



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 08:11 PM EDT

PDB ID : 3DYM  
Title : E. coli (lacZ) beta-galactosidase (H418E)  
Authors : Juers, D.H.; Huber, R.E.; Matthews, B.W.  
Deposited on : 2008-07-28  
Resolution : 2.05 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

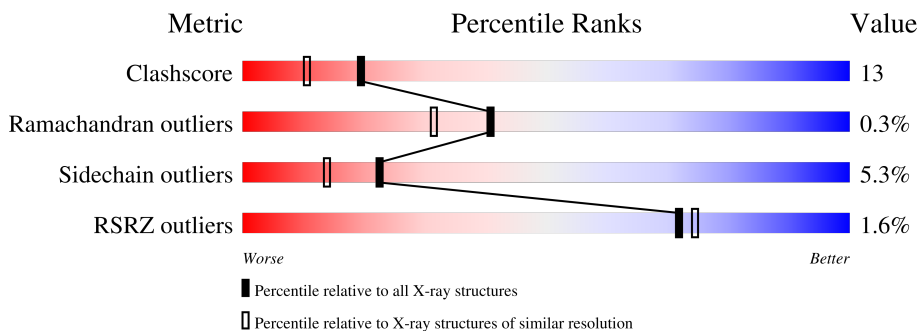
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	 2% (poor fit), 64% (0 outliers), 27% (1 outlier), 7% (2 outliers), 2% (3+ outliers)
1	B	1023	 % (poor fit), 62% (0 outliers), 29% (1 outlier), 7% (2 outliers), % (3+ outliers)
1	C	1023	 % (poor fit), 63% (0 outliers), 28% (1 outlier), 8% (2 outliers), % (3+ outliers)
1	D	1023	 2% (poor fit), 64% (0 outliers), 29% (1 outlier), 5% (2 outliers), % (3+ outliers)

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	DMS	A	8412	-	-	X	-
4	DMS	D	8419	-	-	X	-
4	DMS	D	8703	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 36314 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1011	8124	5137	1438	1511	38	0	0	0
1	B	1011	8124	5137	1438	1511	38	0	0	0
1	C	1011	8124	5137	1438	1511	38	0	0	0
1	D	1011	8124	5137	1438	1511	38	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P00722
A	2	SER	-	expression tag	UNP P00722
A	3	HIS	-	expression tag	UNP P00722
A	4	MET	-	expression tag	UNP P00722
A	5	LEU	-	expression tag	UNP P00722
A	6	GLU	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	418	GLU	HIS	engineered mutation	UNP P00722
B	1	GLY	-	expression tag	UNP P00722
B	2	SER	-	expression tag	UNP P00722
B	3	HIS	-	expression tag	UNP P00722
B	4	MET	-	expression tag	UNP P00722
B	5	LEU	-	expression tag	UNP P00722
B	6	GLU	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	418	GLU	HIS	engineered mutation	UNP P00722
C	1	GLY	-	expression tag	UNP P00722
C	2	SER	-	expression tag	UNP P00722
C	3	HIS	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	expression tag	UNP P00722
C	5	LEU	-	expression tag	UNP P00722
C	6	GLU	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	418	GLU	HIS	engineered mutation	UNP P00722
D	1	GLY	-	expression tag	UNP P00722
D	2	SER	-	expression tag	UNP P00722
D	3	HIS	-	expression tag	UNP P00722
D	4	MET	-	expression tag	UNP P00722
D	5	LEU	-	expression tag	UNP P00722
D	6	GLU	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	418	GLU	HIS	engineered mutation	UNP P00722

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

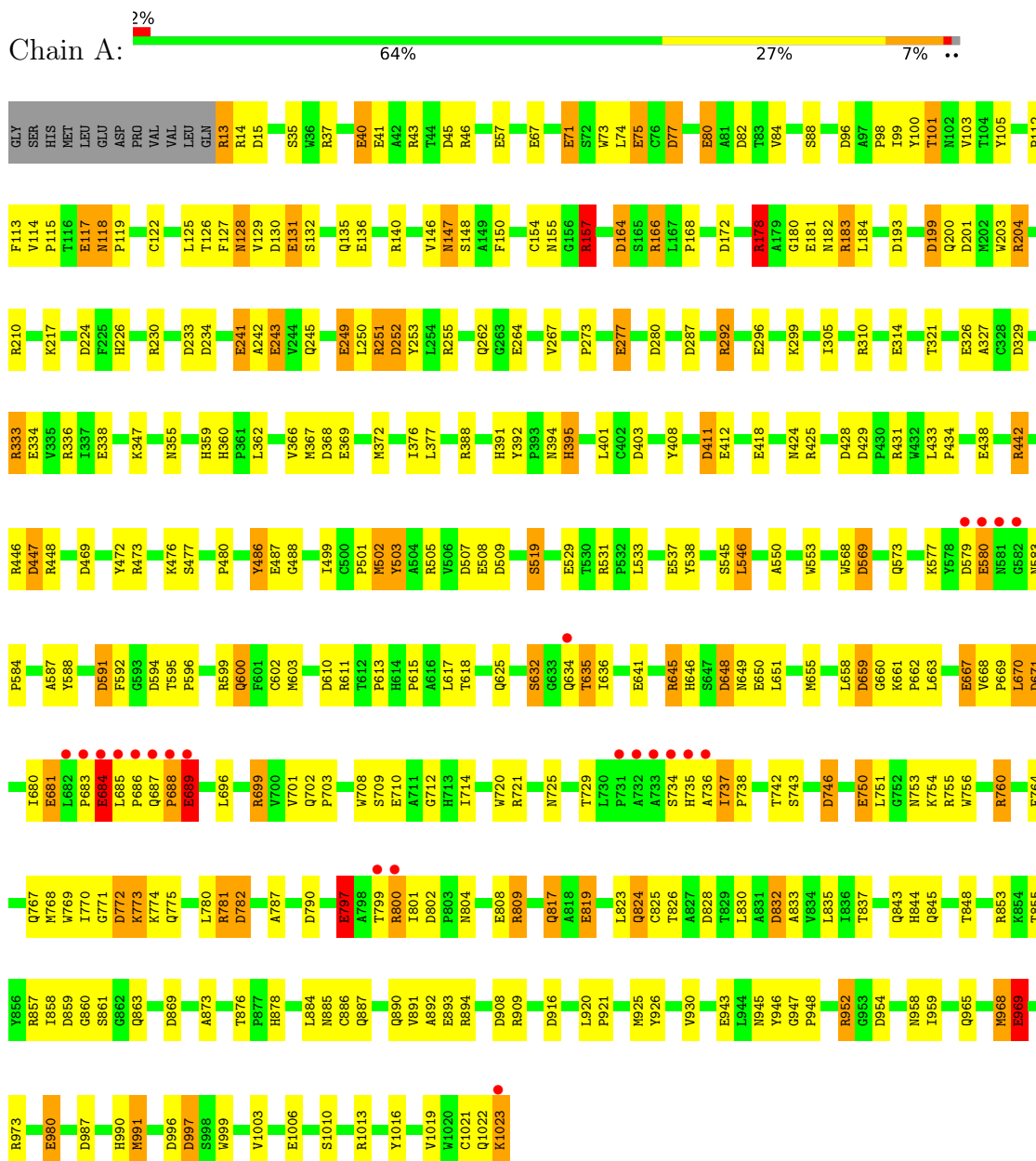
- Molecule 5 is water.

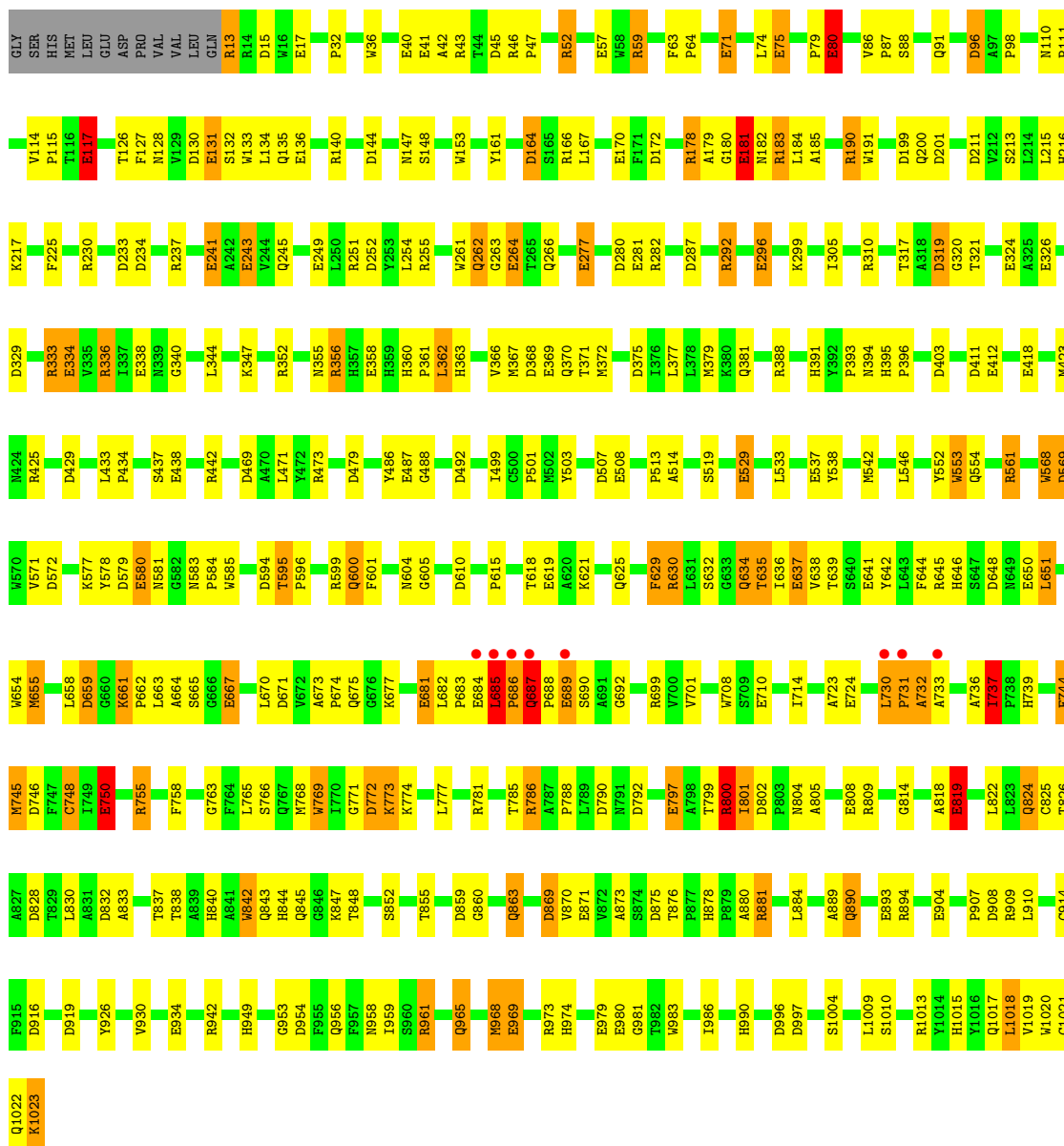
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	871	Total	O	0	0
			871	871		
5	B	864	Total	O	0	0
			864	864		
5	C	838	Total	O	0	0
			838	838		
5	D	891	Total	O	0	0
			891	891		

### 3 Residue-property plots [i](#)

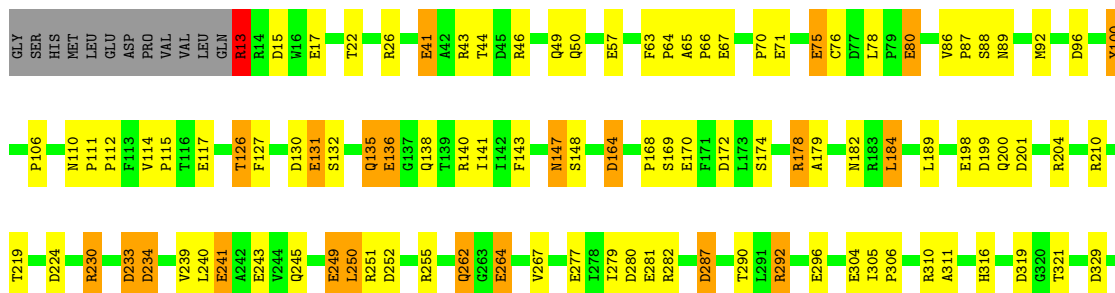
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

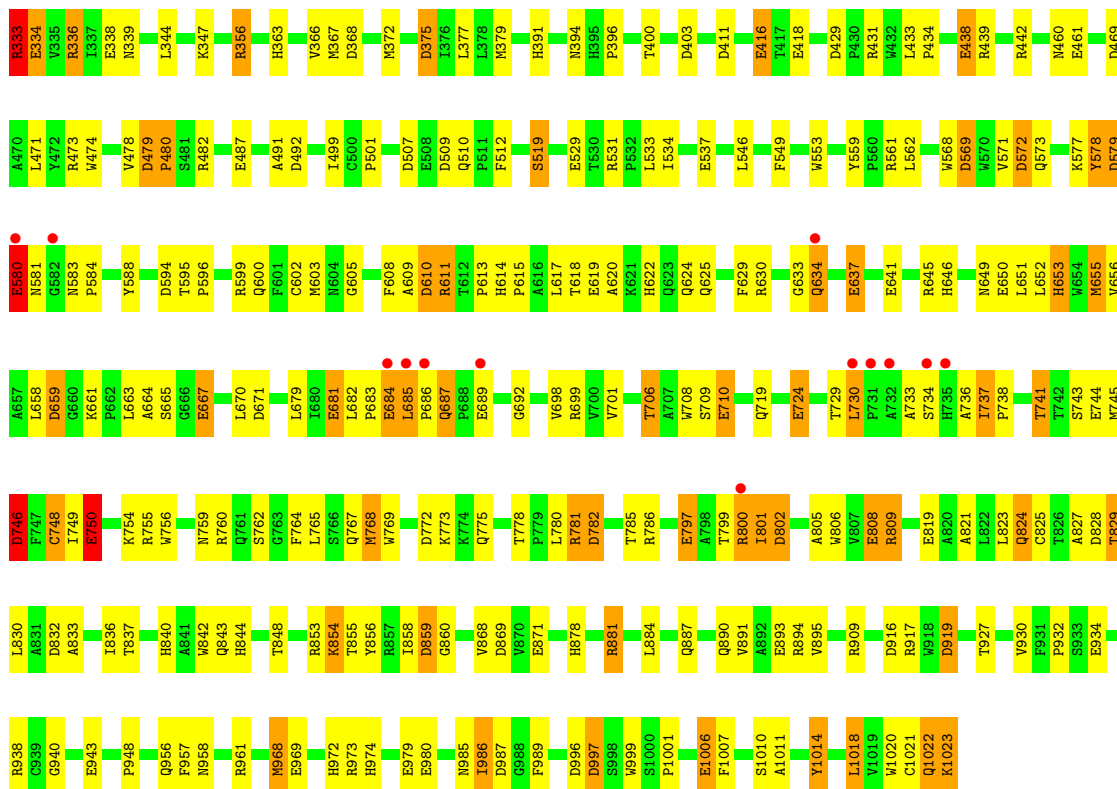
- Molecule 1: Beta-galactosidase



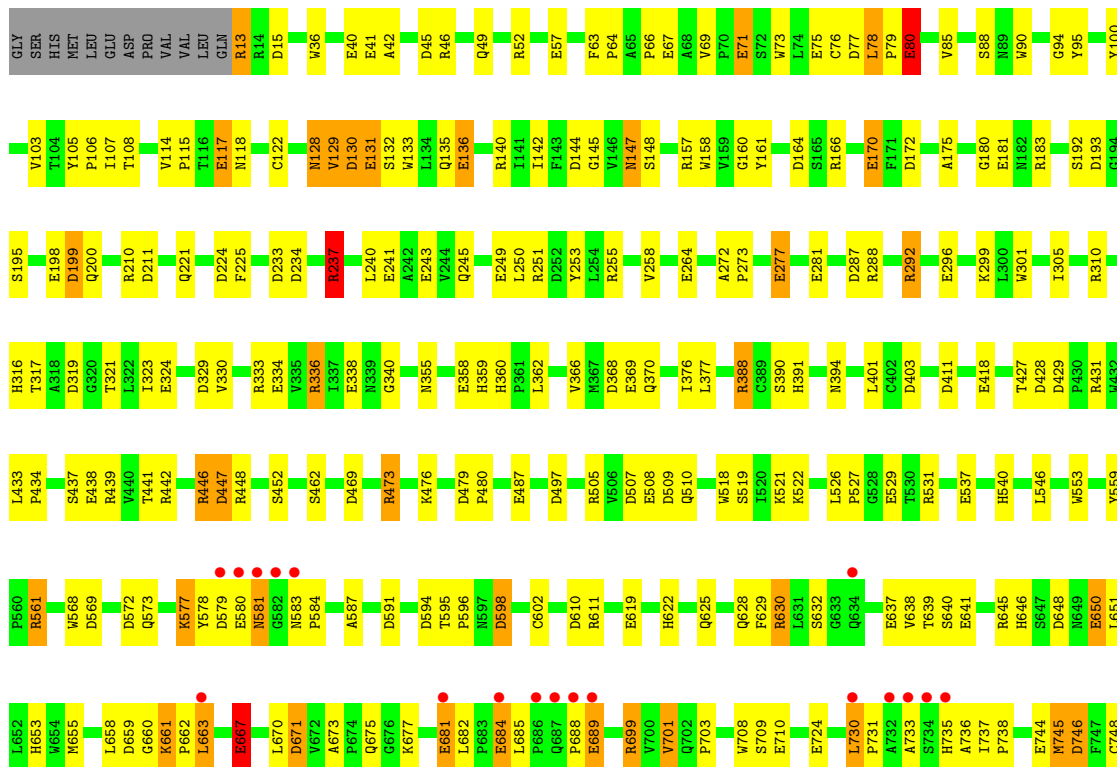


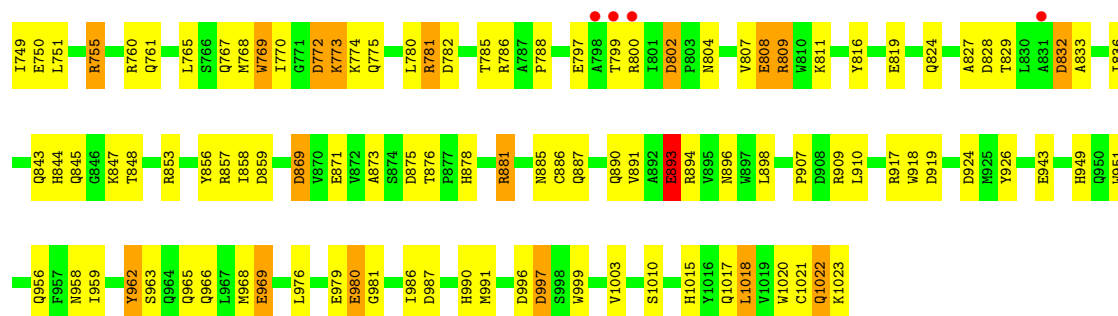
• Molecule 1: Beta-galactosidase





● Molecule 1: Beta-galactosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.34Å 167.16Å 200.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.05 34.55 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.50-2.05) 99.3 (34.55-2.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.05Å)	Xtrriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.158 , 0.251 0.158 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtrriage
Anisotropy	0.484	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 116.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	36314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0670e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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: DMS, NA, MG

