



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:51 PM GMT

PDB ID : 1CT9  
Title : CRYSTAL STRUCTURE OF ASPARAGINE SYNTHETASE B FROM ES-  
CHERICHIA COLI  
Authors : Larsen, T.M.; Boehlein, S.K.; Schuster, S.M.; Richards, N.G.J.; Thoden, J.B.;  
Holden, H.M.; Rayment, I.  
Deposited on : 1999-08-20  
Resolution : 2.00 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](mailto: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

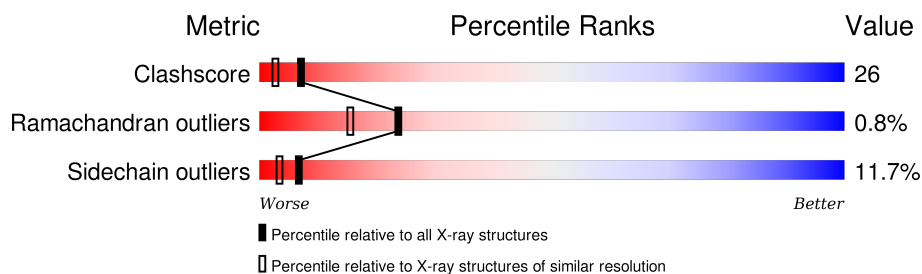
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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  $\geq 3$ , 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	553	
1	B	553	
1	C	553	
1	D	553	

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
4	AMP	C	1114	-	-	X	-
4	AMP	D	1121	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16980 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.

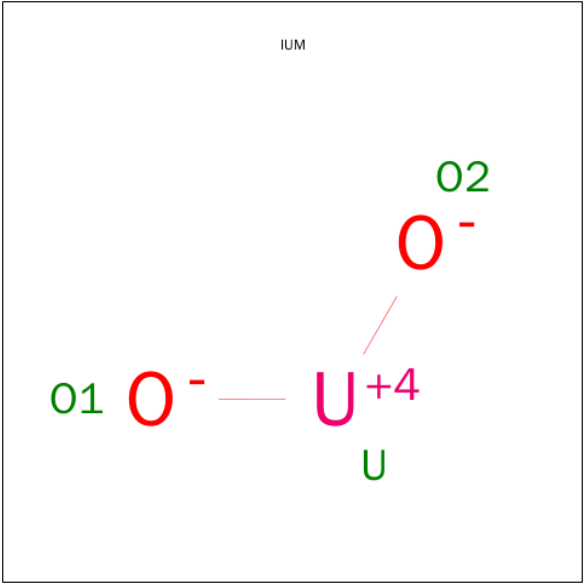
- Molecule 1 is a protein called ASPARAGINE SYNTHETASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3966	2530	671	745	20			
1	B	495	Total	C	N	O	S	0	0	0
			3942	2518	665	739	20			
1	C	495	Total	C	N	O	S	0	0	0
			3942	2518	665	739	20			
1	D	495	Total	C	N	O	S	0	0	0
			3930	2507	664	739	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	ENGINEERED	UNP P22106
B	1	ALA	CYS	ENGINEERED	UNP P22106
C	1	ALA	CYS	ENGINEERED	UNP P22106
D	1	ALA	CYS	ENGINEERED	UNP P22106

- Molecule 2 is URANYL (VI) ION (three-letter code: IUM) (formula: O<sub>2</sub>U).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total U 1 1	0	0
2	A	1	Total O U 2 1 1	0	0
2	A	1	Total U 1 1	0	0
2	A	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	D	1	Total O U 2 1 1	0	0
2	D	1	Total U 1 1	0	0

Continued on next page...

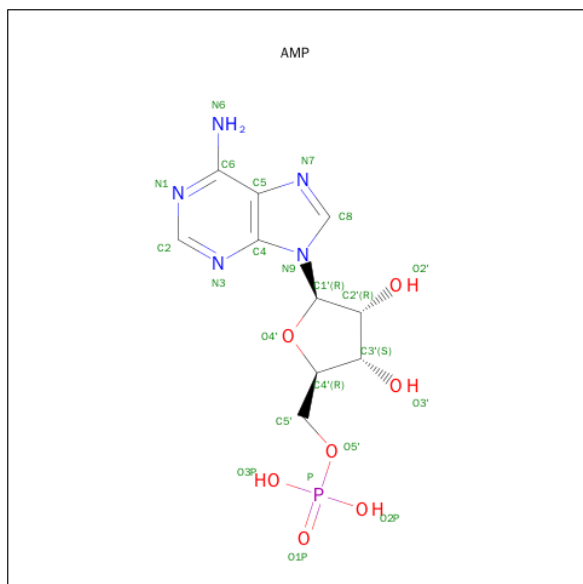
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	U	0	0
			1	1		
2	D	1	Total	U	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



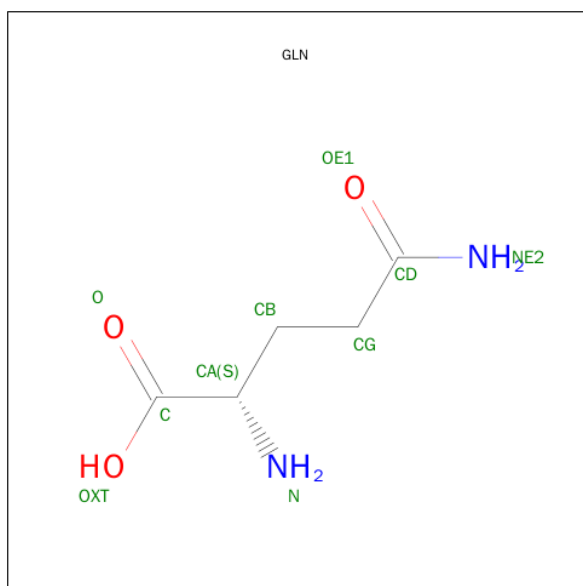
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	5	2	3		
5	B	1	Total	C	N	O	0	0
			10	5	2	3		
5	C	1	Total	C	N	O	0	0
			10	5	2	3		
5	D	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 6 is water.

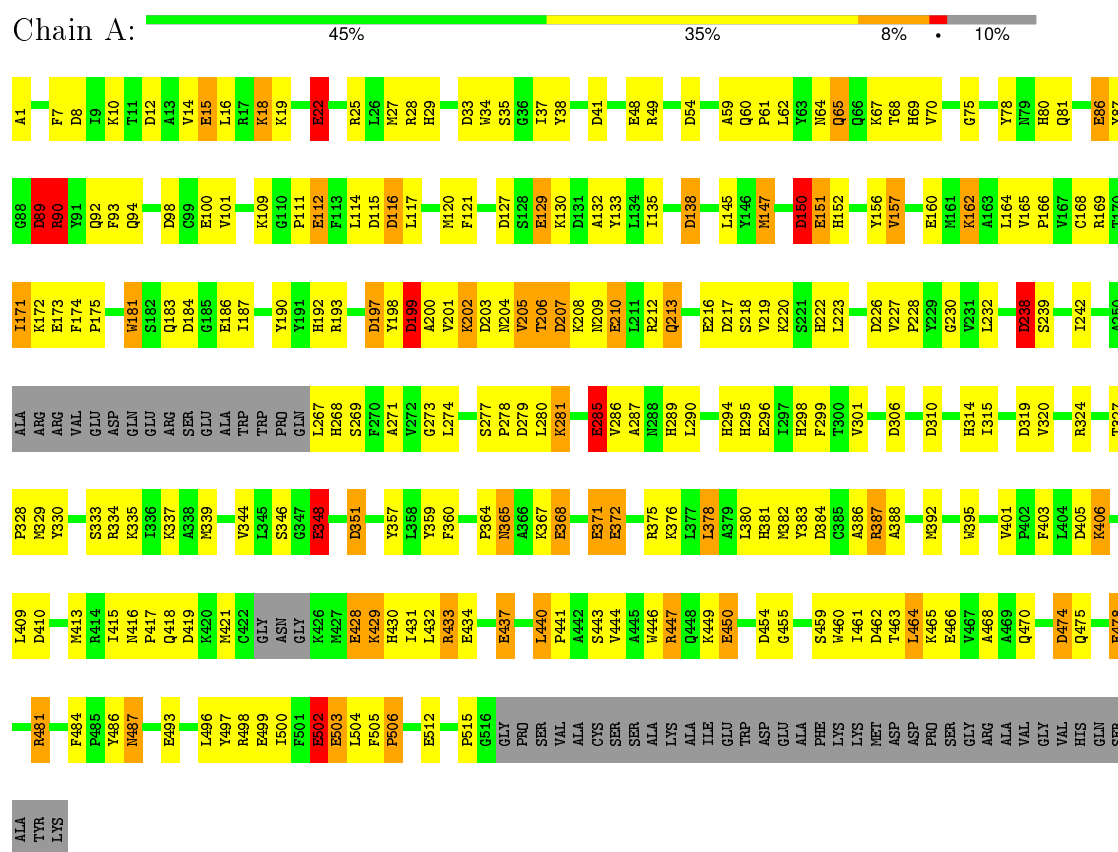
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total	O	0	0
			292	292		
6	B	235	Total	O	0	0
			235	235		
6	C	223	Total	O	0	0
			223	223		
6	D	296	Total	O	0	0
			296	296		

### 3 Residue-property plots

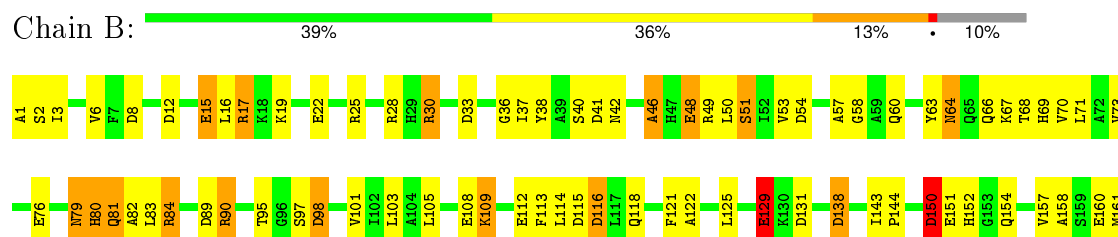
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

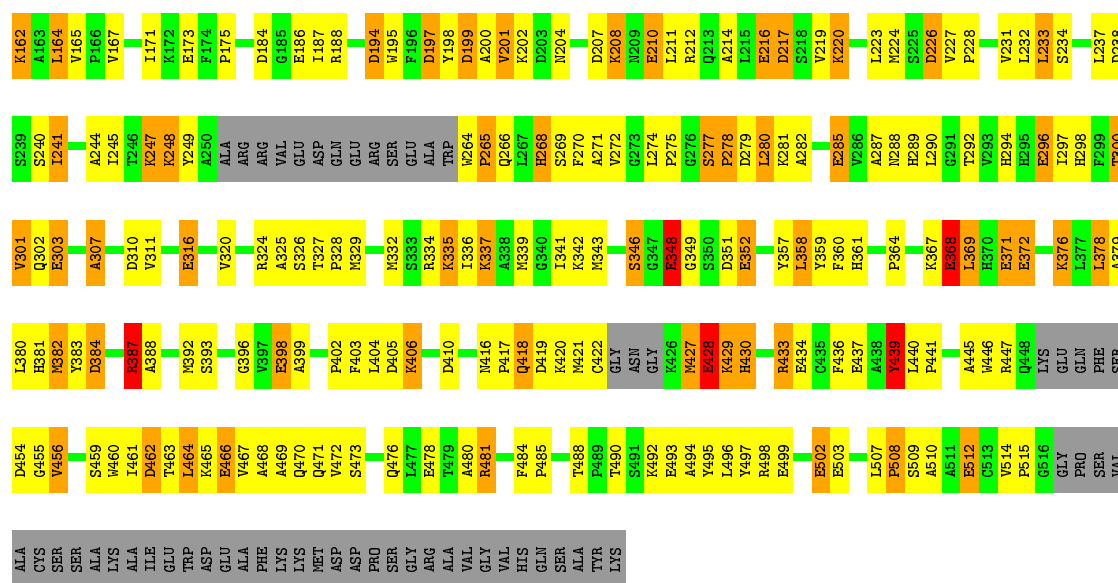
Note EDS was not executed.

