



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 03:26 PM EDT

PDB ID : 3DYP  
Title : E. coli (lacZ) beta-galactosidase (H418N)  
Authors : Juers, D.H.; Huber, R.E.; Matthews, B.W.  
Deposited on : 2008-07-28  
Resolution : 1.75 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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

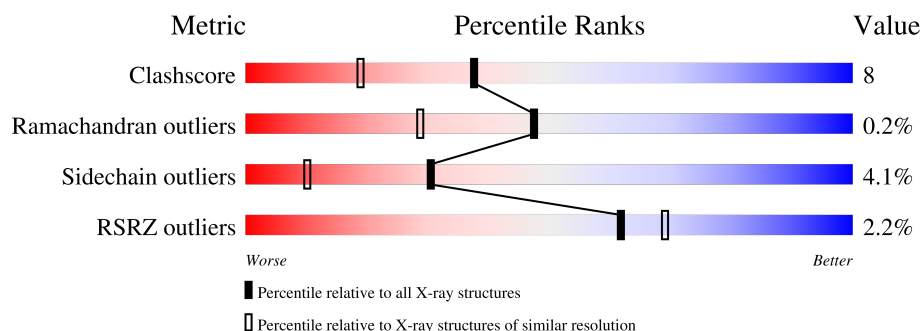
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	1023	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	C	1023	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>5% •</div> </div> </div>
1	D	1023	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>

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	8427	-	-	X	-
4	DMS	B	8506	-	-	X	-
4	DMS	C	8506	-	-	X	-
4	DMS	D	8701	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37221 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
1	A	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			

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	ASN	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	ASN	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	ASN	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	ASN	HIS	engineered mutation	UNP P00722

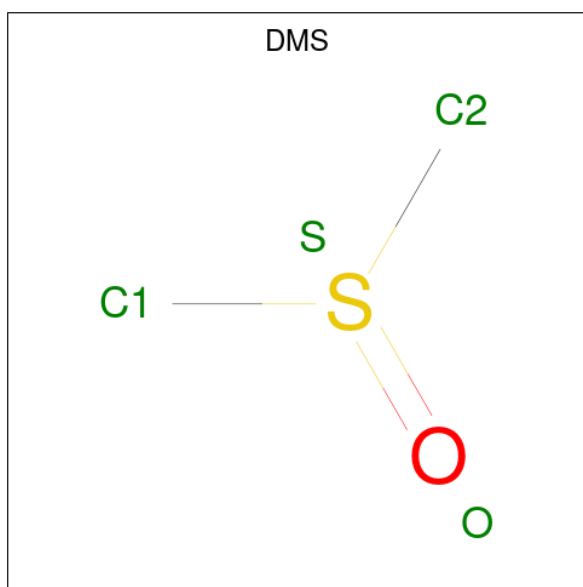
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Mg 5 5	0	0
2	B	3	Total Mg 3 3	0	0
2	C	5	Total Mg 5 5	0	0
2	D	3	Total Mg 3 3	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		

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

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

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

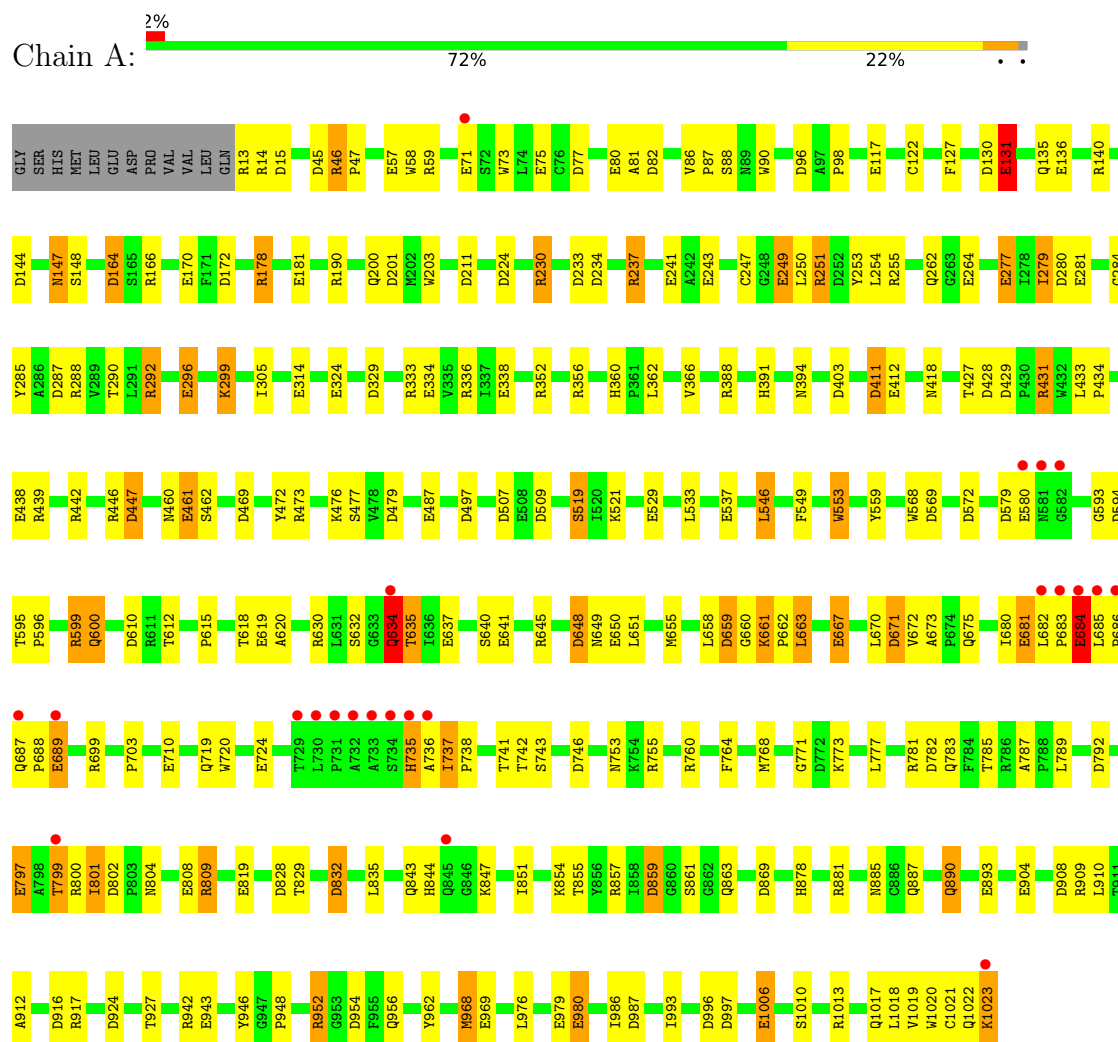
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1088	Total O 1088 1088	0	0
5	B	1078	Total O 1078 1078	0	0
5	C	1033	Total O 1033 1033	0	0
5	D	1070	Total O 1070 1070	0	0

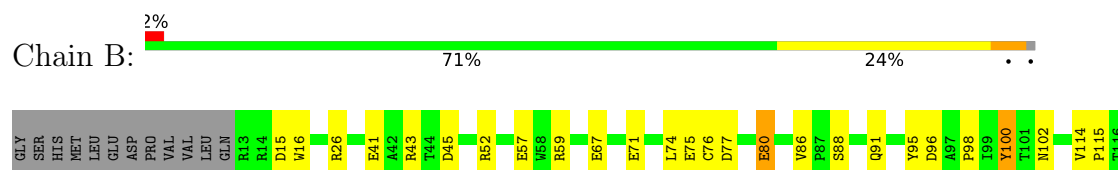
### 3 Residue-property plots

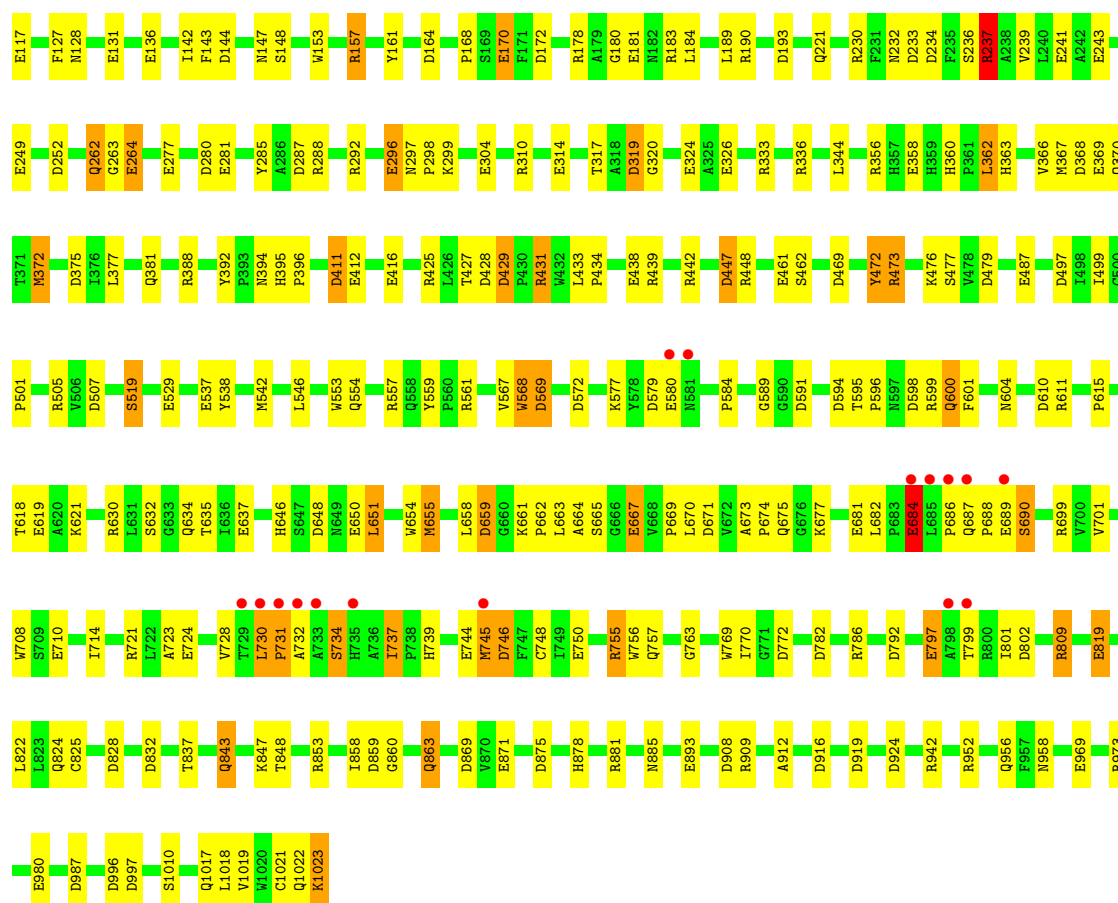
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