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	1.06	45/8365 (0.5%)	1.66	163/11412 (1.4%)
1	B	1.08	53/8365 (0.6%)	1.66	160/11412 (1.4%)
1	C	1.07	50/8365 (0.6%)	1.65	160/11412 (1.4%)
1	D	1.08	51/8365 (0.6%)	1.68	169/11412 (1.5%)
All	All	1.07	199/33460 (0.6%)	1.66	652/45648 (1.4%)

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	681	GLU	CD-OE2	9.01	1.35	1.25
1	C	170	GLU	CD-OE2	8.98	1.35	1.25
1	A	681	GLU	CD-OE2	8.76	1.35	1.25
1	A	249	GLU	CD-OE2	8.37	1.34	1.25
1	D	893	GLU	CD-OE2	8.29	1.34	1.25
1	D	819	GLU	CD-OE2	8.07	1.34	1.25
1	B	418	GLU	CD-OE2	8.05	1.34	1.25
1	B	57	GLU	CD-OE2	7.95	1.34	1.25
1	D	808	GLU	CD-OE2	7.89	1.34	1.25
1	A	750	GLU	CD-OE2	7.69	1.34	1.25
1	A	487	GLU	CD-OE2	7.67	1.34	1.25
1	B	117	GLU	CD-OE2	7.66	1.34	1.25
1	B	667	GLU	CD-OE2	7.65	1.34	1.25
1	D	281	GLU	CD-OE2	7.62	1.34	1.25
1	B	537	GLU	CD-OE2	7.58	1.33	1.25
1	A	641	GLU	CD-OE2	7.57	1.33	1.25
1	B	326	GLU	CD-OE2	7.55	1.33	1.25
1	C	80	GLU	CD-OE2	7.53	1.33	1.25
1	A	667	GLU	CD-OE2	7.43	1.33	1.25
1	C	893	GLU	CD-OE2	7.39	1.33	1.25
1	B	819	GLU	CD-OE2	7.39	1.33	1.25
1	A	684	GLU	CD-OE2	7.36	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	418	GLU	CD-OE2	7.31	1.33	1.25
1	B	979	GLU	CD-OE2	7.29	1.33	1.25
1	A	117	GLU	CD-OE2	7.26	1.33	1.25
1	B	637	GLU	CD-OE2	7.26	1.33	1.25
1	C	537	GLU	CD-OE1	-7.23	1.17	1.25
1	D	170	GLU	CD-OE2	7.23	1.33	1.25
1	A	580	GLU	CD-OE2	7.21	1.33	1.25
1	B	281	GLU	CD-OE2	7.21	1.33	1.25
1	D	41	GLU	CD-OE2	7.20	1.33	1.25
1	D	80	GLU	CD-OE2	7.18	1.33	1.25
1	A	131	GLU	CD-OE2	7.16	1.33	1.25
1	C	710	GLU	CD-OE2	7.14	1.33	1.25
1	B	689	GLU	CD-OE2	7.12	1.33	1.25
1	C	819	GLU	CD-OE2	7.11	1.33	1.25
1	B	170	GLU	CD-OE2	7.09	1.33	1.25
1	B	249	GLU	CD-OE2	7.04	1.33	1.25
1	A	650	GLU	CD-OE2	7.03	1.33	1.25
1	B	580	GLU	CD-OE2	7.02	1.33	1.25
1	C	667	GLU	CD-OE2	7.02	1.33	1.25
1	C	249	GLU	CD-OE2	6.99	1.33	1.25
1	D	369	GLU	CD-OE2	6.99	1.33	1.25
1	D	249	GLU	CD-OE2	6.97	1.33	1.25
1	D	667	GLU	CD-OE2	6.94	1.33	1.25
1	D	689	GLU	CD-OE2	6.94	1.33	1.25
1	C	744	GLU	CD-OE2	6.91	1.33	1.25
1	A	943	GLU	CD-OE2	6.91	1.33	1.25
1	B	980	GLU	CD-OE2	6.89	1.33	1.25
1	D	181	GLU	CD-OE2	6.88	1.33	1.25
1	D	684	GLU	CD-OE2	6.88	1.33	1.25
1	D	117	GLU	CD-OE2	6.88	1.33	1.25
1	D	71	GLU	CD-OE2	6.86	1.33	1.25
1	D	136	GLU	CD-OE2	6.84	1.33	1.25
1	C	338	GLU	CD-OE2	6.80	1.33	1.25
1	C	537	GLU	CD-OE2	6.80	1.33	1.25
1	B	969	GLU	CD-OE2	6.79	1.33	1.25
1	D	277	GLU	CD-OE2	6.79	1.33	1.25
1	B	71	GLU	CD-OE2	6.78	1.33	1.25
1	A	819	GLU	CD-OE2	6.78	1.33	1.25
1	C	461	GLU	CD-OE2	6.78	1.33	1.25
1	C	684	GLU	CD-OE2	6.77	1.33	1.25
1	A	710	GLU	CD-OE2	6.77	1.33	1.25
1	C	71	GLU	CD-OE2	6.77	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	619	GLU	CD-OE2	6.76	1.33	1.25
1	D	980	GLU	CD-OE2	6.74	1.33	1.25
1	A	314	GLU	CD-OE2	6.72	1.33	1.25
1	C	580	GLU	CD-OE2	6.72	1.33	1.25
1	D	57	GLU	CD-OE2	6.67	1.32	1.25
1	A	296	GLU	CD-OE2	6.67	1.32	1.25
1	C	264	GLU	CD-OE2	6.66	1.32	1.25
1	D	710	GLU	CD-OE2	6.66	1.32	1.25
1	D	580	GLU	CD-OE2	6.66	1.32	1.25
1	B	684	GLU	CD-OE2	6.66	1.32	1.25
1	C	277	GLU	CD-OE2	6.61	1.32	1.25
1	B	904	GLU	CD-OE2	6.60	1.32	1.25
1	B	710	GLU	CD-OE2	6.60	1.32	1.25
1	C	681	GLU	CD-OE2	6.60	1.32	1.25
1	A	980	GLU	CD-OE2	6.60	1.32	1.25
1	B	136	GLU	CD-OE2	6.58	1.32	1.25
1	B	241	GLU	CD-OE2	6.58	1.32	1.25
1	D	131	GLU	CD-OE2	6.57	1.32	1.25
1	D	438	GLU	CD-OE2	6.56	1.32	1.25
1	B	369	GLU	CD-OE2	6.56	1.32	1.25
1	C	689	GLU	CD-OE2	6.55	1.32	1.25
1	D	296	GLU	CD-OE2	6.51	1.32	1.25
1	C	980	GLU	CD-OE2	6.51	1.32	1.25
1	A	75	GLU	CD-OE2	6.50	1.32	1.25
1	D	487	GLU	CD-OE2	6.49	1.32	1.25
1	D	241	GLU	CD-OE2	6.49	1.32	1.25
1	C	75	GLU	CD-OE2	6.48	1.32	1.25
1	A	136	GLU	CD-OE2	6.47	1.32	1.25
1	C	198	GLU	CD-OE2	6.43	1.32	1.25
1	B	277	GLU	CD-OE2	6.42	1.32	1.25
1	B	529	GLU	CD-OE2	6.41	1.32	1.25
1	D	750	GLU	CD-OE2	6.41	1.32	1.25
1	D	979	GLU	CD-OE2	6.40	1.32	1.25
1	A	893	GLU	CD-OE2	6.38	1.32	1.25
1	C	296	GLU	CD-OE2	6.38	1.32	1.25
1	D	338	GLU	CD-OE2	6.38	1.32	1.25
1	A	67	GLU	CD-OE2	6.37	1.32	1.25
1	A	969	GLU	CD-OE2	6.37	1.32	1.25
1	C	57	GLU	CD-OE2	6.36	1.32	1.25
1	B	724	GLU	CD-OE2	6.35	1.32	1.25
1	D	650	GLU	CD-OE2	6.34	1.32	1.25
1	C	117	GLU	CD-OE2	6.33	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	GLU	CD-OE2	6.31	1.32	1.25
1	B	893	GLU	CD-OE2	6.28	1.32	1.25
1	B	41	GLU	CD-OE2	6.26	1.32	1.25
1	B	296	GLU	CD-OE2	6.26	1.32	1.25
1	D	264	GLU	CD-OE2	6.25	1.32	1.25
1	C	1006	GLU	CD-OE2	6.23	1.32	1.25
1	C	797	GLU	CD-OE2	6.23	1.32	1.25
1	A	689	GLU	CD-OE2	6.19	1.32	1.25
1	C	136	GLU	CD-OE2	6.16	1.32	1.25
1	D	508	GLU	CD-OE2	6.14	1.32	1.25
1	B	80	GLU	CD-OE2	6.13	1.32	1.25
1	B	808	GLU	CD-OE2	6.13	1.32	1.25
1	B	508	GLU	CD-OE2	6.12	1.32	1.25
1	A	264	GLU	CD-OE2	6.11	1.32	1.25
1	B	934	GLU	CD-OE2	6.11	1.32	1.25
1	C	979	GLU	CD-OE2	6.10	1.32	1.25
1	D	637	GLU	CD-OE2	6.07	1.32	1.25
1	A	243	GLU	CD-OE2	6.03	1.32	1.25
1	B	681	GLU	CD-OE2	6.02	1.32	1.25
1	C	934	GLU	CD-OE2	6.00	1.32	1.25
1	A	537	GLU	CD-OE2	6.00	1.32	1.25
1	A	277	GLU	CD-OE2	6.00	1.32	1.25
1	A	71	GLU	CD-OE2	5.98	1.32	1.25
1	A	41	GLU	CD-OE2	5.98	1.32	1.25
1	A	529	GLU	CD-OE2	5.95	1.32	1.25
1	C	281	GLU	CD-OE2	5.95	1.32	1.25
1	D	40	GLU	CD-OE2	5.92	1.32	1.25
1	B	744	GLU	CD-OE2	5.92	1.32	1.25
1	C	17	GLU	CD-OE2	5.90	1.32	1.25
1	A	40	GLU	CD-OE2	5.89	1.32	1.25
1	A	369	GLU	CD-OE2	5.86	1.32	1.25
1	B	487	GLU	CD-OE2	5.85	1.32	1.25
1	B	181	GLU	CD-OE2	5.72	1.31	1.25
1	B	871	GLU	CD-OE2	5.71	1.31	1.25
1	B	131	GLU	CD-OE2	5.70	1.31	1.25
1	D	537	GLU	CD-OE2	5.69	1.31	1.25
1	C	750	GLU	CD-OE2	5.66	1.31	1.25
1	D	529	GLU	CD-OE2	5.61	1.31	1.25
1	A	808	GLU	CD-OE2	5.61	1.31	1.25
1	D	724	GLU	CD-OE2	5.61	1.31	1.25
1	C	241	GLU	CD-OE2	5.61	1.31	1.25
1	C	969	GLU	CD-OE2	5.59	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	797	GLU	CD-OE2	5.59	1.31	1.25
1	D	744	GLU	CD-OE2	5.59	1.31	1.25
1	C	724	GLU	CD-OE2	5.57	1.31	1.25
1	A	181	GLU	CD-OE2	5.55	1.31	1.25
1	A	334	GLU	CD-OE2	5.52	1.31	1.25
1	A	1006	GLU	CD-OE2	5.52	1.31	1.25
1	B	438	GLU	CD-OE2	5.51	1.31	1.25
1	B	334	GLU	CD-OE2	5.49	1.31	1.25
1	A	508	GLU	CD-OE2	5.47	1.31	1.25
1	D	418	GLU	CD-OE2	5.44	1.31	1.25
1	C	438	GLU	CD-OE2	5.42	1.31	1.25
1	B	338	GLU	CD-OE2	5.42	1.31	1.25
1	C	416	GLU	CD-OE2	5.40	1.31	1.25
1	B	324	GLU	CD-OE2	5.39	1.31	1.25
1	A	438	GLU	CD-OE2	5.38	1.31	1.25
1	A	80	GLU	CD-OE2	5.36	1.31	1.25
1	C	619	GLU	CD-OE1	-5.36	1.19	1.25
1	D	943	GLU	CD-OE2	5.35	1.31	1.25
1	B	243	GLU	CD-OE2	5.33	1.31	1.25
1	B	17	GLU	CD-OE2	5.33	1.31	1.25
1	A	241	GLU	CD-OE2	5.33	1.31	1.25
1	B	358	GLU	CD-OE2	5.32	1.31	1.25
1	D	198	GLU	CD-OE2	5.31	1.31	1.25
1	D	324	GLU	CD-OE1	-5.30	1.19	1.25
1	B	619	GLU	CD-OE2	5.29	1.31	1.25
1	B	264	GLU	CD-OE2	5.29	1.31	1.25
1	C	641	GLU	CD-OE1	-5.28	1.19	1.25
1	B	750	GLU	CD-OE2	5.28	1.31	1.25
1	A	326	GLU	CD-OE2	5.27	1.31	1.25
1	C	808	GLU	CD-OE2	5.22	1.31	1.25
1	D	969	GLU	CD-OE2	5.21	1.31	1.25
1	D	641	GLU	CD-OE1	-5.21	1.20	1.25
1	A	412	GLU	CD-OE2	5.21	1.31	1.25
1	B	75	GLU	CD-OE2	5.21	1.31	1.25
1	C	131	GLU	CD-OE2	5.20	1.31	1.25
1	D	358	GLU	CD-OE2	5.20	1.31	1.25
1	D	871	GLU	CD-OE2	5.18	1.31	1.25
1	A	797	GLU	CD-OE2	5.18	1.31	1.25
1	B	641	GLU	CD-OE1	-5.18	1.20	1.25
1	C	871	GLU	CD-OE2	5.14	1.31	1.25
1	C	41	GLU	CD-OE2	5.10	1.31	1.25
1	A	57	GLU	CD-OE2	5.09	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	304	GLU	CD-OE2	5.07	1.31	1.25
1	C	637	GLU	CD-OE2	5.07	1.31	1.25
1	D	641	GLU	CD-OE2	5.07	1.31	1.25
1	C	943	GLU	CD-OE2	5.06	1.31	1.25
1	B	650	GLU	CD-OE2	5.04	1.31	1.25
1	B	40	GLU	CD-OE2	5.02	1.31	1.25
1	D	67	GLU	CD-OE2	5.00	1.31	1.25
1	C	334	GLU	CD-OE2	5.00	1.31	1.25
1	C	650	GLU	CD-OE2	5.00	1.31	1.25