#### • Molecule 1: ASPARAGINE SYNTHETASE B



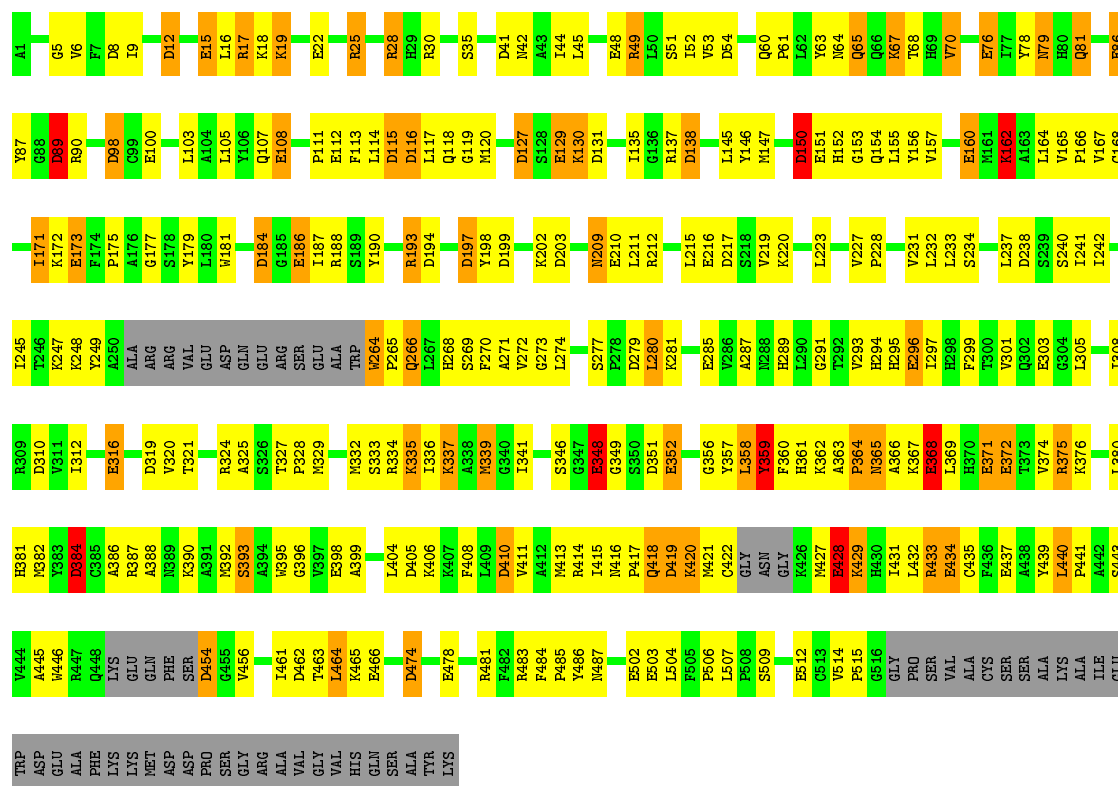
#### • Molecule 1: ASPARAGINE SYNTHETASE B





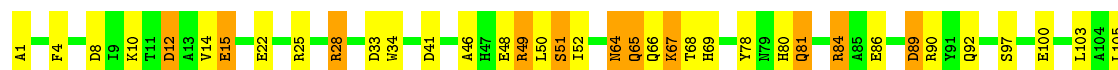
### • Molecule 1: ASPARAGINE SYNTHETASE B

Chain C: 41% 37% 10% 10%



### • Molecule 1: ASPARAGINE SYNTHETASE B

Chain D: 48% 31% 9% 10%



[illegible]

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.93 Å   127.10 Å   204.51 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.0 (30.00-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.197 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16980	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, IUM, CL

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	1.02	24/4060 (0.6%)	1.48	66/5493 (1.2%)
1	B	1.04	32/4037 (0.8%)	1.50	67/5466 (1.2%)
1	C	1.01	33/4037 (0.8%)	1.44	63/5466 (1.2%)
1	D	1.06	30/4022 (0.7%)	1.49	67/5443 (1.2%)
All	All	1.03	119/16156 (0.7%)	1.48	263/21868 (1.2%)

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	478	GLU	CD-OE2	9.23	1.35	1.25
1	D	398	GLU	CD-OE2	8.52	1.35	1.25
1	B	466	GLU	CD-OE2	7.96	1.34	1.25
1	D	48	GLU	CD-OE2	7.61	1.34	1.25
1	B	296	GLU	CD-OE2	7.58	1.33	1.25
1	A	15	GLU	CD-OE2	7.56	1.33	1.25
1	B	352	GLU	CD-OE2	7.49	1.33	1.25
1	C	86	GLU	CD-OE2	7.38	1.33	1.25
1	D	296	GLU	CD-OE2	7.34	1.33	1.25
1	B	316	GLU	CD-OE2	7.29	1.33	1.25
1	D	15	GLU	CD-OE2	7.21	1.33	1.25
1	D	352	GLU	CD-OE2	7.21	1.33	1.25
1	B	348	GLU	CD-OE2	7.17	1.33	1.25
1	B	285	GLU	CD-OE2	7.15	1.33	1.25
1	A	512	GLU	CD-OE2	7.14	1.33	1.25
1	B	437	GLU	CD-OE2	7.09	1.33	1.25
1	A	210	GLU	CD-OE2	7.04	1.33	1.25
1	D	503	GLU	CD-OE2	6.89	1.33	1.25
1	B	478	GLU	CD-OE2	6.89	1.33	1.25
1	B	372	GLU	CD-OE2	6.84	1.33	1.25
1	B	503	GLU	CD-OE2	6.75	1.33	1.25
1	D	512	GLU	CD-OE2	6.72	1.33	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	GLU	CD-OE2	6.71	1.33	1.25
1	C	393	SER	CB-OG	6.70	1.50	1.42
1	D	285	GLU	CD-OE2	6.70	1.33	1.25
1	C	112	GLU	CD-OE2	6.66	1.32	1.25
1	B	398	GLU	CD-OE2	6.66	1.32	1.25
1	C	503	GLU	CD-OE2	6.65	1.32	1.25
1	C	466	GLU	CD-OE2	6.63	1.32	1.25
1	A	186	GLU	CD-OE2	6.61	1.32	1.25
1	C	129	GLU	CD-OE2	6.57	1.32	1.25
1	D	437	GLU	CD-OE2	6.56	1.32	1.25
1	A	129	GLU	CD-OE2	6.51	1.32	1.25
1	D	502	GLU	CD-OE2	6.51	1.32	1.25
1	A	151	GLU	CD-OE2	6.50	1.32	1.25
1	D	466	GLU	CD-OE2	6.47	1.32	1.25
1	C	173	GLU	CD-OE2	6.44	1.32	1.25
1	B	434	GLU	CD-OE2	6.43	1.32	1.25
1	B	108	GLU	CD-OE2	6.43	1.32	1.25
1	C	303	GLU	CD-OE2	6.43	1.32	1.25
1	C	368	GLU	CD-OE2	6.40	1.32	1.25
1	C	151	GLU	CD-OE2	6.38	1.32	1.25
1	B	22	GLU	CD-OE2	6.36	1.32	1.25
1	C	428	GLU	CD-OE2	6.36	1.32	1.25
1	B	112	GLU	CD-OE2	6.36	1.32	1.25
1	A	466	GLU	CD-OE2	6.33	1.32	1.25
1	C	15	GLU	CD-OE2	6.32	1.32	1.25
1	B	151	GLU	CD-OE2	6.31	1.32	1.25
1	C	502	GLU	CD-OE2	6.30	1.32	1.25
1	C	434	GLU	CD-OE2	6.25	1.32	1.25
1	B	499	GLU	CD-OE2	6.25	1.32	1.25
1	A	368	GLU	CD-OE2	6.22	1.32	1.25
1	A	112	GLU	CD-OE2	6.22	1.32	1.25
1	D	372	GLU	CD-OE2	6.15	1.32	1.25
1	C	478	GLU	CD-OE2	6.15	1.32	1.25
1	B	368	GLU	CD-OE2	6.13	1.32	1.25
1	D	22	GLU	CD-OE2	6.11	1.32	1.25
1	B	15	GLU	CD-OE2	6.07	1.32	1.25
1	A	371	GLU	CD-OE2	6.07	1.32	1.25
1	B	186	GLU	CD-OE2	6.03	1.32	1.25
1	A	478	GLU	CD-OE2	6.01	1.32	1.25
1	D	428	GLU	CD-OE2	6.01	1.32	1.25
1	B	129	GLU	CD-OE2	6.01	1.32	1.25
1	D	434	GLU	CD-OE2	6.00	1.32	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	398	GLU	CD-OE2	5.96	1.32	1.25
1	C	437	GLU	CD-OE2	5.95	1.32	1.25
1	D	186	GLU	CD-OE2	5.89	1.32	1.25
1	B	371	GLU	CD-OE2	5.88	1.32	1.25
1	D	129	GLU	CD-OE2	5.88	1.32	1.25
1	C	285	GLU	CD-OE2	5.88	1.32	1.25
1	A	348	GLU	CD-OE2	5.87	1.32	1.25
1	D	210	GLU	CD-OE2	5.84	1.32	1.25
1	B	48	GLU	CD-OE2	5.83	1.32	1.25
1	A	22	GLU	CD-OE2	5.82	1.32	1.25
1	B	428	GLU	CD-OE2	5.82	1.32	1.25
1	C	398	GLU	CD-OE1	-5.80	1.19	1.25
1	C	371	GLU	CD-OE2	5.79	1.32	1.25
1	B	502	GLU	CD-OE2	5.77	1.31	1.25
1	D	151	GLU	CD-OE2	5.74	1.31	1.25
1	A	493	GLU	CD-OE2	5.73	1.31	1.25
1	C	512	GLU	CD-OE2	5.71	1.31	1.25
1	D	368	GLU	CD-OE2	5.71	1.31	1.25
1	D	112	GLU	CD-OE2	5.70	1.31	1.25
1	A	285	GLU	CD-OE2	5.69	1.31	1.25
1	D	348	GLU	CD-OE2	5.68	1.31	1.25
1	C	210	GLU	CD-OE2	5.68	1.31	1.25
1	B	210	GLU	CD-OE2	5.67	1.31	1.25
1	C	186	GLU	CD-OE2	5.67	1.31	1.25
1	B	76	GLU	CD-OE2	5.66	1.31	1.25
1	A	503	GLU	CD-OE2	5.62	1.31	1.25
1	B	512	GLU	CD-OE2	5.61	1.31	1.25
1	B	173	GLU	CD-OE2	5.60	1.31	1.25
1	C	100	GLU	CD-OE2	5.58	1.31	1.25
1	A	502	GLU	CD-OE2	5.53	1.31	1.25
1	A	434	GLU	CD-OE2	5.52	1.31	1.25
1	A	428	GLU	CD-OE2	5.51	1.31	1.25
1	B	216	GLU	CD-OE2	5.50	1.31	1.25
1	A	160	GLU	CD-OE2	5.48	1.31	1.25
1	C	76	GLU	CD-OE2	5.47	1.31	1.25
1	D	160	GLU	CD-OE2	5.41	1.31	1.25
1	D	303	GLU	CD-OE2	5.39	1.31	1.25
1	A	86	GLU	CD-OE2	5.37	1.31	1.25
1	D	100	GLU	CD-OE1	-5.34	1.19	1.25
1	C	296	GLU	CD-OE2	5.32	1.31	1.25
1	D	493	GLU	CD-OE2	5.25	1.31	1.25
1	C	316	GLU	CD-OE2	5.24	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	108	GLU	CD-OE2	5.24	1.31	1.25
1	C	372	GLU	CD-OE2	5.23	1.31	1.25
1	C	352	GLU	CD-OE2	5.22	1.31	1.25
1	D	499	GLU	CD-OE2	5.21	1.31	1.25
1	A	437	GLU	CD-OE2	5.18	1.31	1.25
1	C	160	GLU	CD-OE2	5.12	1.31	1.25
1	A	499	GLU	CD-OE2	5.10	1.31	1.25
1	B	303	GLU	CD-OE2	5.08	1.31	1.25
1	D	216	GLU	CD-OE2	5.08	1.31	1.25
1	C	48	GLU	CD-OE2	5.07	1.31	1.25
1	B	160	GLU	CD-OE2	5.05	1.31	1.25
1	D	173	GLU	CD-OE2	5.02	1.31	1.25
1	C	348	GLU	CD-OE2	5.00	1.31	1.25

