



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:02 pm GMT

PDB ID : 1PX4  
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (G794A) WITH IPTG BOUND  
Authors : Juers, D.H.; Hakda, S.; Matthews, B.W.; Huber, R.E.  
Deposited on : 2003-07-02  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk28620

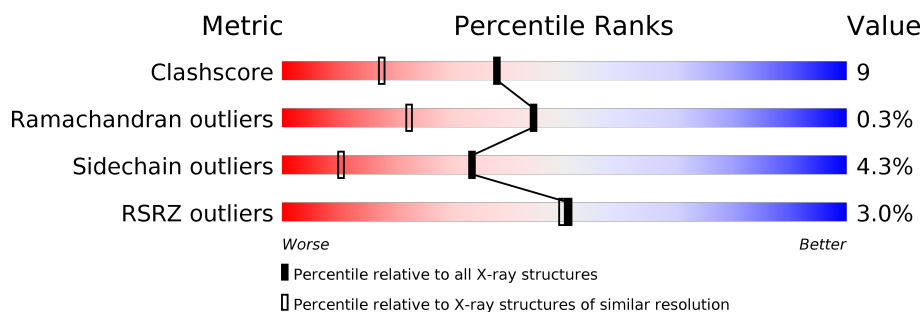
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	1023	<div> <div>3%</div> <div>71%</div> <div>23%</div> <div>5%</div> </div>
1	B	1023	<div> <div>3%</div> <div>71%</div> <div>24%</div> <div>•</div> </div>
1	C	1023	<div> <div>2%</div> <div>68%</div> <div>25%</div> <div>5%</div> <div>••</div> </div>
1	D	1023	<div> <div>4%</div> <div>70%</div> <div>23%</div> <div>5%</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
3	NA	A	3103	-	-	-	X
3	NA	B	3101	-	-	-	X
3	NA	B	3104	-	-	-	X
3	NA	C	3104	-	-	-	X
3	NA	D	3104	-	-	-	X
5	DMS	A	8404	-	-	X	X
5	DMS	A	8405	-	-	-	X
5	DMS	A	8406	-	-	-	X
5	DMS	A	8407	-	-	-	X
5	DMS	A	8411	-	-	-	X
5	DMS	A	8412	-	-	-	X
5	DMS	A	8416	-	-	X	X
5	DMS	A	8417	-	-	-	X
5	DMS	A	8420	-	-	-	X
5	DMS	A	8502	-	-	-	X
5	DMS	A	8504	-	-	-	X
5	DMS	B	8417	-	-	-	X
5	DMS	B	8425	-	-	-	X
5	DMS	B	8502	-	-	-	X
5	DMS	B	8506	-	-	X	X
5	DMS	B	8508	-	-	-	X
5	DMS	C	8404	-	-	-	X
5	DMS	C	8407	-	-	-	X
5	DMS	C	8411	-	-	-	X
5	DMS	C	8412	-	-	-	X
5	DMS	C	8417	-	-	-	X
5	DMS	C	8420	-	-	-	X
5	DMS	C	8423	-	-	-	X
5	DMS	C	8425	-	-	-	X
5	DMS	C	8501	-	-	-	X
5	DMS	C	8506	-	-	X	-
5	DMS	D	8404	-	-	-	X
5	DMS	D	8405	-	-	-	X
5	DMS	D	8417	-	-	-	X
5	DMS	D	8501	-	-	-	X
5	DMS	D	8506	-	-	X	-
5	DMS	D	8508	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36785 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
			8126	5139	1440	1509	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P00722
A	2	SER	-	CLONING ARTIFACT	UNP P00722
A	3	HIS	-	CLONING ARTIFACT	UNP P00722
A	4	MET	-	CLONING ARTIFACT	UNP P00722
A	5	LEU	-	CLONING ARTIFACT	UNP P00722
A	6	GLU	-	CLONING ARTIFACT	UNP P00722
A	7	ASP	-	CLONING ARTIFACT	UNP P00722
A	8	PRO	-	CLONING ARTIFACT	UNP P00722
A	794	ALA	GLY	ENGINEERED	UNP P00722
B	1	GLY	-	CLONING ARTIFACT	UNP P00722
B	2	SER	-	CLONING ARTIFACT	UNP P00722
B	3	HIS	-	CLONING ARTIFACT	UNP P00722
B	4	MET	-	CLONING ARTIFACT	UNP P00722
B	5	LEU	-	CLONING ARTIFACT	UNP P00722
B	6	GLU	-	CLONING ARTIFACT	UNP P00722
B	7	ASP	-	CLONING ARTIFACT	UNP P00722
B	8	PRO	-	CLONING ARTIFACT	UNP P00722
B	794	ALA	GLY	ENGINEERED	UNP P00722
C	1	GLY	-	CLONING ARTIFACT	UNP P00722
C	2	SER	-	CLONING ARTIFACT	UNP P00722
C	3	HIS	-	CLONING ARTIFACT	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	CLONING ARTIFACT	UNP P00722
C	5	LEU	-	CLONING ARTIFACT	UNP P00722
C	6	GLU	-	CLONING ARTIFACT	UNP P00722
C	7	ASP	-	CLONING ARTIFACT	UNP P00722
C	8	PRO	-	CLONING ARTIFACT	UNP P00722
C	794	ALA	GLY	ENGINEERED	UNP P00722
D	1	GLY	-	CLONING ARTIFACT	UNP P00722
D	2	SER	-	CLONING ARTIFACT	UNP P00722
D	3	HIS	-	CLONING ARTIFACT	UNP P00722
D	4	MET	-	CLONING ARTIFACT	UNP P00722
D	5	LEU	-	CLONING ARTIFACT	UNP P00722
D	6	GLU	-	CLONING ARTIFACT	UNP P00722
D	7	ASP	-	CLONING ARTIFACT	UNP P00722
D	8	PRO	-	CLONING ARTIFACT	UNP P00722
D	794	ALA	GLY	ENGINEERED	UNP P00722