All (652) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	ARG	NE-CZ-NH2	-19.36	110.62	120.30
1	C	809	ARG	NE-CZ-NH1	16.16	128.38	120.30
1	D	255	ARG	NE-CZ-NH1	15.41	128.00	120.30
1	A	997	ASP	CB-CG-OD2	-14.81	104.97	118.30
1	D	431	ARG	NE-CZ-NH2	-14.64	112.98	120.30
1	A	853	ARG	NE-CZ-NH2	-14.15	113.23	120.30
1	D	255	ARG	NE-CZ-NH2	-13.83	113.38	120.30
1	B	310	ARG	NE-CZ-NH2	-13.47	113.56	120.30
1	B	442	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	B	442	ARG	NE-CZ-NH2	-12.98	113.81	120.30
1	B	388	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	A	233	ASP	CB-CG-OD2	-12.57	106.99	118.30
1	A	809	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	D	172	ASP	CB-CG-OD2	-12.01	107.50	118.30
1	A	178	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	A	233	ASP	CB-CG-OD1	11.91	129.02	118.30
1	A	853	ARG	NE-CZ-NH1	11.71	126.16	120.30
1	A	403	ASP	CB-CG-OD2	-11.18	108.23	118.30
1	B	388	ARG	NE-CZ-NH2	-11.11	114.75	120.30
1	A	336	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	D	431	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	A	997	ASP	CB-CG-OD1	10.71	127.94	118.30
1	A	909	ARG	NE-CZ-NH1	10.69	125.64	120.30
1	D	699	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	224	ASP	CB-CG-OD1	10.34	127.61	118.30
1	B	786	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	B	172	ASP	CB-CG-OD2	-10.13	109.19	118.30
1	C	909	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	D	172	ASP	CB-CG-OD1	9.98	127.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	469	ASP	CB-CG-OD1	9.93	127.23	118.30
1	B	172	ASP	CB-CG-OD1	9.87	127.19	118.30
1	C	233	ASP	CB-CG-OD2	-9.87	109.41	118.30
1	C	201	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	D	909	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	D	786	ARG	NE-CZ-NH1	9.77	125.19	120.30
1	A	43	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	C	809	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	D	996	ASP	CB-CG-OD1	9.63	126.97	118.30
1	A	987	ASP	CB-CG-OD1	9.61	126.95	118.30
1	D	786	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	D	224	ASP	CB-CG-OD1	9.51	126.86	118.30
1	B	687	GLN	C-N-CD	-9.48	99.75	120.60
1	D	336	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	D	996	ASP	CB-CG-OD2	-9.38	109.85	118.30
1	C	473	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	C	429	ASP	CB-CG-OD2	-9.35	109.89	118.30
1	A	403	ASP	CB-CG-OD1	9.35	126.71	118.30
1	A	280	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	D	447	ASP	CB-CG-OD1	9.28	126.65	118.30
1	C	588	TYR	CB-CG-CD2	-9.23	115.46	121.00
1	B	287	ASP	CB-CG-OD1	9.21	126.59	118.30
1	A	447	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	828	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	D	591	ASP	CB-CG-OD1	9.16	126.54	118.30
1	A	746	ASP	CB-CG-OD2	-9.15	110.07	118.30
1	D	782	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	C	43	ARG	NE-CZ-NH1	9.01	124.80	120.30
1	C	782	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	A	172	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	D	594	ASP	CB-CG-OD2	-8.95	110.25	118.30
1	A	178	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	B	685	LEU	C-N-CD	-8.91	101.00	120.60
1	A	280	ASP	CB-CG-OD1	8.90	126.31	118.30
1	B	199	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	C	429	ASP	CB-CG-OD1	8.88	126.30	118.30
1	A	77	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	A	164	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	C	233	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	569	ASP	CB-CG-OD1	8.74	126.16	118.30
1	B	594	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	251	ARG	NE-CZ-NH1	8.71	124.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	996	ASP	CB-CG-OD1	8.71	126.14	118.30
1	B	473	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	C	13	ARG	NH1-CZ-NH2	8.67	128.94	119.40
1	B	59	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	C	280	ASP	CB-CG-OD2	-8.65	110.51	118.30
1	B	233	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	B	140	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	961	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	D	909	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	B	671	ASP	CB-CG-OD2	-8.57	110.58	118.30
1	C	917	ARG	NE-CZ-NH2	8.57	124.59	120.30
1	D	368	ASP	CB-CG-OD2	-8.57	110.58	118.30
1	B	800	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	D	509	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	D	782	ASP	CB-CG-OD1	8.53	125.97	118.30
1	B	356	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	D	869	ASP	CB-CG-OD1	8.52	125.97	118.30
1	B	356	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	D	411	ASP	CB-CG-OD1	8.51	125.96	118.30
1	A	509	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	D	442	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	D	572	ASP	CB-CG-OD1	8.51	125.96	118.30
1	A	157	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	D	403	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	C	199	ASP	CB-CG-OD1	8.43	125.88	118.30
1	D	859	ASP	CB-CG-OD1	8.41	125.87	118.30
1	D	772	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	B	800	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	D	446	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	C	958	ASN	N-CA-CB	8.36	125.65	110.60
1	D	509	ASP	CB-CG-OD1	8.32	125.78	118.30
1	B	572	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	446	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	594	ASP	CB-CG-OD1	8.30	125.77	118.30
1	B	492	ASP	CB-CG-OD1	8.29	125.76	118.30
1	B	786	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	569	ASP	CB-CG-OD2	-8.26	110.86	118.30
1	A	908	ASP	CB-CG-OD1	8.26	125.73	118.30
1	B	671	ASP	CB-CG-OD1	8.26	125.73	118.30
1	D	857	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	D	610	ASP	CB-CG-OD1	8.22	125.69	118.30
1	A	632	SER	N-CA-CB	8.17	122.75	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	828	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	D	442	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	D	403	ASP	CB-CG-OD1	8.15	125.64	118.30
1	C	204	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	987	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	D	446	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	D	869	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	D	802	ASP	CB-CG-OD2	-8.03	111.08	118.30
1	C	996	ASP	CB-CG-OD1	7.98	125.48	118.30
1	D	233	ASP	CB-CG-OD1	7.97	125.48	118.30
1	C	184	LEU	CB-CA-C	-7.97	95.05	110.20
1	A	828	ASP	CB-CG-OD1	7.94	125.44	118.30
1	C	786	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	224	ASP	CB-CG-OD2	-7.91	111.19	118.30
1	B	166	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	D	13	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	B	832	ASP	CB-CG-OD1	7.88	125.39	118.30
1	D	746	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	B	875	ASP	CB-CG-OD1	7.87	125.39	118.30
1	A	329	ASP	CB-CG-OD1	7.87	125.39	118.30
1	C	869	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	C	869	ASP	CB-CG-OD1	7.83	125.34	118.30
1	B	319	ASP	CB-CG-OD1	7.82	125.33	118.30
1	C	252	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	A	746	ASP	CB-CA-C	-7.78	94.84	110.40
1	B	292	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	C	659	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	588	TYR	CB-CG-CD1	7.68	125.61	121.00
1	B	875	ASP	CB-CG-OD2	-7.66	111.40	118.30
1	B	699	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	492	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	B	233	ASP	CB-CG-OD1	7.62	125.16	118.30
1	B	890	GLN	N-CA-CB	-7.62	96.88	110.60
1	D	859	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	D	856	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	C	746	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	909	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	C	579	ASP	CB-CG-OD1	7.56	125.11	118.30
1	C	611	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	961	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	A	164	ASP	CB-CG-OD1	7.53	125.07	118.30
1	C	201	ASP	CB-CG-OD1	7.52	125.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	448	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	411	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	C	997	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	C	579	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	D	572	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	C	630	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	D	183	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	D	579	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	C	287	ASP	CB-CG-OD1	7.39	124.95	118.30
1	C	772	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	D	210	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	D	659	ASP	CB-CG-OD1	7.38	124.95	118.30
1	B	144	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	C	224	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	411	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	D	926	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	B	818	ALA	N-CA-CB	7.36	120.40	110.10
1	A	553	TRP	CA-CB-CG	-7.33	99.77	113.70
1	C	442	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	D	310	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	201	ASP	CB-CG-OD1	7.33	124.89	118.30
1	B	746	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	190	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	630	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	479	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	C	363	HIS	CA-CB-CG	-7.31	101.18	113.60
1	A	37	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	375	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	781	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	C	333	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	538	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	D	140	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	509	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	140	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	282	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	C	531	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	D	578	TYR	CB-CG-CD1	7.20	125.32	121.00
1	D	166	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	D	429	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	172	ASP	CB-CG-OD1	7.18	124.76	118.30
1	B	329	ASP	CB-CG-OD1	7.17	124.76	118.30
1	B	818	ALA	CB-CA-C	7.17	120.85	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	572	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	C	329	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	D	659	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	C	368	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	D	13	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	958	ASN	N-CA-CB	7.14	123.45	110.60
1	C	319	ASP	CB-CG-OD1	7.13	124.72	118.30
1	D	210	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	D	630	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	356	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	B	429	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	204	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	772	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	832	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	C	319	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	D	15	ASP	CB-CG-OD1	7.05	124.65	118.30
1	D	292	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	D	253	TYR	CB-CG-CD2	7.04	125.22	121.00
1	B	329	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	C	234	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	447	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	755	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	D	329	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	D	591	ASP	CB-CG-OD2	-7.01	112.00	118.30
1	A	659	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	881	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	193	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C	375	ASP	CB-CG-OD1	6.97	124.57	118.30
1	B	579	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	C	569	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	C	561	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	579	ASP	CB-CG-OD1	6.95	124.55	118.30
1	A	329	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	C	280	ASP	CB-CG-OD1	6.94	124.55	118.30
1	A	610	ASP	CB-CG-OD1	6.93	124.54	118.30
1	D	428	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	B	310	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	594	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	D	958	ASN	N-CA-CB	6.90	123.02	110.60
1	C	126	THR	CA-CB-CG2	-6.90	102.74	112.40
1	B	292	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	D	45	ASP	CB-CG-OD1	6.86	124.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	659	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	531	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	884	LEU	CB-CA-C	-6.85	97.19	110.20
1	D	287	ASP	CB-CG-OD1	6.84	124.46	118.30
1	D	199	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	D	772	ASP	CB-CG-OD1	6.83	124.45	118.30
1	D	233	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	C	919	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	82	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	429	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	578	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	C	588	TYR	CB-CG-CD1	6.79	125.07	121.00
1	B	561	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	C	782	ASP	CB-CG-OD1	6.78	124.41	118.30
1	B	164	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	C	15	ASP	CB-CG-OD1	6.78	124.40	118.30
1	C	802	ASP	CB-CG-OD1	6.77	124.39	118.30
1	D	997	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	B	919	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	D	144	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	368	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	C	859	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	C	234	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	172	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	D	164	ASP	CB-CG-OD1	6.69	124.32	118.30
1	D	429	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	A	772	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	403	ASP	CB-CG-OD1	6.66	124.30	118.30
1	A	201	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	140	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	B	479	ASP	CB-CG-OD1	6.65	124.28	118.30
1	B	234	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	D	234	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	505	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	B	507	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	15	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	199	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	579	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	997	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	403	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	C	140	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	594	ASP	CB-CG-OD1	6.60	124.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	TYR	N-CA-CB	6.60	122.48	110.60
1	B	648	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	B	144	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	961	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	569	ASP	CB-CG-OD1	6.56	124.20	118.30
1	C	553	TRP	CA-CB-CG	-6.54	101.27	113.70
1	C	411	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	997	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	287	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	954	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	B	403	ASP	CB-CG-OD2	-6.52	112.44	118.30
1	A	438	GLU	CA-CB-CG	-6.47	99.16	113.40
1	A	519	SER	N-CA-CB	-6.46	100.80	110.50
1	D	448	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	C	671	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	C	136	GLU	CB-CA-C	-6.43	97.54	110.40
1	C	996	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	15	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	671	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	909	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	D	147	ASN	N-CA-CB	-6.40	99.08	110.60
1	D	671	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	507	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	1013	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	43	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	802	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	327	ALA	CB-CA-C	-6.36	100.56	110.10
1	D	648	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	A	996	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	C	310	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	C	333	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	363	HIS	CA-CB-CG	-6.35	102.81	113.60
1	A	292	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	251	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	781	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	239	VAL	CG1-CB-CG2	-6.32	100.79	110.90
1	B	997	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	760	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	B	336	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	781	ARG	N-CA-CB	-6.28	99.31	110.60
1	C	439	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	D	439	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	TYR	N-CA-CB	-6.26	99.33	110.60
1	D	319	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	C	916	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	D	987	ASP	CB-CG-OD1	6.25	123.93	118.30
1	D	832	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	B	869	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	166	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	919	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	46	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	329	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	916	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	333	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	648	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	599	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	411	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	D	224	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	C	473	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	1018	LEU	N-CA-CB	-6.17	98.07	110.40
1	C	653	HIS	N-CA-CB	6.16	121.69	110.60
1	B	237	ARG	CB-CA-C	-6.16	98.08	110.40
1	D	95	TYR	CB-CG-CD2	-6.16	117.31	121.00
1	D	553	TRP	CA-CB-CG	-6.16	102.00	113.70
1	D	987	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	699	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	B	252	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	B	569	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	782	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	781	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	201	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	952	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	684	GLU	CB-CA-C	-6.11	98.18	110.40
1	B	881	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	531	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	746	ASP	CB-CA-C	-6.09	98.22	110.40
1	B	908	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	469	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	193	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	840	HIS	CB-CA-C	-6.07	98.26	110.40
1	B	96	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	D	15	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	C	610	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	B	319	ASP	CB-CG-OD2	-6.05	112.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	782	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	234	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	B	553	TRP	CA-CB-CG	-6.04	102.22	113.70
1	C	507	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	C	746	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	D	857	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	952	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	D	319	ASP	CB-CG-OD1	6.03	123.72	118.30
1	D	164	ASP	N-CA-CB	6.03	121.45	110.60
1	C	578	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	D	77	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	909	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	671	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	403	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	473	ARG	CD-NE-CZ	6.01	132.01	123.60
1	B	792	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	531	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	802	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	164	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	855	THR	N-CA-CB	6.00	121.70	110.30
1	C	748	CYS	CA-CB-SG	-6.00	103.20	114.00
1	B	201	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	336	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	648	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	D	336	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	869	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	492	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	492	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	B	183	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	507	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	503	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	C	828	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	199	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	469	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	161	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	B	748	CYS	CA-CB-SG	-5.92	103.35	114.00
1	D	598	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	853	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	469	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	996	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	219	THR	CA-CB-CG2	-5.90	104.14	112.40
1	D	748	CYS	N-CA-CB	5.89	121.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	164	ASP	N-CA-CB	5.88	121.19	110.60
1	B	45	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	832	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	561	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	44	THR	CA-CB-CG2	-5.86	104.19	112.40
1	D	531	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	954	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	1019	VAL	CA-CB-CG2	-5.85	102.13	110.90
1	B	997	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	968	MET	CB-CA-C	-5.84	98.73	110.40
1	D	330	VAL	CB-CA-C	-5.84	100.31	111.40
1	C	509	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	772	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	809	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	B	411	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	52	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	869	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	741	THR	CA-CB-CG2	-5.80	104.28	112.40
1	D	875	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	909	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	D	828	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	280	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	938	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	610	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	809	ARG	CD-NE-CZ	5.78	131.69	123.60
1	D	1018	LEU	CB-CA-C	-5.78	99.22	110.20
1	D	594	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	184	LEU	CB-CA-C	-5.77	99.23	110.20
1	B	859	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	D	75	GLU	N-CA-CB	5.77	120.99	110.60
1	A	1006	GLU	CG-CD-OE2	-5.77	106.77	118.30
1	D	221	GLN	N-CA-CB	-5.76	100.23	110.60
1	A	869	ASP	N-CA-CB	5.75	120.94	110.60
1	C	287	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	D	473	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	130	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	225	PHE	N-CA-CB	5.72	120.89	110.60
1	A	333	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	635	THR	CA-CB-CG2	-5.71	104.41	112.40
1	B	375	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	D	77	ASP	CB-CG-OD1	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	578	TYR	N-CA-CB	5.70	120.87	110.60
1	D	193	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	126	THR	CA-CB-CG2	-5.70	104.43	112.40
1	C	199	ASP	CB-CG-OD2	-5.69	113.17	118.30
1	A	130	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	916	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	769	TRP	CB-CA-C	-5.69	99.02	110.40
1	B	15	ASP	CB-CG-OD1	5.68	123.42	118.30
1	D	962	TYR	CB-CG-CD1	-5.67	117.59	121.00
1	A	688	PRO	N-CA-C	5.67	126.84	112.10
1	C	255	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	706	THR	CA-CB-CG2	-5.67	104.46	112.40
1	A	429	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	610	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	D	100	TYR	N-CA-CB	5.66	120.78	110.60
1	B	1013	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	844	HIS	CA-CB-CG	-5.65	104.00	113.60
1	A	790	ASP	CA-CB-CG	-5.63	101.00	113.40
1	A	147	ASN	N-CA-CB	-5.63	100.47	110.60
1	B	45	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	D	980	GLU	C-N-CA	-5.59	110.56	122.30
1	A	287	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	829	THR	CA-CB-CG2	-5.58	104.59	112.40
1	C	479	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	829	THR	N-CA-CB	5.58	120.90	110.30
1	B	255	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	869	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	D	166	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	101	THR	N-CA-CB	5.55	120.85	110.30
1	A	310	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	699	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	857	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	45	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	1014	TYR	CB-CG-CD1	5.53	124.32	121.00
1	C	599	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	D	368	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	579	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	802	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	546	LEU	N-CA-CB	5.50	121.39	110.40
1	A	507	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	250	LEU	CB-CG-CD1	-5.48	101.69	111.00
1	A	448	ARG	NE-CZ-NH2	5.47	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	587	ALA	CB-CA-C	-5.47	101.90	110.10
1	A	771	GLY	N-CA-C	-5.46	99.44	113.10
1	D	802	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	96	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	894	ARG	CB-CA-C	-5.44	99.51	110.40
1	A	591	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	538	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	C	917	ARG	CD-NE-CZ	-5.43	115.99	123.60
1	C	507	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	723	ALA	CB-CA-C	-5.43	101.96	110.10
1	C	267	VAL	CA-CB-CG2	-5.43	102.76	110.90
1	C	204	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	164	ASP	CB-CG-OD1	5.42	123.18	118.30
1	D	258	VAL	CA-CB-CG2	-5.42	102.77	110.90
1	C	210	ARG	N-CA-CB	5.42	120.35	110.60
1	A	321	THR	CA-CB-CG2	-5.41	104.82	112.40
1	B	507	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	199	ASP	CB-CG-OD1	5.41	123.17	118.30
1	D	924	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	185	ALA	N-CA-CB	5.41	117.67	110.10
1	C	729	THR	N-CA-CB	5.40	120.56	110.30
1	A	411	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	442	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	C	509	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	C	782	ASP	CB-CA-C	-5.39	99.62	110.40
1	B	641	GLU	OE1-CD-OE2	-5.39	116.84	123.30
1	D	701	VAL	CA-CB-CG2	-5.38	102.82	110.90
1	C	1018	LEU	CB-CA-C	-5.38	99.97	110.20
1	D	673	ALA	N-CA-CB	-5.38	102.57	110.10
1	A	408	TYR	N-CA-CB	-5.38	100.92	110.60
1	A	118	ASN	N-CA-CB	-5.37	100.94	110.60
1	B	1009	LEU	CB-CG-CD2	-5.36	101.88	111.00
1	B	251	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	829	THR	N-CA-CB	5.36	120.48	110.30
1	C	916	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	987	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	D	103	VAL	CA-CB-CG2	-5.36	102.86	110.90
1	C	96	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	949	HIS	CB-CA-C	-5.35	99.71	110.40
1	A	252	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	B	659	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	B	178	ARG	NE-CZ-NH1	5.33	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
1	B	965	GLN	CA-CB-CG	-5.32	101.69	113.40
1	B	842	TRP	CG-CD2-CE3	-5.32	129.11	133.90
1	A	74	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	A	368	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	96	ASP	CB-CA-C	5.31	121.02	110.40
1	A	140	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	856	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	610	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	919	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	768	MET	N-CA-CB	5.28	120.10	110.60
1	C	842	TRP	CB-CG-CD2	-5.28	119.74	126.60
1	B	538	TYR	CB-CG-CD2	5.28	124.17	121.00
1	B	211	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	147	ASN	N-CA-CB	-5.27	101.11	110.60
1	A	659	ASP	CB-CA-C	-5.26	99.87	110.40
1	C	311	ALA	N-CA-CB	5.26	117.47	110.10
1	C	356	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	46	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	991	MET	CG-SD-CE	5.26	108.62	100.20
1	A	550	ALA	CB-CA-C	-5.26	102.22	110.10
1	C	292	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	52	ARG	CB-CA-C	-5.25	99.90	110.40
1	C	853	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	66	PRO	N-CA-CB	5.25	109.60	103.30
1	A	469	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	632	SER	N-CA-CB	5.24	118.36	110.50
1	B	832	ASP	N-CA-CB	-5.24	101.16	110.60
1	C	431	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	611	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	1021	CYS	CA-CB-SG	-5.24	104.58	114.00
1	B	954	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	C	630	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	832	ASP	CB-CG-OD1	5.23	123.00	118.30
1	D	746	ASP	CB-CA-C	-5.23	99.94	110.40
1	B	926	TYR	CB-CG-CD1	5.23	124.14	121.00
1	D	505	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	645	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	230	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	721	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	425	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	355	ASN	CB-CA-C	-5.21	99.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	809	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	480	PRO	CA-N-CD	5.21	118.99	111.70
1	C	802	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	100	TYR	N-CA-CB	5.20	119.96	110.60
1	A	428	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	701	VAL	CA-CB-CG2	-5.20	103.10	110.90
1	A	1013	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	D	140	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	1016	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	D	78	LEU	CA-CB-CG	-5.19	103.36	115.30
1	D	183	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	D	577	LYS	N-CA-CB	5.19	119.94	110.60
1	A	884	LEU	CB-CA-C	-5.19	100.34	110.20
1	C	482	ARG	CB-CA-C	-5.19	100.02	110.40
1	A	13	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	821	ALA	N-CA-CB	5.18	117.35	110.10
1	A	583	ASN	CA-CB-CG	-5.17	102.02	113.40
1	A	611	ARG	CD-NE-CZ	5.17	130.84	123.60
1	C	719	GLN	CB-CA-C	-5.17	100.06	110.40
1	B	569	ASP	CB-CG-OD1	5.16	122.95	118.30
1	D	80	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	B	771	GLY	N-CA-C	-5.16	100.21	113.10
1	D	469	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	638	VAL	CB-CA-C	-5.15	101.62	111.40
1	C	469	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	B	737	ILE	N-CA-CB	5.13	122.61	110.80
1	B	571	VAL	CA-CB-CG2	5.13	118.60	110.90
1	A	395	HIS	N-CA-CB	-5.13	101.36	110.60
1	C	987	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	629	PHE	CB-CA-C	-5.13	100.15	110.40
1	A	667	GLU	CB-CA-C	-5.12	100.16	110.40
1	D	85	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	B	819	GLU	N-CA-CB	-5.12	101.39	110.60
1	C	927	THR	CA-CB-CG2	-5.11	105.25	112.40
1	D	731	PRO	N-CA-CB	5.11	109.43	103.30
1	B	368	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	790	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	503	TYR	CB-CG-CD2	5.10	124.06	121.00
1	C	599	ARG	CD-NE-CZ	5.09	130.73	123.60
1	B	996	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	519	SER	N-CA-CB	-5.09	102.87	110.50
1	B	183	ARG	NE-CZ-NH1	5.09	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	497	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	840	HIS	CB-CA-C	-5.08	100.25	110.40
1	A	183	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	D	78	LEU	CB-CA-C	-5.07	100.56	110.20
1	D	559	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	D	926	TYR	CB-CG-CD1	5.07	124.04	121.00
1	C	842	TRP	CG-CD2-CE3	-5.07	129.34	133.90
1	C	832	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	128	ASN	N-CA-CB	-5.07	101.48	110.60
1	A	925	MET	CG-SD-CE	5.06	108.29	100.20
1	C	842	TRP	CE2-CD2-CE3	5.05	124.76	118.70
1	A	210	ARG	N-CA-CB	5.05	119.69	110.60
1	A	486	TYR	CG-CD1-CE1	5.05	125.34	121.30
1	B	568	TRP	CA-CB-CG	-5.05	104.11	113.70
1	B	648	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	611	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	78	LEU	C-N-CD	-5.03	109.52	120.60
1	D	418	GLU	CA-CB-CG	-5.03	102.35	113.40
1	A	545	SER	N-CA-CB	-5.02	102.97	110.50
1	D	118	ASN	N-CA-CB	-5.02	101.57	110.60
1	D	388	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	502	MET	N-CA-CB	5.01	119.62	110.60
1	A	1016	TYR	N-CA-CB	5.01	119.63	110.60
1	C	469	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	45	ASP	N-CA-CB	5.01	119.62	110.60
1	C	855	THR	N-CA-CB	5.01	119.82	110.30
1	D	129	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	B	552	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	D	130	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	832	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	C	480	PRO	CA-N-CD	5.01	118.71	111.70
1	C	67	GLU	CB-CA-C	-5.00	100.39	110.40
1	C	853	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	D	507	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	8124	0	7715	189	0
1	B	8124	0	7715	222	0
1	C	8124	0	7715	225	0
1	D	8124	0	7715	188	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	68	0	102	8	0
4	B	76	0	114	2	0
4	C	92	0	138	9	0
4	D	92	0	138	18	0
5	A	871	0	0	15	0
5	B	864	0	0	19	0
5	C	838	0	0	16	0
5	D	891	0	0	22	0
All	All	36314	0	31352	824	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 13.

