27,31,32,32	4
3	EDO	3-A	907	4/4	0.97	0.11	1.69	27,30,32,32	4
3	EDO	4-A	907	4/4	0.97	0.11	1.69	27,31,32,32	4
3	EDO	6-A	907	4/4	0.97	0.11	1.54	27,31,32,32	4
3	EDO	8-A	907	4/4	0.97	0.11	1.54	27,30,32,32	4
3	EDO	1-A	907	4/4	0.97	0.11	1.47	27,31,32,32	4
3	EDO	3-B	905	4/4	0.94	0.07	0.67	35,36,39,39	4
3	EDO	7-B	905	4/4	0.94	0.07	0.67	35,36,39,39	4
3	EDO	4-B	905	4/4	0.94	0.07	0.67	35,36,39,39	4
3	EDO	1-B	905	4/4	0.94	0.07	0.67	35,36,39,39	4
3	EDO	5-B	905	4/4	0.94	0.07	0.67	35,36,39,39	4
2	MG	2-A	802	1/1	0.99	0.06	0.15	15,15,15,15	1
2	MG	4-A	802	1/1	0.99	0.06	0.15	12,12,12,12	1
2	MG	3-A	802	1/1	0.99	0.06	-0.18	12,12,12,12	1
2	MG	6-A	802	1/1	0.99	0.06	-0.18	20,20,20,20	1
2	MG	1-A	802	1/1	0.99	0.06	-0.18	12,12,12,12	1
2	MG	8-A	802	1/1	0.99	0.06	-0.25	17,17,17,17	1
3	EDO	2-B	905	4/4	0.94	0.07	-0.25	35,36,39,39	4
3	EDO	7-A	910	4/4	0.91	0.07	-0.26	42,47,47,48	4
3	EDO	8-A	910	4/4	0.91	0.07	-0.26	42,47,47,48	4
3	EDO	2-A	910	4/4	0.91	0.07	-0.26	42,47,47,48	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	5-A	910	4/4	0.91	0.07	-0.26	42,47,47,48	4
3	EDO	1-A	910	4/4	0.91	0.07	-0.26	42,47,47,48	4
3	EDO	6-A	910	4/4	0.91	0.07	-0.26	42,47,47,48	4
3	EDO	3-A	910	4/4	0.91	0.07	-0.26	42,47,47,48	4
3	EDO	4-A	910	4/4	0.91	0.07	-0.26	42,47,47,48	4
2	MG	5-A	802	1/1	0.99	0.06	-0.27	15,15,15,15	1
2	MG	7-A	802	1/1	0.99	0.06	-0.27	15,15,15,15	1
3	EDO	8-B	905	4/4	0.94	0.07	-0.32	35,36,39,39	4
2	MG	7-B	801	1/1	0.99	0.04	-1.27	19,19,19,19	1
2	MG	5-B	801	1/1	0.99	0.04	-1.29	20,20,20,20	1
2	MG	8-B	801	1/1	0.99	0.04	-1.38	17,17,17,17	1
2	MG	6-B	801	1/1	0.99	0.04	-1.38	18,18,18,18	1
2	MG	4-B	801	1/1	0.99	0.04	-1.38	15,15,15,15	1
2	MG	1-B	801	1/1	0.99	0.04	-1.50	15,15,15,15	1
2	MG	2-B	801	1/1	0.99	0.04	-1.50	15,15,15,15	1
2	MG	3-B	801	1/1	0.99	0.04	-1.50	15,15,15,15	1
3	EDO	6-B	905	4/4	0.94	0.07	-	35,36,39,39	4
3	EDO	7-B	909	4/4	0.87	0.23	-	41,42,45,47	4
3	EDO	3-B	909	4/4	0.87	0.23	-	41,42,45,47	4
3	EDO	4-B	909	4/4	0.87	0.23	-	41,42,45,47	4
3	EDO	5-B	909	4/4	0.87	0.23	-	41,42,45,47	4
3	EDO	7-B	912	4/4	0.85	0.22	-	31,34,36,39	4
3	EDO	8-B	912	4/4	0.85	0.22	-	31,34,36,38	4
3	EDO	4-B	912	4/4	0.85	0.22	-	31,34,36,38	4
3	EDO	3-B	912	4/4	0.85	0.22	-	31,34,36,38	4
3	EDO	8-B	909	4/4	0.87	0.23	-	41,42,45,47	4
3	EDO	1-B	909	4/4	0.87	0.23	-	41,42,45,47	4
3	EDO	7-A	902	4/4	0.95	0.12	-	27,27,30,33	4
3	EDO	4-A	902	4/4	0.95	0.12	-	27,27,29,33	4
3	EDO	2-B	912	4/4	0.85	0.22	-	31,34,36,38	4
3	EDO	2-B	909	4/4	0.87	0.23	-	41,42,45,47	4
3	EDO	5-B	912	4/4	0.85	0.22	-	31,34,36,38	4
3	EDO	1-B	912	4/4	0.85	0.22	-	31,34,36,38	4
3	EDO	6-B	909	4/4	0.87	0.23	-	41,42,45,47	4
3	EDO	6-B	912	4/4	0.85	0.22	-	31,34,36,38	4

6.5 Other polymers

There are no such residues in this entry.