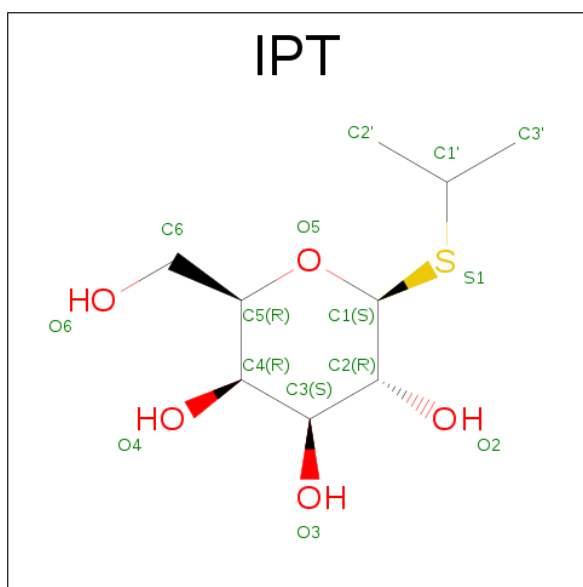
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	4	Total Mg 4 4	0	0
2	D	4	Total Mg 4 4	0	0
2	C	5	Total Mg 5 5	0	0

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

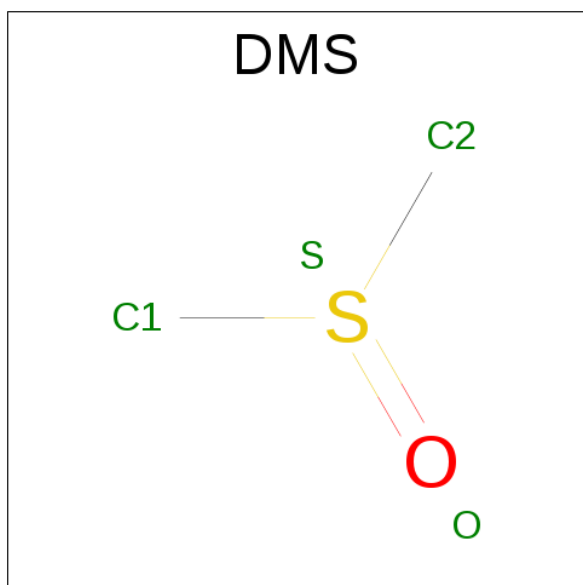
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Na 4 4	0	0
3	A	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0

- Molecule 4 is ISOPROPYL-1-BETA-D-THIOGALACTOSIDE (three-letter code: IPT) (formula: C<sub>9</sub>H<sub>18</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			15	9	5	1		
4	B	1	Total	C	O	S	0	0
			15	9	5	1		
4	C	1	Total	C	O	S	0	0
			15	9	5	1		
4	D	1	Total	C	O	S	0	0
			15	9	5	1		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