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ASP	CB-CG-OD2	-14.12	105.59	118.30
1	A	150	ASP	CB-CG-OD2	-13.62	106.05	118.30
1	C	150	ASP	CB-CG-OD2	-10.79	108.59	118.30
1	D	194	ASP	CB-CG-OD1	10.22	127.50	118.30
1	B	238	ASP	CB-CG-OD2	-10.11	109.20	118.30
1	A	238	ASP	CB-CG-OD1	9.77	127.09	118.30
1	C	238	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	D	410	ASP	CB-CG-OD2	-9.71	109.56	118.30
1	B	351	ASP	CB-CG-OD2	-9.69	109.58	118.30
1	A	238	ASP	CB-CG-OD2	-9.67	109.59	118.30
1	A	481	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	B	387	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	A	474	ASP	CB-CG-OD2	-9.47	109.78	118.30
1	D	150	ASP	CB-CG-OD1	9.15	126.54	118.30
1	D	150	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	B	351	ASP	CB-CG-OD1	8.94	126.35	118.30
1	A	190	TYR	CB-CG-CD2	-8.76	115.75	121.00
1	D	309	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	C	49	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	150	ASP	CB-CG-OD1	8.39	125.85	118.30
1	D	387	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	310	ASP	CB-CG-OD2	-8.36	110.77	118.30
1	C	193	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	194	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	B	439	TYR	CB-CG-CD1	-8.31	116.01	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	306	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	C	138	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	C	410	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	184	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	C	28	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	C	116	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	D	384	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	B	8	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	319	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	B	197	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	A	351	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	C	310	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	B	199	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	197	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	116	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	D	194	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	8	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	D	238	ASP	CB-CG-OD1	7.64	125.18	118.30
1	D	8	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	217	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	C	483	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	D	90	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	184	ASP	CB-CG-OD1	7.57	125.12	118.30
1	C	319	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	D	199	ASP	CB-CG-OD1	7.51	125.06	118.30
1	C	115	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	D	410	ASP	CB-CG-OD1	7.49	125.04	118.30
1	B	405	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	B	8	ASP	CB-CG-OD1	7.43	124.99	118.30
1	D	199	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	64	ASN	N-CA-CB	-7.38	97.31	110.60
1	D	8	ASP	CB-CG-OD1	7.37	124.94	118.30
1	A	8	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	116	ASP	CB-CG-OD1	7.36	124.93	118.30
1	D	157	VAL	CG1-CB-CG2	7.36	122.68	110.90
1	D	184	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	B	498	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	D	147	MET	N-CA-CB	-7.22	97.61	110.60
1	C	387	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	194	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C	54	ASP	CB-CG-OD2	-7.18	111.84	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	B	17	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	D	351	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	199	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	B	138	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	8	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	C	150	ASP	CB-CG-OD1	7.05	124.65	118.30
1	C	454	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	98	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	169	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	197	ASP	CB-CG-OD1	6.99	124.59	118.30
1	D	375	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	162	LYS	N-CA-CB	-6.95	98.10	110.60
1	A	351	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	79	ASN	N-CA-CB	-6.91	98.17	110.60
1	B	188	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	279	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	324	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	405	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	498	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	188	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	41	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	C	131	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	122	ALA	N-CA-CB	6.70	119.48	110.10
1	D	279	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	474	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	184	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	410	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	C	98	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	197	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	D	184	ASP	N-CA-CB	6.56	122.41	110.60
1	C	41	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	B	17	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	C	199	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	199	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	B	430	HIS	CA-CB-CG	-6.51	102.53	113.60
1	B	33	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	310	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	46	ALA	N-CA-CB	6.47	119.16	110.10
1	C	138	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	419	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	D	363	ALA	N-CA-CB	6.46	119.15	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	279	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	410	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	116	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	54	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	98	ASP	CB-CG-OD1	6.39	124.05	118.30
1	C	30	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	49	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	C	79	ASN	N-CA-CB	-6.34	99.19	110.60
1	C	41	ASP	CB-CG-OD1	6.34	124.00	118.30
1	C	116	ASP	CB-CG-OD1	6.33	123.99	118.30
1	C	184	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	212	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	115	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	351	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	D	462	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	C	162	LYS	N-CA-CB	-6.25	99.36	110.60
1	D	319	ASP	CB-CG-OD1	6.22	123.90	118.30
1	D	89	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	197	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	54	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	207	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	41	ASP	CB-CG-OD1	6.13	123.82	118.30
1	D	474	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	310	ASP	CB-CG-OD1	6.13	123.81	118.30
1	D	157	VAL	CA-CB-CG2	6.13	120.09	110.90
1	A	279	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	89	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	498	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	330	TYR	CB-CG-CD2	6.08	124.65	121.00
1	A	33	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	131	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	D	433	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	334	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	84	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	351	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	410	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	25	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	90	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	150	ASP	CA-CB-CG	-5.97	100.26	113.40
1	D	89	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	D	454	ASP	CB-CG-OD2	-5.96	112.94	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	89	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	150	ASP	CA-CB-CG	-5.92	100.37	113.40
1	A	15	GLU	N-CA-CB	-5.92	99.94	110.60
1	D	64	ASN	CA-CB-CG	-5.91	100.39	113.40
1	B	162	LYS	N-CA-CB	-5.91	99.97	110.60
1	A	150	ASP	CB-CA-C	-5.88	98.64	110.40
1	A	314	HIS	CA-CB-CG	-5.87	103.62	113.60
1	B	184	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	197	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	41	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	33	ASP	CB-CG-OD1	5.85	123.56	118.30
1	C	17	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	89	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	B	150	ASP	CB-CA-C	-5.83	98.75	110.40
1	A	319	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	49	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	190	TYR	CB-CG-CD1	5.80	124.48	121.00
1	D	131	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	D	41	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	405	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	439	TYR	CB-CG-CD2	5.78	124.47	121.00
1	D	12	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	115	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	405	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	487	ASN	CB-CA-C	-5.74	98.92	110.40
1	C	150	ASP	CB-CA-C	-5.73	98.94	110.40
1	D	184	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	226	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	C	184	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	89	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	279	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	462	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	116	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	498	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	217	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	131	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	207	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	454	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	226	ASP	CB-CG-OD1	5.63	123.37	118.30
1	D	28	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	217	ASP	CB-CG-OD1	5.60	123.34	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	481	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	D	207	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	199	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	131	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	450	GLU	N-CA-CB	5.58	120.64	110.60
1	C	474	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	203	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	C	419	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	41	ASP	CB-CG-OD1	5.55	123.29	118.30
1	D	147	MET	CA-CB-CG	5.54	122.72	113.30
1	D	422	CYS	CB-CA-C	-5.54	99.33	110.40
1	C	194	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	474	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	138	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	131	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	120	MET	CG-SD-CE	5.50	109.00	100.20
1	A	410	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	98	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	197	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	64	ASN	CB-CA-C	-5.46	99.47	110.40
1	C	193	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	375	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	C	351	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	33	ASP	CB-CG-OD1	5.42	123.17	118.30
1	B	419	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	186	GLU	N-CA-CB	5.40	120.31	110.60
1	C	12	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	138	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	D	238	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	127	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	33	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	C	203	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	30	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	78	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	310	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	405	ASP	CB-CG-OD2	-5.28	113.54	118.30
1	C	8	ASP	CB-CG-OD1	5.28	123.06	118.30
1	D	149	TYR	C-N-CA	5.28	134.91	121.70
1	B	454	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	206	THR	CA-CB-CG2	-5.27	105.02	112.40
1	A	226	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	238	ASP	CB-CG-OD1	5.25	123.02	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	190	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	C	127	ASP	CB-CG-OD1	5.24	123.01	118.30
1	D	339	MET	CB-CA-C	-5.23	99.93	110.40
1	B	217	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	419	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	89	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	25	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	199	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	146	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	B	268	HIS	CA-CB-CG	-5.18	104.79	113.60
1	C	319	ASP	CB-CG-OD1	5.17	122.96	118.30
1	D	419	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	217	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	D	494	ALA	CB-CA-C	-5.15	102.37	110.10
1	B	387	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	447	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	375	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	433	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	112	GLU	N-CA-C	5.10	124.78	111.00
1	D	419	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	384	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	B	307	ALA	CB-CA-C	-5.07	102.49	110.10
1	B	12	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	138	ASP	CB-CG-OD1	5.04	122.84	118.30
1	D	427	MET	CA-CB-CG	5.03	121.84	113.30
1	B	109	LYS	N-CA-CB	-5.02	101.56	110.60
1	D	319	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	A	3966	0	3862	192	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3942	0	3828	247	0
1	C	3942	0	3827	204	0
1	D	3930	0	3818	186	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	11	5	0
4	B	23	0	12	3	0
4	C	23	0	11	7	0
4	D	23	0	12	8	0
5	A	10	0	7	2	0
5	B	10	0	7	4	0
5	C	10	0	7	1	0
5	D	10	0	7	2	0
6	A	292	0	0	8	0
6	B	235	0	0	13	0
6	C	223	0	0	7	0
6	D	296	0	0	19	0
All	All	16980	0	15409	822	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 26.