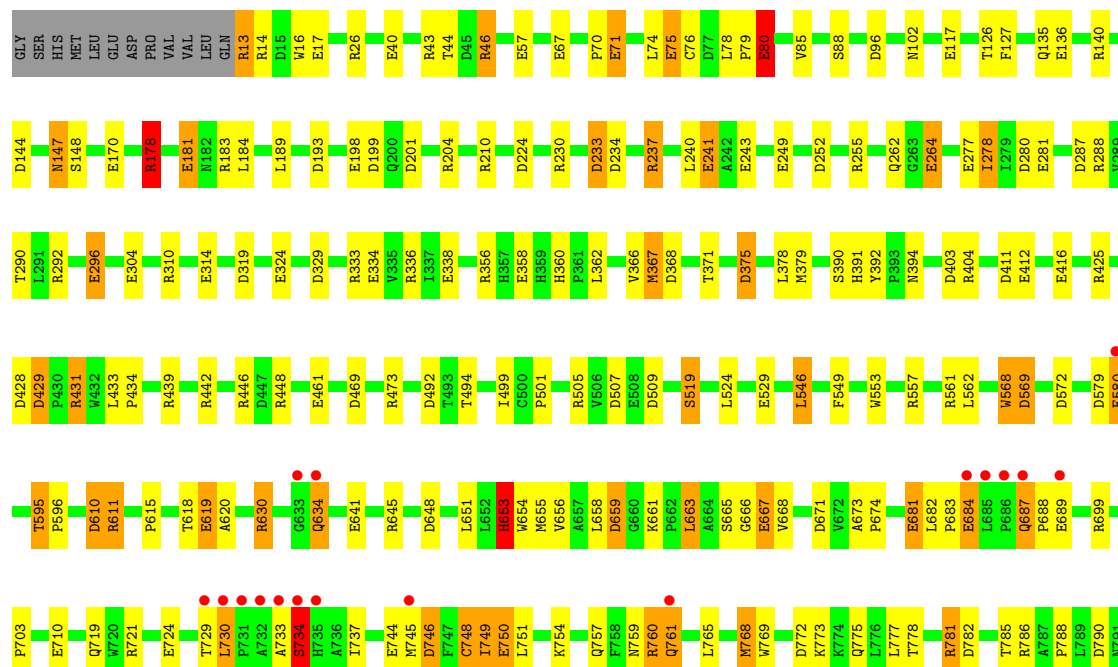


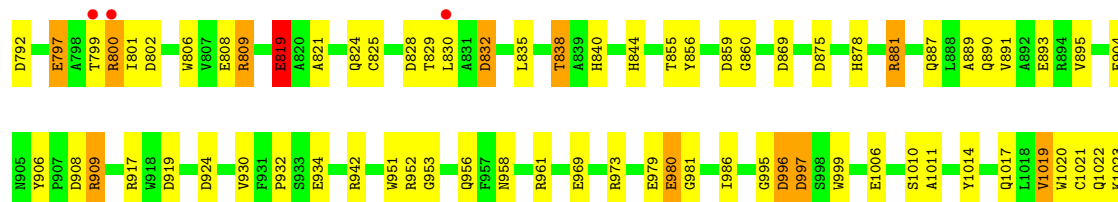
#### • Molecule 1: Beta-galactosidase



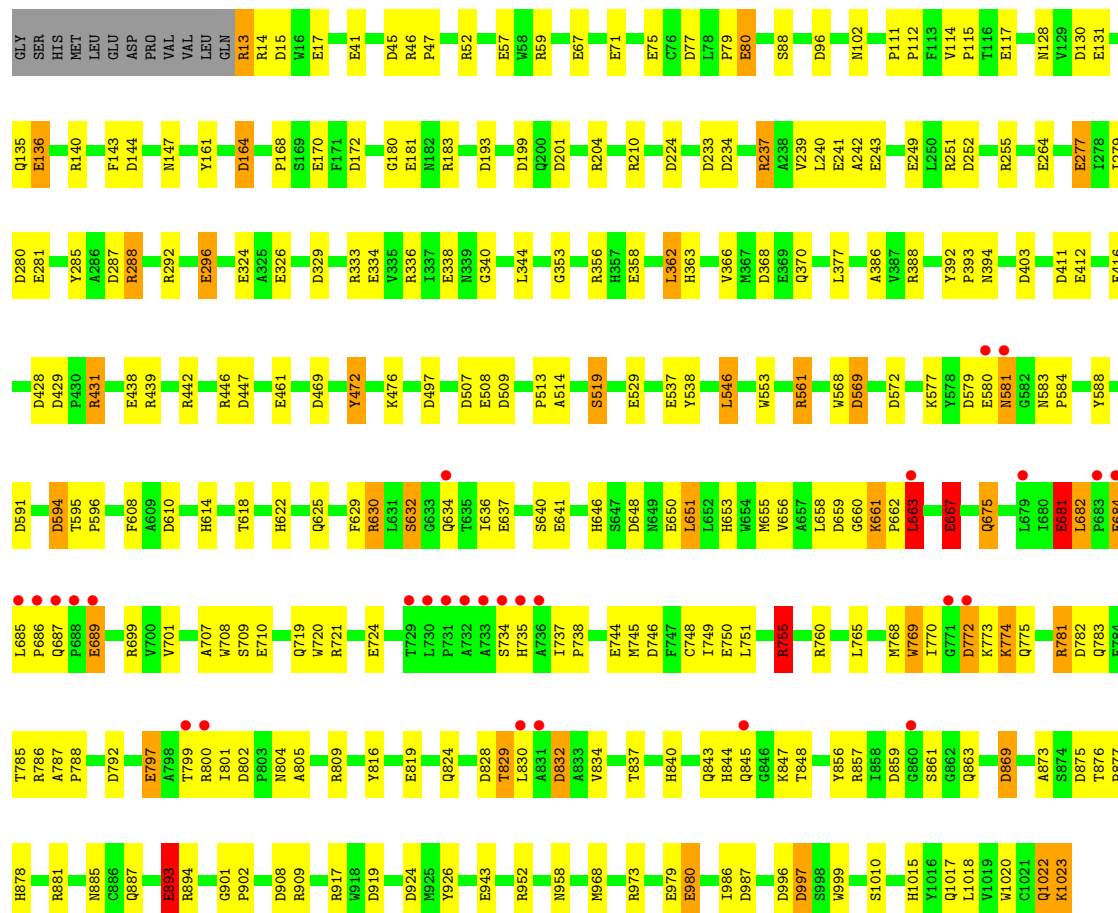


● Molecule 1: Beta-galactosidase





● Molecule 1: Beta-galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.38Å 168.02Å 200.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.70 – 1.75 28.67 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.8 (28.70-1.75) 96.8 (28.67-1.75)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 1.75Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.159 , 0.217 0.158 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 89.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	37221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.53 % 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 6.7230e-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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DMS, 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	1.10	43/8364 (0.5%)	1.65	168/11411 (1.5%)
1	B	1.11	46/8364 (0.5%)	1.62	163/11411 (1.4%)
1	C	1.10	49/8364 (0.6%)	1.64	166/11411 (1.5%)
1	D	1.11	47/8364 (0.6%)	1.63	176/11411 (1.5%)
All	All	1.10	185/33456 (0.6%)	1.64	673/45644 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	GLU	CD-OE2	10.49	1.37	1.25
1	D	893	GLU	CD-OE2	9.54	1.36	1.25
1	C	80	GLU	CD-OE2	8.69	1.35	1.25
1	D	80	GLU	CD-OE2	8.69	1.35	1.25
1	D	170	GLU	CD-OE2	8.44	1.34	1.25
1	D	681	GLU	CD-OE2	8.41	1.34	1.25
1	C	296	GLU	CD-OE2	8.32	1.34	1.25
1	A	296	GLU	CD-OE2	8.26	1.34	1.25
1	D	979	GLU	CD-OE2	8.16	1.34	1.25
1	D	243	GLU	CD-OE2	8.16	1.34	1.25
1	C	934	GLU	CD-OE2	8.03	1.34	1.25
1	A	487	GLU	CD-OE2	7.97	1.34	1.25
1	A	249	GLU	CD-OE2	7.97	1.34	1.25
1	D	75	GLU	CD-OE2	7.91	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	684	GLU	CD-OE2	7.83	1.34	1.25
1	D	650	GLU	CD-OE2	7.67	1.34	1.25
1	A	80	GLU	CD-OE2	7.67	1.34	1.25
1	B	684	GLU	CD-OE2	7.62	1.34	1.25
1	C	281	GLU	CD-OE2	7.61	1.34	1.25
1	B	819	GLU	CD-OE2	7.50	1.33	1.25
1	B	487	GLU	CD-OE2	7.46	1.33	1.25
1	C	277	GLU	CD-OE2	7.43	1.33	1.25
1	B	537	GLU	CD-OE2	7.42	1.33	1.25
1	A	243	GLU	CD-OE2	7.40	1.33	1.25
1	D	296	GLU	CD-OE2	7.40	1.33	1.25
1	D	980	GLU	CD-OE2	7.37	1.33	1.25
1	A	277	GLU	CD-OE2	7.36	1.33	1.25
1	B	281	GLU	CD-OE2	7.34	1.33	1.25
1	A	71	GLU	CD-OE2	7.33	1.33	1.25
1	C	819	GLU	CD-OE2	7.23	1.33	1.25
1	C	580	GLU	CD-OE2	7.21	1.33	1.25
1	B	181	GLU	CD-OE2	7.21	1.33	1.25
1	B	580	GLU	CD-OE2	7.12	1.33	1.25
1	D	710	GLU	CD-OE2	7.12	1.33	1.25
1	C	684	GLU	CD-OE2	7.11	1.33	1.25
1	D	819	GLU	CD-OE2	7.08	1.33	1.25
1	D	580	GLU	CD-OE2	7.07	1.33	1.25
1	C	744	GLU	CD-OE2	7.05	1.33	1.25
1	C	241	GLU	CD-OE2	7.04	1.33	1.25
1	B	243	GLU	CD-OE2	7.04	1.33	1.25
1	C	529	GLU	CD-OE2	7.04	1.33	1.25
1	A	650	GLU	CD-OE2	7.02	1.33	1.25
1	D	689	GLU	CD-OE2	7.00	1.33	1.25
1	B	170	GLU	CD-OE2	7.00	1.33	1.25
1	B	689	GLU	CD-OE2	6.98	1.33	1.25
1	B	710	GLU	CD-OE2	6.97	1.33	1.25
1	A	681	GLU	CD-OE2	6.94	1.33	1.25
1	C	681	GLU	CD-OE2	6.93	1.33	1.25
1	B	724	GLU	CD-OE2	6.91	1.33	1.25
1	C	71	GLU	CD-OE2	6.89	1.33	1.25
1	D	241	GLU	CD-OE2	6.89	1.33	1.25
1	A	1006	GLU	CD-OE2	6.86	1.33	1.25
1	A	969	GLU	CD-OE2	6.83	1.33	1.25
1	B	71	GLU	CD-OE2	6.83	1.33	1.25
1	A	580	GLU	CD-OE2	6.81	1.33	1.25
1	B	980	GLU	CD-OE2	6.81	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	980	GLU	CD-OE2	6.81	1.33	1.25
1	B	667	GLU	CD-OE2	6.79	1.33	1.25
1	C	619	GLU	CD-OE2	6.78	1.33	1.25
1	D	136	GLU	CD-OE2	6.76	1.33	1.25
1	B	969	GLU	CD-OE2	6.74	1.33	1.25
1	B	529	GLU	CD-OE2	6.71	1.33	1.25
1	B	324	GLU	CD-OE2	6.66	1.32	1.25
1	C	667	GLU	CD-OE2	6.66	1.32	1.25
1	A	710	GLU	CD-OE2	6.62	1.32	1.25
1	A	819	GLU	CD-OE2	6.62	1.32	1.25
1	A	980	GLU	CD-OE2	6.60	1.32	1.25
1	C	324	GLU	CD-OE2	6.59	1.32	1.25
1	A	170	GLU	CD-OE2	6.53	1.32	1.25
1	B	296	GLU	CD-OE2	6.52	1.32	1.25
1	B	117	GLU	CD-OE2	6.49	1.32	1.25
1	C	117	GLU	CD-OE2	6.48	1.32	1.25
1	B	264	GLU	CD-OE2	6.48	1.32	1.25
1	D	249	GLU	CD-OE2	6.46	1.32	1.25
1	C	136	GLU	CD-OE2	6.46	1.32	1.25
1	C	893	GLU	CD-OE2	6.46	1.32	1.25
1	A	893	GLU	CD-OE2	6.38	1.32	1.25
1	D	17	GLU	CD-OE2	6.36	1.32	1.25
1	C	75	GLU	CD-OE2	6.36	1.32	1.25
1	B	277	GLU	CD-OE2	6.35	1.32	1.25
1	C	750	GLU	CD-OE2	6.35	1.32	1.25
1	C	710	GLU	CD-OE2	6.33	1.32	1.25
1	D	667	GLU	CD-OE2	6.33	1.32	1.25
1	D	684	GLU	CD-OE2	6.33	1.32	1.25
1	D	797	GLU	CD-OE2	6.33	1.32	1.25
1	A	537	GLU	CD-OE2	6.32	1.32	1.25
1	B	369	GLU	CD-OE2	6.32	1.32	1.25
1	A	979	GLU	CD-OE2	6.29	1.32	1.25
1	D	277	GLU	CD-OE2	6.27	1.32	1.25
1	A	412	GLU	CD-OE2	6.25	1.32	1.25
1	A	338	GLU	CD-OE2	6.25	1.32	1.25
1	D	537	GLU	CD-OE2	6.23	1.32	1.25
1	C	170	GLU	CD-OE2	6.20	1.32	1.25
1	B	241	GLU	CD-OE2	6.18	1.32	1.25
1	C	198	GLU	CD-OE2	6.18	1.32	1.25
1	C	641	GLU	CD-OE1	-6.16	1.18	1.25
1	C	338	GLU	CD-OE2	6.15	1.32	1.25
1	B	326	GLU	CD-OE2	6.08	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	744	GLU	CD-OE2	6.07	1.32	1.25
1	B	75	GLU	CD-OE2	6.07	1.32	1.25
1	B	461	GLU	CD-OE1	-6.07	1.19	1.25
1	C	689	GLU	CD-OE2	6.04	1.32	1.25
1	D	281	GLU	CD-OE2	6.02	1.32	1.25
1	D	264	GLU	CD-OE2	6.01	1.32	1.25
1	C	304	GLU	CD-OE2	6.01	1.32	1.25
1	A	117	GLU	CD-OE2	5.98	1.32	1.25
1	C	797	GLU	CD-OE2	5.97	1.32	1.25
1	C	1006	GLU	CD-OE2	5.96	1.32	1.25
1	B	57	GLU	CD-OE2	5.95	1.32	1.25
1	B	249	GLU	CD-OE2	5.95	1.32	1.25
1	A	131	GLU	CD-OE2	5.95	1.32	1.25
1	A	808	GLU	CD-OE2	5.95	1.32	1.25
1	B	893	GLU	CD-OE2	5.94	1.32	1.25
1	B	131	GLU	CD-OE2	5.93	1.32	1.25
1	D	724	GLU	CD-OE2	5.91	1.32	1.25
1	D	641	GLU	CD-OE1	-5.91	1.19	1.25
1	C	416	GLU	CD-OE2	5.90	1.32	1.25
1	A	943	GLU	CD-OE2	5.90	1.32	1.25
1	B	438	GLU	CD-OE2	5.88	1.32	1.25
1	A	438	GLU	CD-OE2	5.86	1.32	1.25
1	D	181	GLU	CD-OE2	5.83	1.32	1.25
1	A	667	GLU	CD-OE2	5.79	1.32	1.25
1	C	461	GLU	CD-OE1	-5.78	1.19	1.25
1	A	57	GLU	CD-OE2	5.77	1.32	1.25
1	B	41	GLU	CD-OE2	5.77	1.31	1.25
1	D	438	GLU	CD-OE2	5.75	1.31	1.25
1	B	358	GLU	CD-OE2	5.73	1.31	1.25
1	A	75	GLU	CD-OE2	5.73	1.31	1.25
1	A	281	GLU	CD-OE2	5.71	1.31	1.25
1	A	334	GLU	CD-OE2	5.71	1.31	1.25
1	A	264	GLU	CD-OE2	5.70	1.31	1.25
1	B	136	GLU	CD-OE2	5.68	1.31	1.25
1	D	461	GLU	CD-OE2	5.68	1.31	1.25
1	B	650	GLU	CD-OE2	5.67	1.31	1.25
1	D	41	GLU	CD-OE2	5.67	1.31	1.25
1	B	871	GLU	CD-OE1	-5.67	1.19	1.25
1	D	338	GLU	CD-OE2	5.63	1.31	1.25
1	D	131	GLU	CD-OE2	5.61	1.31	1.25
1	D	750	GLU	CD-OE2	5.61	1.31	1.25
1	C	334	GLU	CD-OE2	5.60	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	904	GLU	CD-OE2	5.59	1.31	1.25
1	C	57	GLU	CD-OE2	5.57	1.31	1.25
1	C	264	GLU	CD-OE2	5.56	1.31	1.25
1	B	871	GLU	CD-OE2	5.54	1.31	1.25
1	C	181	GLU	CD-OE2	5.52	1.31	1.25
1	C	979	GLU	CD-OE2	5.50	1.31	1.25
1	A	314	GLU	CD-OE1	-5.48	1.19	1.25
1	A	637	GLU	CD-OE2	5.46	1.31	1.25
1	C	808	GLU	CD-OE1	-5.46	1.19	1.25
1	C	17	GLU	CD-OE2	5.45	1.31	1.25
1	B	681	GLU	CD-OE2	5.45	1.31	1.25
1	D	117	GLU	CD-OE2	5.42	1.31	1.25
1	C	969	GLU	CD-OE2	5.42	1.31	1.25
1	D	326	GLU	CD-OE2	5.42	1.31	1.25
1	D	637	GLU	CD-OE2	5.42	1.31	1.25
1	C	243	GLU	CD-OE1	-5.40	1.19	1.25
1	D	943	GLU	CD-OE2	5.39	1.31	1.25
1	A	461	GLU	CD-OE2	5.37	1.31	1.25
1	C	249	GLU	CD-OE2	5.36	1.31	1.25
1	A	724	GLU	CD-OE2	5.31	1.31	1.25
1	D	508	GLU	CD-OE2	5.29	1.31	1.25
1	B	80	GLU	CD-OE2	5.29	1.31	1.25
1	A	181	GLU	CD-OE2	5.26	1.31	1.25
1	A	136	GLU	CD-OE2	5.24	1.31	1.25
1	B	67	GLU	CD-OE1	-5.24	1.19	1.25
1	A	641	GLU	CD-OE1	-5.22	1.20	1.25
1	C	412	GLU	CD-OE2	5.22	1.31	1.25
1	D	41	GLU	CD-OE1	-5.19	1.20	1.25
1	D	641	GLU	CD-OE2	5.19	1.31	1.25
1	A	529	GLU	CD-OE2	5.17	1.31	1.25
1	C	314	GLU	CD-OE1	-5.17	1.20	1.25
1	D	358	GLU	CD-OE2	5.17	1.31	1.25
1	C	724	GLU	CD-OE2	5.16	1.31	1.25
1	B	412	GLU	CD-OE2	5.13	1.31	1.25
1	B	304	GLU	CD-OE2	5.12	1.31	1.25
1	A	324	GLU	CD-OE1	-5.12	1.20	1.25
1	C	67	GLU	CD-OE2	5.12	1.31	1.25
1	D	744	GLU	CD-OE2	5.11	1.31	1.25
1	B	416	GLU	CD-OE2	5.08	1.31	1.25
1	D	324	GLU	CD-OE1	-5.07	1.20	1.25
1	D	529	GLU	CD-OE2	5.07	1.31	1.25
1	D	57	GLU	CD-OE2	5.04	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	904	GLU	CD-OE2	5.01	1.31	1.25
1	B	797	GLU	CD-OE2	5.01	1.31	1.25
1	C	358	GLU	CD-OE2	5.00	1.31	1.25

