



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:42 PM GMT

PDB ID : 1LKX
Title : MOTOR DOMAIN OF MYOE, A CLASS-I MYOSIN
Authors : Kollmar, M.; Durrwang, U.; Kliche, W.; Manstein, D.J.; Kull, F.J.
Deposited on : 2002-04-26
Resolution : 3.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

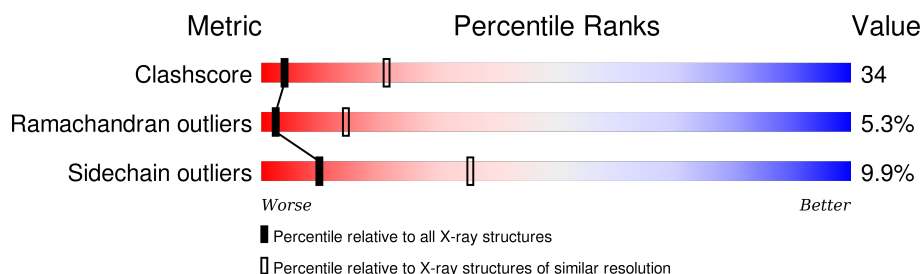
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	697	
1	B	697	
1	C	697	
1	D	697	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21265 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 MYOSIN IE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5192	3285	890	988	29			
1	B	650	Total	C	N	O	S	0	0	0
			5188	3282	889	988	29			
1	C	679	Total	C	N	O	S	0	0	0
			5422	3427	932	1033	30			
1	D	660	Total	C	N	O	S	0	0	0
			5267	3329	903	1005	30			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLU	ASP	SEE REMARK 999	UNP Q03479
A	48	THR	ARG	SEE REMARK 999	UNP Q03479
A	77	MET	ILE	SEE REMARK 999	UNP Q03479
A	?	-	ILE	SEE REMARK 999	UNP Q03479
A	?	-	ARG	SEE REMARK 999	UNP Q03479
A	137	LEU	PHE	SEE REMARK 999	UNP Q03479
A	138	ASP	GLN	SEE REMARK 999	UNP Q03479
A	215	ASP	ASN	SEE REMARK 999	UNP Q03479
A	371	ILE	LEU	SEE REMARK 999	UNP Q03479
A	372	ILE	SER	SEE REMARK 999	UNP Q03479
A	373	ASN	ILE	SEE REMARK 999	UNP Q03479
A	374	CYS	VAL	SEE REMARK 999	UNP Q03479
A	375	THR	HIS	SEE REMARK 999	UNP Q03479
A	376	THR	ARG	SEE REMARK 999	UNP Q03479
A	378	LYS	-	SEE REMARK 999	UNP Q03479
A	380	PRO	THR	SEE REMARK 999	UNP Q03479
A	427	VAL	-	SEE REMARK 999	UNP Q03479
A	428	ARG	-	SEE REMARK 999	UNP Q03479
A	429	GLU	LYS	SEE REMARK 999	UNP Q03479
A	440	ASN	-	SEE REMARK 999	UNP Q03479
A	498	ILE	ASN	SEE REMARK 999	UNP Q03479

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	VAL	ASP	SEE REMARK 999	UNP Q03479
A	681	ASN	ILE	SEE REMARK 999	UNP Q03479
A	683	THR	ARG	SEE REMARK 999	UNP Q03479
B	26	GLU	ASP	SEE REMARK 999	UNP Q03479
B	48	THR	ARG	SEE REMARK 999	UNP Q03479
B	77	MET	ILE	SEE REMARK 999	UNP Q03479
B	?	-	ILE	SEE REMARK 999	UNP Q03479
B	?	-	ARG	SEE REMARK 999	UNP Q03479
B	137	LEU	PHE	SEE REMARK 999	UNP Q03479
B	138	ASP	GLN	SEE REMARK 999	UNP Q03479
B	215	ASP	ASN	SEE REMARK 999	UNP Q03479
B	371	ILE	LEU	SEE REMARK 999	UNP Q03479
B	372	ILE	SER	SEE REMARK 999	UNP Q03479
B	373	ASN	ILE	SEE REMARK 999	UNP Q03479
B	374	CYS	VAL	SEE REMARK 999	UNP Q03479
B	375	THR	HIS	SEE REMARK 999	UNP Q03479
B	376	THR	ARG	SEE REMARK 999	UNP Q03479
B	378	LYS	-	SEE REMARK 999	UNP Q03479
B	380	PRO	THR	SEE REMARK 999	UNP Q03479
B	427	VAL	-	SEE REMARK 999	UNP Q03479
B	428	ARG	-	SEE REMARK 999	UNP Q03479
B	429	GLU	LYS	SEE REMARK 999	UNP Q03479
B	440	ASN	-	SEE REMARK 999	UNP Q03479
B	498	ILE	ASN	SEE REMARK 999	UNP Q03479
B	604	VAL	ASP	SEE REMARK 999	UNP Q03479
B	681	ASN	ILE	SEE REMARK 999	UNP Q03479
B	683	THR	ARG	SEE REMARK 999	UNP Q03479
C	26	GLU	ASP	SEE REMARK 999	UNP Q03479
C	48	THR	ARG	SEE REMARK 999	UNP Q03479
C	77	MET	ILE	SEE REMARK 999	UNP Q03479
C	?	-	ILE	SEE REMARK 999	UNP Q03479
C	?	-	ARG	SEE REMARK 999	UNP Q03479
C	137	LEU	PHE	SEE REMARK 999	UNP Q03479
C	138	ASP	GLN	SEE REMARK 999	UNP Q03479
C	215	ASP	ASN	SEE REMARK 999	UNP Q03479
C	371	ILE	LEU	SEE REMARK 999	UNP Q03479
C	372	ILE	SER	SEE REMARK 999	UNP Q03479
C	373	ASN	ILE	SEE REMARK 999	UNP Q03479
C	374	CYS	VAL	SEE REMARK 999	UNP Q03479
C	375	THR	HIS	SEE REMARK 999	UNP Q03479
C	376	THR	ARG	SEE REMARK 999	UNP Q03479
C	378	LYS	-	SEE REMARK 999	UNP Q03479

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	PRO	THR	SEE REMARK 999	UNP Q03479
C	427	VAL	-	SEE REMARK 999	UNP Q03479
C	428	ARG	-	SEE REMARK 999	UNP Q03479
C	429	GLU	LYS	SEE REMARK 999	UNP Q03479
C	440	ASN	-	SEE REMARK 999	UNP Q03479
C	498	ILE	ASN	SEE REMARK 999	UNP Q03479
C	604	VAL	ASP	SEE REMARK 999	UNP Q03479
C	681	ASN	ILE	SEE REMARK 999	UNP Q03479
C	683	THR	ARG	SEE REMARK 999	UNP Q03479
D	26	GLU	ASP	SEE REMARK 999	UNP Q03479
D	48	THR	ARG	SEE REMARK 999	UNP Q03479
D	77	MET	ILE	SEE REMARK 999	UNP Q03479
D	?	-	ILE	SEE REMARK 999	UNP Q03479
D	?	-	ARG	SEE REMARK 999	UNP Q03479
D	137	LEU	PHE	SEE REMARK 999	UNP Q03479
D	138	ASP	GLN	SEE REMARK 999	UNP Q03479
D	215	ASP	ASN	SEE REMARK 999	UNP Q03479
D	371	ILE	LEU	SEE REMARK 999	UNP Q03479
D	372	ILE	SER	SEE REMARK 999	UNP Q03479
D	373	ASN	ILE	SEE REMARK 999	UNP Q03479
D	374	CYS	VAL	SEE REMARK 999	UNP Q03479
D	375	THR	HIS	SEE REMARK 999	UNP Q03479
D	376	THR	ARG	SEE REMARK 999	UNP Q03479
D	378	LYS	-	SEE REMARK 999	UNP Q03479
D	380	PRO	THR	SEE REMARK 999	UNP Q03479
D	427	VAL	-	SEE REMARK 999	UNP Q03479
D	428	ARG	-	SEE REMARK 999	UNP Q03479
D	429	GLU	LYS	SEE REMARK 999	UNP Q03479
D	440	ASN	-	SEE REMARK 999	UNP Q03479
D	498	ILE	ASN	SEE REMARK 999	UNP Q03479
D	604	VAL	ASP	SEE REMARK 999	UNP Q03479
D	681	ASN	ILE	SEE REMARK 999	UNP Q03479
D	683	THR	ARG	SEE REMARK 999	UNP Q03479

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

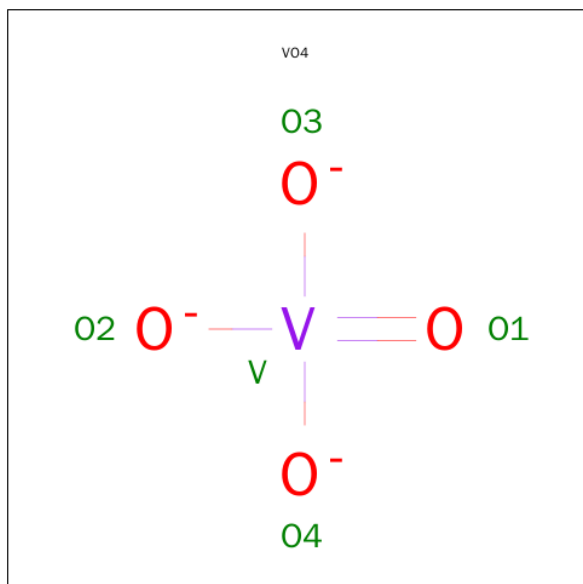
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

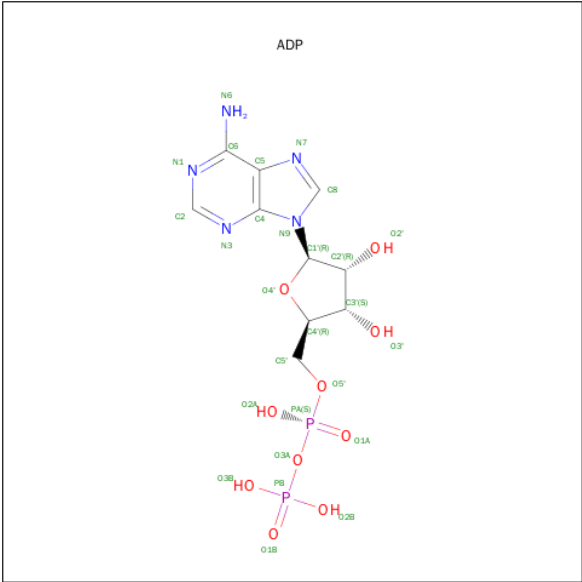
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O₄V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			5	4	1		
3	B	1	Total	O	V	0	0
			5	4	1		
3	C	1	Total	O	V	0	0
			5	4	1		
3	D	1	Total	O	V	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

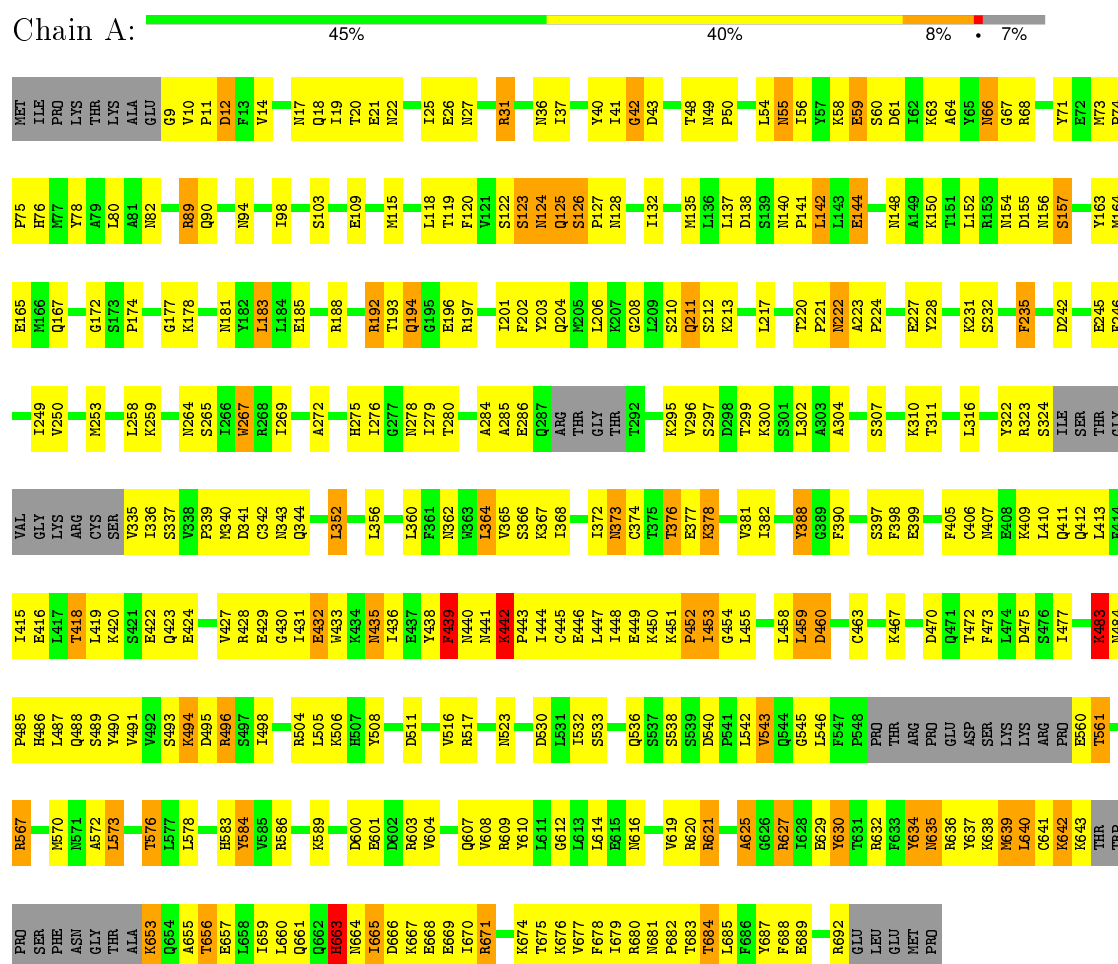
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	16	Total	O	0	0
			16	16		
5	C	19	Total	O	0	0
			19	19		
5	D	11	Total	O	0	0
			11	11		

3 Residue-property plots

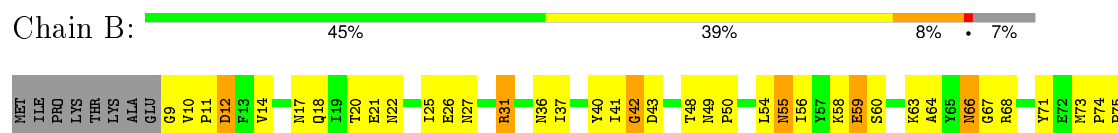
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

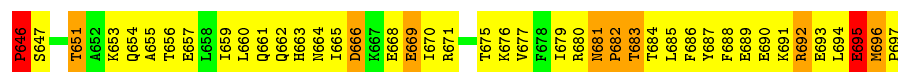
Note EDS was not executed.

• Molecule 1: MYOSIN IE HEAVY CHAIN



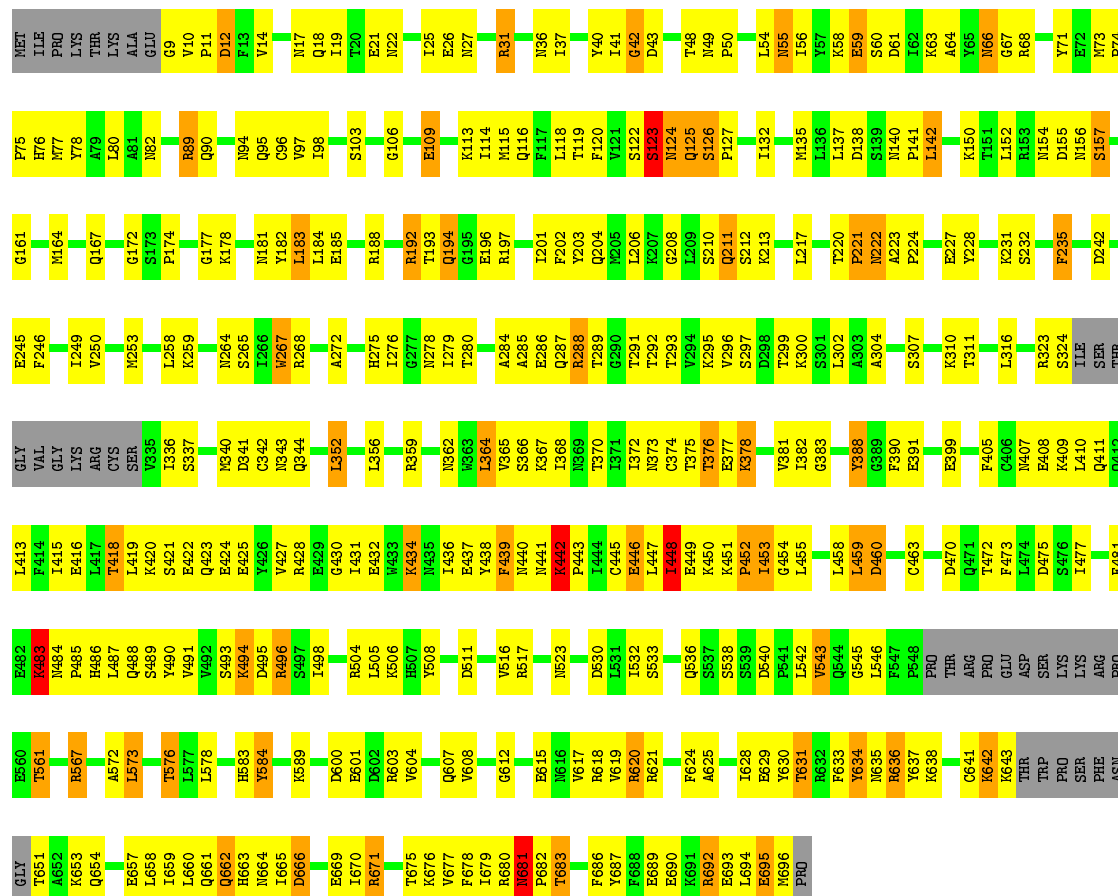
• Molecule 1: MYOSIN IE HEAVY CHAIN





• Molecule 1: MYOSIN IE HEAVY CHAIN

Chain D: 45% 41% 8% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.82Å 143.67Å 236.05Å 90.00° 94.86° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21265	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, MG, ADP

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	A	0.41	0/5280	0.61	1/7108 (0.0%)
1	B	0.41	0/5276	0.61	1/7104 (0.0%)
1	C	0.42	0/5521	0.63	1/7442 (0.0%)
1	D	0.42	0/5356	0.63	2/7212 (0.0%)
All	All	0.42	0/21433	0.62	5/28866 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	LYS	N-CA-C	-6.56	93.30	111.00
1	D	483	LYS	N-CA-C	-6.49	93.49	111.00
1	B	483	LYS	N-CA-C	-6.40	93.72	111.00
1	C	483	LYS	N-CA-C	-6.38	93.77	111.00
1	D	442	LYS	N-CA-C	5.20	125.04	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A	5192	0	5189	366	0
1	B	5188	0	5182	351	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5422	0	5415	417	0
1	D	5267	0	5265	357	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
4	A	27	0	12	2	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	3	0
5	A	18	0	0	4	0
5	B	16	0	0	2	0
5	C	19	0	0	2	0
5	D	11	0	0	2	0
All	All	21265	0	21099	1458	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 34.