All (824) 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:D:804:ASN:ND2	1:D:809:ARG:HH21	1.32	1.26
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.42	1.18
1:C:634:GLN:H	1:C:634:GLN:NE2	1.46	1.11
1:B:804:ASN:ND2	1:B:809:ARG:HH21	1.51	1.06
1:A:600:GLN:H	1:A:600:GLN:HE21	1.07	1.01
1:D:651:LEU:HD11	1:D:653:HIS:CE1	1.97	0.99
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.47	0.96
1:B:804:ASN:HD22	1:B:809:ARG:HH21	1.06	0.96
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.49	0.94
1:C:634:GLN:HE21	1:C:634:GLN:N	1.65	0.93
1:C:634:GLN:H	1:C:634:GLN:HE21	0.94	0.92
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.52	0.90
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.53	0.90
1:B:744:GLU:HB2	1:B:745:MET:HE2	1.53	0.90
1:C:781:ARG:HG2	1:C:781:ARG:HH11	1.38	0.89
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.88	0.88
1:C:827:ALA:HA	1:C:836:ILE:HD13	1.56	0.87
1:D:128:ASN:HB3	1:D:180:GLY:O	1.76	0.86
1:B:655:MET:HE2	1:B:665:SER:HB3	1.56	0.85
1:C:132:SER:HB2	4:C:8504:DMS:H11	1.58	0.85
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.58	0.84
1:B:581:ASN:HB2	1:B:583:ASN:HD22	1.43	0.84
1:D:651:LEU:C	1:D:651:LEU:HD12	1.97	0.84
1:D:629:PHE:O	1:D:630:ARG:HD3	1.77	0.84
1:B:730:LEU:HD12	1:B:730:LEU:H	1.40	0.84
1:B:744:GLU:HB2	1:B:745:MET:CE	2.06	0.83
1:B:804:ASN:HD22	1:B:809:ARG:NH2	1.76	0.83
1:C:633:GLY:HA3	1:C:634:GLN:HE21	1.44	0.81
1:A:615:PRO:O	1:A:618:THR:HG22	1.81	0.79
1:B:634:GLN:HG2	1:B:682:LEU:O	1.81	0.79
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.47	0.79
1:A:787:ALA:HA	1:A:968:MET:HG3	1.64	0.79
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.11	0.79
1:C:634:GLN:NE2	1:C:634:GLN:N	2.27	0.79
1:C:785:THR:O	1:C:881:ARG:HD2	1.83	0.78
1:C:41:GLU:HG2	5:C:4002:HOH:O	1.83	0.78
1:B:600:GLN:H	1:B:600:GLN:HE21	1.31	0.78
5:B:4700:HOH:O	4:C:8420:DMS:H21	1.83	0.78
4:D:8703:DMS:H23	5:D:4835:HOH:O	1.83	0.78
1:D:106:PRO:C	4:D:8419:DMS:H23	2.03	0.78
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.16	0.78
1:D:105:TYR:O	4:D:8419:DMS:H22	1.83	0.77
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.66	0.77
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.00	0.76
1:D:292:ARG:HH12	4:D:8412:DMS:H22	1.48	0.76
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.30	0.76
1:A:965:GLN:O	1:A:969:GLU:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ILE:N	4:D:8419:DMS:H23	2.01	0.75
1:B:367:MET:HE1	1:B:371:THR:HG22	1.69	0.74
1:A:292:ARG:HH12	4:A:8412:DMS:C2	2.00	0.73
1:C:356:ARG:HD2	1:C:379:MET:CE	2.19	0.73
1:B:131:GLU:O	1:B:135:GLN:HG2	1.88	0.72
1:B:615:PRO:O	1:B:618:THR:HG22	1.88	0.72
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.04	0.72
1:B:132:SER:HA	1:B:135:GLN:HG2	1.70	0.72
1:A:178:ARG:HD2	5:A:4741:HOH:O	1.88	0.72
1:A:887:GLN:NE2	1:A:980:GLU:O	2.22	0.72
1:D:595:THR:HA	1:D:596:PRO:C	2.09	0.72
1:C:243:GLU:OE2	1:C:245:GLN:NE2	2.20	0.71
1:C:765:LEU:HD21	1:C:768:MET:CE	2.20	0.71
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.73	0.71
1:A:824:GLN:HG2	1:A:825:CYS:N	2.04	0.71
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.73	0.71
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.54	0.70
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.73	0.70
1:D:1022:GLN:HE21	1:D:1023:LYS:N	1.89	0.70
1:A:277:GLU:H	1:A:277:GLU:CD	1.93	0.70
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.26	0.69
1:A:599:ARG:HH11	1:A:600:GLN:NE2	1.89	0.69
1:C:748:CYS:C	1:C:749:ILE:HD12	2.13	0.69
1:C:799:THR:O	1:C:800:ARG:HG2	1.92	0.69
1:A:183:ARG:HD3	5:A:4302:HOH:O	1.92	0.69
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.24	0.69
1:C:615:PRO:O	1:C:618:THR:HG22	1.92	0.69
1:C:651:LEU:HD12	1:C:651:LEU:O	1.93	0.69
1:A:599:ARG:HG3	1:A:600:GLN:NE2	2.08	0.68
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.29	0.68
1:D:316:HIS:HA	1:D:323:ILE:HD13	1.75	0.68
1:D:577:LYS:O	1:D:584:PRO:HA	1.92	0.68
1:C:633:GLY:HA3	1:C:634:GLN:NE2	2.08	0.68
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.74	0.68
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.75	0.68
1:A:843:GLN:HG2	1:A:848:THR:HA	1.76	0.68
1:C:878:HIS:HD2	5:C:4094:HOH:O	1.76	0.68
1:B:701:VAL:HG22	1:B:714:ILE:HG12	1.75	0.67
1:B:687:GLN:NE2	1:B:687:GLN:HA	2.10	0.67
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.75	0.67
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.16	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLU:HG3	1:C:135:GLN:NE2	2.09	0.67
1:C:843:GLN:NE2	1:C:848:THR:OG1	2.27	0.67
1:D:887:GLN:NE2	1:D:980:GLU:O	2.27	0.67
1:B:132:SER:HA	1:B:135:GLN:CG	2.24	0.67
1:A:128:ASN:HA	1:A:180:GLY:O	1.94	0.67
1:A:685:LEU:HD23	5:A:4839:HOH:O	1.94	0.67
1:B:1018:LEU:HD23	1:B:1019:VAL:N	2.08	0.67
1:A:168:PRO:O	1:A:442:ARG:NH2	2.28	0.66
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.30	0.66
1:B:296:GLU:HB2	4:B:8601:DMS:O	1.94	0.66
1:B:595:THR:HA	1:B:596:PRO:C	2.16	0.66
1:D:292:ARG:HH12	4:D:8412:DMS:C2	2.07	0.66
1:B:200:GLN:HG2	1:B:391:HIS:HB2	1.77	0.66
1:D:781:ARG:NH1	5:D:4692:HOH:O	2.27	0.66
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.77	0.66
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.60	0.66
1:C:356:ARG:HD2	1:C:379:MET:HE3	1.77	0.66
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.11	0.66
1:C:781:ARG:HG2	1:C:781:ARG:NH1	2.11	0.66
1:B:655:MET:CE	1:B:665:SER:HB3	2.24	0.65
1:A:600:GLN:HE21	1:A:600:GLN:N	1.89	0.65
1:C:646:HIS:HB3	5:C:4747:HOH:O	1.96	0.65
1:C:658:LEU:HG	1:C:661:LYS:NZ	2.12	0.65
1:B:659:ASP:OD2	1:B:692:GLY:HA3	1.97	0.65
1:B:878:HIS:HD2	5:B:4087:HOH:O	1.79	0.65
1:C:827:ALA:HA	1:C:836:ILE:CD1	2.25	0.65
1:C:802:ASP:O	1:C:808:GLU:HG3	1.96	0.65
1:B:581:ASN:HB2	1:B:583:ASN:ND2	2.10	0.65
1:D:660:GLY:O	1:D:662:PRO:HD3	1.97	0.65
1:D:1022:GLN:NE2	1:D:1023:LYS:HG2	2.11	0.65
1:B:117:GLU:HB2	5:B:4415:HOH:O	1.95	0.65
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.95	0.65
1:D:277:GLU:CD	1:D:277:GLU:H	1.99	0.65
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.79	0.64
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.79	0.64
1:D:749:ILE:HD12	1:D:749:ILE:N	2.13	0.64
1:D:573:GLN:HB2	1:D:602:CYS:O	1.98	0.63
1:B:181:GLU:OE2	1:B:181:GLU:HA	1.98	0.63
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.32	0.63
1:C:132:SER:CB	4:C:8504:DMS:H11	2.29	0.63
1:C:687:GLN:HA	1:C:687:GLN:NE2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:658:LEU:O	1:D:661:LYS:HG3	1.99	0.63
1:B:381:GLN:O	1:B:621:LYS:HE3	1.98	0.63
1:C:573:GLN:HB2	1:C:602:CYS:O	1.99	0.63
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.28	0.63
1:C:651:LEU:HD12	1:C:651:LEU:C	2.19	0.63
1:D:893:GLU:HG2	1:D:894:ARG:CD	2.28	0.62
1:B:634:GLN:NE2	1:B:683:PRO:O	2.31	0.62
1:C:633:GLY:CA	1:C:634:GLN:HE21	2.11	0.62
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.34	0.62
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.34	0.62
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.29	0.62
1:B:651:LEU:HD22	1:B:651:LEU:O	1.99	0.62
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.00	0.62
1:B:262:GLN:HE21	1:B:262:GLN:C	2.03	0.62
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.81	0.62
1:D:88:SER:HA	1:D:366:VAL:HG21	1.80	0.62
1:A:646:HIS:ND1	5:A:4723:HOH:O	2.23	0.61
1:B:367:MET:CE	1:B:371:THR:HG22	2.30	0.61
1:C:986:ILE:HG21	1:C:1018:LEU:HD21	1.82	0.61
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.96	0.61
1:A:249:GLU:OE2	1:A:251:ARG:NH2	2.32	0.61
1:D:1022:GLN:HE21	1:D:1022:GLN:C	2.04	0.61
1:A:595:THR:HA	1:A:596:PRO:C	2.20	0.61
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.81	0.61
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.36	0.61
1:D:133:TRP:HE1	4:D:8703:DMS:C2	2.13	0.61
1:D:737:ILE:HD13	1:D:832:ASP:HA	1.83	0.61
1:A:754:LYS:NZ	5:A:4760:HOH:O	2.34	0.60
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.16	0.60
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.01	0.60
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.83	0.60
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.84	0.60
1:B:132:SER:HA	1:B:135:GLN:CD	2.21	0.60
1:B:890:GLN:HB2	5:B:4808:HOH:O	2.00	0.60
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.30	0.60
1:A:75:GLU:OE1	1:A:75:GLU:HA	2.01	0.60
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.66	0.60
1:B:262:GLN:HE21	1:B:263:GLY:N	1.99	0.60
1:B:755:ARG:HD3	5:B:4833:HOH:O	2.00	0.60
1:C:833:ALA:HB1	1:C:858:ILE:O	2.01	0.60
1:B:797:GLU:O	1:B:801:ILE:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.37	0.60
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.37	0.60
1:B:52:ARG:NH1	5:B:4602:HOH:O	2.34	0.59
1:A:873:ALA:O	1:A:876:THR:HG22	2.02	0.59
1:A:292:ARG:HH12	4:A:8412:DMS:H22	1.66	0.59
1:C:614:HIS:HB3	1:C:615:PRO:HD2	1.84	0.59
1:B:596:PRO:HB3	5:B:4714:HOH:O	2.02	0.59
1:D:896:ASN:HB2	1:D:919:ASP:OD2	2.02	0.59
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.84	0.59
1:A:742:THR:HG22	1:A:743:SER:N	2.16	0.59
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.68	0.59
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.84	0.59
1:D:107:ILE:CA	4:D:8419:DMS:H23	2.33	0.59
1:A:878:HIS:HD2	5:A:4073:HOH:O	1.86	0.59
1:B:132:SER:CA	1:B:135:GLN:HG2	2.32	0.58
1:C:46:ARG:NH2	5:C:4002:HOH:O	2.27	0.58
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.33	0.58
1:C:809:ARG:HH22	1:C:1001:PRO:HB3	1.67	0.58
1:A:577:LYS:O	1:A:584:PRO:HA	2.03	0.58
1:A:648:ASP:OD2	5:A:4772:HOH:O	2.17	0.58
1:B:128:ASN:HB2	5:B:4776:HOH:O	2.04	0.58
1:B:863:GLN:HG3	1:B:1021:CYS:CB	2.31	0.58
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.38	0.58
1:A:863:GLN:NE2	1:A:952:ARG:HH22	2.01	0.58
1:D:584:PRO:HD2	5:D:4674:HOH:O	2.03	0.58
1:D:893:GLU:HG2	1:D:894:ARG:HD2	1.84	0.58
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.84	0.58
1:C:797:GLU:O	1:C:801:ILE:HD13	2.03	0.58
1:B:88:SER:HA	1:B:366:VAL:HG21	1.85	0.58
1:A:688:PRO:O	1:A:689:GLU:HB2	2.03	0.58
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.37	0.58
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.86	0.58
1:C:768:MET:O	1:C:775:GLN:N	2.32	0.58
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.39	0.58
1:D:1022:GLN:O	1:D:1022:GLN:HG3	2.02	0.58
1:C:572:ASP:HB3	1:C:603:MET:HG2	1.86	0.57
1:B:131:GLU:OE2	1:B:134:LEU:HB2	2.05	0.57
1:D:767:GLN:NE2	1:D:774:LYS:HZ3	2.02	0.57
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.85	0.57
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.40	0.57
1:C:250:LEU:O	1:C:251:ARG:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.69	0.57
1:A:587:ALA:HB1	1:A:591:ASP:HB2	1.86	0.57
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.39	0.57
1:A:861:SER:OG	1:A:863:GLN:HG3	2.05	0.57
1:B:637:GLU:CD	1:B:677:LYS:HD3	2.25	0.57
1:B:599:ARG:HH11	1:B:600:GLN:NE2	2.03	0.57
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.36	0.57
1:D:622:HIS:O	1:D:625:GLN:HG3	2.05	0.57
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.05	0.57
1:D:651:LEU:HD12	1:D:651:LEU:O	2.03	0.57
1:B:824:GLN:HG2	1:B:825:CYS:N	2.19	0.56
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.87	0.56
1:D:896:ASN:OD1	1:D:917:ARG:NH1	2.35	0.56
1:B:655:MET:HE2	1:B:664:ALA:O	2.04	0.56
1:A:132:SER:HA	1:A:135:GLN:HG3	1.87	0.56
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.71	0.56
1:D:893:GLU:HG2	1:D:894:ARG:HG2	1.87	0.56
1:A:947:GLY:O	1:A:1023:LYS:HE3	2.05	0.56
1:C:750:GLU:OE2	1:C:755:ARG:HD2	2.04	0.56
1:A:599:ARG:HG3	1:A:600:GLN:HE21	1.68	0.56
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.86	0.56
1:A:84:VAL:HA	4:A:8414:DMS:O	2.06	0.56
1:A:347:LYS:HE3	5:A:4259:HOH:O	2.06	0.56
1:A:359:HIS:N	1:A:367:MET:HE1	2.20	0.56
1:B:634:GLN:HE21	1:B:683:PRO:C	2.07	0.56
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.69	0.56
1:A:71:GLU:HG2	5:A:4655:HOH:O	2.06	0.56
1:A:613:PRO:HB3	1:A:617:LEU:HD23	1.88	0.56
1:B:127:PHE:O	1:B:182:ASN:N	2.36	0.56
1:C:1023:LYS:HE3	1:C:1023:LYS:HA	1.88	0.56
1:A:686:PRO:C	1:A:688:PRO:HD3	2.26	0.56
1:B:243:GLU:OE2	1:B:245:GLN:NE2	2.37	0.56
1:B:356:ARG:HD2	1:B:379:MET:CE	2.36	0.56
1:A:292:ARG:HH12	4:A:8412:DMS:H23	1.71	0.55
1:B:131:GLU:OE1	1:B:179:ALA:HB2	2.06	0.55
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.21	0.55
1:B:797:GLU:O	1:B:800:ARG:N	2.37	0.55
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.06	0.55
1:A:584:PRO:HD2	5:A:4628:HOH:O	2.06	0.55
1:C:781:ARG:HH11	1:C:781:ARG:CG	2.16	0.55
1:D:765:LEU:HD21	1:D:768:MET:SD	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:THR:HG23	1:D:323:ILE:HD11	1.87	0.55
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.88	0.55
1:B:658:LEU:N	1:B:661:LYS:O	2.39	0.55
1:B:822:LEU:HD21	1:B:825:CYS:HB2	1.89	0.55
1:C:634:GLN:H	1:C:634:GLN:CD	1.95	0.55
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.88	0.55
1:A:684:GLU:HG2	1:A:685:LEU:N	2.21	0.55
1:A:88:SER:HA	1:A:366:VAL:HG21	1.89	0.55
1:D:770:ILE:HD12	1:D:775:GLN:NE2	2.22	0.55
1:A:533:LEU:C	1:A:533:LEU:HD23	2.28	0.55
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.89	0.55
1:D:628:GLN:HB3	5:D:4561:HOH:O	2.07	0.54
1:B:499:ILE:HD11	1:B:529:GLU:CD	2.27	0.54
1:B:737:ILE:HD11	5:B:4803:HOH:O	2.07	0.54
1:D:316:HIS:HA	1:D:323:ILE:CD1	2.38	0.54
1:D:738:PRO:HB3	1:D:751:LEU:HB2	1.89	0.54
1:A:252:ASP:HB2	4:A:8416:DMS:O	2.06	0.54
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.42	0.54
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.42	0.54
1:A:472:TYR:O	1:A:476:LYS:HG2	2.08	0.54
1:D:117:GLU:HB2	5:D:4434:HOH:O	2.07	0.54
1:A:738:PRO:HG3	1:A:751:LEU:HD22	1.89	0.54
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.73	0.54
1:C:88:SER:HA	1:C:366:VAL:HG21	1.90	0.54
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.36	0.54
1:B:744:GLU:HB2	1:B:745:MET:HE3	1.90	0.54
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.91	0.54
1:D:288:ARG:NH1	5:D:4461:HOH:O	2.30	0.54
1:C:658:LEU:HD11	1:C:692:GLY:HA3	1.91	0.53
1:A:753:ASN:OD1	1:A:753:ASN:N	2.40	0.53
1:C:782:ASP:HA	1:C:884:LEU:HD23	1.90	0.53
1:D:240:LEU:HD23	1:D:240:LEU:C	2.28	0.53
1:C:749:ILE:HD12	1:C:749:ILE:N	2.21	0.53
1:A:200:GLN:HG2	1:A:391:HIS:HB2	1.90	0.53
1:B:625:GLN:NE2	5:B:4216:HOH:O	2.32	0.53
1:B:1017:GLN:HB2	5:B:4804:HOH:O	2.09	0.53
1:A:737:ILE:C	1:A:737:ILE:HD13	2.29	0.53
1:B:117:GLU:HA	1:B:117:GLU:OE1	2.09	0.53
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.90	0.53
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.77	0.53
1:D:773:LYS:HD2	1:D:774:LYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.09	0.53
1:B:437:SER:HB2	1:B:471:LEU:HD21	1.89	0.53
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.22	0.53
1:D:965:GLN:O	1:D:969:GLU:HG3	2.09	0.53
1:B:585:TRP:CE3	1:B:974:HIS:CE1	2.97	0.53
1:D:730:LEU:HD12	1:D:730:LEU:H	1.73	0.53
1:A:660:GLY:O	1:A:662:PRO:HD3	2.08	0.53
1:A:599:ARG:HH11	1:A:600:GLN:HE22	1.58	0.52
1:B:13:ARG:HG3	1:C:13:ARG:NH1	2.23	0.52
1:C:595:THR:HA	1:C:596:PRO:C	2.28	0.52
1:D:1017:GLN:HB2	5:D:4874:HOH:O	2.09	0.52
1:B:52:ARG:O	1:B:213:SER:HB2	2.08	0.52
1:A:625:GLN:NE2	5:A:4201:HOH:O	2.35	0.52
1:A:725:ASN:HB2	5:A:4834:HOH:O	2.10	0.52
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.74	0.52
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.45	0.52
4:D:8411:DMS:H13	5:D:4286:HOH:O	2.08	0.52
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.91	0.52
1:A:797:GLU:O	1:A:801:ILE:HD13	2.09	0.52
1:D:79:PRO:HG2	1:D:80:GLU:OE2	2.10	0.52
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.27	0.52
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.92	0.52
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.45	0.52
1:B:777:LEU:HG	1:B:889:ALA:HA	1.91	0.52
1:C:106:PRO:O	4:C:8419:DMS:H22	2.10	0.52
1:C:396:PRO:HG3	5:C:4147:HOH:O	2.10	0.52
1:C:499:ILE:HD11	1:C:529:GLU:CG	2.38	0.52
1:C:533:LEU:C	1:C:533:LEU:HD23	2.29	0.52
1:C:930:VAL:O	1:C:932:PRO:HD3	2.10	0.52
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.44	0.52
1:B:360:HIS:CE1	1:B:361:PRO:HD2	2.45	0.52
1:D:237:ARG:HG2	1:D:237:ARG:NH1	2.25	0.52
1:D:891:VAL:HG23	1:D:981:GLY:HA2	1.91	0.52
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.78	0.52
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.92	0.52
1:C:756:TRP:CD2	1:C:858:ILE:HD13	2.45	0.52
1:C:972:HIS:HB3	1:C:974:HIS:HD1	1.75	0.52
1:D:802:ASP:O	1:D:808:GLU:HG3	2.09	0.52
1:D:878:HIS:HD2	5:D:4110:HOH:O	1.93	0.52
1:C:127:PHE:N	1:C:127:PHE:CD2	2.78	0.52
1:C:178:ARG:HD2	5:C:4783:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:893:GLU:CG	1:D:894:ARG:HD2	2.40	0.52
1:A:127:PHE:N	1:A:127:PHE:CD2	2.77	0.51
1:B:533:LEU:HD23	1:B:533:LEU:C	2.30	0.51
1:A:367:MET:HB3	1:A:372:MET:HE2	1.92	0.51
1:A:683:PRO:O	1:A:685:LEU:HG	2.09	0.51
1:C:577:LYS:O	1:C:584:PRO:HA	2.09	0.51
1:C:767:GLN:HG3	1:C:768:MET:N	2.26	0.51
1:D:869:ASP:OD1	1:D:1015:HIS:ND1	2.42	0.51
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.93	0.51
1:A:129:VAL:N	1:A:180:GLY:O	2.41	0.51
1:C:579:ASP:OD1	1:C:583:ASN:HB2	2.09	0.51
1:A:40:GLU:HA	1:A:40:GLU:OE1	2.11	0.51
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.92	0.51
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.92	0.51
1:B:635:THR:HG23	1:B:681:GLU:OE1	2.10	0.51
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.77	0.51
1:A:997:ASP:HB2	1:A:999:TRP:CZ2	2.46	0.51
1:B:730:LEU:HD12	1:B:730:LEU:N	2.17	0.51
1:D:770:ILE:HD12	1:D:775:GLN:CD	2.31	0.51
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.05	0.51
1:A:800:ARG:CZ	1:A:800:ARG:HB2	2.36	0.51
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.11	0.51
1:D:145:GLY:HA2	5:D:4107:HOH:O	2.10	0.51
1:B:577:LYS:O	1:B:584:PRO:HA	2.11	0.51
1:C:655:MET:HE2	1:C:665:SER:HB3	1.93	0.51
1:D:521:LYS:HE2	5:D:4453:HOH:O	2.11	0.51
1:D:890:GLN:HG3	1:D:891:VAL:N	2.25	0.51
1:C:745:MET:O	1:C:746:ASP:OD1	2.29	0.50
1:D:843:GLN:HA	1:D:847:LYS:O	2.11	0.50
1:B:629:PHE:HA	1:B:637:GLU:O	2.11	0.50
1:D:896:ASN:HD21	1:D:917:ARG:HD2	1.77	0.50
1:A:125:LEU:O	1:A:183:ARG:HA	2.12	0.50
1:B:319:ASP:OD1	1:B:321:THR:N	2.42	0.50
1:C:658:LEU:O	1:C:659:ASP:C	2.47	0.50
1:C:765:LEU:HD21	1:C:768:MET:HE1	1.93	0.50
1:D:638:VAL:O	1:D:677:LYS:HA	2.12	0.50
1:B:132:SER:O	1:B:135:GLN:HG3	2.12	0.50
1:B:241:GLU:HG3	1:B:292:ARG:CG	2.42	0.50
1:D:135:GLN:C	1:D:136:GLU:HG2	2.31	0.50
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.46	0.50
1:B:930:VAL:HA	1:B:973:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:844:HIS:HD2	5:C:4734:HOH:O	1.95	0.50
1:A:756:TRP:CD2	1:A:858:ILE:HD13	2.47	0.50
1:B:127:PHE:CD2	1:B:127:PHE:N	2.80	0.50
1:C:829:THR:HG22	1:C:830:LEU:N	2.25	0.50
1:D:785:THR:HB	1:D:816:TYR:CE2	2.47	0.50
1:B:662:PRO:C	1:B:663:LEU:HD23	2.31	0.50
1:C:141:ILE:CD1	1:C:184:LEU:HD11	2.42	0.50
1:A:249:GLU:OE2	1:A:251:ARG:NE	2.43	0.50
1:B:873:ALA:O	1:B:876:THR:HG22	2.11	0.50
1:D:1020:TRP:HD1	1:D:1021:CYS:N	2.10	0.50
1:B:79:PRO:HD2	1:B:80:GLU:OE2	2.12	0.49
1:B:826:THR:OG1	1:B:837:THR:HB	2.12	0.49
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.79	0.49
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.94	0.49
1:A:376:ILE:HD12	1:A:401:LEU:HB3	1.94	0.49
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.47	0.49
1:A:668:VAL:HG12	1:A:669:PRO:O	2.12	0.49
1:A:742:THR:CG2	1:A:743:SER:N	2.74	0.49
1:C:416:GLU:HA	1:C:460:ASN:O	2.11	0.49
1:C:625:GLN:NE2	5:C:4225:HOH:O	2.40	0.49
1:A:699:ARG:NH1	5:A:4837:HOH:O	2.45	0.49
1:B:356:ARG:HD2	1:B:379:MET:HE1	1.94	0.49
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.48	0.49
1:B:788:PRO:HD2	1:B:968:MET:HB2	1.94	0.49
1:B:804:ASN:ND2	1:B:809:ARG:NH2	2.35	0.49
1:C:178:ARG:O	1:C:178:ARG:HG2	2.12	0.49
1:C:287:ASP:OD1	1:C:287:ASP:N	2.37	0.49
1:D:277:GLU:HA	5:D:4563:HOH:O	2.13	0.49
1:D:827:ALA:HB2	1:D:836:ILE:CD1	2.42	0.49
1:A:128:ASN:HB2	5:A:4769:HOH:O	2.11	0.49
1:B:658:LEU:O	1:B:661:LYS:HG3	2.13	0.49