All (673) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	ARG	NE-CZ-NH1	22.98	131.79	120.30
1	B	442	ARG	NE-CZ-NH1	16.31	128.46	120.30
1	B	442	ARG	NE-CZ-NH2	-15.56	112.52	120.30
1	C	442	ARG	NE-CZ-NH2	-14.69	112.95	120.30
1	C	473	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	D	781	ARG	NE-CZ-NH1	14.37	127.48	120.30
1	C	43	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	B	721	ARG	NE-CZ-NH1	12.71	126.66	120.30
1	C	178	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	C	721	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	A	599	ARG	NE-CZ-NH1	-12.16	114.22	120.30
1	A	997	ASP	CB-CG-OD2	-11.87	107.62	118.30
1	A	952	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	D	431	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	C	233	ASP	CB-CG-OD1	11.62	128.76	118.30
1	D	183	ARG	NE-CZ-NH1	-11.60	114.50	120.30
1	A	234	ASP	CB-CG-OD2	-11.56	107.89	118.30
1	D	172	ASP	CB-CG-OD2	-11.45	107.99	118.30
1	A	755	ARG	NE-CZ-NH2	-11.23	114.68	120.30
1	A	594	ASP	CB-CG-OD1	11.05	128.24	118.30
1	C	204	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	D	224	ASP	CB-CG-OD1	10.88	128.09	118.30
1	D	439	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	C	442	ARG	NE-CZ-NH1	10.81	125.71	120.30
1	A	251	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	C	233	ASP	CB-CG-OD2	-10.75	108.63	118.30
1	A	755	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	987	ASP	CB-CG-OD2	-10.57	108.79	118.30
1	C	13	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	B	336	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	D	987	ASP	CB-CG-OD1	10.44	127.69	118.30
1	D	356	ARG	NE-CZ-NH1	10.43	125.51	120.30
1	A	442	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	A	172	ASP	CB-CG-OD2	-10.32	109.02	118.30
1	A	442	ARG	NE-CZ-NH1	10.27	125.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	ASP	CB-CG-OD2	-10.20	109.12	118.30
1	B	319	ASP	CB-CG-OD2	-10.17	109.15	118.30
1	C	255	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	B	557	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	D	561	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	D	172	ASP	CB-CG-OD1	10.06	127.36	118.30
1	D	869	ASP	CB-CG-OD1	9.98	127.28	118.30
1	C	809	ARG	NE-CZ-NH2	-9.97	115.31	120.30
1	D	255	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	A	659	ASP	CB-CG-OD2	-9.88	109.40	118.30
1	B	772	ASP	CB-CG-OD2	-9.87	109.42	118.30
1	B	368	ASP	CB-CG-OD1	9.78	127.10	118.30
1	B	448	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	A	634	GLN	N-CA-CB	9.69	128.05	110.60
1	B	388	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	B	611	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	A	671	ASP	CB-CG-OD2	-9.66	109.61	118.30
1	C	909	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	D	781	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	224	ASP	CB-CG-OD1	9.61	126.95	118.30
1	A	610	ASP	CB-CG-OD1	9.61	126.95	118.30
1	A	234	ASP	CB-CG-OD1	9.60	126.94	118.30
1	B	368	ASP	CB-CG-OD2	-9.59	109.67	118.30
1	D	859	ASP	CB-CG-OD2	-9.56	109.69	118.30
1	C	425	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	D	648	ASP	CB-CG-OD2	-9.41	109.83	118.30
1	C	561	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	B	942	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	C	448	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	D	699	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	D	234	ASP	CB-CG-OD1	9.27	126.64	118.30
1	D	429	ASP	CB-CG-OD2	-9.24	109.98	118.30
1	B	671	ASP	CB-CG-OD2	-9.21	110.01	118.30
1	B	319	ASP	CB-CG-OD1	9.18	126.57	118.30
1	C	368	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	B	772	ASP	CB-CG-OD1	9.14	126.52	118.30
1	C	201	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	A	178	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	D	996	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	D	403	ASP	CB-CG-OD1	9.04	126.44	118.30
1	C	199	ASP	CB-CG-OD1	9.03	126.43	118.30
1	B	610	ASP	CB-CG-OD2	-8.97	110.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	917	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	C	579	ASP	CB-CG-OD2	-8.92	110.27	118.30
1	B	59	ARG	NE-CZ-NH1	-8.90	115.85	120.30
1	C	224	ASP	CB-CG-OD1	8.83	126.25	118.30
1	B	233	ASP	CB-CG-OD1	8.83	126.24	118.30
1	D	287	ASP	CB-CG-OD1	8.83	126.24	118.30
1	D	579	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	A	233	ASP	CB-CG-OD1	8.81	126.23	118.30
1	A	509	ASP	CB-CG-OD1	8.81	126.23	118.30
1	A	287	ASP	CB-CG-OD1	8.80	126.22	118.30
1	D	15	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	D	869	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	A	46	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	B	252	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	B	832	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	A	172	ASP	CB-CG-OD1	8.64	126.07	118.30
1	D	234	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	A	648	ASP	CB-CG-OD1	8.62	126.06	118.30
1	A	201	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	A	356	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	D	429	ASP	CB-CG-OD1	8.57	126.02	118.30
1	B	237	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	446	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	469	ASP	CB-CG-OD1	8.56	126.00	118.30
1	B	572	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	A	909	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	A	233	ASP	CB-CG-OD2	-8.45	110.70	118.30
1	C	908	ASP	CB-CG-OD1	8.44	125.89	118.30
1	A	987	ASP	CB-CG-OD1	8.41	125.87	118.30
1	B	632	SER	N-CA-CB	8.40	123.10	110.50
1	D	15	ASP	CB-CG-OD1	8.39	125.85	118.30
1	D	439	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	632	SER	N-CA-CB	8.36	123.04	110.50
1	B	648	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	B	648	ASP	CB-CG-OD1	8.31	125.78	118.30
1	D	859	ASP	CB-CG-OD1	8.30	125.77	118.30
1	B	287	ASP	CB-CG-OD1	8.29	125.76	118.30
1	A	201	ASP	CB-CG-OD1	8.28	125.75	118.30
1	C	76	CYS	N-CA-CB	-8.26	95.72	110.60
1	C	473	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	C	659	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	A	144	ASP	CB-CG-OD1	8.20	125.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	782	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	D	193	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	C	234	ASP	CB-CG-OD1	8.18	125.67	118.30
1	A	832	ASP	CB-CG-OD1	8.18	125.66	118.30
1	D	630	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	B	505	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	14	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	954	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	A	431	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	D	446	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	439	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	C	199	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	B	288	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	B	630	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	45	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	C	746	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	671	ASP	CB-CG-OD1	8.02	125.51	118.30
1	C	404	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	A	287	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	D	446	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	A	800	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	D	996	ASP	CB-CG-OD1	7.95	125.45	118.30
1	A	288	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	96	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	A	857	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	561	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	D	193	ASP	CB-CG-OD1	7.89	125.40	118.30
1	D	755	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	B	853	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	B	828	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	B	792	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	A	741	THR	CA-CB-CG2	-7.86	101.40	112.40
1	D	287	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	D	987	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	D	760	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	610	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	952	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	B	288	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	C	875	ASP	CB-CG-OD1	7.80	125.32	118.30
1	D	632	SER	N-CA-CB	7.79	122.18	110.50
1	B	579	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	A	166	ARG	NE-CZ-NH2	-7.78	116.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1019	VAL	CA-CB-CG2	-7.78	99.23	110.90
1	C	492	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	C	428	ASP	CB-CG-OD1	7.77	125.29	118.30
1	B	610	ASP	CB-CG-OD1	7.76	125.28	118.30
1	B	193	ASP	CB-CG-OD1	7.75	125.27	118.30
1	C	924	ASP	CB-CG-OD2	-7.74	111.33	118.30
1	B	356	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	D	772	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	D	800	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	C	43	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	857	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	183	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	869	ASP	CB-CG-OD1	7.64	125.17	118.30
1	D	201	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	875	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	411	ASP	CB-CG-OD1	7.61	125.15	118.30
1	D	591	ASP	CB-CG-OD1	7.59	125.13	118.30
1	C	610	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	C	821	ALA	N-CA-CB	7.57	120.69	110.10
1	B	356	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	C	802	ASP	CB-CG-OD1	7.54	125.08	118.30
1	C	368	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	832	ASP	N-CA-CB	-7.53	97.05	110.60
1	A	782	ASP	CB-CG-OD1	7.53	125.08	118.30
1	B	869	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	859	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	924	ASP	CB-CG-OD1	7.50	125.05	118.30
1	C	126	THR	CA-CB-CG2	-7.49	101.92	112.40
1	B	569	ASP	CB-CG-OD1	7.48	125.03	118.30
1	D	594	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	D	255	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	859	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	B	594	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	B	919	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	A	403	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	96	ASP	CB-CG-OD1	7.39	124.95	118.30
1	D	388	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	428	ASP	CB-CG-OD1	7.38	124.95	118.30
1	D	45	ASP	CB-CG-OD1	7.38	124.95	118.30
1	B	579	ASP	CB-CG-OD1	7.38	124.94	118.30
1	C	610	ASP	CB-CG-OD1	7.36	124.92	118.30
1	C	859	ASP	CB-CG-OD2	-7.35	111.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	B	559	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	A	190	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	82	ASP	CB-CG-OD1	7.32	124.89	118.30
1	D	403	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	996	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	A	224	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	B	280	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	B	287	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	446	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	447	ASP	CB-CG-OD1	7.27	124.84	118.30
1	C	782	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	A	594	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	C	809	ARG	CD-NE-CZ	7.26	133.76	123.60
1	D	469	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	C	748	CYS	CA-CB-SG	-7.25	100.95	114.00
1	B	958	ASN	N-CA-CB	7.24	123.63	110.60
1	D	659	ASP	CB-CG-OD1	7.23	124.81	118.30
1	C	26	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	C	13	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	C	85	VAL	CA-CB-CG2	-7.22	100.08	110.90
1	B	507	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	924	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	439	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	469	ASP	CB-CG-OD1	7.19	124.77	118.30
1	B	792	ASP	CB-CG-OD1	7.18	124.76	118.30
1	B	659	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	648	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	B	469	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	B	809	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	D	144	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	336	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	579	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	A	292	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	D	952	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	800	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	507	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	204	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	D	356	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	B	439	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	B	659	ASP	CB-CG-OD1	7.08	124.67	118.30
1	D	280	ASP	CB-CG-OD1	7.07	124.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	234	ASP	CB-CG-OD2	-7.03	111.98	118.30
1	B	144	ASP	CB-CG-OD1	7.02	124.62	118.30
1	D	164	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	B	310	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	D	469	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	428	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	802	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	829	THR	N-CA-CB	7.00	123.61	110.30
1	C	772	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	802	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	997	ASP	CB-CG-OD1	6.99	124.59	118.30
1	D	52	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	D	919	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	C	659	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	285	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	B	832	ASP	CB-CG-OD1	6.95	124.55	118.30
1	B	594	ASP	CB-CG-OD1	6.94	124.55	118.30
1	A	255	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	572	ASP	CB-CG-OD1	6.92	124.53	118.30
1	C	579	ASP	CB-CG-OD1	6.91	124.52	118.30
1	D	924	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	329	ASP	CB-CG-OD1	6.90	124.51	118.30
1	B	853	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	C	280	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	15	ASP	CB-CG-OD1	6.88	124.49	118.30
1	D	164	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	439	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	996	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	598	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	579	ASP	CB-CG-OD1	6.85	124.47	118.30
1	B	428	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	802	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	425	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	D	13	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	507	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	D	952	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	746	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	D	997	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	C	828	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	C	237	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	D	252	ASP	CB-CG-OD2	-6.78	112.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	828	ASP	CB-CG-OD1	6.78	124.40	118.30
1	D	288	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	553	TRP	CA-CB-CG	-6.77	100.83	113.70
1	A	388	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	D	509	ASP	CB-CG-OD1	6.76	124.39	118.30
1	C	201	ASP	CB-CG-OD1	6.75	124.37	118.30
1	B	1018	LEU	CB-CA-C	-6.74	97.39	110.20
1	D	832	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	411	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	828	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	144	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	425	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	689	GLU	CB-CA-C	6.69	123.78	110.40
1	D	251	ARG	CD-NE-CZ	6.68	132.96	123.60
1	C	906	TYR	CB-CG-CD1	6.68	125.01	121.00
1	D	610	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	919	ASP	CB-CG-OD1	6.65	124.29	118.30
1	D	800	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	403	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	C	140	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	906	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	C	494	THR	CA-CB-CG2	-6.62	103.13	112.40
1	B	557	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	411	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	509	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	D	1018	LEU	CB-CA-C	-6.58	97.71	110.20
1	C	611	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	C	917	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	B	95	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	D	431	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	809	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	771	GLY	N-CA-C	-6.55	96.73	113.10
1	D	428	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	477	SER	N-CA-CB	6.53	120.29	110.50
1	C	859	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	164	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	946	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	D	926	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	D	472	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	B	431	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	916	ASP	CB-CG-OD1	6.49	124.14	118.30
1	C	193	ASP	CB-CG-OD1	6.49	124.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	144	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	917	ARG	CD-NE-CZ	-6.48	114.53	123.60
1	C	997	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	429	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	140	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	D	781	ARG	CD-NE-CZ	6.46	132.64	123.60
1	D	594	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	635	THR	CA-CB-CG2	-6.43	103.40	112.40
1	C	280	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	659	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	C	569	ASP	CB-CG-OD1	6.38	124.04	118.30
1	D	96	ASP	CB-CG-OD1	6.38	124.04	118.30
1	D	442	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	962	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	A	230	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	336	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	546	LEU	N-CA-CB	6.32	123.04	110.40
1	B	233	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	746	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	C	572	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	D	80	GLU	OE1-CD-OE2	6.29	130.85	123.30
1	D	746	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	C	509	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	924	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	C	875	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	C	832	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	B	372	MET	CG-SD-CE	6.26	110.22	100.20
1	D	997	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	363	HIS	CA-CB-CG	-6.25	102.97	113.60
1	B	802	ASP	CB-CG-OD1	6.25	123.92	118.30
1	D	280	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	280	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	B	77	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	572	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	B	996	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	746	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	D	828	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	D	497	ASP	CB-CG-OD1	6.23	123.90	118.30
1	A	832	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	A	760	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	538	TYR	CB-CG-CD2	6.22	124.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	572	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	C	569	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	996	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	924	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	B	172	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	14	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	719	GLN	CB-CA-C	-6.19	98.02	110.40
1	C	961	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	962	TYR	CB-CG-CD2	6.18	124.71	121.00
1	D	77	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	375	ASP	CB-CG-OD1	6.17	123.85	118.30
1	D	802	ASP	CB-CG-OD1	6.16	123.85	118.30
1	B	924	ASP	CB-CG-OD1	6.16	123.84	118.30
1	D	699	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	D	569	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	C	909	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	505	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	519	SER	N-CA-CB	-6.14	101.30	110.50
1	A	890	GLN	N-CA-CB	-6.13	99.57	110.60
1	C	429	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	828	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	782	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	497	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	840	HIS	CB-CA-C	-6.10	98.20	110.40
1	C	404	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	292	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	367	MET	CB-CA-C	-6.09	98.22	110.40
1	B	599	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	C	719	GLN	CB-CA-C	-6.07	98.26	110.40
1	A	968	MET	CB-CA-C	-6.07	98.27	110.40
1	B	973	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	A	13	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	77	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	B	859	ASP	CB-CG-OD1	6.04	123.74	118.30
1	D	251	ARG	CG-CD-NE	-6.04	99.12	111.80
1	C	546	LEU	N-CA-CB	6.03	122.47	110.40
1	D	572	ASP	CB-CG-OD1	6.03	123.73	118.30
1	D	755	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	D	721	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	729	THR	N-CA-CB	6.01	121.73	110.30
1	B	553	TRP	CA-CB-CG	-6.01	102.28	113.70
1	B	786	ARG	NE-CZ-NH2	-6.01	117.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	519	SER	N-CA-CB	-6.00	101.50	110.50
1	C	507	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	130	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	136	GLU	CB-CA-C	-5.99	98.42	110.40
1	A	144	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	497	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	997	ASP	N-CA-CB	5.98	121.36	110.60
1	D	919	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	569	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	875	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	C	648	ASP	CB-CG-OD1	5.95	123.66	118.30
1	C	252	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	C	733	ALA	N-CA-CB	5.93	118.41	110.10
1	C	958	ASN	N-CA-CB	5.93	121.27	110.60
1	C	809	ARG	NH1-CZ-NH2	-5.92	112.89	119.40
1	A	630	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	733	ALA	CB-CA-C	5.92	118.97	110.10
1	A	746	ASP	CB-CA-C	-5.90	98.60	110.40
1	B	157	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	C	140	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	45	ASP	CB-CG-OD1	5.89	123.60	118.30
1	C	403	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	681	GLU	CB-CG-CD	-5.89	98.29	114.20
1	D	388	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	1021	CYS	CA-CB-SG	-5.88	103.41	114.00
1	B	869	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	C	46	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	C	840	HIS	CB-CA-C	-5.87	98.65	110.40
1	B	26	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	B	909	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	723	ALA	CB-CA-C	-5.86	101.31	110.10
1	D	252	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	255	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	D	553	TRP	CA-CB-CG	-5.83	102.63	113.70
1	B	76	CYS	CA-CB-SG	-5.82	103.53	114.00
1	D	980	GLU	C-N-CA	-5.82	110.08	122.30
1	C	671	ASP	CB-CG-OD2	-5.82	113.07	118.30
1	D	630	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	285	TYR	CD1-CE1-CZ	-5.80	114.58	119.80
1	B	568	TRP	CA-CB-CG	-5.80	102.68	113.70
1	A	909	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	375	ASP	CB-CG-OD1	5.79	123.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	856	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	D	579	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	190	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	447	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	1017	GLN	CA-CB-CG	5.78	126.10	113.40
1	B	909	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	997	ASP	N-CA-CB	5.77	120.99	110.60
1	D	368	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	859	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	43	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	737	ILE	N-CA-CB	5.77	124.06	110.80
1	A	164	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	519	SER	N-CA-CB	-5.75	101.88	110.50
1	D	917	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	B	429	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	569	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	96	ASP	N-CA-CB	5.73	120.91	110.60
1	A	45	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	356	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	446	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	746	ASP	CB-CG-OD1	5.72	123.44	118.30
1	C	952	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	473	ARG	CD-NE-CZ	5.70	131.59	123.60
1	C	772	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	247	CYS	CA-CB-SG	-5.69	103.75	114.00
1	C	790	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	140	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	721	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	673	ALA	N-CA-CB	-5.67	102.16	110.10
1	C	319	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	416	GLU	CG-CD-OE1	5.67	129.64	118.30
1	B	782	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	15	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	C	371	THR	CA-CB-CG2	-5.66	104.47	112.40
1	D	656	VAL	CA-CB-CG2	-5.66	102.41	110.90
1	B	52	ARG	CB-CA-C	-5.66	99.08	110.40
1	B	429	ASP	CB-CG-OD1	5.66	123.39	118.30
1	D	288	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	52	ARG	CB-CA-C	-5.66	99.09	110.40
1	A	942	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	B	987	ASP	CB-CG-OD1	5.65	123.39	118.30
1	D	909	ARG	NE-CZ-NH2	-5.65	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	591	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	908	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	926	TYR	CB-CG-CD1	5.64	124.38	121.00
1	C	799	THR	CA-CB-CG2	-5.64	104.51	112.40
1	D	958	ASN	N-CA-CB	5.63	120.74	110.60
1	C	210	ARG	N-CA-CB	5.63	120.73	110.60
1	D	224	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	D	45	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	908	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	411	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	561	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	869	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	230	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	329	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	14	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	439	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	786	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	279	ILE	CA-CB-CG2	5.58	122.06	110.90
1	B	234	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	211	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	448	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	961	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	689	GLU	O-C-N	5.54	131.56	122.70
1	A	77	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	D	572	ASP	CB-CA-C	-5.54	99.33	110.40
1	B	748	CYS	CA-CB-SG	-5.53	104.05	114.00
1	D	746	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	630	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	507	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	553	TRP	CA-CB-CG	-5.52	103.22	113.70
1	B	237	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	572	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	829	THR	CA-CB-CG2	-5.50	104.69	112.40
1	B	881	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	973	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	996	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	147	ASN	N-CA-CB	-5.48	100.73	110.60
1	D	416	GLU	CG-CD-OE2	-5.48	107.33	118.30
1	A	477	SER	CB-CA-C	-5.48	99.69	110.10
1	C	505	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	838	THR	CA-CB-CG2	-5.48	104.73	112.40
1	D	648	ASP	CB-CG-OD1	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	916	ASP	CB-CG-OD1	5.47	123.23	118.30
1	D	210	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	C	832	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	792	ASP	CB-CG-OD1	5.46	123.22	118.30
1	D	233	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	A	429	ASP	CB-CG-OD1	5.45	123.20	118.30
1	D	787	ALA	N-CA-CB	-5.45	102.47	110.10
1	B	472	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	D	769	TRP	CB-CA-C	-5.43	99.54	110.40
1	C	856	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	C	781	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	411	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	559	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	411	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	479	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	411	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	568	TRP	CA-CB-CG	-5.40	103.44	113.70
1	B	591	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	D	472	TYR	CB-CG-CD1	5.39	124.23	121.00
1	B	221	GLN	N-CA-CB	-5.39	100.91	110.60
1	A	479	ASP	CB-CG-OD1	5.38	123.15	118.30
1	D	161	TYR	N-CA-CB	-5.38	100.91	110.60
1	D	875	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	D	770	ILE	N-CA-C	-5.38	96.48	111.00
1	D	721	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	147	ASN	N-CA-CB	-5.37	100.94	110.60
1	C	768	MET	N-CA-CB	5.36	120.25	110.60
1	C	74	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	D	324	GLU	N-CA-CB	5.35	120.23	110.60
1	A	147	ASN	N-CA-CB	-5.35	100.98	110.60
1	C	431	ARG	CA-CB-CG	-5.35	101.64	113.40
1	A	14	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	B	100	TYR	CA-CB-CG	-5.34	103.25	113.40
1	D	59	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	653	HIS	N-CA-CB	5.34	120.21	110.60
1	B	559	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
1	C	183	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	D	663	LEU	CB-CA-C	-5.32	100.09	110.20
1	B	670	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	C	277	GLU	CA-CB-CG	-5.32	101.70	113.40
1	A	13	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	843	GLN	O-C-N	5.29	131.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	832	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	746	ASP	CB-CA-C	-5.29	99.83	110.40
1	A	507	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	299	LYS	CA-CB-CG	-5.28	101.79	113.40
1	A	546	LEU	N-CA-CB	5.28	120.95	110.40
1	D	588	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	C	96	ASP	N-CA-CB	5.27	120.09	110.60
1	B	479	ASP	CB-CG-OD1	5.27	123.04	118.30
1	D	144	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	659	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	770	ILE	CA-CB-CG1	-5.25	101.02	111.00
1	C	310	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	D	242	ALA	CB-CA-C	-5.25	102.22	110.10
1	D	857	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	C	329	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	C	881	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	D	204	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	671	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	428	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	719	GLN	CB-CA-C	-5.22	99.97	110.40
1	A	648	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	761	GLN	CB-CG-CD	5.21	125.15	111.60
1	A	689	GLU	N-CA-CB	5.21	119.98	110.60
1	D	96	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	612	THR	CA-CB-CG2	-5.20	105.11	112.40
1	B	819	GLU	O-C-N	5.20	131.01	122.70
1	B	802	ASP	CB-CG-OD2	-5.19	113.62	118.30
1	D	183	ARG	CD-NE-CZ	-5.19	116.33	123.60
1	C	40	GLU	CG-CD-OE1	5.19	128.68	118.30
1	B	690	SER	N-CA-CB	5.19	118.28	110.50
1	B	924	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	362	LEU	CB-CA-C	-5.19	100.34	110.20
1	D	792	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	969	GLU	CA-CB-CG	-5.18	102.01	113.40
1	B	952	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	645	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	869	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	183	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	336	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	927	THR	CA-CB-CG2	-5.16	105.18	112.40
1	A	497	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	438	GLU	CG-CD-OE2	-5.15	107.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	C	645	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	234	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	86	VAL	CG1-CB-CG2	-5.15	102.67	110.90
1	D	786	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	1019	VAL	CA-CB-CG1	-5.14	103.19	110.90
1	B	314	GLU	CB-CA-C	-5.14	100.12	110.40
1	B	447	ASP	CB-CG-OD1	5.14	122.92	118.30
1	C	183	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	C	760	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	D	96	ASP	N-CA-CB	5.13	119.83	110.60
1	D	782	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	14	ARG	N-CA-CB	-5.12	101.38	110.60
1	C	1019	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	D	675	GLN	CB-CA-C	-5.12	100.17	110.40
1	B	280	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	287	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	782	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	707	ALA	CB-CA-C	-5.11	102.44	110.10
1	A	329	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	800	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	375	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	C	469	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	255	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	1018	LEU	CB-CA-C	-5.10	100.51	110.20
1	C	792	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	82	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	D	519	SER	N-CA-CB	-5.09	102.86	110.50
1	B	161	TYR	N-CA-CB	-5.09	101.44	110.60
1	A	854	LYS	CB-CA-C	-5.08	100.24	110.40
1	D	199	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	190	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	A	277	GLU	CG-CD-OE1	5.07	128.44	118.30
1	C	375	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	C	786	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	908	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	C	210	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	67	GLU	CG-CD-OE2	-5.05	108.19	118.30
1	D	746	ASP	CB-CA-C	-5.05	100.29	110.40
1	B	611	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	557	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	546	LEU	N-CA-CB	5.04	120.48	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	VAL	CA-CB-CG2	-5.04	103.34	110.90
1	C	230	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	239	VAL	CA-CB-CG2	-5.03	103.36	110.90
1	A	670	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	C	568	TRP	CA-CB-CG	-5.02	104.16	113.70
1	A	946	TYR	CB-CG-CD1	5.01	124.00	121.00
1	C	288	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	C	630	ARG	NE-CZ-NH1	5.01	122.80	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	634	GLN	CA
1	A	689	GLU	CA