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

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

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

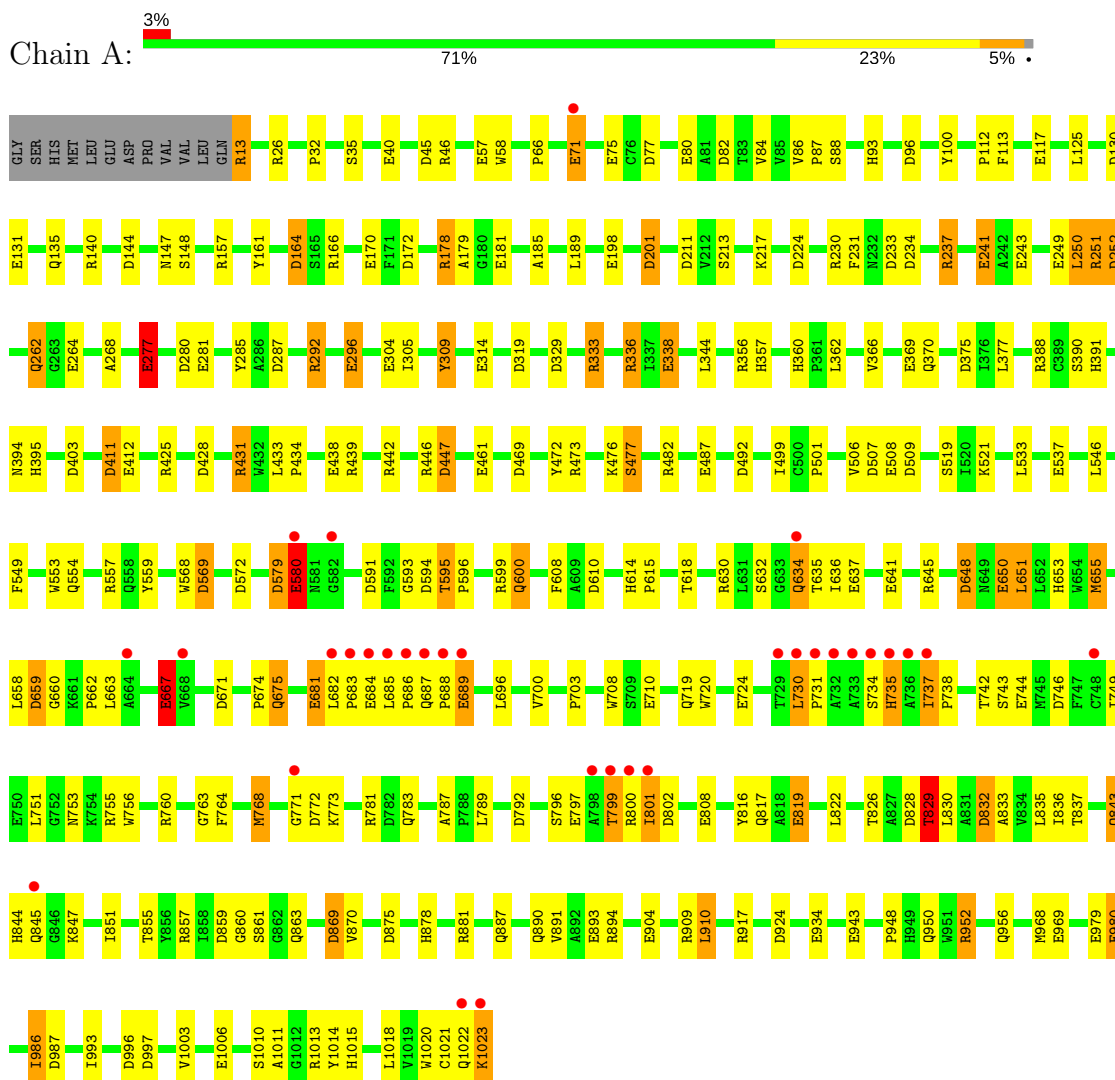
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	950	Total O 950 950	0	0
6	B	971	Total O 971 971	0	0
6	C	943	Total O 943 943	0	0
6	D	949	Total O 949 949	0	0