All (1458) 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:C:131:ARG:HD3	1:D:259:LYS:HE2	1.24	1.17
1:C:635:ASN:HA	1:C:638:LYS:HD2	1.28	1.16
1:D:642:LYS:HD2	1:D:642:LYS:H	1.00	1.09
1:B:656:THR:HG21	1:B:677:VAL:HG21	1.37	1.06
1:C:288:ARG:H	1:C:288:ARG:HD3	1.22	1.03
1:C:376:THR:HG23	1:D:373:ASN:O	1.60	1.01
1:B:76:HIS:HD2	1:B:78:TYR:H	1.00	1.00
1:B:635:ASN:HD22	1:B:636:ARG:H	1.09	0.99
1:C:629:GLU:CD	1:C:629:GLU:H	1.61	0.99
1:B:634:TYR:HB2	1:B:655:ALA:HB3	1.43	0.98
1:A:125:GLN:NE2	1:C:68:ARG:HE	1.60	0.98
1:D:651:THR:HB	1:D:654:GLN:HG3	1.44	0.97
1:A:76:HIS:HD2	1:A:78:TYR:H	0.97	0.96
1:C:295:LYS:HD3	1:C:296:VAL:H	1.31	0.96
1:A:67:GLY:H	1:A:82:ASN:HD21	1.10	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:GLU:H	1:D:278:ASN:HD21	1.12	0.95
1:D:486:HIS:HA	1:D:506:LYS:HB2	1.49	0.95
1:A:37:ILE:HD11	1:A:54:LEU:HD22	1.49	0.95
1:C:67:GLY:H	1:C:82:ASN:HD21	1.12	0.94
1:A:125:GLN:HB3	1:C:68:ARG:NH2	1.81	0.94
1:C:76:HIS:HD2	1:C:78:TYR:H	1.00	0.94
1:A:295:LYS:HD3	1:A:296:VAL:H	1.30	0.94
1:B:295:LYS:HD3	1:B:296:VAL:H	1.31	0.93
1:B:67:GLY:H	1:B:82:ASN:HD21	1.11	0.93
1:B:627:ARG:HG2	1:B:676:LYS:HE2	1.48	0.93
1:D:295:LYS:HD3	1:D:296:VAL:H	1.32	0.92
1:D:76:HIS:HD2	1:D:78:TYR:H	0.96	0.92
1:B:37:ILE:HD11	1:B:54:LEU:HD22	1.52	0.92
1:D:642:LYS:HD2	1:D:642:LYS:N	1.84	0.92
1:B:227:GLU:H	1:B:278:ASN:HD21	1.17	0.91
1:D:67:GLY:H	1:D:82:ASN:HD21	1.10	0.91
1:C:227:GLU:H	1:C:278:ASN:HD21	1.15	0.91
1:D:448:ILE:HG12	1:D:448:ILE:O	1.71	0.91
1:D:37:ILE:HD11	1:D:54:LEU:HD22	1.52	0.91
1:D:291:THR:HG22	1:D:292:THR:HG22	1.52	0.91
1:B:620:ARG:NE	1:B:620:ARG:HA	1.84	0.91
1:D:76:HIS:CD2	1:D:78:TYR:H	1.88	0.90
1:C:181:ASN:HD21	1:C:362:ASN:ND2	1.70	0.90
1:A:589:LYS:H	1:A:607:GLN:HE22	1.19	0.89
1:A:486:HIS:HA	1:A:506:LYS:HB2	1.55	0.89
1:A:227:GLU:H	1:A:278:ASN:HD21	1.17	0.89
1:A:125:GLN:HB3	1:C:68:ARG:HH21	1.38	0.88
1:C:645:TRP:HB3	1:C:646:PRO:HD2	1.53	0.88
1:A:76:HIS:CD2	1:A:78:TYR:H	1.89	0.88
1:A:423:GLN:HE21	1:A:433:TRP:HE1	1.17	0.88
1:C:288:ARG:N	1:C:288:ARG:HD3	1.88	0.88
1:A:451:LYS:HB3	1:A:452:PRO:HD2	1.56	0.88
1:C:259:LYS:H	1:C:259:LYS:HD2	1.38	0.88
1:C:76:HIS:CD2	1:C:78:TYR:H	1.91	0.88
1:C:589:LYS:H	1:C:607:GLN:HE22	1.21	0.88
1:C:37:ILE:HD11	1:C:54:LEU:HD22	1.56	0.87
1:C:451:LYS:HB3	1:C:452:PRO:HD2	1.56	0.87
1:A:11:PRO:HA	1:A:31:ARG:HH21	1.40	0.87
1:D:451:LYS:HB3	1:D:452:PRO:HD2	1.56	0.86
1:B:76:HIS:CD2	1:B:78:TYR:H	1.92	0.86
1:B:486:HIS:HA	1:B:506:LYS:HB2	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:LYS:HD2	1:D:259:LYS:H	1.41	0.85
1:B:639:MET:O	1:B:640:LEU:HG	1.77	0.85
1:B:634:TYR:HB2	1:B:655:ALA:CB	2.06	0.85
1:D:181:ASN:HD21	1:D:362:ASN:ND2	1.75	0.85
1:C:486:HIS:HA	1:C:506:LYS:HB2	1.56	0.85
1:A:572:ALA:O	1:A:576:THR:HG22	1.76	0.85
1:B:377:GLU:HG2	1:D:681:ASN:OD1	1.77	0.84
1:B:451:LYS:HB3	1:B:452:PRO:HD2	1.57	0.84
1:D:418:THR:HG23	1:D:419:LEU:HG	1.58	0.84
1:A:259:LYS:H	1:A:259:LYS:HD2	1.43	0.84
1:D:11:PRO:HA	1:D:31:ARG:HH21	1.43	0.84
1:C:572:ALA:O	1:C:576:THR:HG22	1.78	0.84
1:D:629:GLU:HA	1:D:675:THR:O	1.78	0.83
1:B:258:LEU:HD21	1:B:367:LYS:HD2	1.58	0.83
1:A:258:LEU:HD21	1:A:367:LYS:HD2	1.59	0.83
1:A:629:GLU:HA	1:A:676:LYS:HG2	1.58	0.83
1:D:572:ALA:O	1:D:576:THR:HG22	1.78	0.83
1:C:696:MET:H	1:C:697:PRO:HA	1.44	0.82
1:C:408:GLU:HB3	1:C:446:GLU:OE1	1.79	0.82
1:B:11:PRO:HA	1:B:31:ARG:HH21	1.44	0.82
1:D:258:LEU:HD21	1:D:367:LYS:HD2	1.62	0.82
1:B:589:LYS:H	1:B:607:GLN:HE22	1.24	0.82
1:C:635:ASN:HA	1:C:638:LYS:CD	2.08	0.81
1:B:572:ALA:O	1:B:576:THR:HG22	1.79	0.81
1:C:660:LEU:HD13	1:C:670:ILE:HD13	1.62	0.81
1:C:288:ARG:CD	1:C:288:ARG:H	1.89	0.81
1:B:12:ASP:HA	1:B:40:TYR:O	1.81	0.81
1:B:259:LYS:H	1:B:259:LYS:HD2	1.44	0.81
1:D:288:ARG:HB2	1:D:288:ARG:HH11	1.46	0.81
1:D:12:ASP:HA	1:D:40:TYR:O	1.81	0.81
1:D:642:LYS:NZ	1:D:662:GLN:HB3	1.96	0.80
1:C:80:LEU:HD11	1:C:583:HIS:HB3	1.64	0.80
1:A:439:PHE:HD1	1:A:440:ASN:N	1.79	0.80
1:A:156:ASN:ND2	4:A:791:ADP:O3'	2.13	0.80
1:A:10:VAL:HB	1:A:27:ASN:HD21	1.46	0.80
1:D:288:ARG:NH1	1:D:288:ARG:HB2	1.96	0.80
1:B:115:MET:O	1:B:119:THR:HG22	1.81	0.80
1:D:167:GLN:HE22	1:D:374:CYS:H	1.29	0.80
1:A:640:LEU:H	1:A:640:LEU:HD12	1.47	0.80
1:C:31:ARG:HB3	1:C:31:ARG:HH11	1.46	0.80
1:B:31:ARG:HB3	1:B:31:ARG:HH11	1.45	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:MET:O	1:C:119:THR:HG22	1.82	0.80
1:D:589:LYS:H	1:D:607:GLN:HE22	1.26	0.79
1:D:642:LYS:CD	1:D:642:LYS:H	1.84	0.79
1:B:635:ASN:ND2	1:B:636:ARG:H	1.80	0.79
1:B:287:GLN:HB2	1:B:292:THR:HA	1.62	0.79
1:B:211:GLN:CD	1:B:211:GLN:H	1.83	0.79
1:C:10:VAL:HB	1:C:27:ASN:HD21	1.48	0.79
1:C:11:PRO:HA	1:C:31:ARG:HH21	1.48	0.79
1:D:211:GLN:H	1:D:211:GLN:CD	1.86	0.78
1:D:288:ARG:CZ	1:D:288:ARG:H	1.97	0.78
1:B:635:ASN:HD22	1:B:636:ARG:N	1.80	0.78
1:B:506:LYS:HG2	1:B:511:ASP:OD1	1.84	0.78
1:C:258:LEU:HD21	1:C:367:LYS:HD2	1.65	0.78
1:B:181:ASN:HD21	1:B:362:ASN:ND2	1.82	0.78
1:D:506:LYS:HG2	1:D:511:ASP:OD1	1.83	0.77
1:C:131:ARG:HD3	1:D:259:LYS:CE	2.12	0.77
1:C:451:LYS:HB3	1:C:452:PRO:CD	2.15	0.77
1:A:67:GLY:H	1:A:82:ASN:ND2	1.83	0.77
1:C:211:GLN:H	1:C:211:GLN:CD	1.87	0.77
1:A:119:THR:HG23	1:A:119:THR:O	1.84	0.77
1:A:442:LYS:HB2	1:A:442:LYS:NZ	2.00	0.77
1:A:211:GLN:CD	1:A:211:GLN:H	1.87	0.77
1:A:115:MET:O	1:A:119:THR:HG22	1.85	0.77
1:B:418:THR:HG23	1:B:419:LEU:HG	1.68	0.76
1:B:10:VAL:HB	1:B:27:ASN:HD21	1.49	0.76
1:C:418:THR:CG2	1:C:616:ASN:HD21	1.97	0.76
1:D:431:ILE:HD12	1:D:671:ARG:HG2	1.65	0.76
1:C:441:ASN:O	1:C:442:LYS:HD3	1.85	0.76
1:D:67:GLY:H	1:D:82:ASN:ND2	1.83	0.76
1:D:651:THR:HB	1:D:654:GLN:CG	2.14	0.76
1:A:12:ASP:HA	1:A:40:TYR:O	1.86	0.76
1:D:10:VAL:HB	1:D:27:ASN:HD21	1.51	0.75
1:A:37:ILE:HG23	1:A:48:THR:O	1.85	0.75
1:A:436:ILE:HD12	1:A:619:VAL:HA	1.68	0.75
1:D:115:MET:O	1:D:119:THR:HG22	1.87	0.75
1:D:434:LYS:HG2	1:D:434:LYS:O	1.86	0.75
1:D:451:LYS:HB3	1:D:452:PRO:CD	2.16	0.75
1:C:506:LYS:HG2	1:C:511:ASP:OD1	1.87	0.75
1:D:671:ARG:HB3	1:D:678:PHE:HB2	1.69	0.75
1:C:287:GLN:HB3	1:C:291:THR:HG23	1.70	0.74
1:C:639:MET:HG2	1:C:640:LEU:HD12	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:THR:O	1:C:119:THR:HG23	1.86	0.74
1:A:10:VAL:HB	1:A:27:ASN:ND2	2.01	0.74
1:A:439:PHE:CD1	1:A:440:ASN:N	2.54	0.74
1:B:37:ILE:HG23	1:B:48:THR:O	1.87	0.74
1:B:451:LYS:HB3	1:B:452:PRO:CD	2.18	0.74
1:C:37:ILE:HG23	1:C:48:THR:O	1.88	0.74
1:D:660:LEU:HD13	1:D:670:ILE:CD1	2.17	0.74
1:C:636:ARG:HH11	1:C:636:ARG:HG2	1.52	0.74
1:B:67:GLY:H	1:B:82:ASN:ND2	1.85	0.74
1:D:119:THR:HG23	1:D:119:THR:O	1.87	0.74
1:D:641:CYS:HB2	1:D:659:ILE:HG12	1.69	0.74
1:C:418:THR:HG21	1:C:616:ASN:HD21	1.53	0.73
1:A:177:GLY:O	1:A:372:ILE:HG22	1.88	0.73
1:B:630:TYR:CE2	1:B:677:VAL:HG22	2.23	0.73
1:C:167:GLN:HE22	1:C:374:CYS:H	1.34	0.73
1:C:12:ASP:HA	1:C:40:TYR:O	1.89	0.73
1:A:636:ARG:O	1:A:636:ARG:HD2	1.89	0.73
1:A:441:ASN:C	1:A:443:PRO:HD3	2.09	0.73
1:B:423:GLN:HE22	1:B:436:ILE:H	1.37	0.73
1:C:177:GLY:O	1:C:372:ILE:HG22	1.89	0.73
1:A:451:LYS:HB3	1:A:452:PRO:CD	2.18	0.73
1:A:181:ASN:HD21	1:A:362:ASN:ND2	1.86	0.73
1:D:10:VAL:HB	1:D:27:ASN:ND2	2.04	0.72
1:D:31:ARG:HB3	1:D:31:ARG:HH11	1.52	0.72
1:C:320:LEU:HD23	1:C:531:LEU:HD21	1.69	0.72
1:A:125:GLN:HE21	1:C:68:ARG:HE	1.38	0.72
1:A:80:LEU:HD11	1:A:583:HIS:HB3	1.69	0.72
1:C:645:TRP:HB3	1:C:646:PRO:CD	2.18	0.72
1:C:634:TYR:O	1:C:638:LYS:HG3	1.88	0.72
1:D:27:ASN:O	1:D:31:ARG:HG2	1.89	0.72
1:C:636:ARG:HD3	1:C:636:ARG:O	1.89	0.72
1:C:443:PRO:O	1:C:447:LEU:HG	1.90	0.72
1:A:669:GLU:C	1:A:670:ILE:HD12	2.08	0.72
1:C:67:GLY:H	1:C:82:ASN:ND2	1.88	0.71
1:B:119:THR:O	1:B:119:THR:HG23	1.90	0.71
1:D:620:ARG:HA	1:D:620:ARG:CZ	2.20	0.71
1:A:128:ASN:OD1	1:C:73:MET:HA	1.90	0.71
1:C:227:GLU:H	1:C:278:ASN:ND2	1.89	0.71
1:A:423:GLN:HE22	1:A:436:ILE:H	1.39	0.71
1:C:10:VAL:HB	1:C:27:ASN:ND2	2.05	0.71
1:B:448:ILE:HG12	1:B:448:ILE:O	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:THR:HG22	1:B:688:PHE:HE1	1.56	0.71
1:C:289:THR:O	1:C:291:THR:HG22	1.91	0.70
1:C:445:CYS:O	1:C:448:ILE:HG22	1.89	0.70
1:B:80:LEU:HD11	1:B:583:HIS:HB3	1.71	0.70
1:A:506:LYS:HG2	1:A:511:ASP:OD1	1.92	0.70
1:C:90:GLN:CD	1:C:636:ARG:HH21	1.95	0.70
1:D:222:ASN:OD1	1:D:224:PRO:HD2	1.91	0.70
1:B:378:LYS:HG3	1:D:666:ASP:HB2	1.73	0.70
1:B:10:VAL:HB	1:B:27:ASN:ND2	2.05	0.70
1:B:227:GLU:H	1:B:278:ASN:ND2	1.90	0.70
1:C:222:ASN:OD1	1:C:224:PRO:HD2	1.92	0.70
1:A:227:GLU:H	1:A:278:ASN:ND2	1.90	0.70
1:C:444:ILE:H	1:C:444:ILE:HD12	1.57	0.70
1:C:637:TYR:CE2	1:C:688:PHE:HB3	2.27	0.70
1:A:637:TYR:O	1:A:659:ILE:HD13	1.92	0.70
1:D:37:ILE:HG23	1:D:48:THR:O	1.92	0.69
1:A:31:ARG:HH11	1:A:31:ARG:HB3	1.56	0.69
1:B:615:GLU:O	1:B:619:VAL:HG23	1.91	0.69
1:B:473:PHE:CZ	1:B:477:ILE:HD11	2.28	0.69
1:A:444:ILE:HD12	1:A:444:ILE:N	2.08	0.69
1:D:227:GLU:H	1:D:278:ASN:ND2	1.86	0.69
1:D:443:PRO:HA	1:D:446:GLU:HG2	1.75	0.69
1:D:181:ASN:HD21	1:D:362:ASN:HD21	1.40	0.69
1:C:473:PHE:CZ	1:C:477:ILE:HD11	2.27	0.69
1:D:142:LEU:HD11	1:D:364:LEU:HD21	1.75	0.69
1:A:671:ARG:HG2	1:A:671:ARG:HH11	1.58	0.69
1:C:416:GLU:OE2	1:C:420:LYS:HD3	1.93	0.69
1:A:477:ILE:HG22	1:A:487:LEU:HD21	1.75	0.68
1:B:177:GLY:O	1:B:372:ILE:HG22	1.93	0.68
1:B:692:ARG:HA	1:B:692:ARG:HE	1.58	0.68
1:A:144:GLU:HG3	5:A:798:HOH:O	1.94	0.68
1:B:642:LYS:HD2	1:B:642:LYS:N	2.08	0.68
1:C:311:THR:HG22	1:C:538:SER:HA	1.76	0.68
1:D:250:VAL:HA	1:D:253:MET:HG3	1.74	0.68
1:C:441:ASN:C	1:C:443:PRO:HD3	2.13	0.68
1:D:493:SER:O	1:D:495:ASP:N	2.27	0.68
1:A:378:LYS:C	1:A:378:LYS:HD3	2.14	0.68
1:C:620:ARG:HA	1:C:620:ARG:CZ	2.24	0.68
1:B:443:PRO:O	1:B:447:LEU:HG	1.94	0.68
1:D:573:LEU:O	1:D:576:THR:HG23	1.94	0.68
1:C:493:SER:O	1:C:495:ASP:N	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ASN:ND2	4:B:794:ADP:O3'	2.26	0.68
1:B:504:ARG:HD2	1:B:511:ASP:HB3	1.75	0.68
1:B:27:ASN:O	1:B:31:ARG:HG2	1.94	0.68
1:A:641:CYS:HB2	1:A:659:ILE:HG12	1.76	0.67
1:B:477:ILE:HG22	1:B:487:LEU:HD21	1.75	0.67
1:C:27:ASN:O	1:C:31:ARG:HG2	1.94	0.67
1:B:409:LYS:HZ2	1:B:450:LYS:HD3	1.58	0.67
1:B:621:ARG:HG3	1:B:621:ARG:HH21	1.59	0.67
1:A:473:PHE:CZ	1:A:477:ILE:HD11	2.29	0.67
1:A:454:GLY:O	1:A:458:LEU:HD23	1.95	0.67
1:C:630:TYR:CE2	1:C:677:VAL:HG22	2.29	0.67
1:D:683:THR:HA	1:D:686:PHE:CD2	2.30	0.67
1:B:197:ARG:HG2	1:B:203:TYR:CZ	2.29	0.67
1:A:64:ALA:O	1:A:68:ARG:HD2	1.95	0.67
1:A:27:ASN:O	1:A:31:ARG:HG2	1.94	0.67
1:D:177:GLY:O	1:D:372:ILE:HG22	1.95	0.67
1:B:493:SER:O	1:B:495:ASP:N	2.28	0.67
1:C:629:GLU:N	1:C:629:GLU:CD	2.44	0.67
1:A:669:GLU:O	1:A:670:ILE:HD12	1.95	0.66
1:C:436:ILE:HD12	1:C:436:ILE:H	1.61	0.66
1:A:666:ASP:HB3	1:A:668:GLU:HG2	1.77	0.66
1:C:311:THR:HG22	1:C:538:SER:CA	2.25	0.66
1:D:275:HIS:CE1	1:D:304:ALA:HB1	2.30	0.66
1:C:181:ASN:HD21	1:C:362:ASN:HD21	1.40	0.66
1:A:573:LEU:O	1:A:576:THR:HG23	1.95	0.66
1:C:573:LEU:O	1:C:576:THR:HG23	1.96	0.66
1:D:692:ARG:HH11	1:D:692:ARG:HG3	1.60	0.66
1:C:122:SER:OG	1:C:174:PRO:HG3	1.94	0.66
1:A:443:PRO:HD2	1:A:444:ILE:HD13	1.77	0.66
1:B:181:ASN:HD21	1:B:362:ASN:HD21	1.41	0.66
1:A:629:GLU:OE1	1:A:632:ARG:HD2	1.96	0.66
1:D:80:LEU:HD11	1:D:583:HIS:HB3	1.78	0.66
1:C:131:ARG:CD	1:D:259:LYS:HE2	2.15	0.66
1:C:90:GLN:HE22	1:C:636:ARG:NH2	1.94	0.66
1:A:504:ARG:HD2	1:A:511:ASP:HB3	1.77	0.66
1:A:493:SER:O	1:A:495:ASP:N	2.28	0.66
1:C:197:ARG:HG2	1:C:203:TYR:CZ	2.31	0.66
1:B:635:ASN:HA	1:B:638:LYS:HB2	1.78	0.66
1:D:504:ARG:HD2	1:D:511:ASP:HB3	1.78	0.66
1:A:443:PRO:HG2	1:A:444:ILE:HD12	1.77	0.66
1:C:685:LEU:O	1:C:686:PHE:C	2.34	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:LYS:C	1:D:378:LYS:HD3	2.16	0.66
1:B:573:LEU:O	1:B:576:THR:HG23	1.96	0.65
1:A:197:ARG:HG2	1:A:203:TYR:CZ	2.30	0.65
1:D:157:SER:N	5:D:905:HOH:O	2.29	0.65
1:A:423:GLN:HE22	1:A:436:ILE:N	1.93	0.65
1:D:454:GLY:O	1:D:458:LEU:HD23	1.96	0.65
1:C:644:THR:O	1:C:644:THR:HG22	1.95	0.65
1:C:443:PRO:HA	1:C:446:GLU:CG	2.26	0.65
1:D:324:SER:HA	1:D:336:ILE:O	1.96	0.65
1:A:665:ILE:HD11	1:A:688:PHE:HZ	1.62	0.65
1:D:425:GLU:HA	1:D:428:ARG:NH2	2.12	0.64
1:D:259:LYS:HD2	1:D:259:LYS:N	2.13	0.64
1:D:119:THR:HG21	1:D:137:LEU:HD21	1.78	0.64
1:A:670:ILE:HD11	1:A:679:ILE:HG23	1.78	0.64
1:A:125:GLN:NE2	1:C:68:ARG:NE	2.39	0.64
1:C:259:LYS:N	1:C:259:LYS:HD2	2.11	0.64
1:C:423:GLN:HE21	1:C:433:TRP:HE1	1.44	0.64
1:D:89:ARG:HE	1:D:172:GLY:HA3	1.62	0.64
1:C:551:ARG:HD3	1:C:555:SER:OG	1.98	0.64
1:A:627:ARG:H	1:A:627:ARG:HD2	1.62	0.64
1:B:89:ARG:HE	1:B:172:GLY:HA3	1.63	0.64
1:A:295:LYS:HD3	1:A:296:VAL:N	2.09	0.64
1:A:423:GLN:NE2	1:A:436:ILE:H	1.95	0.64
1:C:679:ILE:HG21	1:C:684:THR:HB	1.80	0.64
1:C:504:ARG:HD2	1:C:511:ASP:HB3	1.79	0.64
1:D:680:ARG:O	1:D:681:ASN:HB2	1.98	0.64
1:C:441:ASN:OD1	1:C:443:PRO:HD3	1.98	0.63
1:A:416:GLU:OE2	1:A:420:LYS:HD3	1.99	0.63
1:A:431:ILE:O	1:A:432:GLU:C	2.35	0.63
1:C:295:LYS:HD3	1:C:296:VAL:N	2.10	0.63
1:D:473:PHE:CZ	1:D:477:ILE:HD11	2.33	0.63
1:A:441:ASN:O	1:A:443:PRO:HD3	1.97	0.63
1:C:167:GLN:NE2	1:C:374:CYS:HB3	2.14	0.63
1:C:98:ILE:HD11	1:C:584:TYR:CD2	2.32	0.63
1:C:142:LEU:HD12	1:C:368:ILE:HD11	1.79	0.63
1:B:194:GLN:OE1	1:B:194:GLN:N	2.28	0.63
1:C:477:ILE:HG22	1:C:487:LEU:HD21	1.79	0.63
1:B:443:PRO:O	1:B:446:GLU:HB2	1.99	0.63
1:D:197:ARG:HG2	1:D:203:TYR:CZ	2.33	0.63
1:C:365:VAL:HG23	1:C:366:SER:N	2.14	0.63
1:C:412:GLN:HB2	1:C:442:LYS:HE2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ARG:HG2	1:A:671:ARG:NH1	2.12	0.63
1:B:171:VAL:HG22	1:D:690:GLU:OE2	1.97	0.63
1:C:655:ALA:O	1:C:659:ILE:HG13	1.98	0.63
1:B:222:ASN:OD1	1:B:224:PRO:HD2	1.98	0.63
1:B:412:GLN:HB2	1:B:442:LYS:HE2	1.80	0.63
1:B:439:PHE:CG	1:B:440:ASN:N	2.67	0.63
1:A:103:SER:HA	3:A:792:VO4:O1	1.99	0.62
1:C:694:LEU:O	1:C:695:GLU:HB3	1.98	0.62
1:C:613:LEU:O	1:C:617:VAL:HG23	1.98	0.62
1:A:89:ARG:HE	1:A:172:GLY:HA3	1.64	0.62
1:B:454:GLY:O	1:B:458:LEU:HD23	1.99	0.62
1:A:22:ASN:O	1:A:26:GLU:HG3	1.98	0.62
1:C:259:LYS:H	1:C:259:LYS:CD	2.11	0.62
1:C:438:TYR:O	1:C:439:PHE:O	2.18	0.62
1:B:40:TYR:CZ	1:B:75:PRO:HA	2.33	0.62
1:C:683:THR:HA	1:C:686:PHE:CD2	2.35	0.62
1:D:642:LYS:HZ2	1:D:662:GLN:HB3	1.65	0.62
1:C:443:PRO:HA	1:C:446:GLU:HG2	1.81	0.62
1:A:259:LYS:N	1:A:259:LYS:HD2	2.13	0.62
1:A:444:ILE:CD1	1:A:444:ILE:N	2.61	0.62
1:A:423:GLN:NE2	1:A:433:TRP:HE1	1.94	0.62
1:B:686:PHE:O	1:B:690:GLU:HG2	1.99	0.62
1:B:170:ALA:HB1	1:D:687:TYR:CD1	2.34	0.62
1:C:89:ARG:HE	1:C:172:GLY:HA3	1.65	0.62
1:B:213:LYS:NZ	1:B:264:ASN:HD21	1.98	0.62
1:A:127:PRO:HD2	1:C:73:MET:HG2	1.82	0.62
1:B:378:LYS:HD3	1:B:378:LYS:C	2.20	0.62
1:A:250:VAL:HA	1:A:253:MET:HG3	1.82	0.61
1:D:122:SER:OG	1:D:174:PRO:HG3	1.99	0.61
1:A:76:HIS:HD2	1:A:78:TYR:N	1.82	0.61
1:A:473:PHE:CE2	1:A:477:ILE:HD11	2.35	0.61
1:B:451:LYS:HD2	1:B:451:LYS:N	2.16	0.61
1:D:284:ALA:HB3	1:D:293:THR:C	2.21	0.61
1:C:40:TYR:CZ	1:C:75:PRO:HA	2.35	0.61
1:A:653:LYS:HZ2	1:A:653:LYS:HB2	1.65	0.61
1:D:477:ILE:HG22	1:D:487:LEU:HD21	1.81	0.61
1:A:641:CYS:HB2	1:A:659:ILE:HG23	1.82	0.61
1:C:636:ARG:NH1	1:C:636:ARG:HG2	2.15	0.61
1:C:533:SER:HA	1:C:536:GLN:HE21	1.66	0.61
1:C:641:CYS:SG	1:C:662:GLN:NE2	2.74	0.61
1:D:669:GLU:O	1:D:669:GLU:HG3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ALA:O	1:B:68:ARG:HD2	2.00	0.61
1:D:194:GLN:OE1	1:D:194:GLN:N	2.32	0.61
1:A:451:LYS:N	1:A:451:LYS:HD2	2.16	0.61
1:B:419:LEU:HD22	1:B:619:VAL:HG21	1.82	0.61
1:B:428:ARG:HG2	1:B:428:ARG:HH11	1.66	0.61
1:A:222:ASN:OD1	1:A:224:PRO:HD2	2.01	0.61
1:D:680:ARG:O	1:D:681:ASN:CB	2.49	0.61
1:A:419:LEU:HD13	1:A:438:TYR:CB	2.30	0.61
1:A:448:ILE:O	1:A:448:ILE:HG12	2.00	0.61
1:D:439:PHE:CE2	1:D:612:GLY:HA3	2.35	0.61
1:D:64:ALA:O	1:D:68:ARG:HD2	2.01	0.61
1:B:142:LEU:HD11	1:B:364:LEU:HD21	1.81	0.61
1:B:409:LYS:HD2	1:B:446:GLU:OE1	2.01	0.60
1:C:473:PHE:CE2	1:C:477:ILE:HD11	2.36	0.60
1:D:40:TYR:CZ	1:D:75:PRO:HA	2.36	0.60
1:D:142:LEU:CD1	1:D:364:LEU:HD21	2.30	0.60
1:B:667:LYS:O	1:B:669:GLU:N	2.34	0.60
1:B:22:ASN:O	1:B:26:GLU:HG3	2.00	0.60
1:D:473:PHE:CE2	1:D:477:ILE:HD11	2.36	0.60
1:C:443:PRO:HD2	1:C:444:ILE:CD1	2.31	0.60