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8123	0	7715	126	0
1	B	8123	0	7714	114	0
1	C	8123	0	7714	124	0
1	D	8123	0	7714	115	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
2	C	5	0	0	0	0
2	D	3	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	104	0	156	13	0
4	B	108	0	162	11	0
4	C	112	0	168	9	0
4	D	104	0	156	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1088	0	0	17	2
5	B	1078	0	0	12	1
5	C	1033	0	0	12	1
5	D	1070	0	0	12	0
All	All	37221	0	31499	493	2

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 8.

All (493) 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)
4:B:8407:DMS:C2	4:B:8407:DMS:S	2.04	1.46
4:D:8407:DMS:C2	4:D:8407:DMS:S	2.04	1.46
4:B:8508:DMS:C1	4:B:8508:DMS:S	2.11	1.37
1:C:634:GLN:H	1:C:634:GLN:NE2	1.44	1.15
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.46	1.13
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.48	1.12
1:C:655:MET:HE2	1:C:665:SER:HB3	1.35	1.06
1:C:745:MET:HA	1:C:761:GLN:HE22	1.21	1.03
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.26	0.97
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.31	0.95
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.97	0.94
1:C:102:ASN:HB3	4:C:8506:DMS:H13	1.49	0.92
1:B:600:GLN:H	1:B:600:GLN:HE21	1.16	0.92
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.03	0.91
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.56	0.87
1:C:634:GLN:H	1:C:634:GLN:HE21	1.24	0.86
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.90	0.86
1:B:655:MET:HE2	1:B:665:SER:HB3	1.56	0.85
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.59	0.85
1:D:663:LEU:HD13	1:D:686:PRO:HG2	1.58	0.85
1:C:634:GLN:NE2	1:C:634:GLN:N	2.25	0.84
1:D:658:LEU:O	1:D:661:LYS:HG3	1.78	0.83
1:A:687:GLN:HG3	5:A:4865:HOH:O	1.77	0.83
1:A:720:TRP:HA	4:A:8427:DMS:H13	1.59	0.83
1:A:787:ALA:HA	1:A:968:MET:HG3	1.62	0.82
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.46	0.79
1:B:651:LEU:O	1:B:651:LEU:HD23	1.81	0.79
1:A:797:GLU:O	1:A:801:ILE:HD13	1.81	0.79
1:A:600:GLN:H	1:A:600:GLN:HE21	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:LEU:O	1:A:661:LYS:HG3	1.84	0.78
1:A:634:GLN:HB2	1:A:682:LEU:HB2	1.66	0.78
1:D:629:PHE:O	1:D:630:ARG:HD3	1.83	0.77
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.67	0.77
1:A:720:TRP:HA	4:A:8427:DMS:C1	2.14	0.77
1:B:262:GLN:HE21	1:B:263:GLY:N	1.83	0.77
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.68	0.76
1:A:237:ARG:HB3	1:A:237:ARG:NH1	2.01	0.76
1:D:685:LEU:HB3	1:D:686:PRO:CD	2.15	0.76
1:C:797:GLU:O	1:C:801:ILE:HD13	1.86	0.76
1:B:745:MET:H	1:B:745:MET:CE	1.99	0.76
1:C:748:CYS:C	1:C:749:ILE:HD12	2.07	0.75
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.68	0.75
1:D:292:ARG:HH12	4:D:8412:DMS:H22	1.52	0.75
1:D:651:LEU:O	1:D:651:LEU:HD12	1.87	0.75
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.02	0.74
1:D:128:ASN:HB3	1:D:180:GLY:O	1.86	0.74
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.53	0.74
1:D:663:LEU:CD1	1:D:686:PRO:HG2	2.17	0.74
1:B:863:GLN:HG2	1:B:1019:VAL:HG11	1.70	0.74
1:D:292:ARG:HH12	4:D:8412:DMS:C2	2.01	0.74
1:C:765:LEU:HD21	1:C:768:MET:CE	2.17	0.73
1:B:797:GLU:O	1:B:801:ILE:HD13	1.88	0.73
1:B:734:SER:CB	1:B:860:GLY:HA3	2.19	0.73
1:B:809:ARG:HG2	1:B:809:ARG:NH1	2.03	0.72
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.02	0.72
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.71	0.72
1:B:658:LEU:O	1:B:661:LYS:HE3	1.90	0.72
1:D:663:LEU:HD13	1:D:686:PRO:CG	2.20	0.72
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.19	0.71
5:B:4805:HOH:O	4:C:8420:DMS:H21	1.90	0.71
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.06	0.71
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.03	0.70
1:D:102:ASN:HB3	4:D:8506:DMS:H11	1.72	0.70
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.56	0.70
1:B:878:HIS:HD2	5:B:4088:HOH:O	1.75	0.69
1:D:651:LEU:HD12	1:D:651:LEU:C	2.13	0.69
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.26	0.69
1:A:262:GLN:HE22	1:A:299:LYS:HD3	1.56	0.69
1:A:861:SER:OG	1:A:863:GLN:HG3	1.92	0.69
1:C:745:MET:HA	1:C:761:GLN:NE2	2.03	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.28	0.68
1:A:230:ARG:NH1	1:A:241:GLU:OE2	2.27	0.68
1:D:749:ILE:HD12	1:D:749:ILE:N	2.08	0.67
1:D:748:CYS:C	1:D:749:ILE:HD12	2.14	0.67
1:D:887:GLN:NE2	1:D:980:GLU:O	2.25	0.67
1:C:102:ASN:CB	4:C:8506:DMS:H13	2.21	0.67
1:C:768:MET:HE3	1:C:1020:TRP:CH2	2.28	0.67
1:A:648:ASP:OD2	5:A:4938:HOH:O	2.12	0.67
1:A:887:GLN:NE2	1:A:980:GLU:O	2.26	0.67
1:B:734:SER:HB2	1:B:860:GLY:HA3	1.77	0.67
1:A:809:ARG:HG2	1:A:809:ARG:HH11	1.59	0.67
1:A:178:ARG:HD2	5:A:4890:HOH:O	1.95	0.67
1:C:878:HIS:HD2	5:C:4096:HOH:O	1.77	0.67
1:A:290:THR:HB	4:A:8412:DMS:H22	1.77	0.67
1:A:595:THR:HA	1:A:596:PRO:C	2.15	0.67
1:B:745:MET:H	1:B:745:MET:HE3	1.58	0.66
1:D:102:ASN:CB	4:D:8506:DMS:H11	2.26	0.66
1:A:878:HIS:HD2	5:A:4073:HOH:O	1.79	0.66
1:B:262:GLN:HE21	1:B:262:GLN:C	1.99	0.66
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.77	0.66
1:D:797:GLU:O	1:D:801:ILE:HD13	1.96	0.65
1:C:178:ARG:HG3	5:C:4847:HOH:O	1.95	0.65
4:B:8506:DMS:H12	5:B:5049:HOH:O	1.97	0.65
1:C:824:GLN:HG2	1:C:825:CYS:N	2.12	0.65
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.79	0.65
1:A:685:LEU:O	1:A:687:GLN:NE2	2.29	0.65
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.29	0.65
1:B:595:THR:HA	1:B:596:PRO:C	2.18	0.64
1:D:646:HIS:ND1	5:D:4879:HOH:O	2.29	0.64
1:B:102:ASN:HB3	4:B:8506:DMS:H11	1.79	0.64
1:D:861:SER:OG	1:D:863:GLN:HG3	1.98	0.64
1:B:429:ASP:OD1	1:B:431:ARG:HG3	1.96	0.64
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.78	0.64
1:B:1022:GLN:HG3	1:B:1023:LYS:O	1.97	0.64
1:D:237:ARG:NH1	5:D:4574:HOH:O	2.22	0.64
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.80	0.63
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.28	0.63
1:D:893:GLU:HG2	1:D:894:ARG:HG2	1.79	0.63
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.80	0.63
1:A:277:GLU:H	1:A:277:GLU:CD	2.01	0.63
1:A:431:ARG:HG3	5:A:4780:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:PRO:HB2	5:B:4911:HOH:O	1.99	0.62
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.28	0.62
1:C:356:ARG:HD2	1:C:379:MET:CE	2.28	0.62
1:C:749:ILE:HD12	1:C:749:ILE:N	2.13	0.62
1:D:622:HIS:O	1:D:625:GLN:HG3	1.99	0.62
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.29	0.62
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.12	0.62
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.13	0.62
1:B:320:GLY:O	4:B:8406:DMS:O	2.19	0.61
1:B:863:GLN:HG3	1:B:1021:CYS:CB	2.29	0.61
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.82	0.61
1:D:102:ASN:HB3	4:D:8506:DMS:C1	2.29	0.61
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.35	0.61
1:C:651:LEU:HD12	1:C:651:LEU:O	1.99	0.61
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.07	0.61
1:A:279:ILE:HG23	1:A:284:GLY:HA2	1.82	0.61
1:C:595:THR:HA	1:C:596:PRO:C	2.19	0.61
1:C:687:GLN:HE21	1:C:687:GLN:N	1.98	0.61
1:D:805:ALA:O	1:D:809:ARG:HG3	2.01	0.61
1:D:595:THR:HA	1:D:596:PRO:C	2.20	0.61
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.82	0.60
1:A:262:GLN:NE2	1:A:299:LYS:HD3	2.17	0.60
1:D:765:LEU:HD21	1:D:768:MET:SD	2.42	0.60
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.84	0.59
1:D:781:ARG:NH1	5:D:4780:HOH:O	2.27	0.59
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.84	0.59
1:D:878:HIS:HD2	5:D:4108:HOH:O	1.85	0.59
1:D:809:ARG:HH11	1:D:809:ARG:HG2	1.66	0.59
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.21	0.58
1:A:683:PRO:O	1:A:685:LEU:HG	2.04	0.58
1:A:742:THR:HG22	1:A:743:SER:N	2.18	0.58
1:C:88:SER:HA	1:C:366:VAL:HG21	1.85	0.58
1:B:655:MET:HG3	5:B:4388:HOH:O	2.04	0.57
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.85	0.57
1:D:135:GLN:O	1:D:136:GLU:HG2	2.04	0.57
1:B:236:SER:C	1:B:237:ARG:HG2	2.13	0.56
1:B:299:LYS:HE2	5:B:4704:HOH:O	2.03	0.56
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.86	0.56
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.36	0.56
1:A:262:GLN:HE22	1:A:299:LYS:CD	2.19	0.56
1:A:976:LEU:HB2	4:A:8423:DMS:H11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:980:GLU:HA	5:C:4816:HOH:O	2.05	0.56
1:D:135:GLN:C	1:D:136:GLU:HG2	2.26	0.56
1:C:651:LEU:HD12	1:C:651:LEU:C	2.25	0.56
1:A:663:LEU:HD11	1:A:688:PRO:HG3	1.88	0.56
1:A:663:LEU:HD12	1:A:686:PRO:HG2	1.89	0.55
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.89	0.55
1:C:757:GLN:OE1	1:C:769:TRP:HH2	1.88	0.55
1:D:618:THR:HG21	5:D:4352:HOH:O	2.06	0.55
4:A:8420:DMS:H21	5:D:4823:HOH:O	2.06	0.55
1:B:745:MET:SD	1:B:745:MET:N	2.77	0.55
1:C:181:GLU:OE1	1:C:181:GLU:HA	2.05	0.55
1:C:745:MET:HG2	5:C:4872:HOH:O	2.07	0.55
1:C:844:HIS:HD2	5:C:4878:HOH:O	1.88	0.55
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.42	0.54
1:D:584:PRO:HD2	5:D:4754:HOH:O	2.06	0.54
4:C:8427:DMS:H21	5:C:4462:HOH:O	2.06	0.54
1:A:663:LEU:HD13	1:A:686:PRO:CB	2.37	0.54
1:B:637:GLU:OE2	1:B:677:LYS:HD3	2.06	0.54
1:C:835:LEU:HD11	1:C:855:THR:HB	1.88	0.54
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.72	0.54
1:A:88:SER:HA	1:A:366:VAL:HG21	1.90	0.54
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.89	0.54
1:B:843:GLN:HG2	1:B:848:THR:HA	1.90	0.54
1:A:832:ASP:OD1	1:A:832:ASP:N	2.40	0.54
1:D:738:PRO:HG3	1:D:751:LEU:HD13	1.90	0.54
1:B:1022:GLN:HG3	1:B:1023:LYS:N	2.22	0.53
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.08	0.53
1:A:521:LYS:HE2	5:A:4434:HOH:O	2.09	0.53
1:D:847:LYS:HG3	1:D:848:THR:N	2.16	0.53
1:A:684:GLU:HG2	1:A:685:LEU:N	2.24	0.53
1:A:237:ARG:NH1	5:A:4540:HOH:O	2.32	0.53
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.90	0.53
1:B:88:SER:HA	1:B:366:VAL:HG21	1.90	0.53
1:C:610:ASP:O	1:C:611:ARG:HB2	2.09	0.53
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.91	0.53
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.44	0.53
1:A:890:GLN:OE1	1:A:948:PRO:HD3	2.08	0.53
1:C:429:ASP:OD1	1:C:431:ARG:HG3	2.09	0.53
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.77	0.52
1:B:615:PRO:O	1:B:618:THR:HG22	2.09	0.52
1:C:654:TRP:NE1	1:C:666:GLY:HA3	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:734:SER:CB	1:C:860:GLY:HA3	2.39	0.52
1:A:781:ARG:NH1	5:A:4747:HOH:O	2.42	0.52
1:D:431:ARG:HD2	5:D:4816:HOH:O	2.08	0.52
1:D:749:ILE:N	1:D:749:ILE:CD1	2.72	0.52
1:A:251:ARG:HA	4:A:8416:DMS:S	2.49	0.52
1:A:737:ILE:C	1:A:737:ILE:HD13	2.29	0.52
1:B:1017:GLN:HB2	5:B:4993:HOH:O	2.08	0.52
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.74	0.52
1:A:735:HIS:O	1:A:736:ALA:HB2	2.09	0.52
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.45	0.52
1:D:1022:GLN:O	1:D:1022:GLN:HG3	2.06	0.52
1:C:734:SER:HB3	1:C:860:GLY:C	2.30	0.52
1:D:809:ARG:HG2	1:D:809:ARG:NH1	2.24	0.52
1:A:237:ARG:HG2	1:A:296:GLU:OE1	2.10	0.52
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.74	0.52
1:D:618:THR:HG23	5:D:4367:HOH:O	2.10	0.52
1:C:240:LEU:C	1:C:240:LEU:HD23	2.30	0.51
1:D:237:ARG:NH1	1:D:237:ARG:CG	2.72	0.51
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.11	0.51
1:A:634:GLN:OE1	1:A:683:PRO:O	2.28	0.51
1:B:600:GLN:HE21	1:B:600:GLN:N	1.97	0.51
1:D:681:GLU:HG2	5:D:4769:HOH:O	2.11	0.51
1:D:651:LEU:C	1:D:651:LEU:CD1	2.78	0.51
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.93	0.51
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.11	0.51
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.11	0.51
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.92	0.51
1:C:102:ASN:HD22	4:C:8506:DMS:C1	2.24	0.51
1:A:292:ARG:NH1	4:A:8412:DMS:C2	2.75	0.50
1:C:806:TRP:CE2	1:C:809:ARG:NH2	2.80	0.50
1:C:829:THR:HG22	1:C:830:LEU:O	2.10	0.50
1:C:46:ARG:HG2	5:C:4947:HOH:O	2.12	0.50
1:C:655:MET:SD	1:C:656:VAL:O	2.69	0.50
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.11	0.50
1:A:809:ARG:HG2	1:A:809:ARG:NH1	2.26	0.50
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.46	0.50
1:B:655:MET:HE2	1:B:664:ALA:O	2.12	0.50
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.37	0.50
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.47	0.50
1:D:237:ARG:HG2	1:D:296:GLU:OE1	2.12	0.50
1:C:951:TRP:HA	1:C:1019:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:MET:HE3	1:C:1020:TRP:CZ2	2.46	0.50
1:B:372:MET:CE	1:B:395:HIS:HB3	2.42	0.49
1:B:381:GLN:O	1:B:621:LYS:HE3	2.12	0.49
1:D:843:GLN:HA	1:D:847:LYS:O	2.13	0.49
1:B:651:LEU:HD23	1:B:651:LEU:C	2.32	0.49
1:D:634:GLN:HB2	1:D:682:LEU:HB2	1.94	0.49
1:C:654:TRP:O	1:C:665:SER:HB2	2.12	0.49
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.31	0.49
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.28	0.49
4:A:8502:DMS:H12	5:A:4760:HOH:O	2.12	0.49