### 3 Residue-property plots

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

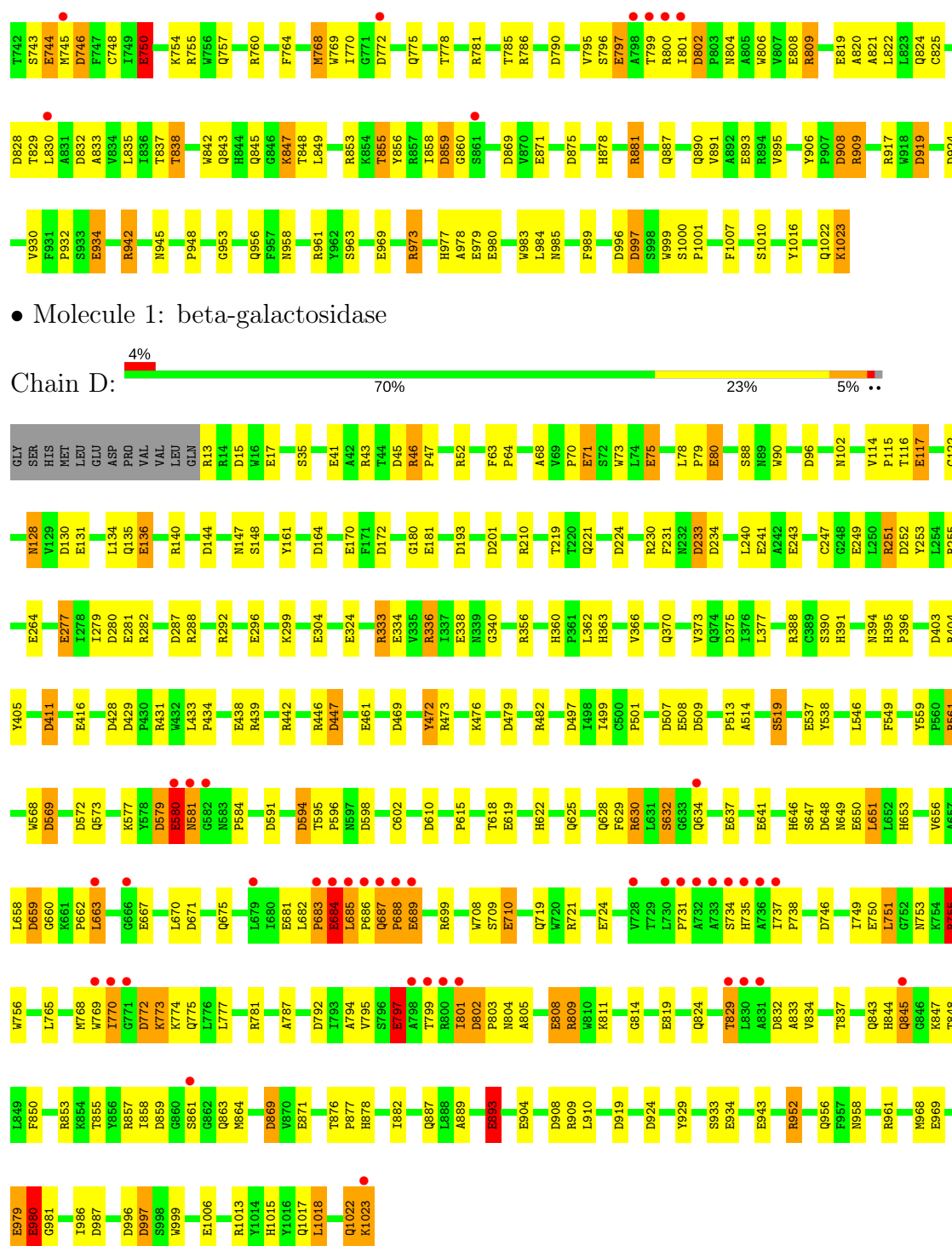
- Molecule 1: beta-galactosidase



- Molecule 1: beta-galactosidase







• Molecule 1: beta-galactosidase

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.49Å 168.29Å 200.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 1.60 31.50 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (31.50-1.60) 90.8 (31.50-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 1.60Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.187 , 0.239 0.200 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 82.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	36785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 36.39 % 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 5.0375e-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, MG, DMS, IPT

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	1.09	48/8368 (0.6%)	1.61	153/11417 (1.3%)
1	B	1.11	49/8368 (0.6%)	1.63	154/11417 (1.3%)
1	C	1.10	46/8368 (0.5%)	1.61	155/11417 (1.4%)
1	D	1.12	48/8368 (0.6%)	1.64	170/11417 (1.5%)
All	All	1.10	191/33472 (0.6%)	1.62	632/45668 (1.4%)