All (822) 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:364:PRO:HG2	1:C:368:GLU:HG2	1.26	1.17
1:D:472:VAL:HB	1:D:492:LYS:HG2	1.22	1.12
1:D:364:PRO:HG2	1:D:368:GLU:HG2	1.40	1.01
1:B:300:THR:HG22	1:B:303:GLU:H	1.29	0.96
1:D:64:ASN:HB3	1:D:67:LYS:N	1.80	0.95
1:D:427:MET:H	1:D:430:HIS:HD2	1.14	0.95
1:C:366:ALA:HA	1:C:421:MET:HE3	1.46	0.95
1:B:198:TYR:CE2	1:B:367:LYS:HB2	2.04	0.92
1:A:387:ARG:HH11	1:A:387:ARG:HB3	1.35	0.90
1:C:211:LEU:HD12	1:C:411:VAL:HG12	1.54	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:H	1:C:81:GLN:NE2	1.69	0.90
1:A:207:ASP:HB3	1:A:210:GLU:HB3	1.56	0.88
1:C:193:ARG:HH22	1:C:406:LYS:HE3	1.38	0.87
1:C:366:ALA:HA	1:C:421:MET:CE	2.04	0.87
1:D:472:VAL:CB	1:D:492:LYS:HG2	2.03	0.87
1:B:83:LEU:HD13	1:B:101:VAL:HG11	1.57	0.86
1:C:168:CYS:HB2	1:C:171:ILE:HD11	1.59	0.85
1:D:64:ASN:HB2	1:D:69:HIS:H	1.41	0.84
1:B:1:ALA:N	5:B:1113:GLN:HE22	1.75	0.84
1:D:272:VAL:H	4:D:1121:AMP:HN62	1.22	0.84
1:D:64:ASN:HB3	1:D:67:LYS:H	1.41	0.82
1:D:279:ASP:OD2	1:D:455:GLY:HA3	1.80	0.82
1:A:175:PRO:HG2	1:A:187:ILE:HG21	1.59	0.82
1:B:300:THR:HG21	6:B:1187:HOH:O	1.80	0.82
1:B:198:TYR:CD2	1:B:367:LYS:HB2	2.15	0.81
1:C:234:SER:HB3	4:C:1114:AMP:C5	2.14	0.81
1:C:422:CYS:SG	1:C:428:GLU:HA	2.21	0.81
1:B:81:GLN:NE2	1:B:82:ALA:H	1.79	0.80
1:C:320:VAL:HG12	1:C:324:ARG:HD2	1.61	0.80
1:C:364:PRO:HG2	1:C:368:GLU:CG	2.10	0.80
1:B:83:LEU:CD1	1:B:101:VAL:HG11	2.12	0.80
1:A:387:ARG:CB	1:A:387:ARG:HH11	1.94	0.79
1:B:150:ASP:HB3	1:B:152:HIS:H	1.45	0.79
1:A:199:ASP:HB3	1:A:202:LYS:NZ	1.96	0.79
1:B:348:GLU:CD	4:B:1107:AMP:H5'1	2.03	0.79
1:B:278:PRO:HG2	1:B:455:GLY:HA2	1.64	0.79
1:D:50:LEU:HG	1:D:52:ILE:HD11	1.64	0.79
1:D:277:SER:O	1:D:281:LYS:HE2	1.83	0.79
1:C:433:ARG:HD2	1:C:446:TRP:CE3	2.19	0.78
1:C:248:LYS:HG2	1:C:249:TYR:CD1	2.18	0.78
1:B:216:GLU:HG2	1:B:249:TYR:HE1	1.48	0.78
1:C:440:LEU:HB3	1:C:441:PRO:HD2	1.66	0.77
1:C:380:LEU:CD2	1:C:384:ASP:HB2	2.14	0.77
1:A:150:ASP:HB3	1:A:152:HIS:H	1.48	0.77
1:B:49:ARG:CZ	1:B:51:SER:HB3	2.14	0.77
1:A:440:LEU:HB3	1:A:441:PRO:HD2	1.65	0.77
1:D:349:GLY:O	1:D:353:VAL:HG23	1.85	0.77
1:C:232:LEU:HD12	1:C:346:SER:HB3	1.65	0.77
1:C:211:LEU:CD1	1:C:411:VAL:HG12	2.15	0.76
1:C:150:ASP:HB3	1:C:152:HIS:H	1.50	0.76
1:A:227:VAL:HB	1:A:228:PRO:HD2	1.66	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:HIS:NE2	1:D:428:GLU:HG3	2.00	0.76
1:B:300:THR:CG2	1:B:303:GLU:H	1.98	0.76
1:B:380:LEU:CD2	1:B:384:ASP:HB2	2.16	0.76
1:C:380:LEU:HD22	1:C:384:ASP:HB2	1.68	0.76
1:B:508:PRO:O	1:B:512:GLU:HG3	1.85	0.76
1:A:199:ASP:HB3	1:A:202:LYS:HZ1	1.50	0.75
1:D:348:GLU:CD	4:D:1121:AMP:H5'1	2.08	0.75
1:D:381:HIS:CE1	1:D:382:MET:HG3	2.22	0.74
1:D:372:GLU:OE2	1:D:375:ARG:HD2	1.87	0.74
1:D:268:HIS:ND1	1:D:295:HIS:NE2	2.34	0.74
1:A:365:ASN:HD21	1:A:368:GLU:HG2	1.53	0.73
1:C:193:ARG:NH2	1:C:406:LYS:HE3	2.04	0.73
1:A:418:GLN:HB2	6:A:1392:HOH:O	1.88	0.73
1:B:336:ILE:HG22	1:B:341:ILE:HB	1.71	0.73
1:D:271:ALA:HA	4:D:1121:AMP:N1	2.04	0.73
1:C:44:ILE:C	1:C:45:LEU:HD12	2.09	0.73
1:D:342:LYS:NZ	6:D:1276:HOH:O	2.22	0.73
1:B:171:ILE:HD12	1:B:507:LEU:CD2	2.19	0.72
1:B:64:ASN:HB3	1:B:67:LYS:H	1.55	0.72
1:C:366:ALA:CA	1:C:421:MET:HE3	2.19	0.72
1:A:64:ASN:HB3	1:A:67:LYS:N	2.05	0.72
1:A:207:ASP:HB3	1:A:210:GLU:CB	2.19	0.72
1:B:64:ASN:HB3	1:B:67:LYS:N	2.05	0.72
1:B:439:TYR:C	1:B:440:LEU:HD23	2.10	0.72
1:A:64:ASN:HB2	1:A:69:HIS:H	1.54	0.72
1:B:358:LEU:HA	1:B:361:HIS:HD2	1.54	0.71
1:A:387:ARG:HG3	1:A:388:ALA:N	2.06	0.71
1:A:132:ALA:HB2	1:A:183:GLN:NE2	2.06	0.71
1:A:268:HIS:ND1	1:A:295:HIS:NE2	2.39	0.71
1:B:80:HIS:CD2	1:B:98:ASP:HA	2.26	0.71
1:A:64:ASN:HB3	1:A:67:LYS:H	1.55	0.71
1:C:248:LYS:HE2	1:C:249:TYR:CZ	2.25	0.71
1:A:267:LEU:N	6:A:1379:HOH:O	2.24	0.71
1:C:81:GLN:N	1:C:81:GLN:HE21	1.88	0.70
1:C:248:LYS:HG2	1:C:249:TYR:CE1	2.26	0.70
1:C:417:PRO:HA	1:C:420:LYS:HG3	1.73	0.70
1:C:89:ASP:OD1	1:C:90:ARG:HG3	1.92	0.70
1:C:364:PRO:HB2	1:C:365:ASN:ND2	2.07	0.70
1:A:109:LYS:HE3	1:A:116:ASP:OD1	1.91	0.69
1:B:113:PHE:O	1:B:116:ASP:HB2	1.92	0.69
1:C:211:LEU:HD12	1:C:411:VAL:CG1	2.21	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:PHE:HE2	1:D:339:MET:CE	2.05	0.69
1:C:308:ILE:O	1:C:312:ILE:HG13	1.92	0.69
1:B:297:ILE:HG23	1:B:335:LYS:HD3	1.74	0.69
1:B:427:MET:O	1:B:430:HIS:HB2	1.92	0.69
1:A:81:GLN:HB2	6:A:1292:HOH:O	1.92	0.69
1:B:194:ASP:OD1	1:B:195:TRP:N	2.25	0.69
1:C:81:GLN:H	1:C:81:GLN:HE21	1.40	0.68
1:C:367:LYS:O	1:C:371:GLU:HG3	1.94	0.68
1:D:281:LYS:HD3	1:D:281:LYS:N	2.07	0.68
1:D:199:ASP:HA	1:D:202:LYS:HE2	1.74	0.68
1:D:201:VAL:HA	1:D:204:ASN:ND2	2.09	0.68
1:A:168:CYS:HB2	1:A:171:ILE:HD12	1.74	0.68
1:D:496:LEU:O	1:D:496:LEU:HD12	1.93	0.68
1:A:173:GLU:OE1	1:A:381:HIS:ND1	2.23	0.68
1:D:318:TYR:OH	1:D:487:ASN:ND2	2.26	0.68
1:D:193:ARG:HH11	1:D:193:ARG:HG2	1.59	0.68
1:A:86:GLU:HG2	1:A:87:TYR:CD1	2.29	0.68
1:D:364:PRO:HG2	1:D:368:GLU:CG	2.22	0.68
1:B:233:LEU:O	1:B:271:ALA:HB2	1.94	0.68
1:D:493:GLU:HG2	1:D:497:TYR:CE2	2.29	0.67
1:A:289:HIS:CD2	1:A:441:PRO:HD3	2.29	0.67
1:B:211:LEU:O	1:B:214:ALA:HB3	1.94	0.67
1:D:272:VAL:H	4:D:1121:AMP:N6	1.93	0.67
1:C:63:TYR:CE2	1:C:70:VAL:HG13	2.30	0.67
1:A:365:ASN:HA	1:A:421:MET:CE	2.25	0.67
1:B:336:ILE:CG2	1:B:341:ILE:HB	2.24	0.67
1:D:81:GLN:HB2	6:D:1256:HOH:O	1.95	0.67
1:D:232:LEU:HB3	4:D:1121:AMP:N3	2.10	0.67
1:C:232:LEU:HD22	1:C:332:MET:HE1	1.75	0.67
1:C:410:ASP:O	1:C:414:ARG:HD2	1.94	0.67
1:C:171:ILE:HD12	1:C:507:LEU:CD2	2.26	0.66
1:C:173:GLU:O	1:C:175:PRO:HD3	1.95	0.66
1:D:332:MET:O	1:D:336:ILE:HG13	1.95	0.66
1:B:472:VAL:HG21	1:B:492:LYS:O	1.96	0.66
1:D:78:TYR:HA	1:D:224:MET:HE1	1.77	0.66
1:C:209:ASN:OD1	1:C:212:ARG:NH1	2.28	0.66
1:B:63:TYR:CD2	1:B:70:VAL:HG22	2.31	0.66
1:B:227:VAL:HB	1:B:228:PRO:HD2	1.77	0.66
1:C:115:ASP:OD2	1:C:193:ARG:NH2	2.28	0.66
1:A:360:PHE:CZ	1:A:372:GLU:HG3	2.30	0.66
1:B:1:ALA:H1	5:B:1113:GLN:HE22	1.43	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:HIS:HE2	1:D:428:GLU:HG3	1.59	0.65
1:D:320:VAL:HG22	1:D:497:TYR:CD2	2.30	0.65
1:B:388:ALA:O	1:B:392:MET:HG2	1.95	0.65
1:C:392:MET:HG3	1:C:399:ALA:HB2	1.79	0.65
1:C:232:LEU:HD22	1:C:332:MET:CE	2.26	0.65
1:C:348:GLU:CD	4:C:1114:AMP:H5'1	2.16	0.65
1:C:454:ASP:N	6:C:1309:HOH:O	2.30	0.65
1:A:348:GLU:CD	4:A:1100:AMP:H5'1	2.17	0.65
1:D:473:SER:OG	1:D:475:GLN:N	2.30	0.65
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.61	0.65
1:C:117:LEU:O	1:C:406:LYS:NZ	2.26	0.65
1:C:198:TYR:CD2	1:C:367:LYS:HG3	2.31	0.65
1:C:81:GLN:N	1:C:81:GLN:NE2	2.43	0.65
1:D:361:HIS:NE2	1:D:428:GLU:OE2	2.30	0.64
1:A:199:ASP:HB3	1:A:202:LYS:CE	2.27	0.64
1:B:427:MET:HE1	1:B:447:ARG:N	2.12	0.64
1:B:300:THR:HG22	1:B:303:GLU:N	2.08	0.64
1:B:81:GLN:NE2	6:B:1255:HOH:O	2.27	0.64
1:B:440:LEU:HD23	1:B:440:LEU:N	2.13	0.64
1:B:264:TRP:O	1:B:266:GLN:N	2.28	0.64
1:C:364:PRO:CG	1:C:368:GLU:HG2	2.17	0.64
1:C:281:LYS:HE3	6:C:1288:HOH:O	1.98	0.64
1:B:80:HIS:HD2	1:B:84:ARG:HE	1.46	0.64
1:D:64:ASN:HB3	1:D:67:LYS:CA	2.28	0.64
1:C:289:HIS:NE2	1:C:439:TYR:O	2.31	0.64
1:B:418:GLN:O	1:B:421:MET:HB2	1.97	0.64
1:B:1:ALA:H3	5:B:1113:GLN:HE22	1.46	0.64
1:D:49:ARG:HD3	6:D:1173:HOH:O	1.97	0.63
1:C:415:ILE:HD11	1:C:420:LYS:HE3	1.81	0.63
1:D:277:SER:O	1:D:280:LEU:HB2	1.97	0.63
1:B:307:ALA:O	1:B:311:VAL:HG23	1.98	0.63
1:C:416:ASN:HB3	1:C:419:ASP:OD2	1.98	0.63
1:B:83:LEU:HD13	1:B:101:VAL:CG1	2.28	0.63
1:C:271:ALA:HA	4:C:1114:AMP:N1	2.13	0.63
1:C:44:ILE:O	1:C:45:LEU:HD12	1.99	0.63
1:A:12:ASP:HB3	1:A:15:GLU:CB	2.28	0.63
1:B:199:ASP:HA	1:B:202:LYS:HD3	1.81	0.63
1:C:64:ASN:OD1	1:C:67:LYS:N	2.31	0.63
1:B:358:LEU:HA	1:B:361:HIS:CD2	2.33	0.63
1:A:277:SER:HB2	1:A:278:PRO:HD2	1.80	0.63
1:B:81:GLN:HE21	1:B:81:GLN:N	1.97	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ARG:NH2	1:D:97:SER:O	2.28	0.63
1:A:382:MET:SD	1:A:515:PRO:HG3	2.38	0.62
1:D:12:ASP:OD1	1:D:14:VAL:HB	2.00	0.62
1:C:234:SER:HB3	4:C:1114:AMP:N7	2.15	0.62
1:D:52:ILE:HD12	1:D:52:ILE:N	2.14	0.62
1:C:168:CYS:HB2	1:C:171:ILE:CD1	2.29	0.62
1:C:219:VAL:O	1:C:223:LEU:HG	2.00	0.62
1:A:359:TYR:OH	1:A:376:LYS:HE3	1.99	0.62
1:C:415:ILE:HD11	1:C:420:LYS:CE	2.29	0.62
1:D:12:ASP:OD1	1:D:15:GLU:N	2.27	0.62
1:B:232:LEU:HD12	1:B:346:SER:HB2	1.82	0.62
1:A:500:ILE:O	1:A:503:GLU:HB3	1.99	0.62
1:C:287:ALA:O	1:C:291:GLY:N	2.32	0.62
1:B:461:ILE:O	1:B:464:LEU:N	2.33	0.61
1:A:86:GLU:HG2	1:A:87:TYR:CE1	2.35	0.61
1:B:216:GLU:HG2	1:B:249:TYR:CE1	2.32	0.61
1:D:473:SER:HG	1:D:475:GLN:H	1.45	0.61
1:A:365:ASN:HA	1:A:421:MET:HE1	1.81	0.61
1:D:64:ASN:CB	1:D:68:THR:H	2.14	0.61
1:B:461:ILE:HG22	1:B:465:LYS:HE2	1.83	0.61
1:D:1:ALA:N	5:D:1127:GLN:HE22	1.99	0.61
1:A:365:ASN:HD21	1:A:368:GLU:CG	2.13	0.61
1:B:514:VAL:CG1	1:B:515:PRO:HD2	2.31	0.61
1:B:287:ALA:HB1	1:B:294:HIS:HB2	1.83	0.61
1:A:461:ILE:HG22	1:A:465:LYS:HE2	1.82	0.61
1:D:353:VAL:O	1:D:420:LYS:HE2	2.01	0.60
1:C:63:TYR:CD2	1:C:70:VAL:HG13	2.36	0.60
1:A:351:ASP:HB2	1:A:357:TYR:CZ	2.36	0.60
1:C:211:LEU:HA	1:C:411:VAL:HG11	1.83	0.60
1:D:65:GLN:HG2	1:D:92:GLN:O	2.01	0.60
1:C:6:VAL:HA	1:C:155:LEU:O	2.01	0.60
1:A:168:CYS:HB2	1:A:171:ILE:CD1	2.32	0.60