1:B:654:TRP:O	1:B:665:SER:HB2	2.12	0.49
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.95	0.49
1:D:720:TRP:HA	4:D:8427:DMS:C1	2.43	0.49
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.12	0.49
1:C:569:ASP:HB2	5:C:4828:HOH:O	2.12	0.49
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.61	0.49
1:D:783:GLN:HG2	1:D:881:ARG:HD2	1.95	0.48
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.96	0.48
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.48	0.48
1:C:667:GLU:C	1:C:668:VAL:HG23	2.33	0.48
1:A:473:ARG:HH12	1:A:476:LYS:HB2	1.74	0.48
1:A:835:LEU:HD11	1:A:855:THR:HB	1.95	0.48
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.94	0.48
1:C:824:GLN:CG	1:C:825:CYS:N	2.77	0.48
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.48	0.48
1:A:699:ARG:NH1	5:A:5038:HOH:O	2.47	0.48
1:B:297:ASN:N	1:B:298:PRO:CD	2.77	0.48
4:A:8427:DMS:H22	5:A:5025:HOH:O	2.13	0.48
1:B:367:MET:HE2	1:B:372:MET:HG3	1.94	0.48
1:D:844:HIS:N	1:D:847:LYS:O	2.42	0.48
1:B:637:GLU:OE2	1:B:677:LYS:HE3	2.14	0.48
1:B:730:LEU:H	1:B:730:LEU:CD1	2.14	0.48
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.96	0.48
1:C:703:PRO:HG2	4:C:8425:DMS:C1	2.43	0.48
1:C:367:MET:HE3	1:C:367:MET:HA	1.96	0.47
1:A:147:ASN:HA	1:A:148:SER:HA	1.51	0.47
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.50	0.47
1:B:157:ARG:HD3	5:B:4879:HOH:O	2.14	0.47
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.97	0.47
4:C:8427:DMS:H12	5:C:4462:HOH:O	2.14	0.47
1:A:640:SER:O	1:A:675:GLN:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LEU:CD1	1:A:686:PRO:HB2	2.45	0.47
1:C:102:ASN:ND2	4:C:8506:DMS:C1	2.77	0.47
1:D:88:SER:HA	1:D:366:VAL:HG21	1.96	0.47
1:A:127:PHE:N	1:A:127:PHE:CD2	2.82	0.47
1:C:824:GLN:O	1:C:838:THR:HA	2.15	0.47
1:A:615:PRO:O	1:A:618:THR:HG22	2.15	0.47
4:A:8503:DMS:O	5:A:4234:HOH:O	2.17	0.47
1:D:240:LEU:HD23	1:D:240:LEU:C	2.35	0.47
1:D:640:SER:O	1:D:675:GLN:HA	2.15	0.47
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.50	0.47
1:B:809:ARG:NH1	5:B:4770:HOH:O	2.48	0.46
4:A:8409:DMS:O	5:A:4514:HOH:O	2.21	0.46
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.38	0.46
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.51	0.46
1:D:788:PRO:CD	1:D:968:MET:HG3	2.45	0.46
1:A:433:LEU:N	1:A:434:PRO:CD	2.79	0.46
1:D:285:TYR:HB3	1:D:288:ARG:HG3	1.97	0.46
4:D:8427:DMS:H23	5:D:4411:HOH:O	2.15	0.46
1:B:634:GLN:CG	1:B:682:LEU:O	2.63	0.46
1:B:262:GLN:NE2	1:B:263:GLY:N	2.58	0.46
1:D:393:PRO:HD3	1:D:412:GLU:O	2.15	0.46
1:B:542:MET:HA	1:B:604:ASN:HA	1.96	0.46
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.79	0.46
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.31	0.46
1:A:735:HIS:ND1	1:A:735:HIS:N	2.33	0.46
1:A:742:THR:CG2	1:A:743:SER:N	2.79	0.46
1:B:634:GLN:HG3	1:B:682:LEU:O	2.15	0.46
1:B:1023:LYS:HB3	1:B:1023:LYS:HE3	1.53	0.46
1:D:513:PRO:O	1:D:514:ALA:HB3	2.15	0.46
1:D:773:LYS:HG2	1:D:775:GLN:NE2	2.30	0.46
1:B:16:TRP:CG	1:B:189:LEU:HD13	2.50	0.46
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.97	0.46
1:B:655:MET:CE	1:B:665:SER:HB3	2.37	0.45
1:C:895:VAL:O	1:C:919:ASP:HA	2.15	0.45
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.14	0.45
1:B:699:ARG:NH2	4:B:8415:DMS:C1	2.79	0.45
1:C:296:GLU:OE1	1:C:296:GLU:HA	2.15	0.45
1:D:829:THR:O	1:D:830:LEU:HD23	2.16	0.45
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.49	0.45
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.30	0.45
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:LYS:HA	1:B:662:PRO:HD3	1.71	0.45
1:C:730:LEU:H	1:C:730:LEU:HG	1.33	0.45
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.98	0.45
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.76	0.45
1:C:431:ARG:HG3	5:C:4809:HOH:O	2.16	0.45
1:A:131:GLU:O	1:A:135:GLN:HG2	2.16	0.45
1:A:279:ILE:HG21	1:A:279:ILE:HD13	1.45	0.45
1:A:533:LEU:C	1:A:533:LEU:HD23	2.36	0.45
1:A:660:GLY:O	1:A:662:PRO:HD3	2.16	0.45
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.43	0.45
1:C:751:LEU:HD21	1:C:860:GLY:O	2.17	0.45
1:D:832:ASP:OD1	1:D:832:ASP:N	2.50	0.45
1:A:844:HIS:HD2	5:A:4856:HOH:O	1.99	0.45
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.80	0.45
1:C:930:VAL:O	1:C:932:PRO:HD3	2.17	0.45
1:D:577:LYS:O	1:D:584:PRO:HA	2.17	0.45
1:C:16:TRP:CG	1:C:189:LEU:CD1	3.00	0.44
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.53	0.44
1:C:615:PRO:O	1:C:618:THR:HG22	2.16	0.44
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.17	0.44
1:C:734:SER:HB3	1:C:860:GLY:CA	2.48	0.44
1:C:278:ILE:HD13	1:C:278:ILE:N	2.31	0.44
1:C:655:MET:CE	1:C:665:SER:HB3	2.26	0.44
1:C:658:LEU:O	1:C:659:ASP:C	2.54	0.44
1:A:200:GLN:HG2	1:A:391:HIS:HB2	2.00	0.44
1:A:433:LEU:N	1:A:434:PRO:HD2	2.33	0.44
1:A:685:LEU:CB	1:A:686:PRO:CD	2.92	0.44
1:B:699:ARG:HH21	4:B:8415:DMS:C1	2.31	0.44
1:C:16:TRP:CG	1:C:189:LEU:HD13	2.53	0.44
1:C:832:ASP:OD1	1:C:832:ASP:N	2.51	0.44
1:D:472:TYR:O	1:D:476:LYS:HG2	2.16	0.44
1:D:660:GLY:O	1:D:662:PRO:HD3	2.18	0.44
1:A:427:THR:HG21	1:A:462:SER:HB3	1.99	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.59	0.44
1:B:372:MET:HE2	5:B:4205:HOH:O	2.18	0.44
1:B:15:ASP:OD2	5:B:4188:HOH:O	2.21	0.44
1:B:658:LEU:O	1:B:659:ASP:C	2.55	0.43
1:C:890:GLN:HG3	1:C:891:VAL:N	2.33	0.43
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.48	0.43
1:C:375:ASP:O	1:C:379:MET:HG3	2.17	0.43
1:A:783:GLN:HG2	1:A:881:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:ILE:HD11	1:B:728:VAL:HG12	2.01	0.43
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.00	0.43
1:B:699:ARG:HE	1:B:714:ILE:HD13	1.82	0.43
1:C:687:GLN:CG	1:C:688:PRO:HD2	2.44	0.43
1:D:636:ILE:HG21	1:D:636:ILE:HD13	1.79	0.43
1:D:745:MET:HE3	1:D:745:MET:HB2	1.86	0.43
1:C:768:MET:O	1:C:775:GLN:N	2.48	0.43
1:A:460:ASN:O	1:A:461:GLU:C	2.57	0.43
1:A:472:TYR:O	1:A:476:LYS:HG2	2.18	0.43
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.89	0.43
1:D:292:ARG:HH12	4:D:8412:DMS:H23	1.80	0.43
1:C:658:LEU:HG	1:C:661:LYS:HZ2	1.84	0.43
1:C:658:LEU:HG	1:C:661:LYS:NZ	2.33	0.43
1:C:673:ALA:HB1	1:C:674:PRO:HD2	2.00	0.43
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.54	0.43
1:D:353:GLY:HA2	1:D:386:ALA:O	2.19	0.43
1:D:785:THR:HB	1:D:816:TYR:CE2	2.53	0.43
1:D:824:GLN:HE21	1:D:837:THR:HG22	1.84	0.43
1:A:737:ILE:HD13	1:A:737:ILE:O	2.18	0.43
1:B:237:ARG:HD2	1:B:296:GLU:OE1	2.18	0.43
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.34	0.43
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.54	0.43
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.54	0.43
1:A:859:ASP:OD1	1:A:861:SER:OG	2.23	0.43
1:B:377:LEU:HD22	1:B:708:TRP:HA	2.00	0.43
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.53	0.43
1:D:755:ARG:HB2	1:D:769:TRP:CE3	2.54	0.43
1:D:893:GLU:HG2	1:D:894:ARG:CG	2.48	0.43
1:B:142:ILE:HG12	1:B:170:GLU:HG2	2.00	0.43
1:B:427:THR:HG21	1:B:462:SER:HB3	2.00	0.43
1:B:730:LEU:H	1:B:730:LEU:HD12	1.83	0.43
1:A:600:GLN:HE21	1:A:600:GLN:N	2.09	0.42
1:A:663:LEU:CD1	1:A:686:PRO:CG	2.97	0.42
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.82	0.42
1:B:114:VAL:HB	1:B:115:PRO:HD2	2.00	0.42
1:B:178:ARG:O	1:B:178:ARG:HG3	2.18	0.42
1:B:473:ARG:NH1	1:B:477:SER:HB2	2.34	0.42
1:C:687:GLN:HE21	1:C:687:GLN:CA	2.32	0.42
1:C:777:LEU:HG	1:C:889:ALA:HA	2.01	0.42
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.39	0.42
1:C:44:THR:OG1	1:C:46:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD13	1:C:653:HIS:ND1	2.34	0.42
1:C:759:ASN:OD1	1:C:761:GLN:N	2.51	0.42
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.36	0.42
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.54	0.42
1:A:663:LEU:CD1	1:A:686:PRO:CB	2.97	0.42
1:A:764:PHE:CD1	1:A:781:ARG:NH1	2.88	0.42
1:A:843:GLN:HA	1:A:847:LYS:O	2.19	0.42
1:A:863:GLN:NE2	1:A:952:ARG:HH22	2.18	0.42
4:A:8427:DMS:C2	5:A:5025:HOH:O	2.67	0.42
1:B:577:LYS:O	1:B:584:PRO:HA	2.19	0.42
1:B:763:GLY:HA3	1:B:822:LEU:HD13	2.00	0.42
1:A:658:LEU:O	1:A:659:ASP:C	2.57	0.42
1:A:785:THR:O	1:A:881:ARG:HD2	2.20	0.42
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.49	0.42
1:C:433:LEU:HD12	1:C:433:LEU:O	2.20	0.42
1:C:778:THR:HG23	1:C:887:GLN:HB3	2.01	0.42
1:C:942:ARG:HA	1:C:953:GLY:O	2.20	0.42
1:D:608:PHE:CD1	1:D:614:HIS:HD2	2.38	0.42
1:D:873:ALA:O	1:D:876:THR:HG22	2.20	0.42
1:A:619:GLU:HA	1:A:912:ALA:HB2	2.02	0.41
1:B:601:PHE:CD2	4:B:8506:DMS:C2	3.03	0.41
1:B:601:PHE:CD2	4:B:8506:DMS:H23	2.55	0.41
1:C:237:ARG:NH1	1:C:237:ARG:CB	2.83	0.41
1:C:749:ILE:N	1:C:749:ILE:CD1	2.80	0.41
1:C:781:ARG:NH1	5:C:4771:HOH:O	2.52	0.41
1:D:773:LYS:HG3	1:D:774:LYS:N	2.35	0.41
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.55	0.41
1:A:593:GLY:O	1:A:595:THR:HG22	2.21	0.41
1:C:785:THR:O	1:C:881:ARG:HD2	2.20	0.41
1:C:995:GLY:O	1:C:996:ASP:C	2.58	0.41
1:A:680:ILE:HG12	5:A:4650:HOH:O	2.20	0.41
1:A:1006:GLU:OE1	5:A:5044:HOH:O	2.22	0.41
1:C:524:LEU:HD11	1:C:562:LEU:HG	2.02	0.41
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.55	0.41
1:A:58:TRP:CD1	1:A:86:VAL:HB	2.56	0.41
1:A:352:ARG:HG2	1:A:553:TRP:CH2	2.56	0.41
1:A:768:MET:CE	1:A:1020:TRP:CZ2	3.03	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.92	0.41
1:C:619:GLU:HG2	1:C:909:ARG:HG3	2.02	0.41
1:D:111:PRO:HA	1:D:112:PRO:HA	1.78	0.41
1:D:362:LEU:HA	1:D:362:LEU:HD23	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:829:THR:HG23	1:D:834:VAL:HG22	2.02	0.41
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.56	0.41
1:B:538:TYR:O	1:B:567:VAL:HA	2.21	0.41
1:C:765:LEU:CD2	1:C:768:MET:CE	2.95	0.41
1:C:819:GLU:H	1:C:819:GLU:HG2	1.49	0.41
1:D:869:ASP:OD1	1:D:1015:HIS:ND1	2.54	0.41
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.86	0.41
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.03	0.41
1:D:114:VAL:HB	1:D:115:PRO:CD	2.50	0.41
1:D:720:TRP:HA	4:D:8427:DMS:H12	2.02	0.41
1:D:785:THR:O	1:D:881:ARG:HD2	2.20	0.41
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.74	0.41
1:B:102:ASN:HD22	4:B:8506:DMS:C2	2.34	0.41
1:B:127:PHE:N	1:B:127:PHE:CD2	2.89	0.41
1:B:128:ASN:HA	1:B:180:GLY:O	2.21	0.41
1:B:431:ARG:HD3	5:B:4493:HOH:O	2.21	0.41
1:B:674:PRO:O	1:B:675:GLN:HB2	2.21	0.41
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.56	0.41
1:D:143:PHE:O	1:D:168:PRO:HA	2.21	0.41
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.56	0.41
1:A:292:ARG:HH12	4:A:8412:DMS:C2	2.34	0.41
4:D:8407:DMS:C2	4:D:8407:DMS:C1	2.94	0.41
1:A:59:ARG:NH2	1:A:81:ALA:HB3	2.35	0.40
1:A:253:TYR:CD1	1:A:253:TYR:C	2.94	0.40
1:A:753:ASN:OD1	1:A:753:ASN:N	2.50	0.40
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.56	0.40
1:B:755:ARG:HB3	1:B:769:TRP:CE3	2.56	0.40
1:D:340:GLY:O	1:D:561:ARG:HG2	2.22	0.40
1:D:363:HIS:HD2	5:D:4623:HOH:O	2.03	0.40
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.56	0.40
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.51	0.40
1:A:249:GLU:O	1:A:254:LEU:HD11	2.21	0.40
1:B:100:TYR:HB3	1:B:589:GLY:HA2	2.03	0.40
1:B:262:GLN:NE2	1:B:262:GLN:CA	2.85	0.40
1:B:684:GLU:O	1:B:686:PRO:HD3	2.21	0.40
1:B:701:VAL:HG22	1:B:714:ILE:HG12	2.03	0.40
1:C:233:ASP:HA	4:C:8417:DMS:S	2.61	0.40
1:D:130:ASP:OD2	4:D:8703:DMS:H22	2.19	0.40
1:D:583:ASN:HA	1:D:584:PRO:HD3	1.98	0.40
1:B:143:PHE:O	1:B:168:PRO:HA	2.20	0.40
1:B:472:TYR:O	1:B:476:LYS:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.57	0.40
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.57	0.40
4:B:8407:DMS:C2	4:B:8407:DMS:C1	2.92	0.40
1:C:147:ASN:HA	1:C:148:SER:HA	1.59	0.40
1:D:738:PRO:HB3	1:D:751:LEU:HB2	2.02	0.40
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.84	0.40
1:B:824:GLN:HG2	1:B:825:CYS:N	2.35	0.40
1:C:663:LEU:HD22	1:C:663:LEU:HA	1.87	0.40
1:D:893:GLU:HG2	1:D:894:ARG:CD	2.51	0.40
1:B:433:LEU:N	1:B:434:PRO:CD	2.85	0.40
1:C:278:ILE:HD12	1:C:278:ILE:HA	1.92	0.40
1:C:981:GLY:N	5:C:4816:HOH:O	2.36	0.40
1:D:893:GLU:CG	1:D:894:ARG:HD2	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:4934:HOH:O	5:B:5031:HOH:O[2_454]	2.14	0.06
5:A:5071:HOH:O	5:C:5012:HOH:O[2_554]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	971 (96%)	37 (4%)	1 (0%)	51	33
1	B	1009/1023 (99%)	970 (96%)	34 (3%)	5 (0%)	29	12
1	C	1009/1023 (99%)	972 (96%)	36 (4%)	1 (0%)	51	33
1	D	1009/1023 (99%)	970 (96%)	38 (4%)	1 (0%)	51	33
All	All	4036/4092 (99%)	3883 (96%)	145 (4%)	8 (0%)	47	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	ALA
1	B	690	SER
1	C	734	SER
1	B	731	PRO
1	B	164	ASP
1	D	164	ASP
1	A	164	ASP
1	B	688	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	831 (96%)	33 (4%)	33	11
1	B	864/875 (99%)	830 (96%)	34 (4%)	32	11
1	C	864/875 (99%)	828 (96%)	36 (4%)	30	9
1	D	864/875 (99%)	825 (96%)	39 (4%)	27	8
All	All	3456/3500 (99%)	3314 (96%)	142 (4%)	30	10