1:D:630:ARG:NH1	5:D:4561:HOH:O	2.46	0.49
1:A:1022:GLN:NE2	1:A:1023:LYS:O	2.46	0.49
1:D:675:GLN:HG3	5:D:4760:HOH:O	2.11	0.49
1:B:805:ALA:O	1:B:809:ARG:HG3	2.13	0.49
1:B:942:ARG:HA	1:B:953:GLY:O	2.13	0.49
1:B:569:ASP:O	1:B:605:GLY:HA2	2.12	0.49
1:B:786:ARG:HG2	1:B:880:ALA:HB1	1.95	0.49
1:C:624:GLN:NE2	5:C:4043:HOH:O	2.46	0.49
1:C:730:LEU:N	1:C:730:LEU:HD23	2.28	0.49
1:C:734:SER:C	1:C:736:ALA:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.48	0.49
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.47	0.49
1:B:731:PRO:O	1:B:732:ALA:HB2	2.12	0.49
1:C:333:ARG:O	1:C:333:ARG:HG2	2.13	0.49
1:C:578:TYR:CE2	1:C:584:PRO:HB3	2.48	0.49
1:C:854:LYS:HD3	1:C:868:VAL:HG22	1.95	0.49
1:A:948:PRO:O	1:A:1022:GLN:HG2	2.12	0.48
1:B:513:PRO:O	1:B:514:ALA:HB3	2.12	0.48
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.95	0.48
1:D:767:GLN:NE2	1:D:774:LYS:NZ	2.61	0.48
1:D:991:MET:HE2	1:D:1003:VAL:HG21	1.94	0.48
1:A:230:ARG:NH1	1:A:241:GLU:HG3	2.28	0.48
1:A:755:ARG:NH2	1:A:772:ASP:HA	2.28	0.48
1:A:832:ASP:OD1	1:A:832:ASP:N	2.45	0.48
1:C:230:ARG:HB3	5:C:4785:HOH:O	2.12	0.48
1:D:893:GLU:HG2	1:D:894:ARG:CG	2.43	0.48
1:C:499:ILE:HD11	1:C:529:GLU:CD	2.33	0.48
1:C:733:ALA:O	1:C:734:SER:C	2.51	0.48
1:D:427:THR:HG21	1:D:462:SER:HB3	1.94	0.48
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.94	0.48
1:A:147:ASN:HA	1:A:148:SER:HA	1.58	0.48
1:A:580:GLU:HA	1:A:580:GLU:OE1	2.14	0.48
1:A:599:ARG:HG3	1:A:600:GLN:H	1.79	0.48
1:A:702:GLN:O	1:A:712:GLY:N	2.44	0.48
1:D:965:GLN:HA	1:D:968:MET:HE3	1.95	0.48
1:A:835:LEU:HD11	1:A:855:THR:HB	1.95	0.48
1:B:819:GLU:H	1:B:819:GLU:HG2	1.30	0.48
1:C:569:ASP:O	1:C:605:GLY:HA2	2.13	0.48
1:C:571:VAL:CG2	1:C:609:ALA:HA	2.43	0.48
1:A:80:GLU:OE1	1:A:80:GLU:N	2.29	0.48
1:B:433:LEU:O	1:B:433:LEU:HD12	2.13	0.48
1:B:683:PRO:O	1:B:685:LEU:HG	2.13	0.48
1:D:893:GLU:O	1:D:893:GLU:HG3	2.11	0.48
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.96	0.48
1:B:730:LEU:HA	1:B:731:PRO:HD3	1.77	0.48
1:B:842:TRP:C	1:B:843:GLN:HG3	2.33	0.48
1:C:347:LYS:HE3	5:C:4277:HOH:O	2.14	0.48
1:C:741:THR:N	1:C:748:CYS:O	2.35	0.48
1:D:142:ILE:CG1	1:D:170:GLU:HG2	2.35	0.48
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.40	0.48
1:B:128:ASN:HB2	1:B:181:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:ARG:HG2	1:B:880:ALA:CB	2.44	0.48
1:C:781:ARG:NH1	1:C:781:ARG:CG	2.76	0.48
1:C:806:TRP:HA	1:C:809:ARG:HE	1.78	0.48
4:C:8412:DMS:H11	5:C:4348:HOH:O	2.13	0.48
1:A:146:VAL:HG11	1:A:150:PHE:CD2	2.49	0.47
1:A:767:GLN:HG3	1:A:768:MET:N	2.28	0.47
1:B:71:GLU:H	1:B:71:GLU:CD	2.17	0.47
1:C:805:ALA:O	1:C:806:TRP:C	2.52	0.47
1:B:360:HIS:ND1	1:B:362:LEU:N	2.49	0.47
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.49	0.47
1:C:781:ARG:HD3	5:C:4276:HOH:O	2.14	0.47
1:D:833:ALA:HB1	1:D:858:ILE:O	2.14	0.47
1:A:126:THR:HA	1:A:182:ASN:O	2.14	0.47
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.96	0.47
1:D:316:HIS:HB2	1:D:321:THR:O	2.14	0.47
1:D:651:LEU:C	1:D:651:LEU:CD1	2.74	0.47
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.58	0.47
4:D:8423:DMS:H13	5:D:4553:HOH:O	2.14	0.47
1:D:976:LEU:HB2	4:D:8423:DMS:H11	1.96	0.47
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.49	0.47
1:C:533:LEU:HD23	1:C:534:ILE:N	2.30	0.47
1:D:476:LYS:HD2	5:D:4236:HOH:O	2.15	0.47
1:A:635:THR:HG22	1:A:636:ILE:N	2.29	0.47
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.49	0.47
1:B:128:ASN:HA	1:B:180:GLY:O	2.14	0.47
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.97	0.47
1:D:437:SER:O	1:D:441:THR:HG23	2.14	0.47
1:D:788:PRO:CD	1:D:968:MET:HG3	2.45	0.47
1:B:377:LEU:O	1:B:381:GLN:HG3	2.15	0.47
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.96	0.47
1:C:375:ASP:O	1:C:379:MET:HG3	2.14	0.47
1:A:685:LEU:O	1:A:687:GLN:OE1	2.33	0.47
1:B:131:GLU:O	1:B:131:GLU:HG3	2.15	0.47
1:B:830:LEU:HD12	1:B:833:ALA:HB3	1.96	0.47
1:D:133:TRP:HE1	4:D:8703:DMS:H23	1.78	0.47
1:D:142:ILE:HG12	1:D:170:GLU:CG	2.35	0.47
1:A:35:SER:HB2	1:A:217:LYS:HD3	1.95	0.47
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.41	0.47
1:C:699:ARG:NH1	5:C:4741:HOH:O	2.47	0.47
1:D:510:GLN:OE1	5:D:4667:HOH:O	2.20	0.47
1:A:103:VAL:HG22	1:A:418:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:914:CYS:HB2	5:B:4378:HOH:O	2.15	0.47
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.94	0.47
1:C:809:ARG:NH2	1:C:1001:PRO:HG3	2.30	0.47
1:A:685:LEU:CB	1:A:686:PRO:CD	2.92	0.46
1:B:131:GLU:O	1:B:135:GLN:N	2.38	0.46
1:B:372:MET:HE2	5:B:4207:HOH:O	2.15	0.46
1:B:730:LEU:H	1:B:730:LEU:CD1	2.13	0.46
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.97	0.46
1:D:640:SER:O	1:D:675:GLN:HA	2.15	0.46
1:D:873:ALA:O	1:D:876:THR:HG22	2.14	0.46
1:C:433:LEU:N	1:C:434:PRO:CD	2.78	0.46
1:C:655:MET:HE2	1:C:664:ALA:O	2.15	0.46
1:D:785:THR:O	1:D:881:ARG:HD2	2.15	0.46
1:A:115:PRO:HB2	1:A:117:GLU:O	2.16	0.46
1:A:826:THR:OG1	1:A:837:THR:HB	2.15	0.46
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.46
1:B:670:LEU:HA	1:B:670:LEU:HD23	1.63	0.46
1:B:685:LEU:HA	1:B:686:PRO:HD3	1.61	0.46
1:B:965:GLN:NE2	5:B:4822:HOH:O	2.48	0.46
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.15	0.46
1:D:251:ARG:NH1	5:D:4790:HOH:O	2.48	0.46
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.15	0.46
1:B:46:ARG:HB3	1:B:47:PRO:HD2	1.98	0.46
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.48	0.46
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.51	0.46
1:B:133:TRP:CE3	1:B:216:HIS:HB2	2.51	0.46
1:C:110:ASN:N	1:C:111:PRO:HD3	2.31	0.46
1:A:945:ASN:HB3	1:A:1023:LYS:NZ	2.31	0.46
1:B:262:GLN:CA	1:B:262:GLN:NE2	2.79	0.46
1:B:685:LEU:O	1:B:686:PRO:C	2.52	0.46
1:C:49:GLN:HB2	1:C:50:GLN:OE1	2.15	0.46
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.50	0.46
1:C:233:ASP:OD1	1:C:234:ASP:N	2.49	0.46
1:C:292:ARG:HG3	1:C:292:ARG:NH1	2.31	0.46
1:A:433:LEU:N	1:A:434:PRO:CD	2.79	0.46
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.78	0.46
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.79	0.46
1:C:22:THR:OG1	1:C:438:GLU:OE2	2.33	0.46
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.16	0.46
1:C:579:ASP:CG	1:C:583:ASN:HB2	2.36	0.46
1:C:655:MET:SD	1:C:656:VAL:N	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.97	0.46
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.50	0.46
1:C:706:THR:OG1	1:C:709:SER:N	2.48	0.46
1:A:262:GLN:HE22	1:A:299:LYS:HG3	1.81	0.45
1:B:360:HIS:CE1	1:B:362:LEU:H	2.29	0.45
1:C:649:ASN:HA	4:C:8425:DMS:C1	2.47	0.45
1:C:658:LEU:HG	1:C:661:LYS:HZ1	1.81	0.45
1:C:658:LEU:HG	1:C:661:LYS:HZ2	1.81	0.45
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.66	0.45
1:A:154:CYS:O	1:A:155:ASN:C	2.54	0.45
1:A:600:GLN:HB2	1:A:603:MET:CE	2.46	0.45
1:B:654:TRP:O	1:B:665:SER:HB2	2.16	0.45
1:B:910:LEU:C	1:B:910:LEU:HD12	2.37	0.45
1:C:305:ILE:HA	1:C:306:PRO:HD2	1.82	0.45
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.51	0.45
1:B:651:LEU:C	1:B:651:LEU:CD2	2.85	0.45
1:A:991:MET:HE2	1:A:1003:VAL:HG21	1.99	0.45
1:C:824:GLN:CG	1:C:825:CYS:N	2.78	0.45
1:D:158:TRP:CZ2	1:D:160:GLY:HA2	2.52	0.45
1:A:127:PHE:N	1:A:182:ASN:O	2.46	0.45
1:A:200:GLN:CG	1:A:391:HIS:HB2	2.46	0.45
1:A:734:SER:OG	1:A:860:GLY:HA3	2.16	0.45
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.98	0.45
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.17	0.45
1:B:46:ARG:HB3	1:B:47:PRO:CD	2.47	0.45
1:B:568:TRP:CG	1:B:569:ASP:HB3	2.52	0.45
1:C:824:GLN:HG2	1:C:825:CYS:N	2.31	0.45
1:C:890:GLN:HG3	1:C:891:VAL:N	2.30	0.45
1:D:301:TRP:CH2	1:D:452:SER:HA	2.52	0.45
1:C:829:THR:HG22	1:C:830:LEU:O	2.16	0.45
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.47	0.44
1:C:339:ASN:O	1:D:527:PRO:HB3	2.17	0.44
1:C:724:GLU:O	1:D:847:LYS:NZ	2.49	0.44
1:D:94:GLY:HA2	5:D:4199:HOH:O	2.17	0.44
1:D:446:ARG:NE	1:D:447:ASP:OD1	2.47	0.44
1:A:253:TYR:CD1	1:A:253:TYR:C	2.91	0.44
1:A:959:ILE:HD13	1:A:959:ILE:HG21	1.65	0.44
1:B:340:GLY:O	1:B:561:ARG:HG2	2.18	0.44
1:A:577:LYS:HD3	1:A:587:ALA:HB2	2.00	0.44
1:A:890:GLN:HG3	1:A:891:VAL:N	2.32	0.44
1:B:662:PRO:O	1:B:663:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:TRP:CD1	1:B:774:LYS:HG3	2.52	0.44
1:B:797:GLU:O	1:B:800:ARG:C	2.56	0.44
1:C:510:GLN:HB3	1:C:512:PHE:CZ	2.53	0.44
1:D:133:TRP:NE1	4:D:8703:DMS:C2	2.79	0.44
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.53	0.44
1:B:959:ILE:HA	1:B:983:TRP:O	2.18	0.44
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.80	0.44
1:C:968:MET:O	1:C:968:MET:HG3	2.18	0.44
1:D:107:ILE:N	4:D:8419:DMS:C2	2.78	0.44
1:D:192:SER:O	1:D:195:SER:HB2	2.18	0.44
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.99	0.44
1:D:962:TYR:CE2	1:D:976:LEU:HB3	2.53	0.44
1:A:433:LEU:N	1:A:434:PRO:HD2	2.32	0.44
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.17	0.44
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.44
1:D:595:THR:OG1	1:D:596:PRO:HA	2.18	0.44
1:A:99:ILE:HB	1:A:204:ARG:HB2	1.99	0.44
1:A:473:ARG:HH12	1:A:477:SER:N	2.15	0.44
1:B:801:ILE:HD13	1:B:801:ILE:N	2.33	0.44
1:B:843:GLN:HG2	1:B:848:THR:HA	2.00	0.44
5:B:4578:HOH:O	4:C:8420:DMS:H11	2.18	0.44
1:C:610:ASP:O	1:C:611:ARG:HB2	2.17	0.44
1:C:743:SER:HB3	5:C:4618:HOH:O	2.18	0.44
1:D:808:GLU:HA	1:D:811:LYS:HD3	2.00	0.44
1:A:990:HIS:HD2	1:A:991:MET:O	2.00	0.44
1:B:634:GLN:HG2	1:B:682:LEU:C	2.37	0.44
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.52	0.44
1:C:580:GLU:H	1:C:580:GLU:HG3	1.54	0.44
1:C:1023:LYS:HA	1:C:1023:LYS:CE	2.48	0.44
1:D:130:ASP:O	1:D:131:GLU:C	2.56	0.44
1:D:243:GLU:OE2	1:D:245:GLN:NE2	2.42	0.44
1:A:577:LYS:HD2	1:A:592:PHE:CE2	2.53	0.44
1:B:772:ASP:OD1	1:B:773:LYS:HD3	2.18	0.44
1:C:111:PRO:HA	1:C:112:PRO:HA	1.71	0.44
1:C:755:ARG:HH11	1:C:755:ARG:HD3	1.64	0.44
1:D:130:ASP:OD1	1:D:132:SER:OG	2.30	0.44
1:D:376:ILE:CD1	1:D:401:LEU:HB3	2.48	0.44
1:D:1022:GLN:HE22	1:D:1023:LYS:HG2	1.80	0.44
1:A:118:ASN:HA	1:A:119:PRO:HD2	1.83	0.43
1:B:852:SER:HA	1:B:870:VAL:HG22	2.00	0.43
1:B:965:GLN:HA	1:B:968:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:THR:HA	1:C:182:ASN:O	2.18	0.43
1:C:147:ASN:HA	1:C:148:SER:HA	1.80	0.43
1:C:614:HIS:HB3	1:C:615:PRO:CD	2.46	0.43
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.18	0.43
1:D:653:HIS:ND1	1:D:701:VAL:CG2	2.74	0.43
1:A:292:ARG:NH1	4:A:8412:DMS:H23	2.31	0.43
1:B:642:TYR:O	1:B:675:GLN:OE1	2.36	0.43
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.76	0.43
1:C:737:ILE:CD1	1:C:738:PRO:HD2	2.32	0.43
1:C:1006:GLU:HG2	1:C:1007:PHE:CD1	2.53	0.43
1:B:183:ARG:HB3	5:B:4316:HOH:O	2.18	0.43
1:B:299:LYS:HE2	5:B:4633:HOH:O	2.18	0.43
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.52	0.43
1:B:393:PRO:HD3	1:B:412:GLU:O	2.17	0.43
1:B:639:THR:OG1	1:B:677:LYS:HG2	2.19	0.43
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.36	0.43
1:D:827:ALA:CB	1:D:836:ILE:CD1	2.97	0.43
1:A:755:ARG:HH22	1:A:772:ASP:HA	1.84	0.43
1:B:261:TRP:CZ3	1:B:266:GLN:HB2	2.54	0.43
1:C:131:GLU:OE1	1:C:179:ALA:HB2	2.19	0.43
1:C:780:LEU:C	1:C:781:ARG:HG3	2.38	0.43
1:C:823:LEU:O	1:D:730:LEU:HD21	2.18	0.43
4:D:8419:DMS:H21	5:D:4366:HOH:O	2.17	0.43
1:B:377:LEU:HD22	1:B:708:TRP:CA	2.47	0.43
1:D:581:ASN:HD22	1:D:583:ASN:ND2	2.07	0.43
1:D:598:ASP:CG	4:D:8506:DMS:H11	2.39	0.43
1:D:890:GLN:HB2	5:D:4743:HOH:O	2.17	0.43
1:A:780:LEU:HA	1:A:886:CYS:HB3	2.00	0.43
1:A:830:LEU:HD12	1:A:833:ALA:HB3	2.01	0.43
1:A:930:VAL:HA	1:A:973:ARG:HD3	2.00	0.43
1:B:486:TYR:CZ	1:B:488:GLY:HA3	2.54	0.43
1:B:578:TYR:HA	1:B:583:ASN:O	2.18	0.43
1:C:989:PHE:CE1	1:C:1014:TYR:HB3	2.54	0.43
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.53	0.43
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.34	0.43
1:B:663:LEU:HD23	1:B:663:LEU:N	2.34	0.43
1:B:961:ARG:NE	1:B:981:GLY:O	2.49	0.43
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.53	0.43
1:C:579:ASP:OD1	1:C:583:ASN:N	2.42	0.43
1:C:759:ASN:HB3	1:C:762:SER:OG	2.19	0.43
1:D:827:ALA:HB2	1:D:836:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.54	0.43
1:C:367:MET:HB3	1:C:372:MET:CE	2.49	0.43
1:D:769:TRP:HA	1:D:773:LYS:O	2.19	0.43
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.54	0.42
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.19	0.42
1:B:59:ARG:HA	1:B:59:ARG:HD2	1.88	0.42
1:B:637:GLU:OE2	1:B:677:LYS:HD3	2.18	0.42
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.99	0.42
1:C:997:ASP:HB2	1:C:999:TRP:CE2	2.54	0.42
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.80	0.42
1:D:595:THR:HA	1:D:596:PRO:O	2.17	0.42
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.48	0.42
1:A:367:MET:HB3	1:A:372:MET:CE	2.48	0.42
1:A:801:ILE:HD13	1:A:801:ILE:HA	1.71	0.42
1:A:823:LEU:O	1:B:730:LEU:HD23	2.19	0.42
1:B:215:LEU:HD21	1:B:217:LYS:HD3	2.01	0.42
1:B:661:LYS:NZ	5:B:4774:HOH:O	2.47	0.42
1:C:479:ASP:HA	1:C:480:PRO:HD3	1.51	0.42
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.01	0.42
1:D:663:LEU:HD22	1:D:663:LEU:HA	1.84	0.42
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.82	0.42
1:D:211:ASP:HB3	5:D:4335:HOH:O	2.18	0.42
1:D:359:HIS:CD2	1:D:573:GLN:HA	2.55	0.42
1:D:703:PRO:HG2	4:D:8425:DMS:H11	2.02	0.42
1:A:736:ALA:HB1	1:A:751:LEU:HD11	2.01	0.42
1:B:262:GLN:NE2	1:B:263:GLY:N	2.67	0.42
1:A:424:ASN:O	1:A:425:ARG:C	2.57	0.42
1:B:320:GLY:HA2	4:B:8406:DMS:O	2.19	0.42
1:C:487:GLU:O	1:C:491:ALA:N	2.50	0.42
1:D:518:TRP:CD1	1:D:526:LEU:HD11	2.55	0.42
1:D:583:ASN:HA	1:D:584:PRO:HD3	1.75	0.42
1:A:226:HIS:O	1:A:242:ALA:HA	2.19	0.42
1:A:255:ARG:HD3	1:A:273:PRO:HA	2.01	0.42
1:B:167:LEU:HD23	1:B:167:LEU:HA	1.94	0.42
1:C:262:GLN:HE21	1:C:262:GLN:HB3	1.56	0.42
1:C:651:LEU:C	1:C:651:LEU:CD1	2.88	0.42
1:C:734:SER:CB	1:C:860:GLY:HA3	2.50	0.42
1:C:768:MET:HB2	1:C:775:GLN:HB2	2.02	0.42
1:C:799:THR:H	1:C:799:THR:HG23	1.41	0.42
1:C:894:ARG:NE	1:C:919:ASP:OD1	2.50	0.42
1:A:734:SER:C	1:A:736:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.82	0.42
1:D:157:ARG:NH1	1:D:175:ALA:O	2.52	0.42
1:D:200:GLN:HG2	1:D:391:HIS:HB2	2.01	0.42
1:D:737:ILE:CD1	1:D:832:ASP:HA	2.47	0.42
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.55	0.42
1:D:898:LEU:HD12	1:D:898:LEU:HA	1.82	0.42
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.83	0.42
1:A:817:GLN:HE21	1:A:817:GLN:HB3	1.24	0.42
1:B:499:ILE:HD11	1:B:529:GLU:CG	2.49	0.42
1:A:127:PHE:O	1:A:182:ASN:N	2.33	0.42
1:A:770:ILE:HD12	1:A:775:GLN:CD	2.39	0.42
4:A:8425:DMS:H21	5:A:4695:HOH:O	2.19	0.42
1:C:26:ARG:HD2	1:C:169:SER:HA	2.01	0.42
1:C:200:GLN:HG2	1:C:391:HIS:HB2	2.01	0.42
1:C:957:PHE:HA	1:C:985:ASN:O	2.20	0.42
1:A:13:ARG:HB3	1:A:14:ARG:H	1.59	0.42
1:A:863:GLN:HE22	1:A:952:ARG:HH22	1.66	0.42
1:B:542:MET:HE3	1:B:601:PHE:HA	2.01	0.42
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.55	0.42
1:B:658:LEU:HG	1:B:659:ASP:OD2	2.20	0.42
1:B:731:PRO:HB2	1:B:732:ALA:H	1.69	0.42
1:C:895:VAL:O	1:C:919:ASP:HA	2.19	0.42
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.55	0.42
1:D:340:GLY:O	1:D:561:ARG:HG2	2.20	0.42
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.55	0.42
1:A:114:VAL:HB	1:A:115:PRO:HD2	2.02	0.41
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.55	0.41
1:B:114:VAL:HB	1:B:115:PRO:CD	2.49	0.41
1:B:261:TRP:CH2	1:B:266:GLN:HB2	2.55	0.41
1:C:114:VAL:HB	1:C:115:PRO:HD2	2.02	0.41
1:A:103:VAL:HG13	1:A:418:GLU:HG2	2.02	0.41
1:A:157:ARG:NH1	1:A:157:ARG:CG	2.81	0.41
1:A:769:TRP:HA	1:A:773:LYS:O	2.20	0.41
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.51	0.41
1:C:940:GLY:O	5:C:4357:HOH:O	2.22	0.41
1:D:639:THR:OG1	1:D:677:LYS:HD3	2.19	0.41
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.55	0.41
1:B:200:GLN:CG	1:B:391:HIS:HB2	2.49	0.41
1:B:651:LEU:HD22	1:B:651:LEU:C	2.40	0.41
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.50	0.41
1:A:658:LEU:O	1:A:659:ASP:C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:O	1:B:178:ARG:HG3	2.17	0.41
1:B:986:ILE:HG23	1:B:986:ILE:O	2.20	0.41
1:C:63:PHE:HB3	1:C:64:PRO:HD2	2.02	0.41
1:C:240:LEU:C	1:C:240:LEU:HD23	2.40	0.41
1:D:323:ILE:HD12	1:D:323:ILE:N	2.35	0.41
1:B:190:ARG:HG2	1:B:191:TRP:CE2	2.54	0.41
1:B:758:PHE:CZ	1:B:765:LEU:HD13	2.55	0.41
1:C:138:GLN:HA	1:C:174:SER:OG	2.20	0.41
1:C:356:ARG:HH22	1:C:367:MET:CE	2.32	0.41
1:C:279:ILE:HA	1:C:279:ILE:HD13	1.78	0.41
1:C:629:PHE:HA	1:C:637:GLU:O	2.20	0.41
1:A:241:GLU:OE2	1:A:292:ARG:NE	2.46	0.41
1:A:696:LEU:HD23	1:A:720:TRP:CE3	2.55	0.41
1:B:869:ASP:OD1	1:B:1015:HIS:ND1	2.36	0.41
1:C:658:LEU:CG	1:C:661:LYS:NZ	2.83	0.41
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.65	0.41
1:D:577:LYS:HB3	1:D:577:LYS:HE3	1.81	0.41
1:D:736:ALA:HB1	1:D:737:ILE:H	1.69	0.41
1:D:896:ASN:HA	1:D:918:TRP:O	2.21	0.41
1:B:110:ASN:N	1:B:111:PRO:HD3	2.36	0.41
1:C:778:THR:HG23	1:C:887:GLN:CB	2.50	0.41
1:C:825:CYS:HA	1:C:837:THR:O	2.21	0.41
1:C:972:HIS:HB3	1:C:974:HIS:ND1	2.35	0.41
1:D:36:TRP:CD2	1:D:42:ALA:HA	2.56	0.41
1:D:250:LEU:C	1:D:251:ARG:HG2	2.40	0.41
1:A:73:TRP:O	1:A:183:ARG:NH2	2.47	0.41
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.38	0.41
1:A:699:ARG:HD3	1:A:714:ILE:HD12	2.03	0.41
1:A:701:VAL:HG22	1:A:714:ILE:HD13	2.03	0.41
1:B:63:PHE:HB3	1:B:64:PRO:HD2	2.02	0.41
1:B:262:GLN:NE2	1:B:262:GLN:HA	2.35	0.41
1:B:674:PRO:O	1:B:675:GLN:HB2	2.21	0.41
1:B:785:THR:O	1:B:881:ARG:HD2	2.21	0.41
1:B:907:PRO:HG2	1:B:990:HIS:O	2.21	0.41
1:C:143:PHE:O	1:C:168:PRO:HA	2.20	0.41
1:C:471:LEU:HA	1:C:471:LEU:HD23	1.83	0.41
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.56	0.41
1:C:562:LEU:HD23	1:C:562:LEU:HA	1.95	0.41
1:D:225:PHE:HA	1:D:243:GLU:O	2.21	0.41
1:B:347:LYS:HG3	1:B:644:PHE:CE2	2.55	0.41
1:B:777:LEU:HD23	1:B:777:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:608:PHE:CD1	1:C:614:HIS:HD2	2.39	0.41
1:D:147:ASN:HA	1:D:148:SER:HA	1.52	0.41
1:D:907:PRO:HG2	1:D:990:HIS:O	2.20	0.41
1:B:736:ALA:O	1:B:860:GLY:HA3	2.22	0.40
1:C:708:TRP:CH2	4:C:8403:DMS:H13	2.56	0.40
1:C:745:MET:HE3	1:C:745:MET:HB3	1.77	0.40
1:D:745:MET:HE1	1:D:761:GLN:HB2	2.02	0.40
1:D:963:SER:OG	1:D:966:GLN:HB2	2.22	0.40
1:A:486:TYR:CZ	1:A:488:GLY:HA3	2.56	0.40
1:A:668:VAL:HG11	1:A:680:ILE:HD13	2.02	0.40
1:A:750:GLU:CG	1:A:751:LEU:N	2.84	0.40
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.46	0.40
1:B:1018:LEU:HD23	1:B:1018:LEU:C	2.41	0.40
1:C:89:ASN:O	1:C:92:MET:HB2	2.21	0.40
1:C:622:HIS:CE1	4:C:8402:DMS:C1	3.04	0.40
1:D:949:HIS:HB2	1:D:951:TRP:CH2	2.55	0.40
1:A:101:THR:HG23	1:A:204:ARG:NH2	2.37	0.40
1:A:502:MET:HB2	1:A:503:TYR:CD1	2.56	0.40
1:C:316:HIS:HB2	1:C:321:THR:O	2.21	0.40
1:C:559:TYR:CE2	1:D:522:LYS:HA	2.56	0.40
1:C:972:HIS:CB	1:C:974:HIS:CE1	3.04	0.40
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.04	0.40
1:D:807:VAL:HG13	1:D:808:GLU:N	2.36	0.40
1:D:847:LYS:HG3	1:D:848:THR:N	2.35	0.40
1:A:573:GLN:HB2	1:A:602:CYS:O	2.22	0.40
1:A:703:PRO:HG2	4:A:8425:DMS:H11	2.04	0.40
1:B:32:PRO:HG2	5:B:4208:HOH:O	2.22	0.40
1:B:423:MET:HE2	1:C:282:ARG:HG2	2.03	0.40
1:B:824:GLN:O	1:B:838:THR:HA	2.22	0.40
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.82	0.40
1:C:474:TRP:O	1:C:478:VAL:HG13	2.22	0.40
1:C:600:GLN:HB2	1:C:603:MET:HE2	2.02	0.40
1:C:684:GLU:HG2	1:C:685:LEU:N	2.21	0.40
1:B:894:ARG:HE	1:B:894:ARG:HB3	1.72	0.40
1:C:767:GLN:CG	1:C:768:MET:N	2.85	0.40
1:D:63:PHE:CD1	1:D:69:VAL:HG22	2.56	0.40
1:D:107:ILE:C	4:D:8419:DMS:H21	2.42	0.40
1:D:959:ILE:HG21	1:D:959:ILE:HD13	1.78	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	1009/1023 (99%)	963 (95%)	44 (4%)	2 (0%)	47	39
1	B	1009/1023 (99%)	965 (96%)	36 (4%)	8 (1%)	19	10
1	C	1009/1023 (99%)	961 (95%)	47 (5%)	1 (0%)	51	45
1	D	1009/1023 (99%)	958 (95%)	48 (5%)	3 (0%)	41	31
All	All	4036/4092 (99%)	3847 (95%)	175 (4%)	14 (0%)	41	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	690	SER
1	B	731	PRO
1	A	689	GLU
1	D	688	PRO
1	B	732	ALA
1	B	733	ALA
1	D	733	ALA
1	A	164	ASP
1	B	164	ASP
1	B	686	PRO
1	B	687	GLN
1	D	540	HIS
1	C	164	ASP