1:B:438:TYR:HA	1:B:615:GLU:HG2	1.82	0.60
1:A:636:ARG:HG3	1:A:637:TYR:CD1	2.36	0.60
1:D:55:ASN:HD21	1:D:58:LYS:HD3	1.65	0.60
1:A:21:GLU:O	1:A:25:ILE:HD13	2.02	0.60
1:B:426:TYR:HE2	1:B:623:GLY:HA2	1.65	0.60
1:C:378:LYS:C	1:C:378:LYS:HD3	2.20	0.60
1:D:654:GLN:O	1:D:658:LEU:HG	2.02	0.60
1:A:629:GLU:HG2	1:A:676:LYS:NZ	2.16	0.60
1:A:40:TYR:CZ	1:A:75:PRO:HA	2.36	0.60
1:C:194:GLN:OE1	1:C:194:GLN:N	2.29	0.60
1:A:280:THR:OG1	1:A:297:SER:HB2	2.02	0.60
1:A:148:ASN:ND2	5:A:798:HOH:O	2.34	0.60
1:D:55:ASN:ND2	1:D:58:LYS:HD3	2.16	0.60
1:B:250:VAL:HA	1:B:253:MET:HG3	1.84	0.60
1:B:621:ARG:NH2	1:B:621:ARG:HG3	2.17	0.60
1:B:122:SER:OG	1:B:174:PRO:HG3	2.02	0.60
1:C:66:ASN:HD22	1:C:67:GLY:N	2.00	0.60
1:C:156:ASN:ND2	4:C:891:ADP:O3'	2.35	0.60
1:D:451:LYS:N	1:D:451:LYS:HD2	2.17	0.60
1:C:194:GLN:H	1:C:194:GLN:CD	2.03	0.60
1:B:473:PHE:CE2	1:B:477:ILE:HD11	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ARG:HH11	1:B:504:ARG:HG2	1.67	0.60
1:B:442:LYS:HE3	1:B:442:LYS:O	2.02	0.60
1:B:662:GLN:C	1:B:664:ASN:H	2.04	0.60
1:D:288:ARG:NE	1:D:288:ARG:H	1.99	0.59
1:A:670:ILE:HG13	1:A:679:ILE:HA	1.84	0.59
1:D:416:GLU:OE2	1:D:420:LYS:HD3	2.01	0.59
1:C:376:THR:HG22	1:C:377:GLU:N	2.16	0.59
1:C:64:ALA:O	1:C:68:ARG:HD2	2.02	0.59
1:B:295:LYS:HD3	1:B:296:VAL:N	2.11	0.59
1:A:409:LYS:HD2	1:A:446:GLU:OE1	2.02	0.59
1:A:11:PRO:CA	1:A:31:ARG:HH21	2.13	0.59
1:A:412:GLN:HB2	1:A:442:LYS:HE3	1.83	0.59
1:B:378:LYS:HG3	1:D:666:ASP:CB	2.32	0.59
1:A:653:LYS:NZ	1:A:653:LYS:HB2	2.17	0.59
1:A:533:SER:HA	1:A:536:GLN:HE21	1.67	0.59
1:C:41:ILE:HG22	1:C:41:ILE:O	2.03	0.59
1:D:441:ASN:O	1:D:442:LYS:HD3	2.02	0.59
1:C:90:GLN:NE2	1:C:636:ARG:HH21	2.00	0.59
1:C:98:ILE:HD11	1:C:584:TYR:HD2	1.66	0.59
1:A:620:ARG:NE	1:A:620:ARG:HA	2.17	0.59
1:B:634:TYR:CB	1:B:655:ALA:HB3	2.28	0.59
1:D:295:LYS:HD3	1:D:296:VAL:N	2.11	0.59
1:A:181:ASN:HD21	1:A:362:ASN:HD21	1.49	0.59
1:C:142:LEU:HD11	1:C:364:LEU:HD21	1.84	0.59
1:B:17:ASN:CG	1:B:18:GLN:H	2.05	0.59
1:C:158:SER:N	3:C:892:VO4:O2	2.33	0.59
1:A:635:ASN:HB3	1:C:642:LYS:HG2	1.84	0.59
1:A:440:ASN:ND2	1:A:442:LYS:HB3	2.18	0.59
1:A:411:GLN:HG2	1:A:508:TYR:CD2	2.37	0.59
1:A:679:ILE:N	1:A:679:ILE:HD12	2.18	0.59
1:B:390:PHE:N	1:B:407:ASN:OD1	2.36	0.59
1:D:642:LYS:HZ3	1:D:662:GLN:HB3	1.68	0.59
1:C:640:LEU:HD21	1:C:691:LYS:HB3	1.83	0.59
1:A:55:ASN:HD21	1:A:58:LYS:HD3	1.68	0.59
1:D:259:LYS:CD	1:D:259:LYS:H	2.13	0.58
1:C:90:GLN:OE1	1:C:636:ARG:NH2	2.30	0.58
1:B:341:ASP:OD2	1:B:343:ASN:HB2	2.03	0.58
1:B:21:GLU:O	1:B:25:ILE:HD13	2.03	0.58
1:B:411:GLN:HG2	1:B:508:TYR:CD2	2.37	0.58
1:B:119:THR:HG21	1:B:137:LEU:HD21	1.84	0.58
1:A:140:ASN:HB2	1:A:141:PRO:HD3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:GLU:O	1:C:695:GLU:OE1	2.21	0.58
1:B:472:THR:HA	1:B:475:ASP:OD2	2.03	0.58
1:C:442:LYS:C	1:C:444:ILE:H	2.06	0.58
1:C:309:LEU:HD13	1:C:535:MET:SD	2.43	0.58
1:B:311:THR:HG22	1:B:538:SER:HA	1.86	0.58
1:A:567:ARG:HG2	1:A:567:ARG:HH11	1.67	0.58
1:C:472:THR:HA	1:C:475:ASP:OD2	2.03	0.58
1:C:438:TYR:HA	1:C:615:GLU:HG2	1.86	0.58
1:B:486:HIS:O	1:B:505:LEU:HD12	2.03	0.58
1:B:140:ASN:HB2	1:B:141:PRO:HD3	1.85	0.58
1:D:95:GLN:HB2	1:D:382:ILE:HG12	1.86	0.58
1:C:680:ARG:O	1:C:681:ASN:HB2	2.04	0.58
1:A:341:ASP:OD2	1:A:343:ASN:HB2	2.03	0.58
1:C:341:ASP:OD2	1:C:343:ASN:HB2	2.04	0.58
1:C:567:ARG:HG2	1:C:567:ARG:HH11	1.67	0.58
1:D:227:GLU:O	1:D:231:LYS:HG3	2.03	0.58
1:B:259:LYS:HD2	1:B:259:LYS:N	2.14	0.58
1:D:617:VAL:O	1:D:621:ARG:HB2	2.03	0.58
1:A:55:ASN:ND2	1:A:58:LYS:HD3	2.19	0.58
1:C:213:LYS:NZ	1:C:264:ASN:HD21	2.00	0.58
1:D:280:THR:OG1	1:D:297:SER:HB2	2.02	0.58
1:D:192:ARG:HG3	1:D:232:SER:HB3	1.83	0.58
1:B:441:ASN:O	1:B:442:LYS:HD3	2.03	0.58
1:D:140:ASN:HB2	1:D:141:PRO:HD3	1.86	0.58
1:D:21:GLU:O	1:D:25:ILE:HD13	2.04	0.58
1:D:284:ALA:HB3	1:D:293:THR:O	2.04	0.58
1:A:253:MET:HE1	1:A:267:TRP:CH2	2.37	0.58
1:A:192:ARG:HG3	1:A:232:SER:HB3	1.86	0.58
1:D:441:ASN:O	1:D:443:PRO:HD3	2.04	0.58
1:C:454:GLY:O	1:C:458:LEU:HD23	2.03	0.58
1:A:259:LYS:H	1:A:259:LYS:CD	2.14	0.58
1:C:451:LYS:HD2	1:C:451:LYS:N	2.19	0.58
1:B:450:LYS:HB3	1:B:451:LYS:HD2	1.86	0.58
1:D:636:ARG:HH11	1:D:636:ARG:HG2	1.68	0.58
1:D:424:GLU:O	1:D:427:VAL:HG22	2.04	0.58
1:C:645:TRP:O	1:C:647:SER:N	2.37	0.57
1:A:418:THR:HG23	1:A:419:LEU:HG	1.85	0.57
1:D:533:SER:HA	1:D:536:GLN:HE21	1.68	0.57
1:D:295:LYS:CD	1:D:296:VAL:H	2.14	0.57
1:D:660:LEU:CD2	1:D:665:ILE:HD12	2.34	0.57
1:B:670:ILE:N	1:B:670:ILE:HD12	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LYS:HZ3	1:A:442:LYS:HB2	1.68	0.57
1:A:156:ASN:HD22	4:A:791:ADP:HO3'	1.52	0.57
1:C:90:GLN:NE2	1:C:636:ARG:NH2	2.52	0.57
1:A:683:THR:C	1:A:685:LEU:H	2.08	0.57
1:B:259:LYS:H	1:B:259:LYS:CD	2.15	0.57
1:C:250:VAL:HA	1:C:253:MET:HG3	1.86	0.57
1:C:17:ASN:CG	1:C:18:GLN:H	2.08	0.57
1:D:504:ARG:HG2	1:D:504:ARG:HH11	1.70	0.57
1:B:227:GLU:O	1:B:231:LYS:HG3	2.04	0.57
1:C:192:ARG:HG3	1:C:232:SER:HB3	1.86	0.57
1:A:194:GLN:N	1:A:194:GLN:OE1	2.30	0.57
1:D:249:ILE:O	1:D:253:MET:HG2	2.05	0.57
1:C:324:SER:HA	1:C:336:ILE:O	2.04	0.57
1:D:138:ASP:O	1:D:141:PRO:HD2	2.04	0.57
1:D:341:ASP:OD2	1:D:343:ASN:HB2	2.04	0.57
1:B:295:LYS:CD	1:B:296:VAL:H	2.13	0.57
1:B:66:ASN:HD22	1:B:67:GLY:N	2.02	0.57
1:C:227:GLU:O	1:C:231:LYS:HG3	2.04	0.57
1:B:452:PRO:O	1:B:453:ILE:HB	2.05	0.57
1:D:253:MET:HE1	1:D:267:TRP:CH2	2.39	0.57
1:C:558:ARG:HB2	1:C:559:PRO:HD3	1.87	0.57
1:A:142:LEU:HD11	1:A:364:LEU:HD21	1.87	0.57
1:D:542:LEU:O	1:D:545:GLY:N	2.38	0.57
1:B:663:HIS:HB3	1:B:665:ILE:HG13	1.87	0.57
1:A:443:PRO:HG2	1:A:444:ILE:CD1	2.34	0.57
1:B:633:PHE:O	1:B:637:TYR:HB2	2.04	0.56
1:C:434:LYS:H	1:C:434:LYS:CE	2.18	0.56
1:A:157:SER:N	5:A:808:HOH:O	2.37	0.56
1:D:213:LYS:NZ	1:D:264:ASN:HD21	2.03	0.56
1:C:629:GLU:HG3	1:C:676:LYS:HE3	1.87	0.56
1:D:365:VAL:HG23	1:D:366:SER:N	2.19	0.56
1:D:434:LYS:HD2	1:D:434:LYS:H	1.70	0.56
1:C:348:SER:HB3	1:C:531:LEU:HD11	1.86	0.56
1:D:94:ASN:ND2	1:D:381:VAL:H	2.03	0.56
1:A:125:GLN:HE22	1:C:68:ARG:HE	1.48	0.56
1:C:448:ILE:O	1:C:455:LEU:HG	2.04	0.56
1:C:485:PRO:O	1:C:486:HIS:HB2	2.05	0.56
1:A:441:ASN:C	1:A:443:PRO:CD	2.74	0.56
1:A:420:LYS:HE2	1:A:424:GLU:OE1	2.05	0.56
1:C:557:LYS:N	1:C:557:LYS:HZ2	2.03	0.56
1:A:122:SER:OG	1:A:174:PRO:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ASN:ND2	1:B:58:LYS:HD3	2.19	0.56
1:C:504:ARG:HH11	1:C:504:ARG:HG2	1.70	0.56
1:B:11:PRO:CA	1:B:31:ARG:HH21	2.18	0.56
1:A:667:LYS:C	1:A:669:GLU:H	2.09	0.56
1:C:197:ARG:NH1	1:C:242:ASP:OD1	2.39	0.56
1:A:276:ILE:HD13	1:A:352:LEU:HD13	1.88	0.56
1:D:660:LEU:HD23	1:D:665:ILE:HD12	1.87	0.56
1:B:448:ILE:O	1:B:455:LEU:HG	2.05	0.56
1:D:695:GLU:O	1:D:696:MET:HB2	2.05	0.56
1:D:17:ASN:CG	1:D:18:GLN:H	2.09	0.56
1:C:140:ASN:HB2	1:C:141:PRO:HD3	1.87	0.56
1:A:604:VAL:O	1:A:608:VAL:HG23	2.05	0.56
1:A:41:ILE:HG22	1:A:41:ILE:O	2.06	0.56
1:D:642:LYS:HD3	1:D:662:GLN:HG2	1.86	0.56
1:D:438:TYR:O	1:D:440:ASN:N	2.39	0.56
1:C:253:MET:HE1	1:C:267:TRP:CH2	2.41	0.56
1:D:54:LEU:O	1:D:56:ILE:N	2.39	0.56
1:C:486:HIS:O	1:C:505:LEU:HD12	2.06	0.56
1:C:22:ASN:O	1:C:26:GLU:HG3	2.06	0.56
1:B:167:GLN:HE22	1:B:374:CYS:H	1.53	0.56
1:B:653:LYS:CE	1:B:653:LYS:H	2.19	0.56
1:D:66:ASN:HD22	1:D:67:GLY:N	2.04	0.56
1:A:227:GLU:O	1:A:231:LYS:HG3	2.05	0.56
1:C:450:LYS:HB3	1:C:451:LYS:HD2	1.88	0.56
1:C:204:GLN:HE22	1:C:245:GLU:HG2	1.70	0.56
1:D:485:PRO:O	1:D:486:HIS:HB2	2.06	0.56
1:A:452:PRO:O	1:A:453:ILE:HB	2.06	0.56
1:C:488:GLN:HB2	1:C:504:ARG:HB3	1.87	0.56
1:D:9:GLY:HA3	1:D:31:ARG:HD3	1.88	0.56
1:C:656:THR:O	1:C:660:LEU:HG	2.05	0.56
1:D:19:ILE:HD11	1:D:618:ARG:HG2	1.88	0.56
1:C:690:GLU:O	1:C:694:LEU:HD23	2.06	0.56
1:D:484:ASN:OD1	1:D:485:PRO:O	2.24	0.55
1:A:295:LYS:CD	1:A:296:VAL:H	2.12	0.55
1:D:452:PRO:O	1:D:453:ILE:HB	2.06	0.55
1:D:291:THR:HG22	1:D:292:THR:N	2.20	0.55
1:B:671:ARG:HH11	1:B:671:ARG:HG2	1.71	0.55
1:C:362:ASN:O	1:C:365:VAL:HG22	2.06	0.55
1:B:488:GLN:HB2	1:B:504:ARG:HB3	1.87	0.55
1:B:118:LEU:O	1:B:122:SER:HB2	2.05	0.55
1:C:634:TYR:CZ	1:C:638:LYS:HG2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:HG23	1:A:366:SER:N	2.21	0.55
1:C:624:PHE:CZ	1:C:680:ARG:NH2	2.73	0.55
1:B:55:ASN:HD21	1:B:58:LYS:HD3	1.71	0.55
1:D:472:THR:HA	1:D:475:ASP:OD2	2.06	0.55
1:D:422:GLU:HG2	1:D:619:VAL:HG11	1.87	0.55
1:B:567:ARG:HH11	1:B:567:ARG:HG2	1.71	0.55
1:C:31:ARG:NH1	1:C:36:ASN:HB3	2.21	0.55
1:B:211:GLN:NE2	1:B:211:GLN:H	2.04	0.55
1:A:17:ASN:CG	1:A:18:GLN:H	2.09	0.55
1:C:288:ARG:NH2	1:C:289:THR:OG1	2.39	0.55
1:B:498:ILE:HD12	1:B:504:ARG:HB2	1.88	0.55
1:C:448:ILE:O	1:C:448:ILE:HG12	2.06	0.55
1:C:670:ILE:HG22	1:C:671:ARG:H	1.71	0.55
1:D:567:ARG:HG2	1:D:567:ARG:HH11	1.70	0.55
1:A:419:LEU:HD13	1:A:438:TYR:HB2	1.88	0.55
1:C:679:ILE:HD12	1:C:685:LEU:HD21	1.88	0.55
1:B:533:SER:HA	1:B:536:GLN:HE21	1.72	0.55
1:B:675:THR:HG22	1:B:675:THR:O	2.05	0.55
1:A:150:LYS:HG3	1:A:155:ASP:HA	1.89	0.55
1:B:604:VAL:O	1:B:608:VAL:HG23	2.07	0.55
1:C:76:HIS:HD2	1:C:78:TYR:N	1.85	0.55
1:A:678:PHE:C	1:A:679:ILE:HD12	2.27	0.55
1:B:246:PHE:O	1:B:250:VAL:HG23	2.07	0.55
1:B:125:GLN:O	1:B:126:SER:C	2.45	0.55
1:D:635:ASN:HA	1:D:638:LYS:HD3	1.89	0.55
1:B:652:ALA:O	1:B:654:GLN:N	2.40	0.55
1:B:523:ASN:OD1	1:B:561:THR:HB	2.07	0.55
1:D:11:PRO:CA	1:D:31:ARG:HH21	2.14	0.55
1:D:434:LYS:O	1:D:436:ILE:HD12	2.07	0.55
1:A:213:LYS:NZ	1:A:264:ASN:HD21	2.04	0.55
1:D:150:LYS:HG3	1:D:155:ASP:HA	1.87	0.55
1:A:441:ASN:OD1	1:A:443:PRO:HD3	2.07	0.54
1:C:211:GLN:H	1:C:211:GLN:NE2	2.05	0.54
1:B:637:TYR:HE2	1:B:688:PHE:HB3	1.72	0.54
1:B:150:LYS:HG3	1:B:155:ASP:HA	1.88	0.54
1:B:680:ARG:HG2	1:B:681:ASN:OD1	2.07	0.54
1:A:442:LYS:HB2	1:A:442:LYS:HZ2	1.69	0.54
1:D:411:GLN:HG2	1:D:508:TYR:CD2	2.43	0.54
1:B:41:ILE:O	1:B:41:ILE:HG22	2.07	0.54
1:C:484:ASN:OD1	1:C:485:PRO:O	2.25	0.54
1:D:376:THR:HG22	1:D:377:GLU:N	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:HIS:HD2	1:B:78:TYR:N	1.86	0.54
1:B:12:ASP:OD1	1:B:14:VAL:HG23	2.08	0.54
1:D:436:ILE:HG12	1:D:618:ARG:HB3	1.89	0.54
1:A:634:TYR:O	1:A:638:LYS:HG3	2.06	0.54
1:D:489:SER:HA	1:D:498:ILE:HG21	1.89	0.54
1:A:211:GLN:NE2	1:A:211:GLN:H	2.06	0.54
1:C:434:LYS:H	1:C:434:LYS:HE3	1.71	0.54
1:C:375:THR:O	1:D:376:THR:OG1	2.17	0.54
1:A:459:LEU:HD13	1:A:523:ASN:ND2	2.23	0.54
1:B:272:ALA:O	1:B:276:ILE:HG13	2.07	0.54
1:B:276:ILE:HD13	1:B:352:LEU:HD13	1.90	0.54
1:B:192:ARG:HG3	1:B:232:SER:HB3	1.90	0.54
1:A:485:PRO:O	1:A:486:HIS:HB2	2.08	0.54
1:B:679:ILE:CG2	1:B:684:THR:HB	2.37	0.54
1:C:434:LYS:O	1:C:434:LYS:HD2	2.07	0.54
1:B:132:ILE:HA	1:B:135:MET:CE	2.38	0.54
1:C:557:LYS:HZ2	1:C:557:LYS:H	1.55	0.54
1:B:59:GLU:OE1	1:B:60:SER:N	2.41	0.54
1:C:322:TYR:CE2	1:C:339:PRO:HG3	2.43	0.54
1:C:376:THR:O	1:D:375:THR:HB	2.07	0.54
1:D:227:GLU:N	1:D:278:ASN:HD21	1.95	0.54
1:D:246:PHE:O	1:D:250:VAL:HG23	2.07	0.54
1:C:680:ARG:HH11	1:C:680:ARG:HG3	1.71	0.54
1:A:31:ARG:NH1	1:A:36:ASN:HB3	2.23	0.54
1:C:418:THR:CG2	1:C:616:ASN:ND2	2.67	0.54
1:D:634:TYR:CD2	1:D:634:TYR:C	2.81	0.54
1:A:472:THR:HA	1:A:475:ASP:OD2	2.08	0.54
1:C:21:GLU:O	1:C:25:ILE:HD13	2.08	0.54
1:D:498:ILE:HD12	1:D:504:ARG:HB2	1.90	0.53
1:C:620:ARG:HA	1:C:620:ARG:NE	2.23	0.53
1:D:22:ASN:O	1:D:26:GLU:HG3	2.08	0.53
1:C:95:GLN:HB2	1:C:382:ILE:HG12	1.90	0.53
1:B:434:LYS:O	1:B:434:LYS:HG2	2.06	0.53
1:A:486:HIS:O	1:A:505:LEU:HD12	2.08	0.53
1:C:452:PRO:O	1:C:453:ILE:HB	2.08	0.53
1:D:14:VAL:HG13	1:D:621:ARG:HA	1.90	0.53
1:A:627:ARG:HG2	1:A:627:ARG:O	2.08	0.53
1:A:629:GLU:HG2	1:A:676:LYS:HZ1	1.72	0.53
1:C:636:ARG:HD2	1:C:637:TYR:CE1	2.43	0.53
1:A:324:SER:HA	1:A:336:ILE:O	2.07	0.53
1:D:388:TYR:N	1:D:388:TYR:CD1	2.77	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LYS:CD	1:C:296:VAL:H	2.13	0.53
1:D:487:LEU:HD12	1:D:488:GLN:N	2.24	0.53
1:C:444:ILE:N	1:C:444:ILE:HD12	2.23	0.53
1:B:378:LYS:HG3	1:D:666:ASP:CG	2.28	0.53
1:C:542:LEU:O	1:C:545:GLY:N	2.41	0.53
1:C:272:ALA:O	1:C:276:ILE:HG13	2.09	0.53
1:D:41:ILE:O	1:D:41:ILE:HG22	2.07	0.53
1:A:589:LYS:N	1:A:607:GLN:HE22	1.99	0.53
1:C:498:ILE:HD12	1:C:504:ARG:HB2	1.89	0.53
1:C:182:TYR:OH	1:C:573:LEU:HD23	2.08	0.53
1:D:276:ILE:HD13	1:D:352:LEU:HD13	1.91	0.53
1:C:629:GLU:HA	1:C:675:THR:O	2.08	0.53
1:A:484:ASN:OD1	1:A:485:PRO:O	2.27	0.53
1:A:411:GLN:HG3	1:A:442:LYS:HE2	1.90	0.53
1:A:272:ALA:O	1:A:276:ILE:HG13	2.09	0.53
1:C:359:ARG:HB3	1:C:546:LEU:HD12	1.90	0.53
1:C:181:ASN:HD21	1:C:362:ASN:HD22	1.53	0.53
1:C:627:ARG:HG2	1:C:627:ARG:O	2.08	0.53
1:A:119:THR:CG2	1:A:119:THR:O	2.56	0.53
1:B:253:MET:HE1	1:B:267:TRP:CH2	2.44	0.53
1:D:192:ARG:NH2	1:D:228:TYR:O	2.42	0.53
1:C:88:MET:HG3	1:C:380:PRO:HB2	1.91	0.53
1:C:669:GLU:HA	1:C:669:GLU:OE1	2.09	0.53
1:D:442:LYS:HE3	1:D:446:GLU:OE2	2.09	0.53
1:B:204:GLN:HE22	1:B:245:GLU:HG2	1.73	0.53
1:B:489:SER:HA	1:B:498:ILE:HG21	1.90	0.53
1:B:9:GLY:HA3	1:B:31:ARG:HD3	1.91	0.53
1:D:19:ILE:CD1	1:D:618:ARG:HG2	2.38	0.53
1:D:448:ILE:O	1:D:455:LEU:HG	2.08	0.52
1:A:436:ILE:CD1	1:A:619:VAL:HA	2.37	0.52
1:C:459:LEU:HD11	1:C:523:ASN:HB2	1.92	0.52
1:D:572:ALA:O	1:D:576:THR:CG2	2.56	0.52
1:C:696:MET:HB2	1:C:697:PRO:C	2.29	0.52
1:C:11:PRO:CA	1:C:31:ARG:HH21	2.21	0.52
1:A:142:LEU:HD12	1:A:368:ILE:HD11	1.91	0.52
1:B:416:GLU:OE2	1:B:420:LYS:HD3	2.09	0.52
1:A:681:ASN:ND2	1:A:682:PRO:HD2	2.24	0.52
1:A:390:PHE:N	1:A:407:ASN:OD1	2.42	0.52
1:A:125:GLN:O	1:A:126:SER:C	2.47	0.52
1:C:246:PHE:O	1:C:250:VAL:HG23	2.08	0.52
1:B:636:ARG:HD3	1:B:636:ARG:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ALA:O	1:A:576:THR:CG2	2.53	0.52
1:C:603:ARG:NH1	1:C:603:ARG:HG3	2.24	0.52
1:D:441:ASN:C	1:D:443:PRO:HD3	2.30	0.52
1:C:589:LYS:N	1:C:607:GLN:HE22	2.00	0.52
1:B:459:LEU:HD13	1:B:523:ASN:ND2	2.24	0.52
1:B:154:ASN:HB3	1:B:157:SER:HB2	1.91	0.52
1:C:142:LEU:CD1	1:C:364:LEU:HD21	2.40	0.52
1:A:9:GLY:HA3	1:A:31:ARG:HD3	1.91	0.52
1:B:484:ASN:OD1	1:B:485:PRO:O	2.28	0.52
1:A:59:GLU:O	1:A:63:LYS:HG3	2.10	0.52
1:A:118:LEU:O	1:A:122:SER:HB2	2.10	0.52
1:B:185:GLU:OE1	1:B:188:ARG:NE	2.34	0.52
1:B:640:LEU:HD13	1:B:663:HIS:CD2	2.45	0.52
1:A:448:ILE:O	1:A:455:LEU:HG	2.09	0.52
1:B:408:GLU:HB3	1:B:446:GLU:OE2	2.09	0.52
1:B:378:LYS:CG	1:D:666:ASP:HB2	2.39	0.52
1:D:204:GLN:HE22	1:D:245:GLU:HG2	1.75	0.52
1:D:603:ARG:HG3	1:D:603:ARG:NH1	2.25	0.52
1:B:653:LYS:HE2	1:B:653:LYS:H	1.74	0.52
1:A:125:GLN:HE21	1:C:68:ARG:NE	2.03	0.52
1:A:125:GLN:CB	1:C:68:ARG:HH21	2.17	0.52
1:C:320:LEU:CD2	1:C:531:LEU:HD21	2.39	0.52
1:A:422:GLU:OE1	1:A:620:ARG:NH2	2.43	0.52
1:C:204:GLN:NE2	1:C:245:GLU:HG2	2.24	0.52
1:B:125:GLN:O	1:B:127:PRO:N	2.43	0.52
1:A:429:GLU:O	1:A:674:LYS:HG3	2.10	0.52
1:D:642:LYS:O	1:D:643:LYS:HB2	2.10	0.52
1:D:167:GLN:HE22	1:D:374:CYS:N	2.05	0.52
1:D:167:GLN:NE2	1:D:374:CYS:HB3	2.24	0.52
1:C:138:ASP:O	1:C:141:PRO:HD2	2.09	0.52
1:B:197:ARG:NH1	1:B:242:ASP:OD1	2.43	0.52
1:D:633:PHE:O	1:D:636:ARG:HB2	2.10	0.52
1:B:427:VAL:C	1:B:429:GLU:H	2.13	0.52
1:C:290:GLY:O	1:C:291:THR:HB	2.10	0.52
1:D:211:GLN:H	1:D:211:GLN:NE2	2.08	0.52
1:A:670:ILE:CG1	1:A:679:ILE:HG13	2.40	0.52
1:C:634:TYR:CE1	1:C:638:LYS:HG2	2.45	0.51
1:C:376:THR:HG21	1:D:370:THR:O	2.10	0.51
1:D:488:GLN:HB2	1:D:504:ARG:HB3	1.92	0.51
1:D:415:ILE:HD12	1:D:442:LYS:HD2	1.92	0.51
1:B:376:THR:HG22	1:B:377:GLU:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:NH1	1:B:36:ASN:HB3	2.23	0.51
1:A:119:THR:HG21	1:A:137:LEU:HD21	1.91	0.51
1:D:532:ILE:O	1:D:536:GLN:HG3	2.10	0.51
1:A:204:GLN:HE22	1:A:245:GLU:HG2	1.75	0.51
1:C:627:ARG:HA	1:C:677:VAL:O	2.11	0.51
1:C:22:ASN:OD1	1:C:605:ARG:NH1	2.40	0.51
1:A:54:LEU:O	1:A:56:ILE:N	2.43	0.51
1:C:572:ALA:O	1:C:576:THR:CG2	2.55	0.51
1:C:119:THR:HG21	1:C:137:LEU:HD21	1.93	0.51
1:D:197:ARG:NH1	1:D:242:ASP:OD1	2.44	0.51
1:B:670:ILE:HG23	1:B:678:PHE:O	2.10	0.51
1:D:390:PHE:N	1:D:407:ASN:OD1	2.43	0.51
1:B:490:TYR:O	1:B:494:LYS:HA	2.09	0.51
1:D:405:PHE:CE1	1:D:409:LYS:HD3	2.46	0.51
1:D:14:VAL:CG1	1:D:621:ARG:HA	2.40	0.51
1:A:415:ILE:HD12	1:A:442:LYS:HD2	1.93	0.51
1:B:671:ARG:NH1	1:B:671:ARG:HG2	2.26	0.51