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TRP
1	A	131	GLU
1	A	237	ARG
1	A	250	LEU
1	A	279	ILE
1	A	333	ARG
1	A	394	ASN
1	A	418	ASN
1	A	519	SER
1	A	546	LEU
1	A	600	GLN
1	A	634	GLN

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Mol	Chain	Res	Type
1	A	655	MET
1	A	661	LYS
1	A	663	LEU
1	A	667	GLU
1	A	671	ASP
1	A	672	VAL
1	A	684	GLU
1	A	689	GLU
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	797	GLU
1	A	799	THR
1	A	801	ILE
1	A	885	ASN
1	A	910	LEU
1	A	956	GLN
1	A	986	ILE
1	A	1013	ARG
1	A	1017	GLN
1	A	1023	LYS
1	B	80	GLU
1	B	230	ARG
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
1	B	370	GLN
1	B	392	TYR
1	B	394	ASN
1	B	519	SER
1	B	554	GLN
1	B	600	GLN
1	B	635	THR
1	B	651	LEU
1	B	655	MET
1	B	663	LEU
1	B	667	GLU
1	B	684	GLU
1	B	687	GLN

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Mol	Chain	Res	Type
1	B	730	LEU
1	B	731	PRO
1	B	734	SER
1	B	737	ILE
1	B	745	MET
1	B	755	ARG
1	B	799	THR
1	B	819	GLU
1	B	847	LYS
1	B	863	GLN
1	B	885	ASN
1	B	956	GLN
1	B	1023	LYS
1	C	13	ARG
1	C	71	GLU
1	C	75	GLU
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	262	GLN
1	C	264	GLU
1	C	278	ILE
1	C	333	ARG
1	C	392	TYR
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	595	THR
1	C	630	ARG
1	C	634	GLN
1	C	653	HIS
1	C	663	LEU
1	C	681	GLU
1	C	684	GLU
1	C	687	GLN
1	C	699	ARG
1	C	730	LEU
1	C	734	SER
1	C	737	ILE
1	C	749	ILE
1	C	750	GLU

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Mol	Chain	Res	Type
1	C	773	LYS
1	C	788	PRO
1	C	800	ARG
1	C	819	GLU
1	C	956	GLN
1	C	986	ILE
1	C	1023	LYS
1	D	13	ARG
1	D	79	PRO
1	D	80	GLU
1	D	237	ARG
1	D	277	GLU
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	392	TYR
1	D	394	ASN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	594	ASP
1	D	632	SER
1	D	651	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	667	GLU
1	D	681	GLU
1	D	682	LEU
1	D	684	GLU
1	D	687	GLN
1	D	689	GLU
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	774	LYS
1	D	799	THR
1	D	845	GLN
1	D	885	ASN
1	D	893	GLU

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Mol	Chain	Res	Type
1	D	986	ILE
1	D	1017	GLN
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	262	GLN
1	A	600	GLN
1	A	624	GLN
1	A	675	GLN
1	A	687	GLN
1	A	824	GLN
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	B	262	GLN
1	B	363	HIS
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	878	HIS
1	B	965	GLN
1	B	977	HIS
1	B	1017	GLN
1	C	102	ASN
1	C	266	GLN
1	C	624	GLN
1	C	634	GLN
1	C	646	HIS
1	C	687	GLN
1	C	702	GLN
1	C	761	GLN
1	C	824	GLN
1	C	844	HIS
1	C	878	HIS
1	C	977	HIS
1	D	363	HIS
1	D	583	ASN

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Mol	Chain	Res	Type
1	D	624	GLN
1	D	628	GLN
1	D	757	GLN
1	D	804	ASN
1	D	824	GLN
1	D	878	HIS
1	D	977	HIS
1	D	1022	GLN