1:A:460:TRP:CZ2	1:A:464:LEU:HD21	2.37	0.60
1:D:427:MET:H	1:D:430:HIS:CD2	2.05	0.60
1:C:241:ILE:O	1:C:245:ILE:HG13	2.02	0.60
1:B:463:THR:O	1:B:467:VAL:HG23	2.00	0.60
1:D:466:GLU:O	1:D:470:GLN:HG3	2.02	0.60
1:D:51:SER:C	1:D:52:ILE:HD12	2.22	0.60
1:D:507:LEU:HD12	1:D:508:PRO:HD2	1.82	0.60
1:D:466:GLU:O	1:D:466:GLU:HG2	2.00	0.59
1:A:213:GLN:C	1:A:213:GLN:HE21	2.06	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ASP:O	1:D:200:ALA:HB3	2.02	0.59
1:B:216:GLU:O	1:B:220:LYS:HD3	2.02	0.59
1:B:165:VAL:HB	6:B:1164:HOH:O	2.01	0.59
1:B:282:ALA:O	1:B:285:GLU:HB2	2.01	0.59
1:A:111:PRO:HG3	1:A:181:TRP:CD1	2.37	0.59
1:C:336:ILE:O	1:C:339:MET:HB2	2.03	0.59
1:B:428:GLU:HB2	1:B:433:ARG:HH21	1.67	0.59
1:C:431:ILE:O	1:C:434:GLU:HB3	2.02	0.59
1:B:248:LYS:HE2	1:B:249:TYR:CZ	2.38	0.58
1:C:150:ASP:HB3	1:C:152:HIS:N	2.17	0.58
1:A:381:HIS:CE1	1:A:382:MET:HG3	2.38	0.58
1:A:329:MET:HE3	1:A:388:ALA:HA	1.85	0.58
1:B:199:ASP:HB2	1:B:202:LYS:NZ	2.18	0.58
1:B:278:PRO:HD2	1:B:455:GLY:O	2.04	0.58
1:B:279:ASP:HB2	1:B:455:GLY:O	2.04	0.58
1:B:237:LEU:O	1:B:241:ILE:HG13	2.04	0.58
1:B:105:LEU:O	1:B:109:LYS:HB2	2.03	0.58
1:D:387:ARG:HG2	1:D:388:ALA:N	2.18	0.58
1:B:81:GLN:H	1:B:81:GLN:HE21	1.50	0.58
1:B:64:ASN:HD22	1:B:68:THR:H	1.50	0.58
1:B:358:LEU:CA	1:B:361:HIS:HD2	2.15	0.58
1:B:81:GLN:NE2	6:B:1152:HOH:O	2.29	0.58
1:B:358:LEU:O	1:B:361:HIS:HB2	2.03	0.58
1:A:281:LYS:HD3	1:A:285:GLU:OE1	2.04	0.58
1:C:19:LYS:HE3	1:C:167:VAL:CG1	2.33	0.58
1:B:79:ASN:HD22	1:B:118:GLN:CB	2.16	0.58
1:C:365:ASN:N	1:C:365:ASN:ND2	2.52	0.58
1:C:357:TYR:O	1:C:360:PHE:HB2	2.04	0.58
1:B:277:SER:HB2	1:B:278:PRO:HD2	1.86	0.57
1:C:440:LEU:HB3	1:C:441:PRO:CD	2.32	0.57
1:D:358:LEU:HA	1:D:361:HIS:HD2	1.70	0.57
1:A:395:TRP:HH2	1:D:28:ARG:HD3	1.68	0.57
1:A:367:LYS:HE3	1:A:371:GLU:OE1	2.04	0.57
1:D:183:GLN:NE2	6:D:1260:HOH:O	2.35	0.57
1:D:279:ASP:HB3	6:D:1413:HOH:O	2.04	0.57
1:D:50:LEU:CG	1:D:52:ILE:HD11	2.34	0.57
1:D:66:GLN:HB2	6:D:1255:HOH:O	2.05	0.57
1:C:264:TRP:CD1	1:C:265:PRO:HD2	2.39	0.57
1:D:270:PHE:HE2	1:D:339:MET:HE2	1.68	0.57
1:A:89:ASP:OD1	1:A:90:ARG:HG3	2.04	0.57
1:A:416:ASN:OD1	1:A:417:PRO:HD2	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:HIS:HE2	1:D:428:GLU:CG	2.18	0.57
1:B:289:HIS:CG	1:B:441:PRO:HG3	2.39	0.57
1:D:81:GLN:NE2	1:D:81:GLN:HA	2.19	0.57
1:D:50:LEU:HG	1:D:52:ILE:CD1	2.33	0.56
1:A:192:HIS:O	1:A:193:ARG:HD3	2.04	0.56
1:A:199:ASP:HA	1:A:202:LYS:HE2	1.86	0.56
1:D:120:MET:HB2	1:D:143:ILE:HG12	1.86	0.56
1:A:201:VAL:HA	1:A:204:ASN:OD1	2.06	0.56
1:A:280:LEU:HD22	1:A:296:GLU:HG3	1.88	0.56
1:C:212:ARG:HB2	1:C:435:CYS:HB3	1.87	0.56
1:B:30:ARG:HG2	1:B:393:SER:HB3	1.86	0.56
1:A:315:ILE:N	1:A:315:ILE:HD13	2.19	0.56
1:B:300:THR:HG22	1:B:303:GLU:HB2	1.88	0.56
1:A:164:LEU:HB3	1:A:171:ILE:HD11	1.88	0.56
1:B:121:PHE:H	1:B:138:ASP:HB3	1.71	0.56
1:A:199:ASP:CA	1:A:202:LYS:HE2	2.36	0.56
1:B:364:PRO:HG2	1:B:368:GLU:CG	2.36	0.56
1:D:50:LEU:CD2	1:D:52:ILE:HD11	2.35	0.56
1:D:233:LEU:O	1:D:271:ALA:HB2	2.05	0.55
1:C:90:ARG:HD2	1:C:108:GLU:HG3	1.88	0.55
1:D:65:GLN:OE1	1:D:92:GLN:HB2	2.07	0.55
1:B:420:LYS:HE3	6:B:1221:HOH:O	2.06	0.55
1:C:150:ASP:HB2	1:C:154:GLN:H	1.72	0.55
1:A:98:ASP:O	1:A:101:VAL:HG22	2.06	0.55
1:B:427:MET:HE1	1:B:446:TRP:C	2.27	0.55
1:A:301:VAL:HG11	1:A:463:THR:HG21	1.88	0.55
1:A:277:SER:HB2	1:A:455:GLY:O	2.06	0.55
1:A:416:ASN:HB3	1:A:419:ASP:OD2	2.06	0.55
1:B:234:SER:HB3	4:B:1107:AMP:C5	2.41	0.55
1:B:57:ALA:O	1:B:95:THR:HB	2.07	0.55
1:C:337:LYS:HE3	1:C:396:GLY:O	2.06	0.55
1:C:233:LEU:O	1:C:271:ALA:HB2	2.06	0.55
1:A:269:SER:O	1:A:295:HIS:HD2	1.90	0.55
1:C:155:LEU:HD12	1:C:156:TYR:N	2.21	0.55
1:B:325:ALA:O	1:B:328:PRO:HD2	2.07	0.55
1:A:286:VAL:O	1:A:290:LEU:HD13	2.07	0.55
1:D:348:GLU:HG2	1:D:384:ASP:HB3	1.87	0.55
1:B:467:VAL:O	1:B:470:GLN:HB2	2.06	0.55
1:A:60:GLN:HB3	1:A:61:PRO:HA	1.89	0.55
1:A:320:VAL:HG22	1:A:497:TYR:CE2	2.42	0.55
1:A:7:PHE:HB3	1:A:133:TYR:CE2	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:THR:HB	1:C:129:GLU:HG2	1.89	0.55
1:C:105:LEU:HD22	1:C:113:PHE:HB2	1.88	0.55
1:B:352:GLU:OE1	1:B:357:TYR:OH	2.25	0.55
1:B:224:MET:HG3	1:B:224:MET:O	2.08	0.54
1:A:289:HIS:CG	1:A:441:PRO:HD3	2.43	0.54
1:D:277:SER:HB2	1:D:455:GLY:O	2.07	0.54
1:A:274:LEU:HD23	1:A:299:PHE:O	2.07	0.54
1:C:107:GLN:O	1:C:107:GLN:HG2	2.06	0.54
1:B:367:LYS:O	1:B:371:GLU:HG3	2.08	0.54
1:C:301:VAL:HG11	1:C:463:THR:HG21	1.88	0.54
1:C:433:ARG:HD3	1:C:445:ALA:O	2.08	0.54
1:D:192:HIS:O	1:D:193:ARG:HG2	2.08	0.54
1:C:388:ALA:O	1:C:392:MET:HG2	2.07	0.54
1:A:333:SER:HB2	1:A:392:MET:CE	2.37	0.54
1:B:197:ASP:O	1:B:200:ALA:HB3	2.07	0.54
1:B:216:GLU:OE1	1:B:439:TYR:OH	2.25	0.54
1:D:494:ALA:HB1	6:D:1238:HOH:O	2.08	0.54
1:A:468:ALA:HA	1:A:496:LEU:HD12	1.90	0.54
1:A:117:LEU:O	1:A:406:LYS:NZ	2.36	0.54
1:B:90:ARG:HG3	6:B:1312:HOH:O	2.07	0.54
1:D:337:LYS:NZ	6:D:1168:HOH:O	2.31	0.54
1:D:428:GLU:CD	1:D:428:GLU:H	2.10	0.54
1:C:150:ASP:HB2	1:C:154:GLN:N	2.24	0.53
1:B:332:MET:O	1:B:336:ILE:HG13	2.08	0.53
1:B:380:LEU:HD22	1:B:384:ASP:HB2	1.87	0.53
1:A:365:ASN:HD22	1:A:368:GLU:H	1.57	0.53
1:A:365:ASN:ND2	1:A:368:GLU:HG2	2.22	0.53
1:C:334:ARG:HD2	1:C:395:TRP:CZ2	2.44	0.53
1:B:81:GLN:NE2	1:B:81:GLN:N	2.55	0.53
1:D:227:VAL:HB	1:D:228:PRO:CD	2.37	0.53
1:B:201:VAL:CG1	1:B:417:PRO:HD3	2.39	0.53
1:A:12:ASP:HB3	1:A:15:GLU:HB3	1.90	0.53
1:A:242:ILE:HD11	1:A:403:PHE:CE2	2.44	0.53
1:B:468:ALA:HA	1:B:496:LEU:HD12	1.90	0.53
1:D:367:LYS:O	1:D:371:GLU:HG3	2.09	0.53
1:A:268:HIS:HD1	1:A:295:HIS:CE1	2.27	0.53
1:B:199:ASP:HB2	1:B:202:LYS:HE2	1.90	0.53
1:D:361:HIS:HE2	1:D:428:GLU:CD	2.10	0.53
1:C:5:GLY:O	1:C:156:TYR:HA	2.09	0.53
1:D:125:LEU:C	1:D:125:LEU:HD23	2.29	0.53
1:B:199:ASP:HB2	1:B:202:LYS:HZ1	1.72	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLN:NE2	1:A:213:GLN:O	2.42	0.53
1:D:422:CYS:SG	1:D:428:GLU:HA	2.49	0.52
1:B:80:HIS:CG	1:B:98:ASP:HA	2.44	0.52
1:A:415:ILE:HG22	6:A:1398:HOH:O	2.08	0.52
1:B:403:PHE:HB2	6:B:1287:HOH:O	2.08	0.52
1:C:361:HIS:C	1:C:363:ALA:H	2.11	0.52
1:B:247:LYS:HD3	1:B:290:LEU:O	2.10	0.52
1:B:300:THR:HG23	1:B:302:GLN:N	2.24	0.52
1:B:429:LYS:O	1:B:433:ARG:HG2	2.08	0.52
1:A:12:ASP:HB3	1:A:15:GLU:HB2	1.91	0.52
1:D:297:ILE:HG12	1:D:335:LYS:HG2	1.91	0.52
1:C:79:ASN:HB2	1:C:118:GLN:HB3	1.89	0.52
1:A:239:SER:HB3	4:A:1100:AMP:H2'	1.92	0.52
1:C:356:GLY:HA2	1:C:429:LYS:HG3	1.90	0.52
1:B:240:SER:HB3	1:B:440:LEU:HD13	1.92	0.52
1:B:2:SER:OG	1:B:48:GLU:HB2	2.10	0.52
1:D:384:ASP:CG	1:D:387:ARG:HH21	2.12	0.52
1:B:199:ASP:HB2	1:B:202:LYS:CE	2.39	0.52
1:D:358:LEU:O	1:D:361:HIS:HB2	2.09	0.52
1:D:4:PHE:HB3	1:D:46:ALA:HB3	1.92	0.52
1:A:486:TYR:CE1	1:A:487:ASN:ND2	2.78	0.52
1:C:216:GLU:OE1	1:C:439:TYR:OH	2.27	0.52
1:C:264:TRP:CD1	1:C:265:PRO:CD	2.93	0.52
1:D:444:VAL:HG13	6:D:1362:HOH:O	2.09	0.52
1:D:354:PHE:HA	1:D:420:LYS:HE2	1.92	0.51
1:A:504:LEU:C	1:A:506:PRO:HD3	2.30	0.51
1:A:327:THR:HB	1:A:328:PRO:HD3	1.90	0.51
1:A:268:HIS:ND1	1:A:295:HIS:CE1	2.79	0.51
1:D:300:THR:HB	6:D:1226:HOH:O	2.10	0.51
1:B:364:PRO:HG2	1:B:368:GLU:HG2	1.92	0.51
1:B:171:ILE:HD12	1:B:507:LEU:HD21	1.91	0.51
1:C:264:TRP:HD1	1:C:265:PRO:HD3	1.75	0.51
1:C:171:ILE:HD12	1:C:507:LEU:HD22	1.91	0.51
1:D:327:THR:HB	1:D:328:PRO:HD3	1.93	0.51
1:D:229:TYR:C	1:D:341:ILE:HD13	2.31	0.51
1:D:80:HIS:HD2	1:D:84:ARG:HE	1.59	0.51
1:C:358:LEU:O	1:C:361:HIS:N	2.32	0.51
1:D:181:TRP:NE1	1:D:183:GLN:HB2	2.25	0.51
1:B:289:HIS:ND1	1:B:441:PRO:HG3	2.26	0.51
1:B:289:HIS:CB	1:B:441:PRO:HG3	2.41	0.51
1:C:86:GLU:HG2	1:C:87:TYR:CD1	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LEU:HB2	1:C:408:PHE:CE1	2.45	0.51
1:B:379:ALA:O	1:B:383:TYR:HD1	1.93	0.51
1:B:161:MET:HG2	1:B:316:GLU:OE2	2.11	0.51
1:C:19:LYS:O	1:C:22:GLU:HB2	2.11	0.51
1:B:357:TYR:HE2	1:B:376:LYS:HD2	1.75	0.51
1:C:416:ASN:OD1	1:C:418:GLN:HB2	2.11	0.51
1:C:78:TYR:CD1	1:C:119:GLY:HA2	2.46	0.51
1:B:175:PRO:HG2	1:B:187:ILE:HG21	1.93	0.51
1:C:25:ARG:O	1:C:25:ARG:HG3	2.09	0.51
1:D:472:VAL:CG1	1:D:492:LYS:HG2	2.40	0.51
1:B:433:ARG:HB3	1:B:445:ALA:O	2.10	0.51
1:C:359:TYR:CZ	1:C:360:PHE:CE1	2.99	0.51
1:B:125:LEU:C	1:B:125:LEU:HD23	2.32	0.51
1:A:19:LYS:HE3	1:A:22:GLU:OE1	2.11	0.50
1:A:93:PHE:CD2	1:A:100:GLU:HG2	2.46	0.50
1:D:346:SER:OG	1:D:348:GLU:OE2	2.29	0.50
1:B:360:PHE:HD2	1:B:369:LEU:HD12	1.76	0.50
1:B:36:GLY:HA3	1:B:60:GLN:O	2.11	0.50
1:D:387:ARG:NH1	6:D:1342:HOH:O	2.37	0.50
1:D:269:SER:O	1:D:295:HIS:HD2	1.94	0.50
1:C:358:LEU:O	1:C:360:PHE:N	2.45	0.50
1:C:81:GLN:CD	1:C:81:GLN:H	2.13	0.50
1:C:337:LYS:HG2	1:C:395:TRP:O	2.12	0.50
1:B:289:HIS:HB2	1:B:441:PRO:HG3	1.93	0.50
1:B:337:LYS:HE3	1:B:396:GLY:O	2.12	0.50
1:C:127:ASP:OD1	1:C:130:LYS:HD3	2.12	0.50
1:D:320:VAL:HG22	1:D:497:TYR:CE2	2.46	0.50
1:D:1:ALA:H3	5:D:1127:GLN:HE22	1.59	0.50
1:B:204:ASN:O	1:B:416:ASN:ND2	2.44	0.50
1:C:486:TYR:CD1	1:C:487:ASN:HB2	2.47	0.50
1:A:80:HIS:ND1	1:A:98:ASP:HA	2.25	0.50
1:D:205:VAL:O	1:D:205:VAL:HG12	2.11	0.50
1:A:68:THR:HB	1:A:129:GLU:HG2	1.94	0.50
1:B:84:ARG:NH2	1:B:97:SER:O	2.37	0.50
1:B:496:LEU:HD23	1:B:496:LEU:C	2.32	0.50