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	B	1	0

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	537	GLU	CD-OE2	9.16	1.35	1.25
1	C	304	GLU	CD-OE2	8.84	1.35	1.25
1	C	281	GLU	CD-OE2	8.69	1.35	1.25
1	D	281	GLU	CD-OE2	8.64	1.35	1.25
1	D	893	GLU	CD-OE2	8.64	1.35	1.25
1	C	819	GLU	CD-OE2	8.58	1.35	1.25
1	C	296	GLU	CD-OE2	8.50	1.35	1.25
1	D	80	GLU	CD-OE2	8.40	1.34	1.25
1	D	650	GLU	CD-OE2	8.34	1.34	1.25
1	C	934	GLU	CD-OE2	8.27	1.34	1.25
1	D	296	GLU	CD-OE2	8.18	1.34	1.25
1	C	529	GLU	CD-OE2	8.14	1.34	1.25
1	B	243	GLU	CD-OE2	8.13	1.34	1.25
1	C	619	GLU	CD-OE2	8.13	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	GLU	CD-OE2	7.91	1.34	1.25
1	B	684	GLU	CD-OE2	7.84	1.34	1.25
1	A	296	GLU	CD-OE2	7.70	1.34	1.25
1	A	487	GLU	CD-OE2	7.66	1.34	1.25
1	C	71	GLU	CD-OE2	7.57	1.33	1.25
1	A	281	GLU	CD-OE2	7.57	1.33	1.25
1	D	136	GLU	CD-OE2	7.54	1.33	1.25
1	C	75	GLU	CD-OE2	7.49	1.33	1.25
1	C	684	GLU	CD-OE2	7.48	1.33	1.25
1	D	277	GLU	CD-OE2	7.48	1.33	1.25
1	D	243	GLU	CD-OE2	7.38	1.33	1.25
1	C	641	GLU	CD-OE1	-7.34	1.17	1.25
1	A	537	GLU	CD-OE2	7.34	1.33	1.25
1	C	131	GLU	CD-OE2	7.33	1.33	1.25
1	C	80	GLU	CD-OE2	7.31	1.33	1.25
1	D	1006	GLU	CD-OE2	7.30	1.33	1.25
1	D	17	GLU	CD-OE2	7.28	1.33	1.25
1	C	264	GLU	CD-OE2	7.25	1.33	1.25
1	D	979	GLU	CD-OE2	7.24	1.33	1.25
1	A	1006	GLU	CD-OE2	7.22	1.33	1.25
1	A	170	GLU	CD-OE2	7.16	1.33	1.25
1	D	241	GLU	CD-OE2	7.15	1.33	1.25
1	A	412	GLU	CD-OE2	7.14	1.33	1.25
1	B	650	GLU	CD-OE2	7.13	1.33	1.25
1	D	324	GLU	CD-OE2	7.12	1.33	1.25
1	A	80	GLU	CD-OE2	7.10	1.33	1.25
1	A	241	GLU	CD-OE2	7.08	1.33	1.25
1	B	416	GLU	CD-OE2	7.07	1.33	1.25
1	A	934	GLU	CD-OE2	7.06	1.33	1.25
1	A	980	GLU	CD-OE2	7.03	1.33	1.25
1	B	296	GLU	CD-OE2	7.03	1.33	1.25
1	B	461	GLU	CD-OE2	6.97	1.33	1.25
1	B	641	GLU	CD-OE1	-6.95	1.18	1.25
1	B	281	GLU	CD-OE2	6.92	1.33	1.25
1	A	689	GLU	CD-OE2	6.87	1.33	1.25
1	B	744	GLU	CD-OE2	6.87	1.33	1.25
1	C	893	GLU	CD-OE2	6.84	1.33	1.25
1	B	980	GLU	CD-OE2	6.83	1.33	1.25
1	D	750	GLU	CD-OE2	6.83	1.33	1.25
1	A	243	GLU	CD-OE2	6.82	1.33	1.25
1	B	580	GLU	CD-OE2	6.82	1.33	1.25
1	D	819	GLU	CD-OE2	6.80	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	580	GLU	CD-OE2	6.79	1.33	1.25
1	A	249	GLU	CD-OE2	6.75	1.33	1.25
1	B	689	GLU	CD-OE2	6.74	1.33	1.25
1	D	461	GLU	CD-OE2	6.74	1.33	1.25
1	D	41	GLU	CD-OE2	6.72	1.33	1.25