### 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	864/875 (99%)	825 (96%)	39 (4%)	27	20
1	B	864/875 (99%)	809 (94%)	55 (6%)	17	9
1	C	864/875 (99%)	822 (95%)	42 (5%)	25	17
1	D	864/875 (99%)	818 (95%)	46 (5%)	22	14
All	All	3456/3500 (99%)	3274 (95%)	182 (5%)	22	14

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	131	GLU
1	A	157	ARG
1	A	178	ARG
1	A	250	LEU
1	A	267	VAL
1	A	333	ARG
1	A	394	ASN
1	A	431	ARG
1	A	519	SER
1	A	546	LEU
1	A	600	GLN
1	A	632	SER
1	A	634	GLN
1	A	655	MET
1	A	661	LYS
1	A	663	LEU
1	A	667	GLU
1	A	670	LEU
1	A	671	ASP
1	A	684	GLU
1	A	729	THR
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	774	LYS
1	A	782	ASP
1	A	797	GLU
1	A	799	THR
1	A	800	ARG
1	A	817	GLN
1	A	819	GLU
1	A	824	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	859	ASP
1	A	885	ASN
1	A	926	TYR
1	A	958	ASN
1	A	969	GLU
1	A	1023	LYS
1	B	13	ARG
1	B	80	GLU
1	B	117	GLU
1	B	130	ASP
1	B	181	GLU
1	B	230	ARG
1	B	262	GLN
1	B	264	GLU
1	B	277	GLU
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
1	B	370	GLN
1	B	394	ASN
1	B	519	SER
1	B	546	LEU
1	B	554	GLN
1	B	580	GLU
1	B	595	THR
1	B	600	GLN
1	B	604	ASN
1	B	630	ARG
1	B	634	GLN
1	B	635	THR
1	B	636	ILE
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	667	GLU
1	B	685	LEU
1	B	687	GLN
1	B	689	GLU
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	748	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	750	GLU
1	B	766	SER
1	B	768	MET
1	B	769	TRP
1	B	773	LYS
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	801	ILE
1	B	819	GLU
1	B	824	GLN
1	B	845	GLN
1	B	847	LYS
1	B	863	GLN
1	B	956	GLN
1	B	968	MET
1	B	969	GLU
1	B	1004	SER
1	B	1023	LYS
1	C	13	ARG
1	C	75	GLU
1	C	76	CYS
1	C	80	GLU
1	C	135	GLN
1	C	136	GLU
1	C	178	ARG
1	C	249	GLU
1	C	262	GLN
1	C	264	GLU
1	C	333	ARG
1	C	344	LEU
1	C	394	ASN
1	C	400	THR
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	581	ASN
1	C	634	GLN
1	C	655	MET
1	C	663	LEU
1	C	681	GLU
1	C	685	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	687	GLN
1	C	710	GLU
1	C	730	LEU
1	C	737	ILE
1	C	746	ASP
1	C	750	GLU
1	C	773	LYS
1	C	781	ARG
1	C	800	ARG
1	C	801	ILE
1	C	824	GLN
1	C	854	LYS
1	C	859	ASP
1	C	881	ARG
1	C	956	GLN
1	C	968	MET
1	C	986	ILE
1	C	1022	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	49	GLN
1	D	71	GLU
1	D	76	CYS
1	D	80	GLU
1	D	90	TRP
1	D	108	THR
1	D	128	ASN
1	D	129	VAL
1	D	237	ARG
1	D	299	LYS
1	D	333	ARG
1	D	370	GLN
1	D	390	SER
1	D	394	ASN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	632	SER
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	667	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	681	GLU
1	D	682	LEU
1	D	684	GLU
1	D	685	LEU
1	D	689	GLU
1	D	699	ARG
1	D	730	LEU
1	D	735	HIS
1	D	745	MET
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	799	THR
1	D	800	ARG
1	D	824	GLN
1	D	845	GLN
1	D	885	ASN
1	D	893	GLU
1	D	910	LEU
1	D	956	GLN
1	D	986	ILE
1	D	1018	LEU
1	D	1022	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	262	GLN
1	A	363	HIS
1	A	394	ASN
1	A	600	GLN
1	A	761	GLN
1	A	817	GLN
1	A	824	GLN
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	A	977	HIS
1	B	262	GLN
1	B	266	GLN
1	B	297	ASN
1	B	554	GLN