1:D:125:GLN:O	1:D:126:SER:C	2.49	0.51
1:D:604:VAL:O	1:D:608:VAL:HG23	2.10	0.51
1:B:459:LEU:HD11	1:B:523:ASN:HB2	1.93	0.51
1:C:487:LEU:HD12	1:C:488:GLN:N	2.26	0.51
1:C:641:CYS:SG	1:C:644:THR:OG1	2.67	0.51
1:A:459:LEU:HD11	1:A:523:ASN:HB2	1.93	0.51
1:A:488:GLN:HB2	1:A:504:ARG:HB3	1.93	0.51
1:A:11:PRO:HA	1:A:31:ARG:NH2	2.19	0.51
1:D:490:TYR:O	1:D:494:LYS:HA	2.10	0.51
1:B:542:LEU:O	1:B:545:GLY:N	2.44	0.51
1:D:517:ARG:HB2	1:D:517:ARG:CZ	2.41	0.51
1:B:638:LYS:HD3	1:B:638:LYS:O	2.11	0.51
1:D:523:ASN:OD1	1:D:561:THR:HB	2.11	0.51
1:D:450:LYS:HB3	1:D:451:LYS:HD2	1.92	0.51
1:A:640:LEU:CD1	1:A:640:LEU:H	2.22	0.51
1:C:436:ILE:N	1:C:436:ILE:HD12	2.25	0.51
1:C:118:LEU:O	1:C:122:SER:HB2	2.10	0.51
1:A:267:TRP:HE3	1:A:267:TRP:HA	1.76	0.51
1:C:600:ASP:HB3	1:C:603:ARG:HB3	1.93	0.51
1:C:418:THR:HG21	1:C:616:ASN:ND2	2.23	0.51
1:A:641:CYS:CB	1:A:659:ILE:HG12	2.39	0.51
1:D:636:ARG:NH2	1:D:689:GLU:OE2	2.44	0.51
1:B:194:GLN:CD	1:B:194:GLN:H	2.03	0.51
1:B:426:TYR:HD2	1:B:433:TRP:CE3	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:O	1:B:63:LYS:HG3	2.12	0.51
1:A:427:VAL:HG23	1:A:428:ARG:N	2.26	0.51
1:B:659:ILE:O	1:B:663:HIS:HB2	2.11	0.50
1:C:441:ASN:C	1:C:443:PRO:CD	2.80	0.50
1:C:628:ILE:O	1:C:677:VAL:HG23	2.11	0.50
1:D:115:MET:CE	1:D:140:ASN:HD21	2.25	0.50
1:A:665:ILE:CD1	1:A:688:PHE:HZ	2.24	0.50
1:C:192:ARG:NH2	1:C:228:TYR:O	2.44	0.50
1:A:490:TYR:O	1:A:494:LYS:HA	2.10	0.50
1:B:572:ALA:O	1:B:576:THR:CG2	2.55	0.50
1:D:284:ALA:O	1:D:286:GLU:N	2.45	0.50
1:C:434:LYS:O	1:C:436:ILE:HD12	2.11	0.50
1:A:267:TRP:CE3	1:A:267:TRP:HA	2.46	0.50
1:B:142:LEU:HD12	1:B:368:ILE:HD11	1.93	0.50
1:A:194:GLN:H	1:A:194:GLN:CD	2.01	0.50
1:A:681:ASN:CG	1:A:682:PRO:HD2	2.32	0.50
1:C:150:LYS:HG3	1:C:155:ASP:HA	1.92	0.50
1:A:450:LYS:HB3	1:A:451:LYS:HD2	1.93	0.50
1:C:445:CYS:O	1:C:448:ILE:CG2	2.58	0.50
1:B:447:LEU:C	1:B:449:GLU:H	2.13	0.50
1:B:409:LYS:NZ	1:B:450:LYS:HD3	2.27	0.50
1:B:365:VAL:HG23	1:B:366:SER:N	2.26	0.50
1:D:192:ARG:CG	1:D:232:SER:HB3	2.42	0.50
1:A:446:GLU:O	1:A:449:GLU:N	2.45	0.50
1:D:636:ARG:O	1:D:692:ARG:NH1	2.44	0.50
1:A:310:LYS:HD2	1:A:540:ASP:HB2	1.93	0.50
1:B:452:PRO:O	1:B:453:ILE:CB	2.59	0.50
1:C:441:ASN:O	1:C:443:PRO:HD3	2.11	0.50
1:A:438:TYR:O	1:A:439:PHE:O	2.30	0.50
1:B:115:MET:CE	1:B:140:ASN:HD21	2.25	0.50
1:A:197:ARG:NH1	1:A:242:ASP:OD1	2.44	0.50
1:D:657:GLU:O	1:D:661:GLN:HG3	2.11	0.50
1:A:376:THR:HG22	1:A:377:GLU:N	2.26	0.50
1:A:498:ILE:HD12	1:A:504:ARG:HB2	1.93	0.50
1:A:504:ARG:HH11	1:A:504:ARG:HG2	1.77	0.50
1:D:661:GLN:C	1:D:663:HIS:H	2.15	0.50
1:C:125:GLN:O	1:C:126:SER:C	2.49	0.50
1:C:651:THR:HB	1:C:654:GLN:HB2	1.92	0.50
1:A:487:LEU:HD12	1:A:488:GLN:N	2.26	0.50
1:C:12:ASP:OD1	1:C:14:VAL:HG23	2.12	0.50
1:D:154:ASN:HD21	4:D:894:ADP:H5'2	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:ILE:O	1:C:536:GLN:HG3	2.12	0.50
1:A:428:ARG:HG2	1:A:428:ARG:HH11	1.77	0.50
1:C:490:TYR:O	1:C:494:LYS:HA	2.11	0.50
1:C:59:GLU:CD	1:C:60:SER:H	2.16	0.50
1:D:504:ARG:CD	1:D:511:ASP:HB3	2.42	0.50
1:D:31:ARG:NH1	1:D:36:ASN:HB3	2.27	0.50
1:A:440:ASN:HD22	1:A:442:LYS:HB3	1.76	0.50
1:B:682:PRO:C	1:B:684:THR:H	2.15	0.50
1:C:203:TYR:HD2	5:C:907:HOH:O	1.94	0.50
1:A:560:GLU:O	1:A:561:THR:O	2.30	0.50
1:C:37:ILE:HG12	1:C:50:PRO:HG3	1.94	0.49
1:B:221:PRO:O	1:B:222:ASN:HB2	2.12	0.49
1:A:532:ILE:O	1:A:536:GLN:HG3	2.12	0.49
1:A:19:ILE:HD12	1:A:621:ARG:HD2	1.92	0.49
1:A:452:PRO:O	1:A:453:ILE:CB	2.60	0.49
1:C:459:LEU:HD13	1:C:523:ASN:ND2	2.26	0.49
1:C:670:ILE:HG22	1:C:671:ARG:N	2.27	0.49
1:D:154:ASN:HB3	1:D:157:SER:HB2	1.93	0.49
1:D:420:LYS:HE2	1:D:424:GLU:OE1	2.12	0.49
1:C:55:ASN:ND2	1:C:58:LYS:HD3	2.28	0.49
1:C:284:ALA:O	1:C:286:GLU:N	2.45	0.49
1:B:42:GLY:O	1:B:43:ASP:HB2	2.12	0.49
1:A:66:ASN:HD22	1:A:67:GLY:N	2.09	0.49
1:D:37:ILE:HG12	1:D:50:PRO:HG3	1.93	0.49
1:C:443:PRO:HD2	1:C:444:ILE:HD12	1.93	0.49
1:A:58:LYS:HZ2	1:A:61:ASP:CG	2.15	0.49
1:A:125:GLN:HE21	1:C:68:ARG:HH21	1.60	0.49
1:D:447:LEU:C	1:D:449:GLU:H	2.16	0.49
1:D:452:PRO:O	1:D:453:ILE:CB	2.61	0.49
1:B:436:ILE:O	1:B:436:ILE:HG22	2.13	0.49
1:B:284:ALA:HB3	1:B:293:THR:O	2.13	0.49
1:C:388:TYR:N	1:C:388:TYR:CD1	2.79	0.49
1:A:660:LEU:HD22	1:A:665:ILE:HD12	1.93	0.49
1:D:208:GLY:HA3	1:D:246:PHE:CD2	2.47	0.49
1:A:284:ALA:O	1:A:286:GLU:N	2.45	0.49
1:A:655:ALA:O	1:A:656:THR:C	2.51	0.49
1:C:235:PHE:N	1:C:235:PHE:CD1	2.80	0.49
1:A:439:PHE:CE2	1:A:612:GLY:HA2	2.47	0.49
1:A:630:TYR:HE2	1:A:677:VAL:HG22	1.76	0.49
1:A:429:GLU:OE2	1:A:429:GLU:HA	2.13	0.49
1:D:310:LYS:HD2	1:D:540:ASP:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:642:LYS:CD	1:D:642:LYS:N	2.58	0.49
1:C:287:GLN:O	1:C:291:THR:O	2.30	0.49
1:D:420:LYS:HG2	1:D:424:GLU:OE1	2.13	0.49
1:B:59:GLU:CD	1:B:60:SER:H	2.16	0.49
1:B:192:ARG:NH2	1:B:228:TYR:O	2.46	0.49
1:B:73:MET:HB3	1:B:74:PRO:CD	2.42	0.49
1:C:489:SER:HA	1:C:498:ILE:HG21	1.94	0.49
1:D:288:ARG:NH2	1:D:289:THR:H	2.10	0.49
1:A:246:PHE:O	1:A:250:VAL:HG23	2.12	0.49
1:D:439:PHE:HD2	1:D:615:GLU:CD	2.16	0.49
1:B:635:ASN:ND2	1:B:636:ARG:N	2.48	0.49
1:B:473:PHE:O	1:B:477:ILE:HG13	2.12	0.49
1:C:445:CYS:C	1:C:448:ILE:HG22	2.33	0.49
1:A:192:ARG:NH2	1:A:228:TYR:O	2.46	0.49
1:D:603:ARG:HG3	1:D:603:ARG:HH11	1.77	0.49
1:C:125:GLN:O	1:C:127:PRO:N	2.45	0.49
1:D:630:TYR:CE2	1:D:653:LYS:HG3	2.48	0.49
1:A:453:ILE:HA	1:A:458:LEU:HD21	1.95	0.49
1:D:423:GLN:HE22	1:D:436:ILE:H	1.60	0.49
1:B:132:ILE:HA	1:B:135:MET:HE3	1.95	0.49
1:D:311:THR:HG22	1:D:538:SER:HA	1.94	0.49
1:B:627:ARG:HG2	1:B:676:LYS:CE	2.32	0.48
1:A:504:ARG:CD	1:A:511:ASP:HB3	2.42	0.48
1:A:637:TYR:CE2	1:A:688:PHE:HB3	2.48	0.48
1:C:309:LEU:HD13	1:C:535:MET:CE	2.43	0.48
1:D:267:TRP:HE3	1:D:267:TRP:HA	1.78	0.48
1:C:55:ASN:HD21	1:C:58:LYS:HD3	1.77	0.48
1:C:59:GLU:OE1	1:C:60:SER:N	2.46	0.48
1:B:340:MET:HB2	1:B:344:GLN:HB2	1.95	0.48
1:B:485:PRO:O	1:B:486:HIS:HB2	2.13	0.48
1:A:367:LYS:O	1:A:367:LYS:HD3	2.13	0.48
1:A:636:ARG:NH2	1:A:689:GLU:OE1	2.46	0.48
1:B:54:LEU:O	1:B:56:ILE:N	2.46	0.48
1:B:409:LYS:HA	1:B:446:GLU:OE1	2.13	0.48
1:B:362:ASN:O	1:B:365:VAL:HG22	2.13	0.48
1:C:659:ILE:O	1:C:663:HIS:HD2	1.96	0.48
1:D:118:LEU:O	1:D:122:SER:HB2	2.12	0.48
1:A:188:ARG:O	1:A:192:ARG:NH1	2.47	0.48
1:A:132:ILE:HA	1:A:135:MET:CE	2.44	0.48
1:A:523:ASN:OD1	1:A:561:THR:HB	2.13	0.48
1:B:310:LYS:HD2	1:B:540:ASP:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ALA:HB2	1:B:297:SER:OG	2.13	0.48
1:B:235:PHE:CD1	1:B:235:PHE:N	2.80	0.48
1:B:431:ILE:O	1:B:433:TRP:N	2.46	0.48
1:B:17:ASN:CG	1:B:18:GLN:N	2.66	0.48
1:B:311:THR:HG22	1:B:538:SER:CA	2.43	0.48
1:C:267:TRP:CE3	1:C:267:TRP:HA	2.48	0.48
1:C:186:LYS:NZ	1:C:358:GLU:OE2	2.42	0.48
1:D:473:PHE:O	1:D:477:ILE:HG13	2.14	0.48
1:B:687:TYR:CE1	1:B:691:LYS:HD3	2.48	0.48
1:C:417:LEU:HD12	1:C:584:TYR:HE2	1.78	0.48
1:B:460:ASP:O	1:B:463:CYS:HB2	2.13	0.48
1:C:614:LEU:HD12	1:C:614:LEU:O	2.13	0.48
1:D:459:LEU:HD13	1:D:523:ASN:ND2	2.28	0.48
1:B:37:ILE:HG12	1:B:50:PRO:HG3	1.94	0.48
1:A:489:SER:HA	1:A:498:ILE:HG21	1.95	0.48
1:B:504:ARG:CD	1:B:511:ASP:HB3	2.42	0.48
1:D:267:TRP:CE3	1:D:267:TRP:HA	2.48	0.48
1:B:267:TRP:CE3	1:B:267:TRP:HA	2.48	0.48
1:C:323:ARG:NH2	1:C:528:PHE:CE1	2.81	0.48
1:A:542:LEU:O	1:A:546:LEU:HD22	2.14	0.48
1:D:459:LEU:HD11	1:D:523:ASN:HB2	1.94	0.48
1:C:442:LYS:C	1:C:444:ILE:N	2.67	0.48
1:A:669:GLU:HG2	1:A:684:THR:HG21	1.96	0.48
1:B:684:THR:HG22	1:B:688:PHE:CE1	2.44	0.48
1:D:217:LEU:O	1:D:275:HIS:HE1	1.97	0.48
1:C:683:THR:HA	1:C:686:PHE:HD2	1.77	0.48
1:D:188:ARG:O	1:D:192:ARG:NH1	2.46	0.48
1:C:267:TRP:HA	1:C:267:TRP:HE3	1.78	0.48
1:C:414:PHE:CD2	1:C:586:ARG:CZ	2.97	0.48
1:A:642:LYS:HA	1:A:642:LYS:HE3	1.96	0.48
1:D:279:ILE:HG23	1:D:296:VAL:HG13	1.96	0.48
1:D:446:GLU:HB2	1:D:450:LYS:HE2	1.96	0.48
1:C:9:GLY:HA3	1:C:31:ARG:HD3	1.96	0.48
1:C:118:LEU:O	1:C:122:SER:CB	2.62	0.48
1:B:267:TRP:HE3	1:B:267:TRP:HA	1.78	0.48
1:A:154:ASN:HB3	1:A:157:SER:HB2	1.95	0.48
1:D:486:HIS:O	1:D:505:LEU:HD12	2.13	0.48
1:C:504:ARG:CD	1:C:511:ASP:HB3	2.43	0.48
1:B:211:GLN:CD	1:B:211:GLN:N	2.58	0.48
1:A:688:PHE:H	1:A:688:PHE:HD1	1.61	0.48
1:B:532:ILE:O	1:B:536:GLN:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:MET:HB2	1:D:344:GLN:HB2	1.96	0.48
1:C:442:LYS:O	1:C:446:GLU:HG2	2.13	0.48
1:C:167:GLN:HE22	1:C:374:CYS:N	2.09	0.48
1:B:208:GLY:HA3	1:B:246:PHE:CD2	2.49	0.48
1:B:284:ALA:O	1:B:286:GLU:N	2.47	0.48
1:A:542:LEU:O	1:A:545:GLY:N	2.47	0.48
1:B:603:ARG:NH1	1:B:603:ARG:HG3	2.28	0.48
1:A:37:ILE:HD11	1:A:54:LEU:CD2	2.34	0.47
1:B:453:ILE:HA	1:B:458:LEU:HD21	1.96	0.47
1:D:421:SER:HA	1:D:424:GLU:OE2	2.14	0.47
1:D:58:LYS:HZ2	1:D:61:ASP:CG	2.16	0.47
1:A:59:GLU:OE1	1:A:60:SER:N	2.47	0.47
1:C:192:ARG:CG	1:C:232:SER:HB3	2.43	0.47
1:B:653:LYS:O	1:B:655:ALA:N	2.47	0.47
1:C:276:ILE:HD13	1:C:352:LEU:HD13	1.95	0.47
1:A:600:ASP:HB3	1:A:603:ARG:HB3	1.97	0.47
1:D:453:ILE:HA	1:D:458:LEU:HD21	1.95	0.47
1:B:487:LEU:HD12	1:B:488:GLN:N	2.28	0.47
1:B:119:THR:O	1:B:119:THR:CG2	2.61	0.47
1:C:436:ILE:H	1:C:436:ILE:CD1	2.27	0.47
1:C:694:LEU:O	1:C:695:GLU:CB	2.63	0.47
1:C:181:ASN:ND2	1:C:362:ASN:ND2	2.52	0.47
1:D:625:ALA:HB1	1:D:682:PRO:HG3	1.96	0.47
1:D:692:ARG:NH1	1:D:692:ARG:HG3	2.26	0.47
1:C:460:ASP:O	1:C:463:CYS:HB2	2.14	0.47
1:C:411:GLN:HG2	1:C:508:TYR:CD2	2.49	0.47
1:A:208:GLY:HA3	1:A:246:PHE:CD2	2.49	0.47
1:D:201:ILE:HG23	1:D:202:PHE:N	2.30	0.47
1:B:204:GLN:NE2	1:B:245:GLU:HG2	2.29	0.47
1:C:603:ARG:HH11	1:C:603:ARG:HG3	1.78	0.47
1:B:600:ASP:HB3	1:B:603:ARG:HB3	1.97	0.47
1:A:603:ARG:HG3	1:A:603:ARG:NH1	2.30	0.47
1:C:517:ARG:HB2	1:C:517:ARG:CZ	2.44	0.47
1:D:235:PHE:CD1	1:D:235:PHE:N	2.83	0.47
1:D:185:GLU:HG2	1:D:185:GLU:O	2.14	0.47
1:C:288:ARG:N	1:C:288:ARG:CD	2.58	0.47
1:A:446:GLU:HB3	1:A:450:LYS:HE2	1.96	0.47
1:C:54:LEU:O	1:C:56:ILE:N	2.48	0.47
1:B:506:LYS:HD3	5:B:804:HOH:O	2.15	0.47
1:A:438:TYR:O	1:A:439:PHE:C	2.53	0.47
1:C:310:LYS:HD2	1:C:540:ASP:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LYS:O	1:A:424:GLU:HG3	2.15	0.47
1:D:132:ILE:HA	1:D:135:MET:CE	2.44	0.47
1:B:142:LEU:CD1	1:B:364:LEU:HD21	2.44	0.47
1:D:96:CYS:HA	1:D:383:GLY:O	2.14	0.47
1:D:109:GLU:O	1:D:113:LYS:HG2	2.14	0.47
1:B:71:TYR:C	1:B:71:TYR:CD1	2.88	0.47
1:A:460:ASP:O	1:A:463:CYS:HB2	2.15	0.47
1:D:59:GLU:OE1	1:D:60:SER:N	2.48	0.47
1:A:235:PHE:N	1:A:235:PHE:CD1	2.82	0.47
1:C:443:PRO:HD2	1:C:444:ILE:HD11	1.97	0.47
1:C:132:ILE:HD11	1:C:174:PRO:HB2	1.97	0.47
1:D:428:ARG:C	1:D:430:GLY:H	2.18	0.47
1:A:185:GLU:OE1	1:A:188:ARG:NE	2.41	0.47
1:A:409:LYS:HZ2	1:A:450:LYS:HD3	1.79	0.47
1:C:221:PRO:O	1:C:222:ASN:HB2	2.15	0.47
1:D:11:PRO:HA	1:D:31:ARG:NH2	2.22	0.46
1:B:470:ASP:HB3	1:B:516:VAL:HG12	1.96	0.46
1:A:217:LEU:O	1:A:275:HIS:HE1	1.98	0.46
1:B:217:LEU:O	1:B:275:HIS:HE1	1.98	0.46
1:A:37:ILE:HG12	1:A:50:PRO:HG3	1.97	0.46
1:A:443:PRO:O	1:A:447:LEU:HG	2.15	0.46
1:C:154:ASN:HB3	1:C:157:SER:HB2	1.96	0.46
1:C:430:GLY:O	1:C:431:ILE:HD13	2.14	0.46
1:A:517:ARG:CZ	1:A:517:ARG:HB2	2.46	0.46
1:D:118:LEU:O	1:D:122:SER:CB	2.63	0.46
1:A:25:ILE:HD12	1:A:25:ILE:N	2.30	0.46
1:A:142:LEU:CD1	1:A:364:LEU:HD21	2.45	0.46
1:A:17:ASN:CG	1:A:18:GLN:N	2.69	0.46
1:C:689:GLU:O	1:C:693:GLU:HG3	2.14	0.46
1:C:144:GLU:O	1:C:148:ASN:HB2	2.15	0.46
1:A:167:GLN:HE22	1:A:374:CYS:H	1.63	0.46
1:C:448:ILE:HD13	1:C:505:LEU:HD11	1.97	0.46
1:B:405:PHE:CE1	1:B:409:LYS:HD3	2.51	0.46
1:D:221:PRO:O	1:D:222:ASN:HB2	2.14	0.46
1:D:106:GLY:HA2	4:D:894:ADP:O1A	2.16	0.46
1:D:413:LEU:HD11	1:D:578:LEU:HD21	1.96	0.46
1:C:406:CYS:HA	1:C:570:MET:HE2	1.97	0.46
1:D:442:LYS:NZ	1:D:442:LYS:HB2	2.29	0.46
1:C:365:VAL:CG2	1:C:366:SER:N	2.78	0.46
1:D:142:LEU:HD12	1:D:368:ILE:HD11	1.96	0.46
1:D:634:TYR:O	1:D:638:LYS:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:ASP:HB3	1:D:603:ARG:HB3	1.98	0.46
1:C:340:MET:HB2	1:C:344:GLN:HB2	1.97	0.46
1:A:483:LYS:HD2	1:A:483:LYS:HA	1.76	0.46
1:B:411:GLN:HB3	1:B:442:LYS:HZ3	1.80	0.46
1:D:40:TYR:CE2	1:D:75:PRO:HA	2.50	0.46
1:A:639:MET:HG2	1:A:640:LEU:HD12	1.97	0.46
1:D:666:ASP:O	1:D:669:GLU:HB3	2.15	0.46
1:D:425:GLU:HA	1:D:428:ARG:CZ	2.45	0.46
1:C:17:ASN:CG	1:C:18:GLN:N	2.69	0.46
1:C:473:PHE:O	1:C:477:ILE:HG13	2.16	0.46
1:B:40:TYR:CE2	1:B:75:PRO:HA	2.50	0.46
1:B:92:GLN:NE2	1:D:687:TYR:CE1	2.83	0.46
1:A:630:TYR:CD1	1:A:675:THR:HA	2.50	0.46
1:D:125:GLN:O	1:D:127:PRO:N	2.49	0.46
1:C:604:VAL:O	1:C:608:VAL:HG23	2.16	0.46
1:C:71:TYR:C	1:C:71:TYR:CD1	2.89	0.46
1:B:388:TYR:N	1:B:388:TYR:CD1	2.77	0.46
1:B:655:ALA:O	1:B:659:ILE:HG13	2.16	0.46
1:B:37:ILE:HG22	1:B:48:THR:H	1.80	0.46
1:C:367:LYS:HD3	1:C:367:LYS:O	2.16	0.46
1:A:362:ASN:O	1:A:365:VAL:HG22	2.16	0.46
1:A:249:ILE:O	1:A:253:MET:HG2	2.15	0.46
1:B:128:ASN:OD1	1:D:73:MET:HA	2.15	0.46
1:B:603:ARG:HH11	1:B:603:ARG:HG3	1.81	0.46
1:D:123:SER:O	1:D:124:ASN:CG	2.53	0.46
1:D:486:HIS:O	1:D:505:LEU:HA	2.16	0.46
1:D:681:ASN:HD22	1:D:681:ASN:HA	1.62	0.46
1:D:12:ASP:OD1	1:D:14:VAL:HG23	2.15	0.46
1:D:73:MET:HB3	1:D:74:PRO:CD	2.45	0.46
1:C:542:LEU:O	1:C:543:VAL:C	2.52	0.46
1:A:204:GLN:NE2	1:A:245:GLU:HG2	2.31	0.46
1:A:340:MET:HB2	1:A:344:GLN:HB2	1.97	0.46
1:C:653:LYS:NZ	1:C:653:LYS:HB2	2.31	0.46
1:B:660:LEU:HD23	1:B:665:ILE:HB	1.97	0.46
1:A:473:PHE:O	1:A:477:ILE:HG13	2.15	0.46
1:C:615:GLU:OE2	1:C:615:GLU:N	2.36	0.46
1:C:453:ILE:HA	1:C:458:LEU:HD21	1.96	0.46
1:B:423:GLN:NE2	1:B:436:ILE:H	2.10	0.46
1:D:427:VAL:HG23	1:D:428:ARG:N	2.30	0.46
1:A:132:ILE:HD11	1:A:174:PRO:HB2	1.98	0.46
1:B:58:LYS:HB3	1:B:59:GLU:OE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ASN:CG	1:D:18:GLN:N	2.69	0.46
1:C:376:THR:HA	1:D:374:CYS:HA	1.98	0.45
1:B:653:LYS:HG2	1:B:654:GLN:NE2	2.31	0.45
1:D:287:GLN:HB2	1:D:292:THR:HA	1.97	0.45
1:A:642:LYS:O	1:A:643:LYS:HB2	2.16	0.45
1:C:19:ILE:HD11	1:C:618:ARG:HG2	1.99	0.45
1:A:12:ASP:OD1	1:A:14:VAL:HG23	2.16	0.45
1:A:625:ALA:HB3	1:A:679:ILE:O	2.16	0.45
1:A:197:ARG:HG2	1:A:203:TYR:CE1	2.51	0.45
1:A:211:GLN:CD	1:A:211:GLN:N	2.62	0.45
1:B:438:TYR:O	1:B:439:PHE:C	2.54	0.45
1:D:59:GLU:O	1:D:63:LYS:HG3	2.17	0.45
1:B:18:GLN:HG2	1:B:20:THR:HG23	1.97	0.45
1:A:685:LEU:HD23	1:A:685:LEU:O	2.16	0.45
1:A:118:LEU:O	1:A:122:SER:CB	2.65	0.45
1:A:304:ALA:O	1:A:307:SER:HB3	2.16	0.45
1:B:123:SER:O	1:B:124:ASN:CG	2.55	0.45
1:B:659:ILE:O	1:B:659:ILE:HG22	2.17	0.45
1:C:452:PRO:O	1:C:453:ILE:CB	2.64	0.45
1:B:481:PHE:CB	1:B:487:LEU:HD23	2.47	0.45
1:A:670:ILE:HG13	1:A:679:ILE:HG13	1.99	0.45
1:C:132:ILE:HA	1:C:135:MET:CE	2.46	0.45
1:A:221:PRO:O	1:A:222:ASN:HB2	2.15	0.45
1:A:427:VAL:CG2	1:A:428:ARG:N	2.80	0.45
1:A:322:TYR:CE2	1:A:339:PRO:HG3	2.51	0.45
1:C:524:LYS:NZ	5:C:911:HOH:O	2.48	0.45
1:D:193:THR:O	1:D:196:GLU:HB2	2.16	0.45
1:C:211:GLN:CD	1:C:211:GLN:N	2.63	0.45
1:C:309:LEU:O	1:C:538:SER:OG	2.23	0.45
1:C:58:LYS:HB3	1:C:59:GLU:OE2	2.15	0.45
1:A:94:ASN:ND2	1:A:381:VAL:H	2.14	0.45
1:C:635:ASN:CA	1:C:638:LYS:HD2	2.21	0.45
1:A:125:GLN:O	1:A:127:PRO:N	2.50	0.45
1:A:405:PHE:CE1	1:A:409:LYS:HD3	2.52	0.45
1:B:367:LYS:HD3	1:B:367:LYS:O	2.16	0.45
1:C:447:LEU:C	1:C:449:GLU:N	2.70	0.45
1:B:690:GLU:O	1:B:691:LYS:HD2	2.17	0.45
1:B:154:ASN:HD21	4:B:794:ADP:H5'2	1.81	0.45
1:C:433:TRP:HZ3	1:C:622:ALA:C	2.20	0.45
1:D:359:ARG:HB3	1:D:546:LEU:HD12	1.99	0.45
1:B:680:ARG:HG3	1:B:680:ARG:HH11	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LYS:HZ2	1:C:61:ASP:CG	2.20	0.45
1:B:624:PHE:O	1:B:626:GLY:N	2.48	0.45
1:C:217:LEU:O	1:C:275:HIS:HE1	1.98	0.45
1:C:201:ILE:HG23	1:C:202:PHE:N	2.30	0.45
1:D:367:LYS:HD3	1:D:367:LYS:O	2.16	0.45
1:B:138:ASP:O	1:B:141:PRO:HD2	2.17	0.45
1:A:670:ILE:HG13	1:A:678:PHE:O	2.17	0.45
1:A:18:GLN:HG2	1:A:20:THR:HG23	1.99	0.45
1:A:213:LYS:HZ2	1:A:264:ASN:HD21	1.65	0.45
1:B:297:SER:O	1:B:299:THR:HG23	2.16	0.45
1:D:391:GLU:HA	5:D:897:HOH:O	2.17	0.45
1:D:483:LYS:HA	1:D:483:LYS:HD2	1.72	0.45
1:C:409:LYS:HD2	1:C:446:GLU:OE2	2.17	0.45
1:B:607:GLN:HA	1:B:610:TYR:CE2	2.52	0.45
1:A:442:LYS:C	1:A:444:ILE:H	2.18	0.45
1:D:119:THR:O	1:D:119:THR:CG2	2.60	0.45