1	C	181	GLU	CD-OE2	6.67	1.32	1.25
1	C	980	GLU	CD-OE2	6.64	1.32	1.25
1	A	304	GLU	CD-OE2	6.62	1.32	1.25
1	C	241	GLU	CD-OE2	6.58	1.32	1.25
1	C	969	GLU	CD-OE2	6.58	1.32	1.25
1	A	131	GLU	CD-OE2	6.56	1.32	1.25
1	C	744	GLU	CD-OE2	6.56	1.32	1.25
1	B	681	GLU	CD-OE2	6.55	1.32	1.25
1	C	681	GLU	CD-OE2	6.54	1.32	1.25
1	D	249	GLU	CD-OE2	6.53	1.32	1.25
1	C	136	GLU	CD-OE2	6.51	1.32	1.25
1	C	689	GLU	CD-OE2	6.51	1.32	1.25
1	B	819	GLU	CD-OE2	6.50	1.32	1.25
1	C	650	GLU	CD-OE2	6.49	1.32	1.25
1	D	681	GLU	CD-OE2	6.47	1.32	1.25
1	B	326	GLU	CD-OE2	6.47	1.32	1.25
1	A	744	GLU	CD-OE2	6.45	1.32	1.25
1	A	277	GLU	CD-OE2	6.41	1.32	1.25
1	D	264	GLU	CD-OE2	6.41	1.32	1.25
1	D	684	GLU	CD-OE2	6.40	1.32	1.25
1	D	667	GLU	CD-OE2	6.39	1.32	1.25
1	A	684	GLU	CD-OE2	6.38	1.32	1.25
1	A	710	GLU	CD-OE2	6.37	1.32	1.25
1	D	724	GLU	CD-OE2	6.36	1.32	1.25
1	A	969	GLU	CD-OE2	6.36	1.32	1.25
1	B	314	GLU	CD-OE1	-6.34	1.18	1.25
1	B	619	GLU	CD-OE2	6.31	1.32	1.25
1	D	338	GLU	CD-OE2	6.27	1.32	1.25
1	B	41	GLU	CD-OE2	6.26	1.32	1.25
1	D	689	GLU	CD-OE1	-6.26	1.18	1.25
1	B	529	GLU	CD-OE2	6.22	1.32	1.25
1	A	117	GLU	CD-OE2	6.20	1.32	1.25
1	B	324	GLU	CD-OE2	6.20	1.32	1.25
1	C	750	GLU	CD-OE2	6.19	1.32	1.25
1	B	277	GLU	CD-OE2	6.18	1.32	1.25
1	C	324	GLU	CD-OE2	6.13	1.32	1.25
1	D	75	GLU	CD-OE2	6.12	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	GLU	CD-OE2	6.12	1.32	1.25
1	B	264	GLU	CD-OE2	6.11	1.32	1.25
1	C	797	GLU	CD-OE2	6.11	1.32	1.25
1	C	249	GLU	CD-OE2	6.11	1.32	1.25
1	B	75	GLU	CD-OE2	6.10	1.32	1.25
1	C	314	GLU	CD-OE1	-6.09	1.19	1.25
1	D	181	GLU	CD-OE2	6.06	1.32	1.25
1	B	181	GLU	CD-OE2	6.06	1.32	1.25
1	A	40	GLU	CD-OE2	6.04	1.32	1.25
1	D	943	GLU	CD-OE2	6.04	1.32	1.25
1	A	681	GLU	CD-OE2	6.00	1.32	1.25
1	A	71	GLU	CD-OE2	6.00	1.32	1.25
1	B	979	GLU	CD-OE2	5.97	1.32	1.25
1	B	136	GLU	CD-OE2	5.96	1.32	1.25
1	A	314	GLU	CD-OE1	-5.95	1.19	1.25
1	C	667	GLU	CD-OE2	5.95	1.32	1.25
1	B	241	GLU	CD-OE2	5.95	1.32	1.25
1	D	980	GLU	CD-OE2	5.95	1.32	1.25
1	D	637	GLU	CD-OE2	5.91	1.32	1.25
1	B	667	GLU	CD-OE2	5.91	1.32	1.25
1	B	198	GLU	CD-OE2	5.88	1.32	1.25
1	C	314	GLU	CD-OE2	5.85	1.32	1.25
1	C	710	GLU	CD-OE2	5.84	1.32	1.25
1	B	131	GLU	CD-OE2	5.83	1.32	1.25
1	A	979	GLU	CD-OE2	5.82	1.32	1.25
1	B	871	GLU	CD-OE2	5.81	1.32	1.25
1	D	170	GLU	CD-OE2	5.81	1.32	1.25
1	D	969	GLU	CD-OE2	5.80	1.32	1.25
1	C	416	GLU	CD-OE2	5.76	1.31	1.25