### 5.3.3 RNA [i](#)

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 139 ligands modelled in this entry, 32 are monoatomic - leaving 107 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	8421	-	3,3,3	1.09	0	3,3,3	1.25	1 (33%)
4	DMS	B	8504	-	3,3,3	0.62	0	3,3,3	1.01	0
4	DMS	B	8601	-	3,3,3	1.88	1 (33%)	3,3,3	0.86	0
4	DMS	C	8411	-	3,3,3	1.08	0	3,3,3	0.20	0
4	DMS	B	8415	-	3,3,3	2.34	2 (66%)	3,3,3	0.96	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	C	8417	-	3,3,3	0.59	0	3,3,3	0.62	0
4	DMS	C	8405	-	3,3,3	1.24	0	3,3,3	0.51	0
4	DMS	B	8410	-	3,3,3	1.40	1 (33%)	3,3,3	0.58	0
4	DMS	B	8423	-	3,3,3	0.89	0	3,3,3	0.20	0
4	DMS	C	8412	-	3,3,3	1.32	0	3,3,3	0.55	0
4	DMS	C	8404	-	3,3,3	0.92	0	3,3,3	1.18	1 (33%)
4	DMS	A	8502	-	3,3,3	1.85	1 (33%)	3,3,3	1.14	0
4	DMS	D	8506	-	3,3,3	1.30	0	3,3,3	0.16	0
4	DMS	D	8416	-	3,3,3	0.79	0	3,3,3	0.35	0
4	DMS	C	8410	-	3,3,3	0.98	0	3,3,3	0.29	0
4	DMS	B	8508	-	3,3,3	3.12	1 (33%)	3,3,3	0.69	0
4	DMS	B	8402	-	3,3,3	1.36	0	3,3,3	0.20	0
4	DMS	A	8420	-	3,3,3	1.14	0	3,3,3	0.85	0
4	DMS	B	8416	-	3,3,3	1.13	0	3,3,3	0.64	0
4	DMS	B	8403	-	3,3,3	1.60	1 (33%)	3,3,3	0.81	0
4	DMS	C	8407	-	3,3,3	1.50	0	3,3,3	0.13	0
4	DMS	D	8411	-	3,3,3	0.99	0	3,3,3	0.40	0
4	DMS	C	8504	-	3,3,3	0.53	0	3,3,3	0.33	0
4	DMS	C	8501	-	3,3,3	0.59	0	3,3,3	0.90	0
4	DMS	D	8503	-	3,3,3	0.73	0	3,3,3	0.67	0
4	DMS	D	8412	-	3,3,3	0.66	0	3,3,3	0.28	0
4	DMS	A	8419	-	3,3,3	0.40	0	3,3,3	0.25	0
4	DMS	A	8414	-	3,3,3	1.26	1 (33%)	3,3,3	0.52	0
4	DMS	C	8421	-	3,3,3	0.76	0	3,3,3	0.91	0
4	DMS	A	8405	-	3,3,3	0.98	0	3,3,3	0.70	0
4	DMS	D	8410	-	3,3,3	1.02	0	3,3,3	0.39	0
4	DMS	A	8412	-	3,3,3	0.75	0	3,3,3	0.28	0
4	DMS	A	8404	-	3,3,3	1.91	1 (33%)	3,3,3	0.36	0
4	DMS	C	8414	-	3,3,3	1.93	1 (33%)	3,3,3	1.14	0
4	DMS	A	8407	-	3,3,3	1.72	2 (66%)	3,3,3	0.76	0
4	DMS	C	8401	-	3,3,3	0.96	0	3,3,3	0.15	0
4	DMS	A	8503	-	3,3,3	0.94	0	3,3,3	0.21	0
4	DMS	A	8403	-	3,3,3	1.62	1 (33%)	3,3,3	0.47	0
4	DMS	A	8411	-	3,3,3	0.73	0	3,3,3	0.25	0
4	DMS	D	8405	-	3,3,3	0.91	0	3,3,3	0.72	0
4	DMS	B	8412	-	3,3,3	1.12	0	3,3,3	0.36	0
4	DMS	A	8413	-	3,3,3	2.65	2 (66%)	3,3,3	0.57	0
4	DMS	D	8403	-	3,3,3	1.46	1 (33%)	3,3,3	0.20	0
4	DMS	D	8423	-	3,3,3	1.52	0	3,3,3	0.39	0
4	DMS	C	8409	-	3,3,3	1.68	1 (33%)	3,3,3	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	B	8427	-	3,3,3	1.03	0	3,3,3	0.22	0
4	DMS	D	8419	-	3,3,3	0.82	0	3,3,3	0.66	0
4	DMS	B	8401	-	3,3,3	0.53	0	3,3,3	0.62	0
4	DMS	D	8407	-	3,3,3	2.60	2 (66%)	3,3,3	0.21	0
4	DMS	D	8701	-	3,3,3	2.84	3 (100%)	3,3,3	0.84	0
4	DMS	D	8406	-	3,3,3	1.49	1 (33%)	3,3,3	0.59	0
4	DMS	B	8414	-	3,3,3	0.93	0	3,3,3	0.44	0
4	DMS	C	8427	-	3,3,3	0.89	0	3,3,3	0.27	0
4	DMS	C	8601	-	3,3,3	1.18	1 (33%)	3,3,3	1.27	1 (33%)
4	DMS	D	8414	-	3,3,3	0.37	0	3,3,3	0.29	0
4	DMS	D	8413	-	3,3,3	0.79	0	3,3,3	0.68	0
4	DMS	A	8402	-	3,3,3	1.30	0	3,3,3	0.36	0
4	DMS	D	8421	-	3,3,3	0.15	0	3,3,3	0.43	0
4	DMS	A	8504	-	3,3,3	0.42	0	3,3,3	0.39	0
4	DMS	C	8419	-	3,3,3	1.16	0	3,3,3	0.25	0
4	DMS	B	8420	-	3,3,3	1.53	1 (33%)	3,3,3	0.36	0
4	DMS	A	8423	-	3,3,3	1.39	1 (33%)	3,3,3	0.66	0
4	DMS	C	8503	-	3,3,3	0.96	0	3,3,3	0.15	0
4	DMS	B	8506	-	3,3,3	1.78	1 (33%)	3,3,3	0.62	0
4	DMS	B	8425	3	3,3,3	2.16	1 (33%)	3,3,3	0.72	0
4	DMS	B	8408	-	3,3,3	0.89	0	3,3,3	0.10	0
4	DMS	A	8602	-	3,3,3	0.74	0	3,3,3	0.28	0
4	DMS	D	8427	-	3,3,3	0.48	0	3,3,3	0.37	0
4	DMS	D	8409	-	3,3,3	2.46	2 (66%)	3,3,3	0.87	0
4	DMS	C	8423	-	3,3,3	1.05	0	3,3,3	0.27	0
4	DMS	A	8425	3	3,3,3	2.26	1 (33%)	3,3,3	0.52	0
4	DMS	B	8421	-	3,3,3	0.33	0	3,3,3	0.53	0
4	DMS	B	8502	-	3,3,3	1.18	0	3,3,3	1.50	1 (33%)
4	DMS	B	8405	-	3,3,3	1.56	0	3,3,3	0.38	0
4	DMS	D	8408	-	3,3,3	1.70	1 (33%)	3,3,3	0.15	0
4	DMS	C	8415	-	3,3,3	2.11	1 (33%)	3,3,3	0.91	0
4	DMS	C	8420	-	3,3,3	1.43	1 (33%)	3,3,3	0.89	0
4	DMS	C	8413	-	3,3,3	1.65	0	3,3,3	0.17	0
4	DMS	A	8501	-	3,3,3	1.62	1 (33%)	3,3,3	0.35	0
4	DMS	C	8416	-	3,3,3	0.96	0	3,3,3	0.32	0
4	DMS	B	8409	-	3,3,3	1.81	1 (33%)	3,3,3	0.37	0
4	DMS	A	8409	-	3,3,3	1.30	1 (33%)	3,3,3	0.49	0
4	DMS	B	8407	-	3,3,3	2.52	2 (66%)	3,3,3	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	C	8602	-	3,3,3	1.29	1 (33%)	3,3,3	0.98	0
4	DMS	D	8401	-	3,3,3	1.09	0	3,3,3	0.48	0
4	DMS	A	8427	-	3,3,3	1.01	0	3,3,3	0.57	0
4	DMS	C	8402	-	3,3,3	1.64	1 (33%)	3,3,3	0.30	0
4	DMS	C	8408	-	3,3,3	1.15	0	3,3,3	0.99	0
4	DMS	D	8404	-	3,3,3	1.59	1 (33%)	3,3,3	0.14	0
4	DMS	D	8705	-	3,3,3	1.51	1 (33%)	3,3,3	0.44	0
4	DMS	B	8411	-	3,3,3	0.69	0	3,3,3	0.28	0
4	DMS	C	8506	-	3,3,3	0.89	0	3,3,3	0.50	0
4	DMS	D	8508	-	3,3,3	1.78	1 (33%)	3,3,3	0.57	0
4	DMS	D	8703	-	3,3,3	1.21	0	3,3,3	0.51	0
4	DMS	D	8501	-	3,3,3	0.70	0	3,3,3	0.39	0
4	DMS	B	8404	-	3,3,3	0.68	0	3,3,3	0.73	0
4	DMS	B	8406	-	3,3,3	0.86	0	3,3,3	0.60	0
4	DMS	C	8403	-	3,3,3	0.60	0	3,3,3	0.25	0
4	DMS	C	8425	3	3,3,3	1.93	1 (33%)	3,3,3	0.43	0
4	DMS	A	8406	-	3,3,3	0.94	0	3,3,3	1.35	1 (33%)
4	DMS	A	8416	-	3,3,3	1.46	1 (33%)	3,3,3	0.75	0
4	DMS	A	8408	-	3,3,3	0.46	0	3,3,3	0.51	0
4	DMS	A	8410	-	3,3,3	1.06	0	3,3,3	1.24	1 (33%)
4	DMS	B	8417	-	3,3,3	0.36	0	3,3,3	0.68	0
4	DMS	B	8413	-	3,3,3	2.21	1 (33%)	3,3,3	0.61	0
4	DMS	A	8401	-	3,3,3	0.64	0	3,3,3	0.42	0
4	DMS	D	8402	-	3,3,3	1.19	0	3,3,3	0.20	0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8508	DMS	C1-S	4.85	2.11	1.75
4	D	8407	DMS	C2-S	3.83	2.04	1.75
4	B	8407	DMS	C2-S	3.82	2.04	1.75
4	D	8409	DMS	O-S	3.65	1.74	1.50
4	A	8425	DMS	O-S	3.34	1.72	1.50
4	B	8425	DMS	O-S	3.30	1.72	1.50
4	A	8413	DMS	C1-S	3.26	2.00	1.75
4	D	8701	DMS	O-S	3.21	1.71	1.50
4	B	8409	DMS	O-S	3.07	1.71	1.50
4	C	8415	DMS	C2-S	3.06	1.98	1.75
4	B	8413	DMS	O-S	2.99	1.70	1.50
4	D	8508	DMS	O-S	2.90	1.69	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8425	DMS	O-S	2.77	1.68	1.50
4	C	8409	DMS	O-S	2.76	1.68	1.50
4	D	8408	DMS	C1-S	2.74	1.96	1.75
4	D	8701	DMS	C1-S	2.65	1.95	1.75
4	A	8413	DMS	C2-S	2.64	1.95	1.75
4	A	8502	DMS	C1-S	2.63	1.95	1.75
4	D	8701	DMS	C2-S	2.62	1.95	1.75
4	D	8404	DMS	C2-S	2.60	1.95	1.75
4	B	8506	DMS	O-S	2.58	1.67	1.50
4	A	8501	DMS	O-S	2.56	1.67	1.50
4	A	8404	DMS	C2-S	2.54	1.94	1.75
4	B	8415	DMS	O-S	2.54	1.67	1.50
4	B	8420	DMS	C2-S	2.46	1.94	1.75
4	B	8415	DMS	C2-S	2.46	1.94	1.75
4	C	8402	DMS	C2-S	2.45	1.94	1.75
4	C	8414	DMS	C1-S	-2.44	1.57	1.75
4	C	8420	DMS	O-S	2.42	1.66	1.50
4	A	8416	DMS	O-S	-2.36	1.34	1.50
4	D	8407	DMS	O-S	2.27	1.65	1.50
4	B	8601	DMS	C2-S	2.20	1.92	1.75
4	C	8602	DMS	C2-S	-2.18	1.59	1.75
4	D	8403	DMS	O-S	2.15	1.64	1.50
4	A	8407	DMS	O-S	2.14	1.64	1.50
4	D	8409	DMS	C1-S	2.13	1.91	1.75
4	A	8403	DMS	C2-S	2.12	1.91	1.75
4	A	8423	DMS	C1-S	2.11	1.91	1.75
4	A	8414	DMS	O-S	-2.10	1.35	1.50
4	D	8705	DMS	O-S	2.10	1.64	1.50
4	D	8406	DMS	O-S	-2.08	1.36	1.50
4	B	8410	DMS	C1-S	2.07	1.91	1.75
4	A	8407	DMS	C2-S	2.06	1.91	1.75
4	B	8407	DMS	O-S	2.05	1.64	1.50
4	B	8403	DMS	C1-S	2.05	1.91	1.75
4	C	8601	DMS	C2-S	2.03	1.91	1.75
4	A	8409	DMS	O-S	2.00	1.63	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8502	DMS	C2-S-C1	2.59	111.78	98.44
4	A	8406	DMS	C2-S-C1	2.29	110.20	98.44
4	C	8601	DMS	C2-S-C1	2.18	109.66	98.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	8421	DMS	C2-S-C1	2.16	109.53	98.44
4	A	8410	DMS	C2-S-C1	-2.11	87.60	98.44
4	C	8404	DMS	C2-S-C1	2.03	108.89	98.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	8415	DMS	2	0
4	C	8417	DMS	1	0
4	A	8502	DMS	1	0
4	D	8506	DMS	3	0
4	B	8508	DMS	1	0
4	A	8420	DMS	1	0
4	D	8412	DMS	3	0
4	A	8412	DMS	3	0
4	A	8503	DMS	1	0
4	D	8407	DMS	2	0
4	C	8427	DMS	2	0
4	A	8423	DMS	1	0
4	B	8506	DMS	5	0
4	D	8427	DMS	3	0
4	C	8420	DMS	1	0
4	A	8409	DMS	1	0
4	B	8407	DMS	2	0
4	A	8427	DMS	4	0
4	C	8506	DMS	4	0
4	D	8703	DMS	1	0
4	B	8406	DMS	1	0
4	C	8425	DMS	1	0
4	A	8416	DMS	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	-0.44	23 (2%) 60 67	10, 17, 46, 99	0
1	B	1011/1023 (98%)	-0.40	16 (1%) 72 79	10, 17, 45, 94	0
1	C	1011/1023 (98%)	-0.34	20 (1%) 65 72	11, 18, 50, 97	0