1:D:132:ILE:HD11	1:D:174:PRO:HB2	1.98	0.45
1:D:25:ILE:N	1:D:25:ILE:HD12	2.31	0.45
1:B:73:MET:HB3	1:B:74:PRO:HD2	1.99	0.45
1:C:427:VAL:HG23	1:C:428:ARG:N	2.32	0.45
1:B:517:ARG:CZ	1:B:517:ARG:HB2	2.46	0.45
1:A:98:ILE:HD11	1:A:584:TYR:HD2	1.82	0.45
1:B:409:LYS:HZ2	1:B:450:LYS:CD	2.26	0.45
1:B:589:LYS:N	1:B:607:GLN:HE22	2.03	0.45
1:C:551:ARG:HD2	1:C:551:ARG:O	2.17	0.45
1:D:439:PHE:CD1	1:D:440:ASN:N	2.85	0.45
1:A:192:ARG:CG	1:A:232:SER:HB3	2.47	0.45
1:D:272:ALA:O	1:D:276:ILE:HG13	2.17	0.45
1:C:96:CYS:SG	1:C:580:CYS:HB2	2.57	0.45
1:C:42:GLY:O	1:C:43:ASP:HB2	2.15	0.45
1:A:42:GLY:O	1:A:43:ASP:HB2	2.15	0.45
1:C:73:MET:HB3	1:C:74:PRO:CD	2.47	0.45
1:D:449:GLU:HB3	1:D:455:LEU:HB2	1.99	0.45
1:C:488:GLN:OE1	1:C:504:ARG:NH1	2.50	0.45
1:C:40:TYR:CE2	1:C:75:PRO:HA	2.51	0.45
1:B:157:SER:N	5:B:796:HOH:O	2.49	0.45
1:A:297:SER:O	1:A:299:THR:N	2.46	0.45
1:C:657:GLU:O	1:C:661:GLN:HG2	2.17	0.45
1:B:635:ASN:HD22	1:B:635:ASN:H	1.64	0.44
1:A:419:LEU:HD13	1:A:438:TYR:HB3	1.99	0.44
1:D:132:ILE:HA	1:D:135:MET:HE3	1.97	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:PHE:HE2	1:D:612:GLY:HA3	1.81	0.44
1:B:426:TYR:O	1:B:431:ILE:HB	2.17	0.44
1:C:624:PHE:CE2	1:C:680:ARG:NH2	2.85	0.44
1:C:188:ARG:O	1:C:192:ARG:NH1	2.50	0.44
1:D:488:GLN:OE1	1:D:504:ARG:NH1	2.51	0.44
1:C:322:TYR:HE2	1:C:339:PRO:HG3	1.82	0.44
1:A:542:LEU:HG	1:A:546:LEU:HD21	1.98	0.44
1:C:335:VAL:HG22	1:C:335:VAL:O	2.17	0.44
1:C:607:GLN:HA	1:C:610:TYR:CE2	2.52	0.44
1:C:408:GLU:OE2	1:C:442:LYS:NZ	2.49	0.44
1:C:167:GLN:HE22	1:C:374:CYS:HB3	1.79	0.44
1:A:680:ARG:NH1	1:A:680:ARG:HB2	2.33	0.44
1:B:213:LYS:HZ1	1:B:264:ASN:HD21	1.64	0.44
1:B:662:GLN:C	1:B:664:ASN:N	2.69	0.44
1:A:614:LEU:C	1:A:616:ASN:H	2.20	0.44
1:A:152:LEU:HG	1:A:196:GLU:HG3	1.99	0.44
1:D:460:ASP:O	1:D:463:CYS:HB2	2.17	0.44
1:A:279:ILE:HD13	1:A:302:LEU:HD23	1.99	0.44
1:D:451:LYS:CB	1:D:452:PRO:CD	2.90	0.44
1:D:37:ILE:HG22	1:D:48:THR:H	1.83	0.44
1:C:523:ASN:OD1	1:C:561:THR:HB	2.16	0.44
1:C:447:LEU:C	1:C:449:GLU:H	2.20	0.44
1:A:439:PHE:CE2	1:A:609:ARG:O	2.70	0.44
1:A:40:TYR:CE2	1:A:75:PRO:HA	2.52	0.44
1:D:364:LEU:O	1:D:368:ILE:HG13	2.17	0.44
1:D:381:VAL:HG12	1:D:382:ILE:N	2.32	0.44
1:A:413:LEU:HD11	1:A:578:LEU:HD21	1.98	0.44
1:A:388:TYR:CD1	1:A:388:TYR:N	2.77	0.44
1:B:49:ASN:HA	1:B:50:PRO:HD3	1.83	0.44
1:B:118:LEU:O	1:B:122:SER:CB	2.66	0.44
1:D:185:GLU:HG3	1:D:399:GLU:HG2	2.00	0.44
1:A:123:SER:O	1:A:124:ASN:CG	2.56	0.44
1:A:37:ILE:HG22	1:A:48:THR:H	1.82	0.44
1:C:441:ASN:CB	1:C:443:PRO:HD3	2.48	0.44
1:C:441:ASN:CG	1:C:443:PRO:HD3	2.38	0.44
1:A:441:ASN:C	1:A:442:LYS:HG3	2.38	0.44
1:D:428:ARG:HG2	1:D:428:ARG:HH11	1.82	0.44
1:D:194:GLN:H	1:D:194:GLN:CD	2.07	0.44
1:B:25:ILE:HD12	1:B:25:ILE:N	2.33	0.44
1:C:208:GLY:HA3	1:C:246:PHE:CD2	2.53	0.44
1:B:324:SER:HA	1:B:336:ILE:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TYR:CD1	1:A:71:TYR:C	2.91	0.44
1:B:635:ASN:ND2	1:B:635:ASN:H	2.16	0.44
1:D:409:LYS:HZ2	1:D:450:LYS:HD3	1.83	0.44
1:D:443:PRO:HA	1:D:446:GLU:CG	2.47	0.44
1:C:540:ASP:OD2	1:C:541:PRO:HD2	2.17	0.44
1:C:213:LYS:HZ2	1:C:264:ASN:HD21	1.64	0.44
1:A:683:THR:O	1:A:685:LEU:N	2.50	0.44
1:B:297:SER:O	1:B:299:THR:N	2.48	0.44
1:C:19:ILE:CD1	1:C:618:ARG:HG2	2.48	0.44
1:B:381:VAL:HG12	1:B:382:ILE:N	2.33	0.44
1:B:640:LEU:HD22	1:B:663:HIS:NE2	2.33	0.44
1:B:441:ASN:OD1	1:B:443:PRO:HD3	2.18	0.44
1:B:418:THR:CG2	1:B:419:LEU:HG	2.44	0.44
1:A:688:PHE:CD1	1:A:688:PHE:N	2.86	0.44
1:D:204:GLN:OE1	1:D:249:ILE:HD11	2.17	0.44
1:A:630:TYR:CD1	1:A:653:LYS:HB3	2.53	0.44
1:C:59:GLU:CD	1:C:60:SER:N	2.71	0.44
1:D:71:TYR:C	1:D:71:TYR:CD1	2.92	0.44
1:A:311:THR:HG22	1:A:538:SER:HA	2.00	0.44
1:B:627:ARG:HB2	1:B:677:VAL:O	2.18	0.44
1:D:204:GLN:NE2	1:D:245:GLU:HG2	2.32	0.44
1:A:427:VAL:O	1:A:430:GLY:N	2.51	0.44
1:A:470:ASP:HB3	1:A:516:VAL:HG12	2.00	0.44
1:B:496:ARG:NE	1:B:496:ARG:HA	2.33	0.44
1:C:185:GLU:O	1:C:185:GLU:HG2	2.18	0.44
1:C:633:PHE:CD2	1:C:633:PHE:C	2.90	0.43
1:B:663:HIS:C	1:B:665:ILE:H	2.21	0.43
1:D:485:PRO:O	1:D:486:HIS:CB	2.66	0.43
1:B:459:LEU:HB2	1:B:473:PHE:CZ	2.52	0.43
1:D:286:GLU:O	1:D:288:ARG:NE	2.50	0.43
1:C:115:MET:CE	1:C:140:ASN:HD21	2.31	0.43
1:A:115:MET:CE	1:A:140:ASN:HD21	2.31	0.43
1:B:427:VAL:HG23	1:B:428:ARG:N	2.32	0.43
1:A:603:ARG:HG3	1:A:603:ARG:HH11	1.83	0.43
1:B:201:ILE:HG23	1:B:202:PHE:N	2.33	0.43
1:C:665:ILE:O	1:C:666:ASP:C	2.56	0.43
1:A:37:ILE:HG13	1:A:37:ILE:H	1.55	0.43
1:D:441:ASN:OD1	1:D:443:PRO:HD3	2.18	0.43
1:C:181:ASN:OD1	1:C:365:VAL:HG21	2.18	0.43
1:C:415:ILE:HD11	1:C:439:PHE:CZ	2.53	0.43
1:D:625:ALA:HB3	1:D:681:ASN:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:LEU:HD22	1:C:573:LEU:O	2.17	0.43
1:C:447:LEU:O	1:C:449:GLU:N	2.51	0.43
1:A:442:LYS:C	1:A:444:ILE:N	2.71	0.43
1:B:80:LEU:HA	1:B:80:LEU:HD22	1.79	0.43
1:B:378:LYS:HD2	1:D:666:ASP:HB2	1.98	0.43
1:A:163:TYR:HE2	1:A:165:GLU:OE1	2.01	0.43
1:D:437:GLU:O	1:D:437:GLU:HG3	2.18	0.43
1:C:37:ILE:H	1:C:37:ILE:HG13	1.60	0.43
1:C:542:LEU:O	1:C:546:LEU:HD22	2.18	0.43
1:D:516:VAL:O	1:D:516:VAL:HG12	2.18	0.43
1:A:406:CYS:SG	1:A:570:MET:CE	3.06	0.43
1:C:633:PHE:HD2	1:C:634:TYR:N	2.17	0.43
1:D:423:GLN:NE2	1:D:436:ILE:H	2.15	0.43
1:B:127:PRO:HD2	1:D:73:MET:HG2	2.00	0.43
1:B:185:GLU:HG3	1:B:399:GLU:HG2	2.00	0.43
1:A:488:GLN:OE1	1:A:504:ARG:NH1	2.51	0.43
1:D:624:PHE:CZ	1:D:680:ARG:NH2	2.87	0.43
1:C:405:PHE:O	1:C:408:GLU:HB2	2.17	0.43
1:C:443:PRO:HA	1:C:446:GLU:HG3	2.00	0.43
1:A:59:GLU:CD	1:A:60:SER:H	2.22	0.43
1:A:185:GLU:HG3	1:A:399:GLU:HG2	1.99	0.43
1:C:486:HIS:O	1:C:505:LEU:HA	2.19	0.43
1:C:696:MET:N	1:C:697:PRO:HA	2.23	0.43
1:B:197:ARG:HG2	1:B:203:TYR:CE1	2.53	0.43
1:D:542:LEU:O	1:D:543:VAL:C	2.57	0.43
1:A:322:TYR:O	1:A:340:MET:HE2	2.19	0.43
1:C:287:GLN:HB2	1:C:292:THR:HA	1.99	0.43
1:C:66:ASN:HA	1:C:82:ASN:ND2	2.33	0.43
1:A:485:PRO:O	1:A:486:HIS:CB	2.66	0.43
1:B:560:GLU:O	1:B:561:THR:O	2.36	0.43
1:D:681:ASN:HA	1:D:682:PRO:HD3	1.88	0.43
1:D:211:GLN:N	1:D:211:GLN:CD	2.61	0.43
1:D:297:SER:O	1:D:299:THR:N	2.50	0.43
1:B:185:GLU:O	1:B:185:GLU:HG2	2.17	0.43
1:B:188:ARG:O	1:B:192:ARG:NH1	2.51	0.43
1:B:542:LEU:O	1:B:546:LEU:HD22	2.19	0.43
1:B:227:GLU:N	1:B:278:ASN:HD21	2.00	0.43
1:D:14:VAL:CG1	1:D:621:ARG:HG3	2.48	0.43
1:A:445:CYS:O	1:A:448:ILE:HG22	2.19	0.43
1:C:431:ILE:HG22	1:C:432:GLU:N	2.34	0.43
1:C:163:TYR:HE2	1:C:165:GLU:OE1	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:GLN:OE1	1:B:504:ARG:NH1	2.52	0.43
1:C:106:GLY:HA2	4:C:891:ADP:O1A	2.18	0.43
1:C:59:GLU:O	1:C:63:LYS:HG3	2.18	0.43
1:B:66:ASN:HD22	1:B:67:GLY:H	1.65	0.43
1:A:441:ASN:O	1:A:443:PRO:CD	2.66	0.43
1:B:249:ILE:O	1:B:253:MET:HG2	2.19	0.43
1:C:204:GLN:OE1	1:C:249:ILE:HD11	2.19	0.43
1:B:542:LEU:HG	1:B:546:LEU:HD21	2.01	0.43
1:B:77:MET:HE2	1:B:77:MET:O	2.19	0.43
1:C:633:PHE:O	1:C:634:TYR:C	2.57	0.42
1:C:37:ILE:HG22	1:C:48:THR:H	1.83	0.42
1:B:411:GLN:CG	1:B:442:LYS:HZ2	2.32	0.42
1:C:685:LEU:O	1:C:687:TYR:N	2.52	0.42
1:C:390:PHE:N	1:C:407:ASN:OD1	2.51	0.42
1:D:77:MET:HA	1:D:77:MET:HE3	2.01	0.42
1:B:441:ASN:C	1:B:443:PRO:HD3	2.40	0.42
1:C:311:THR:HG22	1:C:538:SER:N	2.35	0.42
1:B:59:GLU:CD	1:B:60:SER:N	2.72	0.42
1:C:123:SER:O	1:C:124:ASN:CG	2.57	0.42
1:B:144:GLU:O	1:B:148:ASN:HB2	2.19	0.42
1:B:31:ARG:HB3	1:B:31:ARG:NH1	2.23	0.42
1:C:694:LEU:N	1:C:694:LEU:HD22	2.34	0.42
1:B:669:GLU:CG	1:B:670:ILE:HD12	2.50	0.42
1:C:25:ILE:HD12	1:C:25:ILE:N	2.33	0.42
1:B:66:ASN:HA	1:B:82:ASN:ND2	2.35	0.42
1:D:365:VAL:CG2	1:D:366:SER:N	2.83	0.42
1:D:428:ARG:C	1:D:430:GLY:N	2.73	0.42
1:B:132:ILE:HD11	1:B:174:PRO:HB2	2.01	0.42
1:B:192:ARG:CG	1:B:232:SER:HB3	2.49	0.42
1:B:322:TYR:CE2	1:B:339:PRO:HG3	2.54	0.42
1:B:516:VAL:HG12	1:B:516:VAL:O	2.19	0.42
1:D:103:SER:HA	3:D:895:VO4:O2	2.19	0.42
1:A:496:ARG:HA	1:A:496:ARG:NE	2.35	0.42
1:D:42:GLY:O	1:D:43:ASP:HB2	2.18	0.42
1:C:459:LEU:HB2	1:C:473:PHE:CZ	2.55	0.42
1:D:59:GLU:CD	1:D:60:SER:H	2.22	0.42
1:B:542:LEU:O	1:B:543:VAL:C	2.58	0.42
1:D:431:ILE:O	1:D:432:GLU:C	2.56	0.42
1:A:636:ARG:HG3	1:A:637:TYR:CE1	2.53	0.42
1:C:641:CYS:HB2	1:C:659:ILE:HG12	2.02	0.42
1:A:627:ARG:HH11	1:A:627:ARG:HG3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLN:HB3	1:B:125:GLN:HE21	1.67	0.42
1:D:470:ASP:HB3	1:D:516:VAL:HG12	2.01	0.42
1:C:210:SER:C	1:C:212:SER:N	2.73	0.42
1:D:98:ILE:HD11	1:D:584:TYR:HD2	1.85	0.42
1:A:125:GLN:HE21	1:C:68:ARG:NH2	2.18	0.42
1:A:125:GLN:CB	1:C:68:ARG:NH2	2.68	0.42
1:B:405:PHE:O	1:B:408:GLU:HB2	2.20	0.42
1:D:223:ALA:N	1:D:224:PRO:CD	2.83	0.42
1:C:692:ARG:O	1:C:695:GLU:HG3	2.19	0.42
1:A:297:SER:O	1:A:299:THR:HG23	2.19	0.42
1:A:132:ILE:HA	1:A:135:MET:HE2	2.00	0.42
1:A:657:GLU:HG2	1:A:661:GLN:OE1	2.20	0.42
1:D:362:ASN:O	1:D:365:VAL:HG22	2.20	0.42
1:B:140:ASN:CB	1:B:141:PRO:HD3	2.50	0.42
1:D:659:ILE:O	1:D:659:ILE:HG22	2.20	0.42
1:A:58:LYS:O	1:A:61:ASP:N	2.53	0.42
1:C:681:ASN:HA	1:C:682:PRO:HD3	1.75	0.42
1:A:663:HIS:CE1	1:A:687:TYR:HE2	2.38	0.42
1:C:516:VAL:HG12	1:C:516:VAL:O	2.19	0.42
1:B:630:TYR:CD2	1:B:677:VAL:HG22	2.54	0.42
1:D:445:CYS:O	1:D:448:ILE:HG22	2.19	0.42
1:D:670:ILE:HD11	1:D:677:VAL:HG21	2.02	0.42
1:C:197:ARG:HG2	1:C:203:TYR:CE1	2.53	0.42
1:A:429:GLU:OE2	1:A:674:LYS:HB2	2.19	0.42
1:A:275:HIS:CE1	1:A:304:ALA:HB1	2.55	0.42
1:A:381:VAL:HG12	1:A:382:ILE:N	2.34	0.42
1:D:642:LYS:O	1:D:643:LYS:CB	2.68	0.42
1:B:639:MET:N	1:B:639:MET:SD	2.83	0.42
1:C:73:MET:HB3	1:C:74:PRO:HD2	2.01	0.42
1:A:66:ASN:HA	1:A:82:ASN:ND2	2.35	0.42
1:B:119:THR:OG1	1:B:133:SER:HB3	2.19	0.42
1:D:439:PHE:CE2	1:D:612:GLY:CA	3.02	0.42
1:B:21:GLU:HB2	1:B:614:LEU:HD22	2.02	0.42
1:D:542:LEU:O	1:D:546:LEU:HD22	2.20	0.42
1:C:88:MET:CG	1:C:380:PRO:HB2	2.49	0.42
1:B:323:ARG:HB3	1:B:324:SER:H	1.62	0.42
1:B:413:LEU:HD11	1:B:578:LEU:HD21	2.02	0.42
1:A:397:SER:OG	1:A:398:PHE:N	2.51	0.42
1:D:161:GLY:HA3	1:D:182:TYR:HB2	2.02	0.42
1:B:660:LEU:C	1:B:660:LEU:HD23	2.40	0.41
1:A:486:HIS:O	1:A:505:LEU:HA	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ASP:HA	1:B:40:TYR:C	2.39	0.41
1:A:660:LEU:HD22	1:A:665:ILE:CD1	2.50	0.41
1:A:223:ALA:N	1:A:224:PRO:CD	2.82	0.41
1:C:496:ARG:HA	1:C:496:ARG:NE	2.35	0.41
1:A:467:LYS:HE2	1:A:467:LYS:HA	2.02	0.41
1:B:444:ILE:C	1:B:446:GLU:N	2.72	0.41
1:A:668:GLU:O	1:A:680:ARG:NH1	2.53	0.41
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.34	0.41
1:C:557:LYS:N	1:C:557:LYS:HD3	2.35	0.41
1:D:152:LEU:HG	1:D:196:GLU:HG3	2.01	0.41
1:B:77:MET:HE3	1:B:77:MET:HA	2.02	0.41
1:B:11:PRO:HA	1:B:31:ARG:NH2	2.25	0.41
1:D:288:ARG:N	1:D:288:ARG:NE	2.67	0.41
1:D:288:ARG:CZ	1:D:289:THR:H	2.33	0.41
1:C:418:THR:HG23	1:C:419:LEU:HG	2.02	0.41
1:B:154:ASN:CG	1:B:157:SER:H	2.24	0.41
1:A:614:LEU:HD12	1:A:614:LEU:HA	1.78	0.41
1:D:459:LEU:HB2	1:D:473:PHE:CZ	2.55	0.41
1:D:481:PHE:CB	1:D:487:LEU:HD23	2.50	0.41
1:D:279:ILE:CD1	1:D:302:LEU:HD23	2.50	0.41
1:D:408:GLU:OE2	1:D:442:LYS:NZ	2.53	0.41
1:D:636:ARG:NH2	1:D:637:TYR:CE2	2.89	0.41
1:D:156:ASN:ND2	4:D:894:ADP:O3'	2.49	0.41
1:B:427:VAL:C	1:B:429:GLU:N	2.73	0.41
1:C:557:LYS:NZ	1:C:557:LYS:HB2	2.35	0.41
1:C:58:LYS:O	1:C:61:ASP:N	2.54	0.41
1:A:73:MET:HB3	1:A:74:PRO:CD	2.51	0.41
1:B:639:MET:O	1:B:640:LEU:CG	2.59	0.41
1:D:405:PHE:O	1:D:408:GLU:HB2	2.21	0.41
1:B:620:ARG:HE	1:B:620:ARG:HA	1.78	0.41
1:A:138:ASP:O	1:A:141:PRO:HD2	2.20	0.41
1:C:567:ARG:HG2	1:C:567:ARG:NH1	2.34	0.41
1:C:323:ARG:HB3	1:C:324:SER:H	1.65	0.41
1:C:434:LYS:H	1:C:434:LYS:CD	2.33	0.41
1:B:373:ASN:HD22	1:B:374:CYS:N	2.19	0.41
1:A:322:TYR:C	1:A:340:MET:HE2	2.40	0.41
1:A:210:SER:C	1:A:212:SER:N	2.74	0.41
1:C:109:GLU:O	1:C:113:LYS:HG2	2.21	0.41
1:D:66:ASN:HA	1:D:82:ASN:ND2	2.35	0.41
1:C:412:GLN:OE1	1:C:442:LYS:HD3	2.21	0.41
1:C:249:ILE:O	1:C:253:MET:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:LEU:HG	1:D:546:LEU:HD21	2.02	0.41
1:B:98:ILE:HD11	1:B:584:TYR:HD2	1.86	0.41
1:C:152:LEU:HG	1:C:196:GLU:HG3	2.02	0.41
1:A:586:ARG:NH1	5:A:793:HOH:O	2.53	0.41
1:D:496:ARG:NE	1:D:496:ARG:HA	2.36	0.41
1:B:335:VAL:O	1:B:335:VAL:HG22	2.20	0.41
1:B:663:HIS:ND1	1:B:663:HIS:O	2.48	0.41
1:C:66:ASN:HD22	1:C:67:GLY:H	1.66	0.41
1:C:365:VAL:HG23	1:C:366:SER:H	1.84	0.41
1:A:418:THR:CG2	1:A:419:LEU:N	2.82	0.41
1:B:683:THR:HA	1:B:686:PHE:HD2	1.86	0.41
1:A:630:TYR:CE2	1:A:677:VAL:CG2	3.04	0.41
1:A:58:LYS:HB3	1:A:59:GLU:OE2	2.20	0.41
1:D:73:MET:HB3	1:D:74:PRO:HD2	2.02	0.41
1:B:293:THR:HG22	1:B:339:PRO:CG	2.50	0.41
1:D:49:ASN:HA	1:D:50:PRO:HD3	1.87	0.41
1:A:227:GLU:N	1:A:278:ASN:HD21	1.99	0.41
1:B:443:PRO:HD2	1:B:444:ILE:HG13	2.02	0.41
1:D:10:VAL:HG12	1:D:10:VAL:O	2.20	0.41
1:C:310:LYS:O	1:C:538:SER:HA	2.21	0.41
1:D:304:ALA:O	1:D:307:SER:HB3	2.21	0.41
1:B:223:ALA:N	1:B:224:PRO:CD	2.83	0.41
1:B:223:ALA:HB3	1:B:224:PRO:HD3	2.03	0.41
1:D:58:LYS:HB3	1:D:59:GLU:OE2	2.20	0.41
1:C:556:LYS:C	1:C:557:LYS:HD3	2.41	0.41
1:A:132:ILE:HD11	1:A:174:PRO:C	2.41	0.41
1:C:542:LEU:HG	1:C:546:LEU:HD21	2.02	0.41
1:A:681:ASN:CG	1:A:682:PRO:CD	2.89	0.41
1:A:373:ASN:HD22	1:A:374:CYS:N	2.19	0.41
1:A:201:ILE:HG23	1:A:202:PHE:N	2.36	0.41
1:B:152:LEU:HG	1:B:196:GLU:HG3	2.02	0.41
1:B:214:LEU:HA	1:B:214:LEU:HD23	1.87	0.41
1:A:335:VAL:HG22	1:A:335:VAL:O	2.21	0.41
1:D:181:ASN:HD21	1:D:362:ASN:HD22	1.63	0.41
1:C:161:GLY:HA3	1:C:182:TYR:HB2	2.03	0.41
1:A:629:GLU:CG	1:A:676:LYS:NZ	2.82	0.41
1:C:441:ASN:C	1:C:442:LYS:HG3	2.41	0.41
1:A:439:PHE:CZ	1:A:612:GLY:CA	3.03	0.41
1:B:684:THR:C	1:B:686:PHE:H	2.24	0.41
1:B:685:LEU:HA	1:B:688:PHE:CD1	2.56	0.41
1:C:434:LYS:NZ	1:C:622:ALA:HB1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ARG:NH1	1:B:428:ARG:HG2	2.34	0.41
1:D:634:TYR:O	1:D:634:TYR:CD2	2.74	0.41
1:D:268:ARG:CZ	1:D:310:LYS:HE2	2.50	0.41
1:B:94:ASN:ND2	1:B:381:VAL:H	2.18	0.41
1:A:516:VAL:O	1:A:516:VAL:HG12	2.19	0.41
1:D:679:ILE:O	1:D:679:ILE:HG22	2.21	0.41
1:C:405:PHE:CE1	1:C:409:LYS:HD3	2.56	0.40
1:C:18:GLN:HG2	1:C:20:THR:HG23	2.03	0.40
1:A:542:LEU:O	1:A:543:VAL:C	2.58	0.40
1:A:98:ILE:HG13	1:A:98:ILE:O	2.20	0.40
1:A:193:THR:O	1:A:196:GLU:HB2	2.22	0.40
1:C:185:GLU:HG3	1:C:399:GLU:HG2	2.01	0.40
1:B:193:THR:O	1:B:196:GLU:HB2	2.21	0.40
1:B:397:SER:OG	1:B:398:PHE:N	2.52	0.40
1:D:441:ASN:C	1:D:443:PRO:CD	2.90	0.40
1:D:443:PRO:O	1:D:447:LEU:HG	2.21	0.40
1:C:439:PHE:CE2	1:C:610:TYR:O	2.74	0.40
1:A:185:GLU:HG2	1:A:185:GLU:O	2.20	0.40
1:D:210:SER:C	1:D:212:SER:N	2.73	0.40
1:D:367:LYS:O	1:D:370:THR:HB	2.22	0.40
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.88	0.40
1:D:76:HIS:CD2	1:D:77:MET:N	2.89	0.40
1:C:656:THR:HG21	1:C:677:VAL:HG21	2.03	0.40
1:C:639:MET:CG	1:C:640:LEU:HD12	2.47	0.40
1:C:637:TYR:CD2	1:C:688:PHE:HB3	2.56	0.40
1:C:167:GLN:OE1	1:C:373:ASN:ND2	2.54	0.40
1:A:80:LEU:CD1	1:A:583:HIS:HB3	2.45	0.40
1:B:662:GLN:O	1:B:664:ASN:N	2.55	0.40
1:D:311:THR:HG22	1:D:538:SER:CA	2.52	0.40
1:C:553:GLU:O	1:C:554:ASP:HB2	2.20	0.40
1:A:269:ILE:HG21	1:A:360:LEU:HD22	2.04	0.40
1:A:279:ILE:HG23	1:A:296:VAL:HG13	2.03	0.40
1:C:450:LYS:CB	1:C:451:LYS:HD2	2.51	0.40
1:B:442:LYS:O	1:B:446:GLU:HG2	2.22	0.40
1:D:115:MET:O	1:D:116:GLN:C	2.60	0.40
1:C:640:LEU:HD12	1:C:640:LEU:N	2.36	0.40
1:C:416:GLU:HA	1:C:420:LYS:HB3	2.03	0.40
1:C:132:ILE:HD11	1:C:174:PRO:C	2.42	0.40
1:B:675:THR:CG2	1:B:675:THR:O	2.69	0.40
1:B:163:TYR:HE2	1:B:165:GLU:OE1	2.05	0.40
1:D:628:ILE:O	1:D:676:LYS:HA	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:TYR:CD1	1:C:635:ASN:N	2.89	0.40
1:A:67:GLY:N	1:A:82:ASN:ND2	2.62	0.40
1:A:607:GLN:HA	1:A:610:TYR:CE2	2.56	0.40
1:A:12:ASP:HA	1:A:40:TYR:C	2.42	0.40
1:B:200:HIS:O	1:B:201:ILE:C	2.60	0.40
1:B:239:THR:C	1:B:240:ILE:HD13	2.42	0.40
1:D:97:VAL:HG11	1:D:114:ILE:CD1	2.51	0.40
1:B:356:LEU:HD12	1:B:356:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	640/697 (92%)	529 (83%)	80 (12%)	31 (5%)	3	17
1	B	640/697 (92%)	541 (84%)	64 (10%)	35 (6%)	2	13
1	C	675/697 (97%)	553 (82%)	80 (12%)	42 (6%)	2	10
1	D	652/697 (94%)	557 (85%)	66 (10%)	29 (4%)	3	18
All	All	2607/2788 (94%)	2180 (84%)	290 (11%)	137 (5%)	2	14