1	A	57	GLU	CD-OE2	5.76	1.31	1.25
1	A	893	GLU	CD-OE2	5.73	1.31	1.25
1	D	619	GLU	CD-OE2	5.72	1.31	1.25
1	B	724	GLU	CD-OE2	5.68	1.31	1.25
1	B	710	GLU	CD-OE2	5.67	1.31	1.25
1	B	249	GLU	CD-OE2	5.67	1.31	1.25
1	C	198	GLU	CD-OE2	5.66	1.31	1.25
1	A	181	GLU	CD-OE2	5.66	1.31	1.25
1	C	338	GLU	CD-OE2	5.66	1.31	1.25
1	B	750	GLU	CD-OE2	5.65	1.31	1.25
1	D	710	GLU	CD-OE2	5.64	1.31	1.25
1	C	41	GLU	CD-OE2	5.64	1.31	1.25
1	A	724	GLU	CD-OE2	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	GLU	CD-OE1	-5.62	1.19	1.25
1	B	487	GLU	CD-OE2	5.62	1.31	1.25
1	A	904	GLU	CD-OE2	5.60	1.31	1.25
1	C	979	GLU	CD-OE2	5.60	1.31	1.25
1	C	243	GLU	CD-OE2	5.59	1.31	1.25
1	B	508	GLU	CD-OE2	5.57	1.31	1.25
1	D	117	GLU	CD-OE2	5.57	1.31	1.25
1	A	650	GLU	CD-OE2	5.56	1.31	1.25
1	D	808	GLU	CD-OE2	5.56	1.31	1.25
1	A	943	GLU	CD-OE2	5.55	1.31	1.25
1	B	438	GLU	CD-OE2	5.50	1.31	1.25
1	A	264	GLU	CD-OE2	5.49	1.31	1.25
1	D	438	GLU	CD-OE2	5.47	1.31	1.25
1	D	797	GLU	CD-OE2	5.47	1.31	1.25
1	A	637	GLU	CD-OE2	5.46	1.31	1.25
1	A	75	GLU	CD-OE2	5.46	1.31	1.25
1	C	117	GLU	CD-OE2	5.45	1.31	1.25
1	A	641	GLU	CD-OE1	-5.45	1.19	1.25
1	D	71	GLU	CD-OE2	5.40	1.31	1.25
1	B	893	GLU	CD-OE2	5.37	1.31	1.25
1	D	131	GLU	CD-OE2	5.37	1.31	1.25
1	A	819	GLU	CD-OE2	5.35	1.31	1.25
1	A	580	GLU	CD-OE2	5.34	1.31	1.25
1	C	326	GLU	CD-OE2	5.34	1.31	1.25
1	D	904	GLU	CD-OE2	5.29	1.31	1.25
1	A	667	GLU	CD-OE2	5.29	1.31	1.25
1	B	17	GLU	CD-OE2	5.29	1.31	1.25
1	B	170	GLU	CD-OE2	5.28	1.31	1.25
1	D	580	GLU	CD-OE2	5.28	1.31	1.25
1	D	508	GLU	CD-OE2	5.27	1.31	1.25
1	A	338	GLU	CD-OE2	5.26	1.31	1.25
1	D	304	GLU	CD-OE1	-5.24	1.19	1.25
1	A	461	GLU	CD-OE2	5.24	1.31	1.25
1	B	1006	GLU	CD-OE2	5.22	1.31	1.25
1	D	416	GLU	CD-OE1	-5.21	1.20	1.25
1	D	689	GLU	CD-OE2	5.20	1.31	1.25
1	C	461	GLU	CD-OE2	5.19	1.31	1.25
1	B	304	GLU	CD-OE2	5.18	1.31	1.25
1	A	909	ARG	NE-CZ	5.18	1.39	1.33
1	B	461	GLU	CD-OE1	-5.17	1.20	1.25
1	A	296	GLU	CD-OE1	-5.16	1.20	1.25
1	A	198	GLU	CD-OE2	5.15	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	GLU	CD-OE2	5.14	1.31	1.25
1	D	641	GLU	CD-OE1	-5.13	1.20	1.25
1	A	369	GLU	CD-OE2	5.12	1.31	1.25
1	C	724	GLU	CD-OE2	5.11	1.31	1.25
1	B	338	GLU	CD-OE2	5.08	1.31	1.25
1	C	17	GLU	CD-OE2	5.07	1.31	1.25
1	C	537	GLU	CD-OE2	5.06	1.31	1.25
1	A	508	GLU	CD-OE2	5.06	1.31	1.25
1	B	969	GLU	CD-OE2	5.02	1.31	1.25