1	D	1011/1023 (98%)	-0.37	28 (2%) 53 58	11, 18, 48, 99	0
All	All	4044/4092 (98%)	-0.39	87 (2%) 62 69	10, 18, 48, 99	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	8.7
1	D	735	HIS	7.4
1	D	732	ALA	7.2
1	C	732	ALA	7.2
1	C	730	LEU	6.9
1	A	686	PRO	6.9
1	D	733	ALA	6.5
1	C	731	PRO	6.4
1	D	686	PRO	6.1
1	D	734	SER	6.1
1	C	735	HIS	5.9
1	B	731	PRO	5.9
1	B	685	LEU	5.8
1	C	733	ALA	5.6
1	C	689	GLU	5.6
1	B	730	LEU	5.3
1	D	730	LEU	5.2
1	B	733	ALA	4.9
1	B	689	GLU	4.8
1	A	730	LEU	4.8
1	A	687	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	689	GLU	4.4
1	A	733	ALA	4.4
1	D	687	GLN	4.4
1	A	732	ALA	4.2
1	C	685	LEU	4.2
1	A	580	GLU	4.1
1	D	683	PRO	4.1
1	D	684	GLU	4.1
1	B	732	ALA	4.0
1	B	684	GLU	3.8
1	C	745	MET	3.7
1	C	734	SER	3.7
1	D	580	GLU	3.7
1	A	734	SER	3.7
1	B	686	PRO	3.7
1	A	689	GLU	3.6
1	C	687	GLN	3.6
1	A	685	LEU	3.5
1	D	731	PRO	3.4
1	D	581	ASN	3.3
1	C	686	PRO	3.3
1	C	634	GLN	3.2
1	D	685	LEU	3.2
1	B	799	THR	3.2
1	D	772	ASP	3.1
1	A	736	ALA	3.1
1	C	800	ARG	3.0
1	D	845	GLN	3.0
1	B	687	GLN	3.0
1	A	582	GLY	3.0
1	D	634	GLN	3.0
1	A	1023	LYS	2.8
1	D	800	ARG	2.8
1	B	745	MET	2.7
1	A	684	GLU	2.7
1	C	684	GLU	2.7
1	B	735	HIS	2.6
1	B	798	ALA	2.6
1	A	731	PRO	2.6
1	C	830	LEU	2.6
1	D	688	PRO	2.6
1	D	799	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	771	GLY	2.5
1	A	729	THR	2.5
1	C	799	THR	2.5
1	C	729	THR	2.5
1	C	580	GLU	2.5
1	D	729	THR	2.5
1	A	799	THR	2.4
1	A	683	PRO	2.4
1	D	663	LEU	2.3
1	A	71	GLU	2.2
1	C	633	GLY	2.2
1	A	682	LEU	2.2
1	D	679	LEU	2.2
1	A	634	GLN	2.2
1	C	761	GLN	2.2
1	D	860	GLY	2.2
1	B	729	THR	2.1
1	D	736	ALA	2.1
1	D	831	ALA	2.1
1	D	830	LEU	2.1
1	A	581	ASN	2.1
1	A	845	GLN	2.0
1	B	580	GLU	2.0
1	B	581	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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( $\text{\AA}^2$ )	Q<0.9
2	MG	A	3105	1/1	0.84	0.17	48,48,48,48	1
4	DMS	B	8406	4/4	0.84	0.19	35,47,68,69	0
2	MG	D	3105	1/1	0.85	0.19	37,37,37,37	1
4	DMS	D	8703	4/4	0.87	0.20	53,59,62,79	0
4	DMS	D	8427	4/4	0.88	0.21	62,67,91,100	0
3	NA	D	3104	1/1	0.89	0.09	37,37,37,37	0
4	DMS	D	8503	4/4	0.89	0.14	40,56,68,76	0
4	DMS	C	8416	4/4	0.89	0.26	48,50,55,66	0
4	DMS	A	8416	4/4	0.90	0.18	24,33,39,100	0
4	DMS	C	8602	4/4	0.91	0.12	29,55,76,88	0
4	DMS	D	8423	4/4	0.91	0.14	39,49,68,80	0
4	DMS	B	8420	4/4	0.91	0.17	58,64,77,92	0
4	DMS	A	8423	4/4	0.91	0.19	36,70,71,72	0
4	DMS	C	8417	4/4	0.91	0.16	29,38,43,70	0
4	DMS	C	8419	4/4	0.92	0.18	43,63,65,71	0
4	DMS	B	8413	4/4	0.92	0.18	39,48,50,61	0
2	MG	A	3005	1/1	0.92	0.06	34,34,34,34	0
4	DMS	B	8423	4/4	0.92	0.13	43,54,70,91	0
4	DMS	A	8425	4/4	0.92	0.15	36,37,38,47	0
3	NA	B	3104	1/1	0.92	0.10	34,34,34,34	0
2	MG	B	3105	1/1	0.93	0.13	28,28,28,28	1
4	DMS	C	8423	4/4	0.93	0.10	38,40,53,59	0
4	DMS	C	8503	4/4	0.93	0.14	38,57,100,100	0
4	DMS	D	8506	4/4	0.93	0.17	50,62,100,100	0
4	DMS	A	8502	4/4	0.93	0.15	25,25,66,100	0
4	DMS	D	8705	4/4	0.93	0.12	28,40,43,47	0
4	DMS	C	8415	4/4	0.94	0.10	25,32,38,52	0
4	DMS	D	8407	4/4	0.94	0.13	30,47,55,73	0
2	MG	C	3004	1/1	0.94	0.09	43,43,43,43	0
4	DMS	B	8415	4/4	0.94	0.10	25,34,39,48	0
4	DMS	A	8503	4/4	0.94	0.12	34,43,54,55	0
4	DMS	A	8427	4/4	0.94	0.19	40,41,100,100	0
4	DMS	B	8425	4/4	0.94	0.17	24,33,41,48	0
4	DMS	C	8506	4/4	0.94	0.16	52,58,99,100	0
4	DMS	B	8427	4/4	0.95	0.09	34,43,57,87	0
4	DMS	B	8506	4/4	0.95	0.15	45,59,100,100	0
4	DMS	D	8404	4/4	0.95	0.10	21,26,44,100	0
4	DMS	B	8508	4/4	0.95	0.10	26,36,52,56	0
4	DMS	D	8416	4/4	0.95	0.17	28,31,46,100	0
4	DMS	A	8406	4/4	0.95	0.19	16,44,64,66	0
4	DMS	B	8416	4/4	0.95	0.16	35,50,50,55	0
4	DMS	D	8501	4/4	0.95	0.08	28,32,41,51	0
4	DMS	B	8417	4/4	0.95	0.16	27,41,72,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	A	8421	4/4	0.95	0.16	49,55,74,97	0
4	DMS	B	8407	4/4	0.95	0.13	35,36,41,100	0
4	DMS	A	8413	4/4	0.95	0.13	30,39,41,45	0
4	DMS	C	8425	4/4	0.96	0.16	40,46,47,100	0
4	DMS	C	8501	4/4	0.96	0.09	30,34,39,48	0
2	MG	C	3105	1/1	0.96	0.09	28,28,28,28	1
4	DMS	C	8504	4/4	0.96	0.08	36,37,52,60	0
4	DMS	A	8409	4/4	0.96	0.10	30,35,51,51	0
4	DMS	C	8601	4/4	0.96	0.12	40,42,48,54	0
4	DMS	B	8504	4/4	0.96	0.08	24,39,45,51	0
4	DMS	B	8408	4/4	0.96	0.10	24,44,47,100	0
3	NA	C	3104	1/1	0.96	0.12	33,33,33,33	0
4	DMS	D	8409	4/4	0.96	0.11	31,31,37,40	0
4	DMS	B	8601	4/4	0.96	0.10	32,43,46,56	0
4	DMS	A	8414	4/4	0.96	0.13	30,35,54,100	0
4	DMS	A	8501	4/4	0.96	0.10	18,25,31,35	0
3	NA	A	3104	1/1	0.96	0.11	27,27,27,27	0
4	DMS	A	8420	4/4	0.96	0.12	41,46,58,60	0
4	DMS	C	8420	4/4	0.96	0.13	45,48,53,100	0
4	DMS	D	8508	4/4	0.96	0.09	41,45,49,70	0
4	DMS	C	8421	4/4	0.96	0.09	40,46,61,100	0
4	DMS	A	8602	4/4	0.96	0.17	41,49,98,100	0
4	DMS	A	8419	4/4	0.97	0.10	48,49,54,90	0
4	DMS	D	8419	4/4	0.97	0.09	28,36,48,58	0
4	DMS	B	8409	4/4	0.97	0.10	33,33,40,43	0
4	DMS	C	8407	4/4	0.97	0.14	29,36,38,51	0
4	DMS	C	8409	4/4	0.97	0.11	29,36,40,41	0
4	DMS	C	8413	4/4	0.97	0.15	32,35,37,37	0
2	MG	A	3106	1/1	0.97	0.06	24,24,24,24	0
4	DMS	D	8406	4/4	0.97	0.10	25,25,26,36	0
4	DMS	C	8427	4/4	0.97	0.07	47,47,55,63	0
4	DMS	A	8407	4/4	0.97	0.11	22,32,33,39	0
4	DMS	B	8412	4/4	0.98	0.09	30,34,36,39	0
4	DMS	A	8412	4/4	0.98	0.17	36,38,42,100	0
4	DMS	C	8402	4/4	0.98	0.06	17,23,24,31	0
4	DMS	C	8405	4/4	0.98	0.08	24,25,29,31	0
4	DMS	B	8414	4/4	0.98	0.08	27,47,76,100	0
4	DMS	C	8408	4/4	0.98	0.07	22,37,40,56	0
4	DMS	A	8504	4/4	0.98	0.08	22,36,37,86	0
4	DMS	C	8410	4/4	0.98	0.09	28,35,36,37	0
4	DMS	C	8412	4/4	0.98	0.12	35,36,37,100	0
4	DMS	D	8408	4/4	0.98	0.08	19,33,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	D	3103	1/1	0.98	0.05	32,32,32,32	0
4	DMS	D	8411	4/4	0.98	0.07	22,31,32,68	0
4	DMS	D	8413	4/4	0.98	0.14	30,36,38,54	0
4	DMS	C	8414	4/4	0.98	0.08	24,32,43,49	0
4	DMS	B	8404	4/4	0.98	0.06	22,25,35,36	0
4	DMS	D	8421	4/4	0.98	0.10	37,51,76,100	0
4	DMS	B	8405	4/4	0.98	0.10	31,31,31,32	0
4	DMS	B	8421	4/4	0.98	0.12	31,47,52,60	0
4	DMS	A	8402	4/4	0.98	0.07	17,20,25,36	0
4	DMS	A	8408	4/4	0.98	0.07	17,37,38,49	0
4	DMS	A	8404	4/4	0.98	0.08	21,28,33,33	0
4	DMS	B	8502	4/4	0.98	0.09	25,29,39,41	0
4	DMS	D	8701	4/4	0.98	0.09	15,16,21,37	0
4	DMS	A	8410	4/4	0.98	0.10	22,33,34,41	0
4	DMS	B	8410	4/4	0.98	0.12	25,33,36,40	0
4	DMS	A	8411	4/4	0.99	0.08	29,31,35,52	0
3	NA	C	3102	1/1	0.99	0.04	18,18,18,18	0
3	NA	C	3103	1/1	0.99	0.06	29,29,29,29	0
4	DMS	C	8403	4/4	0.99	0.07	22,23,24,27	0
4	DMS	C	8404	4/4	0.99	0.06	20,21,26,29	0
4	DMS	D	8401	4/4	0.99	0.06	15,17,18,21	0
4	DMS	D	8402	4/4	0.99	0.05	18,22,23,24	0
4	DMS	D	8403	4/4	0.99	0.06	18,28,29,32	0
2	MG	A	3002	1/1	0.99	0.04	17,17,17,17	0
4	DMS	D	8405	4/4	0.99	0.08	24,25,36,37	0
3	NA	D	3102	1/1	0.99	0.06	15,15,15,15	0
2	MG	D	3001	1/1	0.99	0.03	15,15,15,15	0
4	DMS	B	8411	4/4	0.99	0.06	22,28,29,87	0
2	MG	D	3002	1/1	0.99	0.07	17,17,17,17	0
4	DMS	D	8410	4/4	0.99	0.08	27,34,35,37	0
4	DMS	C	8411	4/4	0.99	0.12	23,29,30,46	0
4	DMS	D	8412	4/4	0.99	0.09	23,29,32,40	0
4	DMS	A	8401	4/4	0.99	0.06	13,13,15,18	0
4	DMS	D	8414	4/4	0.99	0.13	25,42,96,100	0
2	MG	C	3002	1/1	0.99	0.06	17,17,17,17	0
4	DMS	A	8403	4/4	0.99	0.07	23,24,24,26	0
3	NA	A	3103	1/1	0.99	0.04	28,28,28,28	0
4	DMS	A	8405	4/4	0.99	0.08	20,26,29,49	0
2	MG	B	3002	1/1	0.99	0.04	18,18,18,18	0
3	NA	B	3101	1/1	0.99	0.04	17,17,17,17	0
3	NA	B	3103	1/1	0.99	0.04	26,26,26,26	0
2	MG	C	3006	1/1	0.99	0.14	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	B	8401	4/4	0.99	0.08	17,21,21,22	0
4	DMS	B	8402	4/4	0.99	0.06	15,19,22,24	0
4	DMS	B	8403	4/4	0.99	0.10	16,22,27,27	0
3	NA	C	3101	1/1	0.99	0.05	15,15,15,15	0
3	NA	B	3102	1/1	1.00	0.03	15,15,15,15	0
3	NA	D	3101	1/1	1.00	0.05	19,19,19,19	0
4	DMS	C	8401	4/4	1.00	0.05	15,18,21,25	0
3	NA	A	3101	1/1	1.00	0.04	19,19,19,19	0
3	NA	A	3102	1/1	1.00	0.05	14,14,14,14	0
2	MG	B	3001	1/1	1.00	0.03	14,14,14,14	0
2	MG	C	3001	1/1	1.00	0.02	15,15,15,15	0
2	MG	A	3001	1/1	1.00	0.04	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.