1:D:192:HIS:C	1:D:193:ARG:HG2	2.32	0.50
1:A:209:ASN:HA	1:A:212:ARG:NH1	2.27	0.50
1:B:342:LYS:N	6:B:1274:HOH:O	2.42	0.50
1:A:147:MET:HE2	1:A:174:PHE:HA	1.93	0.50
1:D:64:ASN:CB	1:D:68:THR:N	2.75	0.49
1:A:329:MET:HE2	1:A:387:ARG:HD2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ASN:HA	1:A:421:MET:HE2	1.92	0.49
1:A:227:VAL:HB	1:A:228:PRO:CD	2.40	0.49
1:A:365:ASN:ND2	1:A:368:GLU:CG	2.75	0.49
1:C:175:PRO:HG2	1:C:187:ILE:HG21	1.94	0.49
1:C:352:GLU:OE1	1:C:357:TYR:OH	2.31	0.49
1:B:38:TYR:OH	1:B:40:SER:HB3	2.12	0.49
1:B:115:ASP:OD2	1:B:406:LYS:HE2	2.11	0.49
1:D:371:GLU:O	1:D:375:ARG:HB2	2.13	0.49
1:C:217:ASP:HA	1:C:220:LYS:HD3	1.94	0.49
1:B:81:GLN:CD	1:B:82:ALA:H	2.16	0.49
1:A:218:SER:O	1:A:222:HIS:ND1	2.46	0.49
1:A:401:VAL:HG23	1:A:401:VAL:O	2.13	0.49
1:D:147:MET:HA	1:D:156:TYR:O	2.13	0.49
1:B:270:PHE:HE2	1:B:339:MET:HE2	1.78	0.49
1:B:349:GLY:HA3	1:B:404:LEU:HD21	1.95	0.49
1:A:289:HIS:CD2	1:A:290:LEU:HD12	2.47	0.49
1:A:1:ALA:HB1	1:A:48:GLU:O	2.12	0.49
1:C:186:GLU:HB2	1:C:188:ARG:NH2	2.27	0.49
1:A:199:ASP:HA	1:A:202:LYS:CE	2.42	0.49
1:A:474:ASP:O	1:A:478:GLU:HG3	2.13	0.49
1:C:234:SER:HB3	4:C:1114:AMP:C8	2.48	0.49
1:A:238:ASP:CG	1:A:429:LYS:HZ1	2.15	0.49
1:B:79:ASN:HD22	1:B:118:GLN:HB2	1.78	0.49
1:B:201:VAL:HA	1:B:204:ASN:OD1	2.13	0.49
1:C:504:LEU:C	1:C:506:PRO:HD3	2.33	0.48
1:C:365:ASN:O	1:C:421:MET:HE1	2.13	0.48
1:B:285:GLU:O	1:B:288:ASN:HB2	2.13	0.48
1:D:348:GLU:CG	4:D:1121:AMP:H5'1	2.43	0.48
1:A:64:ASN:ND2	1:A:68:THR:OG1	2.45	0.48
1:A:320:VAL:HG22	1:A:497:TYR:CD2	2.49	0.48
1:A:440:LEU:HB3	1:A:441:PRO:CD	2.41	0.48
1:C:111:PRO:HG3	1:C:181:TRP:CE2	2.48	0.48
1:C:418:GLN:O	1:C:421:MET:HB2	2.14	0.48
1:B:167:VAL:HG22	1:B:167:VAL:O	2.14	0.48
1:D:464:LEU:HA	1:D:464:LEU:HD12	1.62	0.48
1:B:430:HIS:CD2	1:B:446:TRP:HZ3	2.31	0.48
1:D:81:GLN:CA	1:D:81:GLN:NE2	2.76	0.48
1:D:274:LEU:HD23	1:D:299:PHE:O	2.14	0.48
1:D:165:VAL:N	1:D:166:PRO:CD	2.77	0.48
1:A:60:GLN:HA	1:A:61:PRO:C	2.35	0.48
1:A:431:ILE:HG23	1:A:432:LEU:N	2.29	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:HG13	1:A:206:THR:N	2.29	0.48
1:B:357:TYR:O	1:B:360:PHE:HB2	2.14	0.48
1:A:242:ILE:HD11	1:A:403:PHE:CD2	2.49	0.48
1:B:68:THR:O	1:B:69:HIS:HD2	1.97	0.47
1:C:264:TRP:HD1	1:C:265:PRO:CD	2.26	0.47
1:D:80:HIS:O	1:D:84:ARG:HG3	2.14	0.47
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.79	0.47
1:B:49:ARG:NH2	1:B:51:SER:HB3	2.29	0.47
1:D:387:ARG:CG	1:D:388:ALA:N	2.77	0.47
1:A:199:ASP:HB3	1:A:202:LYS:HE2	1.95	0.47
1:B:158:ALA:HB3	1:B:164:LEU:HD13	1.96	0.47
1:B:17:ARG:HD3	6:B:1121:HOH:O	2.14	0.47
1:B:484:PHE:O	1:B:488:THR:HG23	2.14	0.47
1:A:383:TYR:O	1:A:386:ALA:HB3	2.14	0.47
1:A:387:ARG:CG	1:A:388:ALA:N	2.77	0.47
1:A:209:ASN:O	1:A:213:GLN:HB2	2.14	0.47
1:B:334:ARG:NH1	1:C:35:SER:OG	2.48	0.47
1:B:301:VAL:HG12	1:B:302:GLN:N	2.30	0.47
1:B:83:LEU:CB	1:B:101:VAL:HG11	2.43	0.47
1:B:467:VAL:O	1:B:467:VAL:HG12	2.14	0.47
1:C:147:MET:SD	1:C:172:LYS:HE3	2.55	0.47
1:A:381:HIS:CE1	1:A:382:MET:CG	2.98	0.47
1:C:264:TRP:C	1:C:266:GLN:H	2.18	0.47
1:D:210:GLU:HA	6:D:1273:HOH:O	2.14	0.47
1:C:321:THR:HB	6:C:1343:HOH:O	2.14	0.47
1:A:378:LEU:CD1	1:A:378:LEU:N	2.77	0.47
1:B:207:ASP:CG	1:B:210:GLU:HB2	2.35	0.47
1:C:272:VAL:HA	1:C:297:ILE:O	2.14	0.47
1:A:28:ARG:HD3	1:D:395:TRP:HH2	1.80	0.47
1:D:273:GLY:O	1:D:298:HIS:HA	2.14	0.47
1:C:358:LEU:H	1:C:358:LEU:HG	1.44	0.47
1:B:81:GLN:NE2	1:B:82:ALA:N	2.58	0.47
1:C:410:ASP:O	1:C:414:ARG:HB2	2.14	0.47
1:B:514:VAL:HG12	1:B:515:PRO:HD2	1.95	0.47
1:C:386:ALA:O	1:C:390:LYS:HB2	2.15	0.47
1:B:219:VAL:O	1:B:223:LEU:HG	2.15	0.47
1:D:233:LEU:HD22	1:D:235:GLY:H	1.80	0.47
1:B:79:ASN:HB2	1:B:118:GLN:HB3	1.96	0.47
1:B:289:HIS:CG	1:B:441:PRO:HD3	2.50	0.47
1:A:333:SER:HB2	1:A:392:MET:HE3	1.95	0.47
1:C:162:LYS:HB2	1:C:316:GLU:OE1	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:VAL:HG23	1:C:413:MET:CE	2.45	0.47
1:B:372:GLU:HA	1:B:372:GLU:OE2	2.15	0.47
1:C:268:HIS:HA	1:C:293:VAL:O	2.15	0.47
1:D:280:LEU:HD12	1:D:280:LEU:HA	1.78	0.46
1:D:193:ARG:HH11	1:D:193:ARG:CG	2.28	0.46
1:D:334:ARG:HB2	1:D:395:TRP:CE2	2.50	0.46
1:B:1:ALA:HB1	1:B:48:GLU:O	2.16	0.46
1:A:289:HIS:HD2	1:A:290:LEU:HD12	1.79	0.46
1:D:268:HIS:CE1	1:D:293:VAL:HG11	2.51	0.46
1:B:507:LEU:O	1:B:510:ALA:N	2.37	0.46
1:B:324:ARG:NH2	1:B:461:ILE:CG2	2.78	0.46
1:C:184:ASP:OD1	1:C:188:ARG:NH2	2.39	0.46
1:A:335:LYS:HE3	1:D:34:TRP:CZ3	2.50	0.46
1:D:118:GLN:NE2	1:D:405:ASP:OD1	2.48	0.46
1:A:287:ALA:HB1	1:A:294:HIS:HB2	1.97	0.46
1:C:433:ARG:HD2	1:C:446:TRP:CZ3	2.49	0.46
1:B:240:SER:HB3	1:B:440:LEU:CD1	2.46	0.46
1:D:12:ASP:OD1	1:D:15:GLU:HG3	2.15	0.46
1:B:245:ILE:HG23	1:B:249:TYR:CE1	2.50	0.46
1:B:241:ILE:HD13	1:B:436:PHE:HB2	1.97	0.46
1:A:409:LEU:O	1:A:413:MET:HB2	2.14	0.46
1:B:494:ALA:HB2	6:B:1298:HOH:O	2.15	0.46
1:D:64:ASN:C	1:D:67:LYS:H	2.18	0.46
1:B:277:SER:HB2	1:B:455:GLY:O	2.16	0.46
1:B:427:MET:SD	1:B:433:ARG:NE	2.89	0.46
1:A:464:LEU:HD12	6:A:1342:HOH:O	2.15	0.46
1:A:280:LEU:CD1	1:A:298:HIS:CD2	2.98	0.46
1:D:364:PRO:CG	1:D:368:GLU:HG2	2.29	0.46
1:D:78:TYR:CD2	1:D:224:MET:HE2	2.50	0.46
1:B:199:ASP:CB	1:B:202:LYS:NZ	2.78	0.46
1:C:227:VAL:HB	1:C:228:PRO:HD2	1.98	0.46
1:D:406:LYS:NZ	6:D:1196:HOH:O	2.33	0.46
1:D:472:VAL:HB	1:D:492:LYS:CG	2.16	0.46
1:B:248:LYS:HG2	1:B:249:TYR:N	2.31	0.46
1:B:79:ASN:HD22	1:B:118:GLN:N	2.14	0.46
1:D:351:ASP:OD2	1:D:429:LYS:HE3	2.16	0.46
1:B:81:GLN:CD	1:B:82:ALA:N	2.70	0.46
1:A:277:SER:HB2	1:A:278:PRO:CD	2.46	0.46
1:A:213:GLN:NE2	1:A:213:GLN:CA	2.79	0.46
1:C:335:LYS:HG3	6:C:1328:HOH:O	2.16	0.46
1:D:129:GLU:HA	1:D:129: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:173:GLU:O	1:D:175:PRO:HD3	2.15	0.46
1:B:49:ARG:NH1	1:B:58:GLY:HA3	2.31	0.46
1:B:64:ASN:HB2	1:B:69:HIS:H	1.81	0.45
1:D:224:MET:O	1:D:400:ARG:NH1	2.43	0.45
1:A:475:GLN:HA	1:A:478:GLU:CD	2.37	0.45
1:A:430:HIS:O	1:A:433:ARG:HB2	2.16	0.45
1:A:437:GLU:OE1	1:A:446:TRP:NE1	2.49	0.45
1:B:300:THR:HG22	1:B:303:GLU:CB	2.46	0.45
1:D:357:TYR:O	1:D:360:PHE:HB2	2.16	0.45
1:A:165:VAL:N	1:A:166:PRO:CD	2.79	0.45
1:D:514:VAL:HG13	1:D:515:PRO:HD2	1.97	0.45
1:A:351:ASP:OD2	1:A:429:LYS:NZ	2.43	0.45
1:C:280:LEU:HG	1:C:296:GLU:HG3	1.99	0.45
1:C:171:ILE:CD1	1:C:507:LEU:HD22	2.46	0.45
1:B:28:ARG:HG3	1:B:48:GLU:OE2	2.15	0.45
1:C:198:TYR:CD2	1:C:367:LYS:CG	2.99	0.45
1:A:165:VAL:N	1:A:166:PRO:HD2	2.32	0.45
1:B:269:SER:OG	1:B:294:HIS:ND1	2.43	0.45
1:C:19:LYS:HE3	1:C:167:VAL:HG11	1.98	0.45
1:A:1:ALA:N	5:A:1106:GLN:HE22	2.14	0.45
1:D:64:ASN:HB2	1:D:68:THR:N	2.32	0.45
1:B:150:ASP:HB2	1:B:154:GLN:H	1.82	0.45
1:B:248:LYS:CG	1:B:249:TYR:N	2.78	0.45
1:D:496:LEU:C	1:D:496:LEU:HD12	2.37	0.45
1:D:78:TYR:HD2	1:D:224:MET:HE2	1.82	0.45
1:A:464:LEU:HA	1:A:464:LEU:HD13	1.80	0.45
1:C:358:LEU:C	1:C:360:PHE:H	2.20	0.45
1:B:296:GLU:HG2	1:B:298:HIS:NE2	2.32	0.45
1:A:428:GLU:CD	1:A:428:GLU:H	2.20	0.45
1:B:300:THR:HG23	1:B:302:GLN:H	1.82	0.45
1:B:105:LEU:O	1:B:109:LYS:N	2.45	0.45
1:B:79:ASN:ND2	1:B:118:GLN:CB	2.79	0.45
1:C:76:GLU:O	1:C:119:GLY:HA3	2.16	0.45
1:D:509:SER:HB2	6:D:1211:HOH:O	2.17	0.45
1:C:135:ILE:O	1:C:179:TYR:HA	2.17	0.45
1:D:234:SER:HB3	4:D:1121:AMP:C5	2.51	0.45
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.57	0.45
1:A:25:ARG:NH1	1:A:25:ARG:HG2	2.30	0.45
1:B:201:VAL:O	1:B:204:ASN:OD1	2.34	0.45
1:A:34:TRP:CE3	1:D:335:LYS:HD2	2.51	0.45
1:B:481:ARG:N	1:B:488:THR:HG21	2.32	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:VAL:HG11	1:B:16:LEU:HD13	1.99	0.45
1:C:270:PHE:CD2	1:C:295:HIS:HB2	2.51	0.45
1:D:232:LEU:O	1:D:239:SER:HB2	2.17	0.45
1:B:427:MET:SD	1:B:433:ARG:HD2	2.56	0.45
1:D:380:LEU:CD2	1:D:384:ASP:HB2	2.47	0.45
1:A:59:ALA:O	1:A:62:LEU:HD23	2.17	0.45
1:D:64:ASN:HB3	1:D:68:THR:H	1.82	0.44
1:C:150:ASP:OD1	1:C:154:GLN:NE2	2.39	0.44
1:D:361:HIS:CD2	1:D:428:GLU:HG3	2.52	0.44
1:C:358:LEU:O	1:C:361:HIS:HB2	2.17	0.44
1:D:125:LEU:HD23	1:D:126:TYR:N	2.33	0.44
1:A:475:GLN:HA	1:A:478:GLU:OE2	2.17	0.44
1:D:319:ASP:O	1:D:323:ILE:HD12	2.17	0.44
1:C:514:VAL:CG1	1:C:515:PRO:HD2	2.46	0.44
1:C:198:TYR:CD2	1:C:367:LYS:HA	2.53	0.44
1:D:514:VAL:CG1	1:D:515:PRO:HD2	2.47	0.44
1:A:372:GLU:OE2	1:A:372:GLU:HA	2.17	0.44
1:B:49:ARG:NH2	1:B:53:VAL:O	2.51	0.44
1:D:227:VAL:HB	1:D:228:PRO:HD2	1.99	0.44
1:B:367:LYS:HG2	1:B:368:GLU:OE2	2.17	0.44
1:B:28:ARG:HB3	6:B:1344:HOH:O	2.16	0.44
1:C:333:SER:OG	1:C:395:TRP:HB2	2.18	0.44
1:B:327:THR:N	1:B:328:PRO:CD	2.81	0.44
1:C:146:TYR:OH	1:C:390:LYS:NZ	2.51	0.44
1:C:165:VAL:N	1:C:166:PRO:CD	2.79	0.44
1:A:65:GLN:OE1	1:A:92:GLN:N	2.36	0.44
1:D:427:MET:HB3	1:D:433:ARG:NE	2.32	0.44
1:A:290:LEU:N	1:A:290:LEU:HD12	2.33	0.44
1:B:472:VAL:HB	1:B:492:LYS:HB3	1.98	0.44
1:B:461:ILE:O	1:B:464:LEU:HB2	2.18	0.44
1:B:241:ILE:HD13	1:B:436:PHE:CB	2.48	0.44
1:A:395:TRP:CH2	1:D:28:ARG:HD3	2.50	0.44
1:B:357:TYR:CD2	1:B:359:TYR:CE1	3.05	0.44
1:B:244:ALA:HA	1:B:290:LEU:HD21	1.99	0.44
1:D:207:ASP:O	1:D:210:GLU:HB3	2.18	0.44
1:B:49:ARG:HG2	1:B:50:LEU:N	2.32	0.44
1:C:356:GLY:HA3	1:C:429:LYS:HE3	1.98	0.44
1:C:165:VAL:N	1:C:166:PRO:HD2	2.33	0.44