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	157	SER
1	A	376	THR
1	A	439	PHE
1	A	442	LYS
1	A	483	LYS
1	A	494	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	561	THR
1	A	664	ASN
1	B	124	ASN
1	B	157	SER
1	B	376	THR
1	B	439	PHE
1	B	442	LYS
1	B	449	GLU
1	B	483	LYS
1	B	494	LYS
1	B	561	THR
1	B	621	ARG
1	B	640	LEU
1	B	653	LYS
1	B	668	GLU
1	C	124	ASN
1	C	157	SER
1	C	376	THR
1	C	439	PHE
1	C	442	LYS
1	C	483	LYS
1	C	494	LYS
1	C	554	ASP
1	C	561	THR
1	C	646	PRO
1	C	695	GLU
1	D	124	ASN
1	D	157	SER
1	D	376	THR
1	D	439	PHE
1	D	442	LYS
1	D	483	LYS
1	D	494	LYS
1	D	561	THR
1	A	120	PHE
1	A	183	LEU
1	A	285	ALA
1	A	453	ILE
1	A	491	VAL
1	A	625	ALA
1	A	663	HIS
1	A	684	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	120	PHE
1	B	183	LEU
1	B	285	ALA
1	B	448	ILE
1	B	453	ILE
1	B	491	VAL
1	B	625	ALA
1	B	654	GLN
1	C	12	ASP
1	C	120	PHE
1	C	183	LEU
1	C	285	ALA
1	C	418	THR
1	C	440	ASN
1	C	453	ILE
1	C	491	VAL
1	C	549	PRO
1	C	550	THR
1	C	621	ARG
1	C	666	ASP
1	C	683	THR
1	D	120	PHE
1	D	183	LEU
1	D	285	ALA
1	D	453	ILE
1	D	491	VAL
1	D	694	LEU
1	A	12	ASP
1	A	432	GLU
1	A	621	ARG
1	A	635	ASN
1	A	656	THR
1	B	12	ASP
1	B	222	ASN
1	B	432	GLU
1	B	663	HIS
1	B	669	GLU
1	C	222	ASN
1	C	430	GLY
1	C	634	TYR
1	C	651	THR
1	C	664	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	696	MET
1	D	12	ASP
1	D	42	GLY
1	D	55	ASN
1	D	222	ASN
1	D	664	ASN
1	D	681	ASN
1	A	42	GLY
1	A	222	ASN
1	A	435	ASN
1	A	601	GLU
1	A	634	TYR
1	B	123	SER
1	B	601	GLU
1	B	675	THR
1	C	42	GLY
1	C	55	ASN
1	C	551	ARG
1	C	601	GLU
1	C	681	ASN
1	D	543	VAL
1	D	601	GLU
1	A	55	ASN
1	B	42	GLY
1	B	55	ASN
1	B	680	ARG
1	C	452	PRO
1	C	682	PRO
1	C	692	ARG
1	D	123	SER
1	D	448	ILE
1	D	631	THR
1	A	452	PRO
1	B	452	PRO
1	B	543	VAL
1	C	126	SER
1	C	421	SER
1	C	543	VAL
1	C	636	ARG
1	D	126	SER
1	D	636	ARG
1	A	126	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	126	SER
1	D	452	PRO
1	A	543	VAL
1	D	221	PRO