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Mol	Chain	Res	Type
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	653	HIS
1	B	675	GLN
1	B	687	GLN
1	B	757	GLN
1	B	804	ASN
1	B	878	HIS
1	B	965	GLN
1	B	977	HIS
1	C	135	GLN
1	C	226	HIS
1	C	262	GLN
1	C	583	ASN
1	C	614	HIS
1	C	624	GLN
1	C	634	GLN
1	C	687	GLN
1	C	804	ASN
1	C	824	GLN
1	C	843	GLN
1	C	878	HIS
1	D	135	GLN
1	D	583	ASN
1	D	628	GLN
1	D	634	GLN
1	D	761	GLN
1	D	767	GLN
1	D	804	ASN
1	D	824	GLN
1	D	878	HIS
1	D	903	GLN
1	D	977	HIS
1	D	1022	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 26 are monoatomic - leaving 82 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	DMS	A	8602	-	3,3,3	1.16	0	3,3,3	0.21	0
4	DMS	D	8703	-	3,3,3	0.74	0	3,3,3	0.48	0
4	DMS	C	8412	-	3,3,3	0.54	0	3,3,3	0.45	0
4	DMS	A	8416	-	3,3,3	1.05	0	3,3,3	0.49	0
4	DMS	D	8403	-	3,3,3	1.97	1 (33%)	3,3,3	0.36	0
4	DMS	D	8408	-	3,3,3	0.55	0	3,3,3	0.32	0
4	DMS	B	8417	-	3,3,3	0.44	0	3,3,3	0.27	0
4	DMS	C	8405	-	3,3,3	1.67	1 (33%)	3,3,3	0.30	0
4	DMS	B	8403	-	3,3,3	1.74	1 (33%)	3,3,3	0.31	0
4	DMS	C	8409	-	3,3,3	0.92	0	3,3,3	0.27	0
4	DMS	C	8601	-	3,3,3	1.88	1 (33%)	3,3,3	0.63	0
4	DMS	C	8421	-	3,3,3	0.52	0	3,3,3	0.19	0
4	DMS	A	8409	-	3,3,3	1.56	1 (33%)	3,3,3	0.18	0
4	DMS	A	8403	-	3,3,3	2.00	2 (66%)	3,3,3	0.72	0
4	DMS	D	8506	-	3,3,3	1.92	1 (33%)	3,3,3	0.44	0
4	DMS	D	8705	-	3,3,3	0.26	0	3,3,3	1.07	0
4	DMS	D	8409	-	3,3,3	1.24	1 (33%)	3,3,3	0.38	0
4	DMS	B	8412	-	3,3,3	1.20	0	3,3,3	0.26	0
4	DMS	B	8416	-	3,3,3	0.83	0	3,3,3	0.36	0
4	DMS	D	8425	3	3,3,3	0.44	0	3,3,3	0.34	0
4	DMS	D	8501	-	3,3,3	0.51	0	3,3,3	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	A	8425	3	3,3,3	1.06	0	3,3,3	0.19	0
4	DMS	D	8701	-	3,3,3	1.73	1 (33%)	3,3,3	0.99	0
4	DMS	C	8411	-	3,3,3	1.19	0	3,3,3	0.37	0
4	DMS	B	8411	-	3,3,3	1.19	1 (33%)	3,3,3	0.23	0
4	DMS	C	8403	-	3,3,3	1.57	1 (33%)	3,3,3	0.25	0
4	DMS	A	8402	-	3,3,3	1.31	0	3,3,3	0.31	0
4	DMS	C	8414	-	3,3,3	0.93	0	3,3,3	0.23	0
4	DMS	C	8420	-	3,3,3	1.70	1 (33%)	3,3,3	0.08	0
4	DMS	B	8404	-	3,3,3	0.35	0	3,3,3	0.66	0
4	DMS	A	8408	-	3,3,3	0.34	0	3,3,3	0.10	0
4	DMS	A	8421	-	3,3,3	1.09	0	3,3,3	0.23	0
4	DMS	B	8402	-	3,3,3	0.79	0	3,3,3	0.53	0
4	DMS	D	8412	-	3,3,3	0.88	0	3,3,3	0.40	0
4	DMS	A	8501	-	3,3,3	1.42	0	3,3,3	0.52	0
4	DMS	A	8404	-	3,3,3	1.21	0	3,3,3	0.46	0
4	DMS	B	8421	-	3,3,3	0.70	0	3,3,3	0.58	0
4	DMS	D	8416	-	3,3,3	1.19	0	3,3,3	0.23	0
4	DMS	B	8423	-	3,3,3	0.88	0	3,3,3	0.55	0
4	DMS	D	8402	-	3,3,3	0.62	0	3,3,3	0.47	0
4	DMS	A	8405	-	3,3,3	1.58	1 (33%)	3,3,3	0.22	0
4	DMS	C	8419	-	3,3,3	0.79	0	3,3,3	0.30	0
4	DMS	C	8602	-	3,3,3	1.63	1 (33%)	3,3,3	0.24	0
4	DMS	C	8417	-	3,3,3	0.12	0	3,3,3	0.50	0
4	DMS	B	8408	-	3,3,3	0.76	0	3,3,3	1.40	1 (33%)
4	DMS	C	8416	-	3,3,3	0.76	0	3,3,3	0.43	0
4	DMS	C	8425	3	3,3,3	1.50	1 (33%)	3,3,3	0.33	0
4	DMS	B	8405	-	3,3,3	1.72	1 (33%)	3,3,3	0.34	0
4	DMS	D	8420	-	3,3,3	1.56	1 (33%)	3,3,3	0.28	0
4	DMS	C	8402	-	3,3,3	1.39	1 (33%)	3,3,3	0.09	0
4	DMS	B	8601	-	3,3,3	1.17	0	3,3,3	0.45	0
4	DMS	C	8408	-	3,3,3	1.15	0	3,3,3	0.53	0
4	DMS	C	8501	-	3,3,3	1.36	0	3,3,3	0.46	0
4	DMS	C	8401	-	3,3,3	1.60	1 (33%)	3,3,3	0.29	0
4	DMS	D	8508	-	3,3,3	1.02	0	3,3,3	0.27	0
4	DMS	B	8504	-	3,3,3	0.96	0	3,3,3	0.64	0
4	DMS	A	8411	-	3,3,3	0.69	0	3,3,3	0.11	0
4	DMS	A	8504	-	3,3,3	0.48	0	3,3,3	0.33	0
4	DMS	C	8504	-	3,3,3	0.44	0	3,3,3	0.30	0
4	DMS	D	8421	-	3,3,3	0.54	0	3,3,3	0.11	0
4	DMS	A	8414	-	3,3,3	0.81	0	3,3,3	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	D	8411	-	3,3,3	0.85	0	3,3,3	0.13	0
4	DMS	B	8406	-	3,3,3	0.66	0	3,3,3	0.27	0
4	DMS	C	8407	-	3,3,3	2.15	2 (66%)	3,3,3	0.20	0
4	DMS	C	8423	-	3,3,3	0.54	0	3,3,3	0.45	0
4	DMS	D	8404	-	3,3,3	1.16	0	3,3,3	0.16	0
4	DMS	B	8409	-	3,3,3	1.67	1 (33%)	3,3,3	0.38	0
4	DMS	B	8414	-	3,3,3	0.71	0	3,3,3	0.45	0
4	DMS	A	8412	-	3,3,3	0.87	0	3,3,3	0.47	0
4	DMS	D	8423	-	3,3,3	1.13	0	3,3,3	0.26	0
4	DMS	A	8401	-	3,3,3	0.56	0	3,3,3	0.34	0
4	DMS	B	8425	3	3,3,3	1.66	1 (33%)	3,3,3	0.20	0
4	DMS	C	8404	-	3,3,3	1.46	1 (33%)	3,3,3	1.18	1 (33%)
4	DMS	D	8406	-	3,3,3	1.11	0	3,3,3	0.65	0
4	DMS	B	8401	-	3,3,3	1.09	0	3,3,3	0.56	0
4	DMS	B	8508	-	3,3,3	1.64	1 (33%)	3,3,3	0.90	0
4	DMS	D	8401	-	3,3,3	1.36	1 (33%)	3,3,3	0.85	0
4	DMS	A	8406	-	3,3,3	0.76	0	3,3,3	0.92	0
4	DMS	C	8506	-	3,3,3	1.61	1 (33%)	3,3,3	0.25	0
4	DMS	D	8419	-	3,3,3	1.31	1 (33%)	3,3,3	0.91	0
4	DMS	D	8414	-	3,3,3	0.42	0	3,3,3	0.08	0
4	DMS	D	8405	-	3,3,3	1.13	0	3,3,3	1.11	0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8506	DMS	O-S	3.19	1.71	1.50
4	C	8601	DMS	C2-S	3.16	1.99	1.75
4	B	8405	DMS	O-S	2.87	1.69	1.50
4	D	8403	DMS	C2-S	2.79	1.96	1.75
4	B	8409	DMS	O-S	2.78	1.69	1.50
4	B	8403	DMS	C2-S	2.70	1.95	1.75
4	B	8425	DMS	O-S	2.70	1.68	1.50
4	C	8420	DMS	O-S	2.67	1.68	1.50
4	C	8405	DMS	C1-S	2.63	1.95	1.75
4	A	8409	DMS	O-S	2.56	1.67	1.50
4	A	8403	DMS	C2-S	2.54	1.94	1.75
4	C	8602	DMS	C2-S	-2.46	1.57	1.75
4	C	8425	DMS	O-S	2.44	1.66	1.50
4	A	8405	DMS	O-S	2.41	1.66	1.50
4	B	8508	DMS	C1-S	2.39	1.93	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8407	DMS	O-S	2.36	1.66	1.50
4	C	8404	DMS	C2-S	2.36	1.93	1.75
4	C	8401	DMS	O-S	2.35	1.66	1.50
4	D	8420	DMS	C1-S	2.33	1.93	1.75
4	C	8506	DMS	C1-S	2.33	1.93	1.75
4	A	8403	DMS	O-S	2.26	1.65	1.50
4	D	8419	DMS	C2-S	-2.21	1.59	1.75
4	C	8407	DMS	C2-S	2.17	1.92	1.75
4	C	8403	DMS	C2-S	2.14	1.91	1.75
4	C	8402	DMS	C2-S	2.12	1.91	1.75
4	D	8409	DMS	O-S	2.10	1.64	1.50
4	D	8701	DMS	C1-S	2.06	1.91	1.75
4	D	8401	DMS	O-S	2.06	1.64	1.50
4	B	8411	DMS	C1-S	2.01	1.90	1.75