1:A:120:MET:O	1:A:121:PHE:HB3	2.17	0.44
1:A:130:LYS:HG3	6:A:1273:HOH:O	2.17	0.44
1:D:204:ASN:ND2	6:D:1324:HOH:O	2.30	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:VAL:HG22	1:D:497:TYR:HD2	1.78	0.44
1:B:79:ASN:ND2	1:B:118:GLN:HB2	2.33	0.44
1:D:160:GLU:HB3	1:D:316:GLU:OE1	2.18	0.44
1:D:150:ASP:HB3	1:D:152:HIS:H	1.83	0.44
1:D:234:SER:HB3	4:D:1121:AMP:C4	2.53	0.44
1:D:233:LEU:CD2	1:D:235:GLY:H	2.31	0.44
1:B:217:ASP:HA	1:B:220:LYS:HD3	1.99	0.44
1:A:351:ASP:CB	1:A:357:TYR:CE1	3.00	0.44
1:B:343:MET:HA	1:B:398:GLU:O	2.18	0.44
1:B:248:LYS:HE2	1:B:249:TYR:CE1	2.52	0.44
1:B:469:ALA:HA	1:B:492:LYS:HD2	2.00	0.44
1:C:301:VAL:O	1:C:305:LEU:HG	2.18	0.44
1:B:481:ARG:NH2	6:B:1198:HOH:O	2.49	0.44
1:A:37:ILE:HG12	1:A:38:TYR:N	2.33	0.44
1:C:433:ARG:HH11	1:C:433:ARG:HD3	1.69	0.43
1:D:78:TYR:CD2	1:D:224:MET:CE	3.01	0.43
1:B:484:PHE:N	1:B:485:PRO:CD	2.79	0.43
1:B:143:ILE:HG23	1:B:144:PRO:HD2	2.00	0.43
1:C:325:ALA:O	1:C:328:PRO:HD2	2.18	0.43
1:A:216:GLU:O	1:A:220:LYS:HD3	2.18	0.43
1:C:28:ARG:NH2	6:C:1292:HOH:O	2.50	0.43
1:A:289:HIS:CE1	1:A:441:PRO:HD3	2.53	0.43
1:A:165:VAL:HG11	6:A:1156:HOH:O	2.18	0.43
1:A:232:LEU:HB3	4:A:1100:AMP:N3	2.32	0.43
1:A:301:VAL:CG1	1:A:463:THR:HG21	2.48	0.43
1:B:357:TYR:HD2	1:B:359:TYR:CE1	2.35	0.43
1:B:270:PHE:CD1	1:B:270:PHE:N	2.84	0.43
1:C:145:LEU:HG	1:C:146:TYR:N	2.32	0.43
1:D:118:GLN:OE1	1:D:407:LYS:HD2	2.18	0.43
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.79	0.43
1:A:387:ARG:HH11	1:A:387:ARG:CG	2.31	0.43
1:C:138:ASP:O	1:C:177:GLY:N	2.49	0.43
1:A:271:ALA:HA	4:A:1100:AMP:N1	2.34	0.43
1:A:14:VAL:HG12	1:A:15:GLU:N	2.32	0.43
1:B:493:GLU:HG2	1:B:497:TYR:CE2	2.53	0.43
1:D:363:ALA:HA	1:D:364:PRO:HD3	1.73	0.43
1:B:245:ILE:HG22	1:B:249:TYR:HD1	1.84	0.43
1:B:320:VAL:O	1:B:324:ARG:HG3	2.18	0.43
1:C:105:LEU:HB3	1:C:113:PHE:CG	2.53	0.43
1:C:464:LEU:HD12	1:C:464:LEU:HA	1.69	0.43
1:C:65:GLN:HG3	1:C:65:GLN:H	1.14	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:HIS:N	1:B:268:HIS:CD2	2.86	0.43
1:D:64:ASN:ND2	1:D:68:THR:OG1	2.51	0.43
1:B:49:ARG:NH1	1:B:58:GLY:CA	2.82	0.43
1:A:199:ASP:CB	1:A:202:LYS:HE2	2.47	0.43
1:B:277:SER:CB	1:B:278:PRO:HD2	2.48	0.43
1:A:348:GLU:CG	4:A:1100:AMP:H5'1	2.48	0.43
1:A:273:GLY:O	1:A:298:HIS:HA	2.18	0.43
1:B:381:HIS:CE1	1:B:382:MET:HG2	2.54	0.43
1:B:3:ILE:HG21	1:B:3:ILE:HD13	1.68	0.43
1:D:68:THR:O	1:D:69:HIS:HD2	2.01	0.43
1:C:327:THR:N	1:C:328:PRO:CD	2.82	0.43
1:C:17:ARG:HD3	6:C:1144:HOH:O	2.19	0.43
1:D:168:CYS:HB3	1:D:170:THR:O	2.18	0.43
1:A:365:ASN:ND2	1:A:368:GLU:H	2.16	0.43
1:A:238:ASP:OD2	1:A:429:LYS:HE2	2.18	0.43
1:A:280:LEU:HD11	1:A:298:HIS:CD2	2.54	0.43
1:A:268:HIS:CG	1:A:295:HIS:HE2	2.35	0.43
1:D:78:TYR:HD2	1:D:224:MET:CE	2.32	0.43
1:B:49:ARG:NE	1:B:51:SER:HB3	2.34	0.42
1:C:232:LEU:HB3	4:C:1114:AMP:N3	2.34	0.42
1:B:357:TYR:O	1:B:360:PHE:N	2.46	0.42
1:B:38:TYR:CZ	1:B:40:SER:HB3	2.54	0.42
1:C:504:LEU:O	1:C:506:PRO:HD3	2.19	0.42
1:D:152:HIS:HB2	1:D:154:GLN:HG3	2.00	0.42
1:A:145:LEU:HD11	1:A:157:VAL:HG13	2.01	0.42
1:D:105:LEU:HD22	1:D:113:PHE:HB2	2.01	0.42
1:D:476:GLN:HB3	1:D:495:TYR:CZ	2.54	0.42
1:C:248:LYS:HE2	1:C:249:TYR:OH	2.20	0.42
1:B:361:HIS:HA	1:B:422:CYS:SG	2.59	0.42
1:C:60:GLN:HA	1:C:61:PRO:C	2.40	0.42
1:D:52:ILE:CD1	1:D:52:ILE:N	2.82	0.42
1:B:68:THR:HG21	1:B:129:GLU:OE2	2.19	0.42
1:B:480:ALA:HB1	1:B:488:THR:HG22	2.02	0.42
1:C:162:LYS:HZ2	1:C:162:LYS:HB2	1.85	0.42
1:A:135:ILE:HD13	1:A:157:VAL:HG21	2.00	0.42
1:D:230:GLY:O	1:D:344:VAL:HA	2.18	0.42
1:C:234:SER:HB3	4:C:1114:AMP:C4	2.54	0.42
1:A:505:PHE:N	1:A:506:PRO:HD3	2.35	0.42
1:A:147:MET:HE3	1:A:172:LYS:HG3	2.01	0.42
1:C:415:ILE:CD1	1:C:420:LYS:HE3	2.48	0.42
1:C:198:TYR:HD2	1:C:367:LYS:HG3	1.81	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:C	1:A:166:PRO:HD2	2.40	0.42
1:C:114:LEU:HD22	1:C:190:TYR:CE2	2.55	0.42
1:A:280:LEU:HD22	1:A:296:GLU:CG	2.48	0.42
1:C:461:ILE:O	1:C:465:LYS:HG3	2.20	0.42
1:D:410:ASP:O	1:D:414:ARG:HB2	2.20	0.42
1:A:197:ASP:O	1:A:200:ALA:HB3	2.18	0.42
1:A:329:MET:CE	1:A:388:ALA:HA	2.48	0.42
1:B:277:SER:HB2	1:B:278:PRO:CD	2.49	0.42
1:A:364:PRO:HG2	1:A:368:GLU:HG3	2.01	0.42
1:B:264:TRP:HD1	1:B:265:PRO:HD2	1.85	0.42
1:B:464:LEU:HD12	1:B:464:LEU:HA	1.43	0.42
1:A:380:LEU:HD22	1:A:384:ASP:HB2	2.01	0.42
1:C:198:TYR:CE2	1:C:367:LYS:HB2	2.54	0.42
1:B:324:ARG:NH2	1:B:461:ILE:HG21	2.35	0.42
1:B:287:ALA:HA	1:B:292:THR:HG22	2.01	0.42
1:C:111:PRO:HG3	1:C:181:TRP:CD1	2.55	0.42
1:C:231:VAL:O	1:C:269:SER:HA	2.19	0.42
1:C:422:CYS:HG	1:C:428:GLU:HA	1.85	0.42
1:C:433:ARG:HB3	1:C:445:ALA:O	2.19	0.42
1:D:358:LEU:H	1:D:358:LEU:HG	1.61	0.42
1:A:461:ILE:CG2	1:A:465:LYS:HE2	2.48	0.42
1:A:18:LYS:HD2	6:A:1113:HOH:O	2.19	0.42
1:D:132:ALA:HB1	1:D:182:SER:OG	2.20	0.42
1:D:198:TYR:HE1	1:D:417:PRO:HG2	1.85	0.42
1:D:475:GLN:HB2	6:D:1400:HOH:O	2.20	0.42
1:B:324:ARG:CZ	1:B:461:ILE:HG21	2.49	0.42
1:C:160:GLU:HB3	1:C:316:GLU:OE1	2.19	0.42
1:A:330:TYR:HE1	6:D:1134:HOH:O	2.03	0.42
1:C:349:GLY:HA3	1:C:404:LEU:HD21	2.02	0.42
1:C:137:ARG:NH2	6:C:1283:HOH:O	2.52	0.42
1:A:27:MET:HA	1:A:29:HIS:CE1	2.55	0.42
1:C:381:HIS:CE1	1:C:382:MET:HG3	2.55	0.42
1:B:277:SER:CB	1:B:278:PRO:CD	2.98	0.41
1:D:201:VAL:HG12	6:D:1324:HOH:O	2.20	0.41
1:A:75:GLY:N	5:A:1106:GLN:OE1	2.53	0.41
1:C:372:GLU:HA	1:C:375:ARG:NH1	2.35	0.41
1:C:237:LEU:O	1:C:240:SER:HB2	2.20	0.41
1:D:277:SER:OG	1:D:280:LEU:HD22	2.20	0.41
1:D:86:GLU:O	1:D:86:GLU:HG2	2.20	0.41
1:A:129:GLU:HA	1:A:129:GLU:OE2	2.21	0.41
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.79	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:NH2	5:B:1113:GLN:O	2.53	0.41
1:B:245:ILE:CG2	1:B:249:TYR:CD1	3.04	0.41
1:B:464:LEU:HG	1:B:497:TYR:OH	2.20	0.41
1:A:198:TYR:CD2	1:A:367:LYS:HG3	2.55	0.41
1:C:52:ILE:HG22	1:C:53:VAL:HG23	2.02	0.41
1:B:240:SER:CB	1:B:440:LEU:CD1	2.98	0.41
1:C:289:HIS:CD2	1:C:441:PRO:HD3	2.56	0.41
1:B:379:ALA:HB1	1:B:383:TYR:CE1	2.55	0.41
1:A:431:ILE:CG2	1:A:432:LEU:N	2.83	0.41
1:D:137:ARG:HD2	1:D:145:LEU:HB3	2.02	0.41
1:C:15:GLU:O	1:C:18:LYS:HB3	2.20	0.41
1:B:81:GLN:HG3	6:B:1255:HOH:O	2.20	0.41
1:B:216:GLU:C	1:B:220:LYS:HD3	2.41	0.41
1:B:64:ASN:ND2	1:B:68:THR:OG1	2.53	0.41
1:B:231:VAL:O	1:B:269:SER:HA	2.21	0.41
1:A:460:TRP:CE2	1:A:464:LEU:HD21	2.55	0.41
1:D:507:LEU:HA	1:D:508:PRO:HD2	1.79	0.41
1:B:121:PHE:N	1:B:138:ASP:HB3	2.34	0.41
1:B:337:LYS:HA	1:B:337:LYS:HD3	1.75	0.41
1:B:274:LEU:HG	1:B:456:VAL:O	2.20	0.41
1:D:345:LEU:HD23	1:D:402:PRO:HG3	2.02	0.41
1:D:318:TYR:CZ	1:D:514:VAL:HB	2.56	0.41
1:B:326:SER:OG	1:B:387:ARG:HB2	2.20	0.41
1:A:219:VAL:O	1:A:223:LEU:HG	2.21	0.41
1:B:71:LEU:HG	1:B:73:VAL:HG23	2.02	0.41
1:B:49:ARG:NE	1:B:51:SER:CB	2.84	0.41
1:D:281:LYS:CD	1:D:281:LYS:N	2.78	0.41
1:A:199:ASP:CB	1:A:202:LYS:NZ	2.76	0.41
1:A:289:HIS:NE2	1:A:441:PRO:HD3	2.35	0.41
1:A:209:ASN:CG	1:A:212:ARG:HH12	2.24	0.41
1:C:358:LEU:C	1:C:360:PHE:N	2.73	0.41
1:C:86:GLU:HG2	1:C:87:TYR:CE1	2.55	0.41
1:A:147:MET:HA	1:A:156:TYR:O	2.21	0.41
1:B:280:LEU:HA	1:B:280:LEU:HD12	1.90	0.41
1:B:208:LYS:H	1:B:208:LYS:HG2	1.56	0.41
1:C:115:ASP:O	1:C:406:LYS:NZ	2.38	0.41
1:B:234:SER:HB3	4:B:1107:AMP:C4	2.56	0.41
1:C:150:ASP:HB3	1:C:153:GLY:H	1.86	0.41
1:C:45:LEU:N	1:C:45:LEU:HD12	2.36	0.41
1:B:392:MET:HG3	1:B:399:ALA:HB2	2.02	0.41
1:C:273:GLY:HA2	1:C:456:VAL:HG22	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:PHE:HA	1:C:485:PRO:HD2	1.77	0.41
1:A:484:PHE:HD1	1:A:502:GLU:OE1	2.04	0.41
1:C:364:PRO:HG2	1:C:368:GLU:OE2	2.22	0.40
1:C:337:LYS:HD3	1:C:337:LYS:HA	1.64	0.40
1:B:28:ARG:HD3	1:C:395:TRP:HH2	1.86	0.40
1:C:320:VAL:HG12	1:C:324:ARG:CD	2.43	0.40
1:A:441:PRO:O	1:A:444:VAL:N	2.52	0.40
1:C:287:ALA:HB1	1:C:294:HIS:HB2	2.02	0.40
1:C:186:GLU:HB2	1:C:188:ARG:CZ	2.51	0.40
1:A:92:GLN:CD	1:A:94:GLN:HE22	2.25	0.40
1:A:230:GLY:O	1:A:344:VAL:HA	2.21	0.40
1:D:219:VAL:O	1:D:223:LEU:HG	2.21	0.40
1:B:476:GLN:NE2	1:B:495:TYR:CE1	2.89	0.40
1:C:432:LEU:HD12	1:C:432:LEU:HA	1.83	0.40
1:B:245:ILE:CG2	1:B:249:TYR:HD1	2.34	0.40
1:B:199:ASP:CB	1:B:202:LYS:CE	2.99	0.40
1:B:346:SER:O	1:B:402:PRO:HD2	2.22	0.40
1:A:65:GLN:HG3	1:A:65:GLN:H	1.32	0.40
1:C:98:ASP:OD1	5:C:1120:GLN:N	2.55	0.40
1:C:9:ILE:HG23	1:C:16:LEU:HD12	2.03	0.40
1:B:462:ASP:O	1:B:466:GLU:HB2	2.22	0.40
1:C:274:LEU:HD23	1:C:299:PHE:O	2.20	0.40
1:D:139:HIS:HB2	1:D:191:TYR:CG	2.55	0.40
1:C:113:PHE:O	1:C:116:ASP:HB2	2.22	0.40
1:D:165:VAL:HG11	1:D:506:PRO:HD2	2.04	0.40
1:D:140:LEU:HA	1:D:140:LEU:HD23	1.94	0.40
1:A:187:ILE:HD13	1:A:187:ILE:HG21	1.83	0.40
1:B:272:VAL:HG23	1:B:297:ILE:HG22	2.04	0.40
1:C:114:LEU:HB3	1:C:190:TYR:CE2	2.57	0.40
1:D:137:ARG:NH1	1:D:174:PHE:O	2.44	0.40
1:C:12:ASP:OD1	1:C:15:GLU:HB2	2.21	0.40
1:D:418:GLN:NE2	6:D:1286:HOH:O	2.54	0.40
1:B:37:ILE:HD12	1:B:46:ALA:HB2	2.04	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	491/553 (89%)	465 (95%)	24 (5%)	2 (0%)	39	33
1	B	487/553 (88%)	449 (92%)	31 (6%)	7 (1%)	14	6
1	C	487/553 (88%)	450 (92%)	33 (7%)	4 (1%)	24	15
1	D	487/553 (88%)	467 (96%)	18 (4%)	2 (0%)	39	33
All	All	1952/2212 (88%)	1831 (94%)	106 (5%)	15 (1%)	24	15