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	A	575/616 (93%)	520 (90%)	55 (10%)	10	38
1	B	574/616 (93%)	519 (90%)	55 (10%)	10	38
1	C	601/616 (98%)	538 (90%)	63 (10%)	8	32
1	D	583/616 (95%)	525 (90%)	58 (10%)	10	35
All	All	2333/2464 (95%)	2102 (90%)	231 (10%)	10	35

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	59	GLU
1	A	66	ASN
1	A	89	ARG
1	A	90	GLN
1	A	109	GLU
1	A	123	SER
1	A	125	GLN
1	A	142	LEU
1	A	144	GLU
1	A	164	MET
1	A	178	LYS
1	A	183	LEU
1	A	192	ARG
1	A	194	GLN
1	A	206	LEU
1	A	211	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	220	THR
1	A	235	PHE
1	A	265	SER
1	A	267	TRP
1	A	300	LYS
1	A	316	LEU
1	A	323	ARG
1	A	337	SER
1	A	342	CYS
1	A	352	LEU
1	A	356	LEU
1	A	364	LEU
1	A	373	ASN
1	A	378	LYS
1	A	388	TYR
1	A	410	LEU
1	A	418	THR
1	A	435	ASN
1	A	439	PHE
1	A	442	LYS
1	A	459	LEU
1	A	460	ASP
1	A	496	ARG
1	A	530	ASP
1	A	567	ARG
1	A	573	LEU
1	A	576	THR
1	A	584	TYR
1	A	627	ARG
1	A	630	TYR
1	A	639	MET
1	A	640	LEU
1	A	642	LYS
1	A	653	LYS
1	A	663	HIS
1	A	665	ILE
1	A	671	ARG
1	A	692	ARG
1	B	31	ARG
1	B	59	GLU
1	B	66	ASN
1	B	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	109	GLU
1	B	123	SER
1	B	125	GLN
1	B	142	LEU
1	B	164	MET
1	B	178	LYS
1	B	183	LEU
1	B	192	ARG
1	B	194	GLN
1	B	206	LEU
1	B	211	GLN
1	B	220	THR
1	B	235	PHE
1	B	265	SER
1	B	267	TRP
1	B	300	LYS
1	B	316	LEU
1	B	323	ARG
1	B	337	SER
1	B	342	CYS
1	B	352	LEU
1	B	356	LEU
1	B	364	LEU
1	B	373	ASN
1	B	378	LYS
1	B	388	TYR
1	B	410	LEU
1	B	418	THR
1	B	434	LYS
1	B	442	LYS
1	B	459	LEU
1	B	460	ASP
1	B	496	ARG
1	B	530	ASP
1	B	567	ARG
1	B	576	THR
1	B	584	TYR
1	B	620	ARG
1	B	621	ARG
1	B	627	ARG
1	B	628	ILE
1	B	634	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	635	ASN
1	B	636	ARG
1	B	639	MET
1	B	653	LYS
1	B	657	GLU
1	B	671	ARG
1	B	677	VAL
1	B	685	LEU
1	B	692	ARG
1	C	31	ARG
1	C	59	GLU
1	C	66	ASN
1	C	89	ARG
1	C	90	GLN
1	C	109	GLU
1	C	123	SER
1	C	125	GLN
1	C	142	LEU
1	C	144	GLU
1	C	164	MET
1	C	178	LYS
1	C	183	LEU
1	C	192	ARG
1	C	194	GLN
1	C	206	LEU
1	C	211	GLN
1	C	220	THR
1	C	235	PHE
1	C	265	SER
1	C	267	TRP
1	C	288	ARG
1	C	289	THR
1	C	300	LYS
1	C	316	LEU
1	C	323	ARG
1	C	337	SER
1	C	342	CYS
1	C	352	LEU
1	C	356	LEU
1	C	364	LEU
1	C	378	LYS
1	C	388	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	410	LEU
1	C	418	THR
1	C	434	LYS
1	C	439	PHE
1	C	442	LYS
1	C	443	PRO
1	C	459	LEU
1	C	460	ASP
1	C	496	ARG
1	C	530	ASP
1	C	551	ARG
1	C	554	ASP
1	C	557	LYS
1	C	567	ARG
1	C	573	LEU
1	C	576	THR
1	C	584	TYR
1	C	614	LEU
1	C	616	ASN
1	C	620	ARG
1	C	627	ARG
1	C	629	GLU
1	C	636	ARG
1	C	638	LYS
1	C	639	MET
1	C	642	LYS
1	C	646	PRO
1	C	668	GLU
1	C	669	GLU
1	C	695	GLU
1	D	31	ARG
1	D	59	GLU
1	D	66	ASN
1	D	89	ARG
1	D	90	GLN
1	D	109	GLU
1	D	123	SER
1	D	125	GLN
1	D	142	LEU
1	D	164	MET
1	D	178	LYS
1	D	183	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	184	LEU
1	D	192	ARG
1	D	194	GLN
1	D	206	LEU
1	D	211	GLN
1	D	220	THR
1	D	235	PHE
1	D	265	SER
1	D	267	TRP
1	D	288	ARG
1	D	300	LYS
1	D	316	LEU
1	D	323	ARG
1	D	337	SER
1	D	342	CYS
1	D	352	LEU
1	D	356	LEU
1	D	364	LEU
1	D	378	LYS
1	D	388	TYR
1	D	410	LEU
1	D	418	THR
1	D	434	LYS
1	D	442	LYS
1	D	446	GLU
1	D	448	ILE
1	D	459	LEU
1	D	460	ASP
1	D	496	ARG
1	D	530	ASP
1	D	567	ARG
1	D	573	LEU
1	D	576	THR
1	D	584	TYR
1	D	620	ARG
1	D	631	THR
1	D	634	TYR
1	D	642	LYS
1	D	662	GLN
1	D	666	ASP
1	D	671	ARG
1	D	681	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	683	THR
1	D	692	ARG
1	D	693	GLU
1	D	695	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	55	ASN
1	A	66	ASN
1	A	76	HIS
1	A	82	ASN
1	A	90	GLN
1	A	94	ASN
1	A	125	GLN
1	A	140	ASN
1	A	156	ASN
1	A	167	GLN
1	A	211	GLN
1	A	264	ASN
1	A	275	HIS
1	A	278	ASN
1	A	313	GLN
1	A	362	ASN
1	A	373	ASN
1	A	423	GLN
1	A	435	ASN
1	A	440	ASN
1	A	536	GLN
1	A	606	HIS
1	A	607	GLN
1	A	663	HIS
1	A	681	ASN
1	B	27	ASN
1	B	55	ASN
1	B	66	ASN
1	B	76	HIS
1	B	82	ASN
1	B	90	GLN
1	B	94	ASN
1	B	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	140	ASN
1	B	148	ASN
1	B	156	ASN
1	B	167	GLN
1	B	211	GLN
1	B	264	ASN
1	B	275	HIS
1	B	278	ASN
1	B	313	GLN
1	B	362	ASN
1	B	373	ASN
1	B	423	GLN
1	B	536	GLN
1	B	607	GLN
1	B	635	ASN
1	B	654	GLN
1	B	664	ASN
1	C	27	ASN
1	C	55	ASN
1	C	66	ASN
1	C	76	HIS
1	C	82	ASN
1	C	94	ASN
1	C	125	GLN
1	C	140	ASN
1	C	156	ASN
1	C	167	GLN
1	C	211	GLN
1	C	264	ASN
1	C	275	HIS
1	C	278	ASN
1	C	313	GLN
1	C	362	ASN
1	C	373	ASN
1	C	423	GLN
1	C	536	GLN
1	C	607	GLN
1	C	616	ASN
1	C	649	ASN
1	C	662	GLN
1	C	664	ASN
1	D	27	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	55	ASN
1	D	66	ASN
1	D	76	HIS
1	D	82	ASN
1	D	90	GLN
1	D	94	ASN
1	D	125	GLN
1	D	140	ASN
1	D	167	GLN
1	D	211	GLN
1	D	264	ASN
1	D	275	HIS
1	D	278	ASN
1	D	313	GLN
1	D	362	ASN
1	D	373	ASN
1	D	423	GLN
1	D	440	ASN
1	D	536	GLN
1	D	607	GLN
1	D	654	GLN
1	D	662	GLN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	ADP	A	791	3,2	22,29,29	1.63	5 (22%)	27,45,45	1.53	7 (25%)
3	VO4	A	792	2,4	1,4,4	1.64	0	0,6,6	0.00	-
4	ADP	B	794	3,2	22,29,29	1.68	5 (22%)	27,45,45	1.43	6 (22%)
3	VO4	B	795	2,4	1,4,4	1.52	0	0,6,6	0.00	-
4	ADP	C	891	3,2	22,29,29	1.63	5 (22%)	27,45,45	1.37	4 (14%)
3	VO4	C	892	2,4	1,4,4	1.22	0	0,6,6	0.00	-
4	ADP	D	894	3,2	22,29,29	1.63	6 (27%)	27,45,45	1.34	7 (25%)
3	VO4	D	895	2,4	1,4,4	1.60	0	0,6,6	0.00	-