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8408	DMS	C2-S-C1	2.40	110.81	98.44
4	C	8404	DMS	C2-S-C1	2.01	108.77	98.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	8703	DMS	4	0
4	C	8412	DMS	1	0
4	A	8416	DMS	1	0
4	D	8506	DMS	1	0
4	D	8425	DMS	1	0
4	A	8425	DMS	2	0
4	C	8403	DMS	1	0
4	C	8420	DMS	2	0
4	D	8412	DMS	2	0
4	C	8419	DMS	1	0
4	C	8425	DMS	1	0
4	C	8402	DMS	1	0
4	B	8601	DMS	1	0
4	C	8504	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8414	DMS	1	0
4	D	8411	DMS	1	0
4	B	8406	DMS	1	0
4	A	8412	DMS	4	0
4	D	8423	DMS	2	0
4	D	8419	DMS	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1011/1023 (98%)	-0.54	22 (2%) 62 66	9, 22, 53, 100	0
1	B	1011/1023 (98%)	-0.59	8 (0%) 86 88	11, 23, 54, 100	0
1	C	1011/1023 (98%)	-0.63	13 (1%) 77 79	10, 23, 55, 99	0
1	D	1011/1023 (98%)	-0.55	22 (2%) 62 66	10, 23, 53, 100	0
All	All	4044/4092 (98%)	-0.58	65 (1%) 72 74	9, 23, 54, 100	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	8.2
1	A	735	HIS	8.2
1	D	735	HIS	7.1
1	D	686	PRO	6.2
1	D	732	ALA	5.4
1	B	689	GLU	4.8
1	C	731	PRO	4.5
1	A	685	LEU	4.4
1	B	731	PRO	4.1
1	C	730	LEU	4.1
1	D	733	ALA	4.1
1	B	684	GLU	3.9
1	C	732	ALA	3.8
1	B	685	LEU	3.6
1	D	581	ASN	3.5
1	B	733	ALA	3.4
1	C	735	HIS	3.4
1	D	734	SER	3.3
1	A	1023	LYS	3.3
1	D	634	GLN	3.2
1	A	689	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	687	GLN	3.2
1	A	800	ARG	3.1
1	A	582	GLY	3.0
1	A	580	GLU	3.0
1	D	689	GLU	2.9
1	D	684	GLU	2.9
1	D	687	GLN	2.8
1	B	730	LEU	2.7
1	C	689	GLU	2.6
1	C	634	GLN	2.6
1	D	798	ALA	2.6
1	C	686	PRO	2.6
1	A	581	ASN	2.6
1	C	685	LEU	2.6
1	A	736	ALA	2.5
1	C	580	GLU	2.5
1	A	732	ALA	2.5
1	D	730	LEU	2.5
1	A	734	SER	2.5
1	D	831	ALA	2.5
1	C	684	GLU	2.4
1	D	688	PRO	2.4
1	C	800	ARG	2.4
1	A	799	THR	2.4
1	A	688	PRO	2.3
1	B	686	PRO	2.3
1	D	681	GLU	2.3
1	D	800	ARG	2.3
1	A	634	GLN	2.3
1	D	582	GLY	2.3
1	A	682	LEU	2.2
1	A	684	GLU	2.2
1	D	799	THR	2.2
1	D	583	ASN	2.2
1	A	733	ALA	2.2
1	D	580	GLU	2.2
1	A	579	ASP	2.2
1	A	683	PRO	2.2
1	C	582	GLY	2.1
1	D	579	ASP	2.1
1	C	734	SER	2.1
1	D	663	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	731	PRO	2.1
1	B	687	GLN	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	DMS	C	8407	4/4	0.86	0.14	24,32,100,100	0
2	MG	A	3005	1/1	0.87	0.18	44,44,44,44	0
4	DMS	D	8416	4/4	0.88	0.29	49,54,72,100	0
3	NA	D	3104	1/1	0.89	0.09	44,44,44,44	0
4	DMS	B	8508	4/4	0.89	0.14	46,49,56,100	0
4	DMS	B	8417	4/4	0.92	0.14	27,30,49,75	0
4	DMS	A	8406	4/4	0.92	0.16	26,35,53,78	0
4	DMS	A	8416	4/4	0.92	0.29	36,66,91,100	0
4	DMS	C	8416	4/4	0.92	0.33	65,77,100,100	0
4	DMS	C	8506	4/4	0.92	0.17	51,54,73,100	0
4	DMS	B	8406	4/4	0.92	0.20	38,56,100,100	0
4	DMS	D	8423	4/4	0.92	0.15	36,56,77,100	0
4	DMS	D	8703	4/4	0.92	0.14	31,67,78,79	0
4	DMS	D	8506	4/4	0.93	0.14	60,82,100,100	0
4	DMS	A	8421	4/4	0.93	0.18	68,73,83,100	0
4	DMS	C	8417	4/4	0.94	0.15	24,40,50,61	0
4	DMS	B	8416	4/4	0.94	0.23	37,39,76,100	0
4	DMS	C	8601	4/4	0.94	0.11	33,41,60,73	0
4	DMS	A	8414	4/4	0.94	0.14	49,55,92,97	0
4	DMS	A	8501	4/4	0.94	0.13	28,32,54,59	0
4	DMS	A	8602	4/4	0.94	0.22	57,95,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	D	8508	4/4	0.94	0.12	41,50,71,78	0
3	NA	D	3103	1/1	0.94	0.10	35,35,35,35	0
4	DMS	C	8419	4/4	0.95	0.16	61,79,85,100	0
4	DMS	A	8425	4/4	0.95	0.10	37,39,60,70	0
4	DMS	B	8423	4/4	0.95	0.11	53,53,74,80	0
4	DMS	B	8425	4/4	0.95	0.13	30,33,44,55	0
2	MG	A	3105	1/1	0.95	0.05	32,32,32,32	0
4	DMS	B	8408	4/4	0.95	0.20	29,44,44,67	0
4	DMS	B	8414	4/4	0.95	0.23	26,59,70,100	0
4	DMS	A	8504	4/4	0.95	0.13	27,49,100,100	0
4	DMS	D	8705	4/4	0.95	0.11	36,42,50,52	0
4	DMS	C	8423	4/4	0.96	0.10	53,55,57,75	0
4	DMS	B	8504	4/4	0.96	0.11	36,38,60,100	0
4	DMS	B	8404	4/4	0.96	0.12	29,30,56,60	0
4	DMS	C	8602	4/4	0.96	0.13	22,65,100,100	0
4	DMS	D	8420	4/4	0.96	0.12	39,58,78,100	0
4	DMS	B	8601	4/4	0.96	0.12	44,57,68,100	0
4	DMS	D	8421	4/4	0.96	0.15	51,71,100,100	0
3	NA	B	3104	1/1	0.96	0.13	39,39,39,39	0
4	DMS	B	8421	4/4	0.96	0.13	34,52,77,100	0
4	DMS	A	8411	4/4	0.96	0.12	30,45,54,100	0
4	DMS	A	8404	4/4	0.96	0.08	25,37,51,61	0
4	DMS	C	8420	4/4	0.96	0.12	42,62,86,100	0
4	DMS	C	8425	4/4	0.97	0.16	37,50,100,100	0
4	DMS	C	8501	4/4	0.97	0.07	25,30,42,49	0
4	DMS	C	8504	4/4	0.97	0.10	43,75,100,100	0
4	DMS	B	8409	4/4	0.97	0.09	33,37,37,47	0
3	NA	B	3102	1/1	0.97	0.05	19,19,19,19	0
4	DMS	A	8409	4/4	0.97	0.09	39,42,46,48	0
4	DMS	C	8408	4/4	0.97	0.10	23,41,44,44	0
4	DMS	D	8403	4/4	0.97	0.14	31,32,49,67	0
4	DMS	D	8404	4/4	0.97	0.10	22,40,56,100	0
4	DMS	D	8409	4/4	0.97	0.08	41,44,46,57	0
4	DMS	D	8414	4/4	0.97	0.17	43,63,100,100	0
4	DMS	C	8414	4/4	0.97	0.18	26,46,100,100	0
4	DMS	D	8419	4/4	0.97	0.20	47,59,83,92	0
2	MG	A	3002	1/1	0.97	0.05	23,23,23,23	0
4	DMS	A	8412	4/4	0.97	0.15	39,39,50,100	0
4	DMS	D	8425	4/4	0.97	0.17	13,26,31,59	4
2	MG	B	3001	1/1	0.97	0.03	21,21,21,21	0
2	MG	B	3002	1/1	0.97	0.04	18,18,18,18	0
4	DMS	C	8421	4/4	0.97	0.17	52,71,78,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	A	3101	1/1	0.97	0.06	30,30,30,30	0
4	DMS	C	8403	4/4	0.98	0.09	23,30,41,44	0
4	DMS	C	8405	4/4	0.98	0.07	23,36,39,47	0
4	DMS	B	8411	4/4	0.98	0.08	22,42,43,100	0
4	DMS	B	8412	4/4	0.98	0.09	32,46,48,78	0
4	DMS	D	8402	4/4	0.98	0.07	15,32,33,35	0
4	DMS	C	8409	4/4	0.98	0.09	46,50,57,63	0
4	DMS	C	8411	4/4	0.98	0.12	38,38,50,72	0
4	DMS	D	8406	4/4	0.98	0.11	24,25,33,49	0
4	DMS	C	8412	4/4	0.98	0.12	39,43,96,100	0
4	DMS	D	8411	4/4	0.98	0.07	26,29,43,100	0
3	NA	C	3103	1/1	0.98	0.09	37,37,37,37	0
4	DMS	A	8408	4/4	0.98	0.14	32,37,50,100	0
3	NA	C	3104	1/1	0.98	0.18	36,36,36,36	0
3	NA	B	3101	1/1	0.98	0.06	29,29,29,29	0
2	MG	D	3001	1/1	0.98	0.04	26,26,26,26	0
4	DMS	B	8405	4/4	0.98	0.08	38,52,53,63	0
4	DMS	D	8501	4/4	0.98	0.09	42,42,53,66	0
4	DMS	A	8401	4/4	0.98	0.14	14,19,31,33	0
3	NA	A	3103	1/1	0.98	0.04	27,27,27,27	0
4	DMS	D	8701	4/4	0.98	0.10	21,32,32,55	0
4	DMS	A	8405	4/4	0.98	0.09	28,38,39,40	0
4	DMS	C	8402	4/4	0.98	0.10	14,28,30,30	0
4	DMS	D	8401	4/4	0.99	0.07	20,20,27,29	0
2	MG	C	3002	1/1	0.99	0.05	17,17,17,17	0
3	NA	D	3101	1/1	0.99	0.09	27,27,27,27	0
3	NA	D	3102	1/1	0.99	0.04	18,18,18,18	0
4	DMS	D	8405	4/4	0.99	0.11	29,31,31,36	0
3	NA	A	3104	1/1	0.99	0.06	32,32,32,32	0
4	DMS	D	8408	4/4	0.99	0.15	23,36,40,100	0
2	MG	A	3001	1/1	0.99	0.04	30,30,30,30	0
2	MG	D	3002	1/1	0.99	0.04	17,17,17,17	0
4	DMS	D	8412	4/4	0.99	0.12	26,34,45,50	0
4	DMS	A	8402	4/4	0.99	0.08	14,28,31,58	0
4	DMS	A	8403	4/4	0.99	0.13	32,36,46,67	0
3	NA	B	3103	1/1	0.99	0.03	25,25,25,25	0
4	DMS	B	8401	4/4	0.99	0.09	18,20,29,33	0
4	DMS	B	8402	4/4	0.99	0.09	15,23,29,33	0
4	DMS	B	8403	4/4	0.99	0.07	33,35,41,47	0
4	DMS	C	8401	4/4	0.99	0.10	19,21,33,54	0
2	MG	C	3001	1/1	0.99	0.03	20,20,20,20	0
3	NA	C	3101	1/1	0.99	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	C	8404	4/4	0.99	0.08	18,24,38,50	0
3	NA	C	3102	1/1	0.99	0.05	18,18,18,18	0
3	NA	A	3102	1/1	0.99	0.03	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.