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	GLU
1	C	266	GLN
1	A	138	ASP
1	B	265	PRO
1	B	460	TRP
1	C	364	PRO
1	A	506	PRO
1	C	359	TYR
1	D	202	LYS
1	B	248	LYS
1	B	275	PRO
1	C	362	LYS
1	D	460	TRP
1	B	508	PRO
1	B	278	PRO

### 5.3.2 Protein sidechains [i](#)

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	418/462 (90%)	371 (89%)	47 (11%)	7	4
1	B	414/462 (90%)	358 (86%)	56 (14%)	5	2
1	C	414/462 (90%)	364 (88%)	50 (12%)	6	3
1	D	412/462 (89%)	371 (90%)	41 (10%)	9	5
All	All	1658/1848 (90%)	1464 (88%)	194 (12%)	7	3

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	16	LEU
1	A	18	LYS
1	A	22	GLU
1	A	35	SER
1	A	65	GLN
1	A	70	VAL
1	A	89	ASP
1	A	90	ARG
1	A	112	GLU
1	A	114	LEU
1	A	147	MET
1	A	150	ASP
1	A	151	GLU
1	A	157	VAL
1	A	162	LYS
1	A	171	ILE
1	A	181	TRP
1	A	199	ASP
1	A	202	LYS
1	A	205	VAL
1	A	208	LYS
1	A	213	GLN
1	A	238	ASP
1	A	281	LYS
1	A	285	GLU
1	A	337	LYS
1	A	339	MET
1	A	346	SER
1	A	348	GLU
1	A	365	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	375	ARG
1	A	378	LEU
1	A	387	ARG
1	A	406	LYS
1	A	429	LYS
1	A	440	LEU
1	A	443	SER
1	A	447	ARG
1	A	449	LYS
1	A	450	GLU
1	A	459	SER
1	A	462	ASP
1	A	464	LEU
1	A	470	GLN
1	A	481	ARG
1	A	502	GLU
1	B	15	GLU
1	B	19	LYS
1	B	42	ASN
1	B	51	SER
1	B	66	GLN
1	B	80	HIS
1	B	81	GLN
1	B	84	ARG
1	B	90	ARG
1	B	103	LEU
1	B	114	LEU
1	B	129	GLU
1	B	150	ASP
1	B	157	VAL
1	B	162	LYS
1	B	164	LEU
1	B	201	VAL
1	B	208	LYS
1	B	220	LYS
1	B	226	ASP
1	B	233	LEU
1	B	241	ILE
1	B	247	LYS
1	B	277	SER
1	B	280	LEU
1	B	281	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	300	THR
1	B	301	VAL
1	B	329	MET
1	B	335	LYS
1	B	337	LYS
1	B	346	SER
1	B	348	GLU
1	B	358	LEU
1	B	368	GLU
1	B	369	LEU
1	B	376	LYS
1	B	378	LEU
1	B	382	MET
1	B	387	ARG
1	B	406	LYS
1	B	418	GLN
1	B	427	MET
1	B	429	LYS
1	B	433	ARG
1	B	439	TYR
1	B	456	VAL
1	B	459	SER
1	B	462	ASP
1	B	464	LEU
1	B	471	GLN
1	B	473	SER
1	B	481	ARG
1	B	490	THR
1	B	502	GLU
1	B	509	SER
1	C	19	LYS
1	C	25	ARG
1	C	42	ASN
1	C	49	ARG
1	C	51	SER
1	C	65	GLN
1	C	67	LYS
1	C	70	VAL
1	C	81	GLN
1	C	89	ASP
1	C	103	LEU
1	C	130	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	150	ASP
1	C	157	VAL
1	C	162	LYS
1	C	164	LEU
1	C	171	ILE
1	C	197	ASP
1	C	202	LYS
1	C	209	ASN
1	C	242	ILE
1	C	247	LYS
1	C	264	TRP
1	C	277	SER
1	C	280	LEU
1	C	329	MET
1	C	335	LYS
1	C	337	LYS
1	C	339	MET
1	C	341	ILE
1	C	348	GLU
1	C	358	LEU
1	C	359	TYR
1	C	365	ASN
1	C	368	GLU
1	C	369	LEU
1	C	376	LYS
1	C	384	ASP
1	C	393	SER
1	C	418	GLN
1	C	420	LYS
1	C	427	MET
1	C	428	GLU
1	C	429	LYS
1	C	433	ARG
1	C	440	LEU
1	C	443	SER
1	C	464	LEU
1	C	474	ASP
1	C	509	SER
1	D	10	LYS
1	D	25	ARG
1	D	51	SER
1	D	65	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	67	LYS
1	D	81	GLN
1	D	89	ASP
1	D	103	LEU
1	D	129	GLU
1	D	150	ASP
1	D	162	LYS
1	D	166	PRO
1	D	184	ASP
1	D	188	ARG
1	D	199	ASP
1	D	203	ASP
1	D	220	LYS
1	D	222	HIS
1	D	225	SER
1	D	233	LEU
1	D	266	GLN
1	D	280	LEU
1	D	281	LYS
1	D	310	ASP
1	D	335	LYS
1	D	337	LYS
1	D	341	ILE
1	D	357	TYR
1	D	358	LEU
1	D	365	ASN
1	D	387	ARG
1	D	418	GLN
1	D	427	MET
1	D	428	GLU
1	D	429	LYS
1	D	454	ASP
1	D	459	SER
1	D	464	LEU
1	D	473	SER
1	D	496	LEU
1	D	502	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	81	GLN
1	A	94	GLN
1	A	183	GLN
1	A	213	GLN
1	A	284	GLN
1	A	288	ASN
1	A	365	ASN
1	A	448	GLN
1	A	451	GLN
1	A	471	GLN
1	B	64	ASN
1	B	69	HIS
1	B	74	ASN
1	B	79	ASN
1	B	80	HIS
1	B	81	GLN
1	B	183	GLN
1	B	192	HIS
1	B	288	ASN
1	B	302	GLN
1	B	361	HIS
1	B	470	GLN
1	B	476	GLN
1	C	42	ASN
1	C	56	ASN
1	C	65	GLN
1	C	81	GLN
1	C	183	GLN
1	C	288	ASN
1	C	365	ASN
1	C	470	GLN
1	C	471	GLN
1	D	56	ASN
1	D	80	HIS
1	D	81	GLN
1	D	152	HIS
1	D	192	HIS
1	D	284	GLN
1	D	288	ASN
1	D	430	HIS
1	D	470	GLN
1	D	471	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 28 ligands modelled in this entry, 4 are monoatomic and 14 are modelled with single atom - leaving 10 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	AMP	A	1100	-	20,25,25	1.25	3 (15%)	22,38,38	1.90	5 (22%)
2	IUM	A	1102	-	0,1,2	0.00	-	0,0,1	0.00	-
5	GLN	A	1106	-	6,9,9	1.61	1 (16%)	5,11,11	0.30	0
4	AMP	B	1107	2	20,25,25	1.26	3 (15%)	22,38,38	1.29	3 (13%)
5	GLN	B	1113	-	6,9,9	1.29	1 (16%)	5,11,11	0.30	0
4	AMP	C	1114	-	20,25,25	1.23	3 (15%)	22,38,38	2.02	5 (22%)
5	GLN	C	1120	-	6,9,9	1.34	1 (16%)	5,11,11	0.51	0
4	AMP	D	1121	2	20,25,25	1.01	2 (10%)	22,38,38	2.31	7 (31%)
2	IUM	D	1122	4	0,1,2	0.00	-	0,0,1	0.00	-
5	GLN	D	1127	-	6,9,9	1.34	1 (16%)	5,11,11	0.45	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	AMP	A	1100	-	-	0/6/26/26	0/3/3/3
2	IUM	A	1102	-	-	0/0/0/0	0/0/0/0
5	GLN	A	1106	-	-	0/5/9/9	0/0/0/0
4	AMP	B	1107	2	-	0/6/26/26	0/3/3/3
5	GLN	B	1113	-	-	0/5/9/9	0/0/0/0
4	AMP	C	1114	-	-	0/6/26/26	0/3/3/3
5	GLN	C	1120	-	-	0/5/9/9	0/0/0/0
4	AMP	D	1121	2	-	0/6/26/26	0/3/3/3
2	IUM	D	1122	4	-	0/0/0/0	0/0/0/0
5	GLN	D	1127	-	-	0/5/9/9	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1106	GLN	CA-N	-3.81	1.33	1.48
5	B	1113	GLN	CA-N	-3.11	1.35	1.48
5	C	1120	GLN	CA-N	-3.10	1.35	1.48
5	D	1127	GLN	CA-N	-2.99	1.36	1.48
4	B	1107	AMP	C2-N1	2.31	1.38	1.33
4	D	1121	AMP	O3'-C3'	2.36	1.48	1.43
4	C	1114	AMP	C2-N1	2.39	1.38	1.33
4	B	1107	AMP	O2'-C2'	2.43	1.48	1.43
4	A	1100	AMP	C2-N1	2.55	1.38	1.33
4	D	1121	AMP	O2'-C2'	2.97	1.50	1.43
4	B	1107	AMP	O3'-C3'	2.98	1.50	1.43
4	A	1100	AMP	O3'-C3'	3.00	1.50	1.43
4	A	1100	AMP	O2'-C2'	3.02	1.50	1.43
4	C	1114	AMP	O3'-C3'	3.13	1.50	1.43
4	C	1114	AMP	O2'-C2'	3.15	1.50	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1121	AMP	O2P-P-O5'	-5.28	91.36	106.56
4	C	1114	AMP	C2'-C3'-C4'	-5.25	91.82	102.61
4	D	1121	AMP	C2'-C3'-C4'	-4.24	93.90	102.61
4	D	1121	AMP	N6-C6-N1	-4.00	110.63	119.20
4	D	1121	AMP	C4'-O4'-C1'	-3.76	105.59	109.72
4	A	1100	AMP	O2P-P-O5'	-3.33	96.97	106.56
4	C	1114	AMP	O4'-C4'-C3'	-2.52	100.06	105.15
4	A	1100	AMP	C2'-C3'-C4'	-2.52	97.43	102.61
4	B	1107	AMP	C2'-C3'-C4'	-2.37	97.73	102.61
4	A	1100	AMP	C4-C5-N7	2.11	111.42	109.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1121	AMP	O4'-C1'-N9	2.19	112.69	108.10
4	D	1121	AMP	O3P-P-O2P	2.21	115.78	107.38
4	B	1107	AMP	O2P-P-O5'	2.22	112.97	106.56
4	C	1114	AMP	O2'-C2'-C3'	2.28	119.24	111.83
4	A	1100	AMP	O2'-C2'-C3'	3.02	121.64	111.83
4	B	1107	AMP	O3'-C3'-C2'	3.12	121.99	111.83
4	C	1114	AMP	O2P-P-O5'	3.23	115.86	106.56
4	D	1121	AMP	O3'-C3'-C2'	3.52	123.28	111.83
4	C	1114	AMP	O3'-C3'-C2'	4.31	125.83	111.83
4	A	1100	AMP	O3'-C3'-C2'	5.09	128.39	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1100	AMP	5	0
5	A	1106	GLN	2	0
4	B	1107	AMP	3	0
5	B	1113	GLN	4	0
4	C	1114	AMP	7	0
5	C	1120	GLN	1	0
4	D	1121	AMP	8	0
5	D	1127	GLN	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 [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.