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	ADP	A	791	3,2	-	0/12/32/32	0/3/3/3
3	VO4	A	792	2,4	-	0/0/0/0	0/0/0/0
4	ADP	B	794	3,2	-	0/12/32/32	0/3/3/3
3	VO4	B	795	2,4	-	0/0/0/0	0/0/0/0
4	ADP	C	891	3,2	-	0/12/32/32	0/3/3/3
3	VO4	C	892	2,4	-	0/0/0/0	0/0/0/0
4	ADP	D	894	3,2	-	0/12/32/32	0/3/3/3
3	VO4	D	895	2,4	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	794	ADP	C8-N7	-2.86	1.29	1.34
4	C	891	ADP	PB-O2B	-2.58	1.45	1.54
4	C	891	ADP	C8-N7	-2.57	1.29	1.34
4	A	791	ADP	C8-N7	-2.55	1.29	1.34
4	D	894	ADP	PB-O2B	-2.44	1.45	1.54
4	A	791	ADP	PB-O2B	-2.37	1.46	1.54
4	B	794	ADP	PB-O2B	-2.34	1.46	1.54
4	D	894	ADP	C8-N7	-2.26	1.30	1.34
4	A	791	ADP	O4'-C4'	-2.09	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	794	ADP	C2-N3	2.05	1.35	1.32
4	D	894	ADP	C2-N3	2.08	1.35	1.32
4	D	894	ADP	O4'-C1'	2.29	1.44	1.41
4	C	891	ADP	O4'-C1'	2.52	1.44	1.41
4	B	794	ADP	C4-N3	3.28	1.40	1.35
4	C	891	ADP	C4-N3	3.31	1.40	1.35
4	D	894	ADP	C4-N3	3.49	1.40	1.35
4	A	791	ADP	C4-N3	3.63	1.41	1.35
4	C	891	ADP	C2-N1	3.64	1.40	1.33
4	A	791	ADP	C2-N1	3.81	1.41	1.33
4	D	894	ADP	C2-N1	3.85	1.41	1.33
4	B	794	ADP	C2-N1	4.44	1.42	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	791	ADP	N3-C2-N1	-3.54	126.18	128.89
4	B	794	ADP	N3-C2-N1	-3.16	126.47	128.89
4	C	891	ADP	N3-C2-N1	-3.03	126.58	128.89
4	D	894	ADP	N3-C2-N1	-2.78	126.77	128.89
4	B	794	ADP	O3B-PB-O1B	-2.29	103.19	110.58
4	D	894	ADP	O4'-C4'-C3'	-2.17	100.78	105.15
4	A	791	ADP	C1'-N9-C4	-2.16	123.67	126.94
4	A	791	ADP	O3B-PB-O1B	-2.16	103.61	110.58
4	D	894	ADP	O3B-PB-O1B	-2.11	103.77	110.58
4	C	891	ADP	O3B-PB-O1B	-2.07	103.91	110.58
4	D	894	ADP	O2B-PB-O1B	2.00	117.03	110.58
4	D	894	ADP	C4-C5-N7	2.00	111.32	109.48
4	B	794	ADP	O2B-PB-O1B	2.08	117.29	110.58
4	B	794	ADP	C4-C5-N7	2.15	111.46	109.48
4	A	791	ADP	O2B-PB-O1B	2.17	117.55	110.58
4	D	894	ADP	O3'-C3'-C4'	2.30	117.96	111.05
4	A	791	ADP	C4-C5-N7	2.33	111.62	109.48
4	A	791	ADP	O3'-C3'-C4'	2.38	118.19	111.05
4	B	794	ADP	O3'-C3'-C2'	2.40	119.62	111.83
4	C	891	ADP	O3'-C3'-C4'	2.43	118.34	111.05
4	B	794	ADP	O3'-C3'-C4'	2.43	118.34	111.05
4	D	894	ADP	O3'-C3'-C2'	2.46	119.84	111.83
4	C	891	ADP	O3'-C3'-C2'	2.49	119.93	111.83
4	A	791	ADP	O3'-C3'-C2'	2.53	120.06	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	791	ADP	2	0
3	A	792	VO4	1	0
4	B	794	ADP	2	0
4	C	891	ADP	2	0
3	C	892	VO4	1	0
4	D	894	ADP	3	0
3	D	895	VO4	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.