All (632) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	809	ARG	NE-CZ-NH1	21.02	130.81	120.30
1	B	809	ARG	NE-CZ-NH2	-17.60	111.50	120.30
1	D	473	ARG	NE-CZ-NH1	14.07	127.33	120.30
1	C	699	ARG	NE-CZ-NH1	13.78	127.19	120.30
1	B	356	ARG	NE-CZ-NH1	13.66	127.13	120.30
1	D	473	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	D	431	ARG	NE-CZ-NH2	-12.89	113.86	120.30
1	A	166	ARG	NE-CZ-NH2	-12.57	114.01	120.30
1	C	178	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	A	178	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	B	388	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	B	881	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	D	431	ARG	NE-CZ-NH1	11.71	126.16	120.30
1	D	13	ARG	NE-CZ-NH2	-11.65	114.48	120.30
1	B	961	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	B	781	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	B	772	ASP	CB-CG-OD2	-11.30	108.13	118.30
1	C	43	ARG	NE-CZ-NH1	11.29	125.95	120.30
1	D	996	ASP	CB-CG-OD1	11.22	128.40	118.30
1	D	429	ASP	CB-CG-OD2	-11.18	108.24	118.30
1	C	428	ASP	CB-CG-OD1	10.86	128.07	118.30
1	D	15	ASP	CB-CG-OD2	-10.77	108.61	118.30
1	A	431	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	C	482	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	D	13	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	C	809	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	46	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	A	755	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	D	172	ASP	CB-CG-OD2	-10.65	108.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	ARG	NE-CZ-NH2	-10.61	114.99	120.30
1	B	557	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	B	166	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	D	439	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	B	288	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	A	388	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	D	781	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	C	442	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	C	233	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	C	431	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	D	594	ASP	CB-CG-OD2	-9.98	109.31	118.30
1	A	997	ASP	CB-CG-OD2	-9.98	109.32	118.30
1	C	917	ARG	NE-CZ-NH1	-9.95	115.32	120.30
1	D	429	ASP	CB-CG-OD1	9.94	127.24	118.30
1	D	388	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	C	996	ASP	CB-CG-OD1	9.66	127.00	118.30
1	A	336	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	C	46	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	D	442	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	D	446	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	D	45	ASP	CB-CG-OD1	9.52	126.87	118.30
1	C	204	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	A	411	ASP	CB-CG-OD2	-9.45	109.80	118.30
1	A	997	ASP	CB-CG-OD1	9.43	126.78	118.30
1	D	659	ASP	CB-CG-OD2	-9.42	109.83	118.30
1	C	333	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	C	482	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	A	224	ASP	CB-CG-OD1	9.30	126.67	118.30
1	C	881	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	D	594	ASP	CB-CG-OD1	9.28	126.65	118.30
1	B	786	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	C	368	ASP	CB-CG-OD2	-9.13	110.08	118.30
1	B	368	ASP	CB-CG-OD1	9.13	126.52	118.30
1	D	561	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	B	46	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	894	ARG	NE-CZ-NH1	-9.07	115.77	120.30
1	B	1018	LEU	CB-CA-C	-9.06	92.98	110.20
1	D	919	ASP	CB-CG-OD2	-9.06	110.15	118.30
1	B	561	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	B	859	ASP	CB-CG-OD2	-9.05	110.16	118.30
1	A	96	ASP	CB-CG-OD1	9.04	126.44	118.30
1	B	13	ARG	NE-CZ-NH2	-9.04	115.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	828	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	A	233	ASP	CB-CG-OD1	9.02	126.41	118.30
1	A	425	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	252	ASP	CB-CG-OD2	-8.95	110.25	118.30
1	D	746	ASP	CB-CG-OD2	-8.92	110.27	118.30
1	D	996	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	D	1013	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	C	368	ASP	CB-CG-OD1	8.89	126.30	118.30
1	B	760	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	610	ASP	CB-CG-OD1	8.85	126.27	118.30
1	B	875	ASP	CB-CG-OD1	8.85	126.26	118.30
1	D	428	ASP	CB-CG-OD1	8.85	126.26	118.30
1	C	230	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	C	492	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	D	632	SER	N-CA-CB	8.81	123.72	110.50
1	A	800	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	C	594	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	B	569	ASP	CB-CG-OD1	8.74	126.16	118.30
1	D	579	ASP	CB-CG-OD1	8.70	126.13	118.30
1	C	730	LEU	C-N-CD	-8.68	101.50	120.60
1	A	439	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	648	ASP	CB-CG-OD1	8.65	126.08	118.30
1	B	96	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	D	579	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	A	411	ASP	CB-CG-OD1	8.56	126.01	118.30
1	B	594	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	B	287	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	A	292	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	C	869	ASP	CB-CG-OD1	8.51	125.96	118.30
1	B	557	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	D	469	ASP	CB-CG-OD1	8.48	125.93	118.30
1	B	492	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	D	687	GLN	C-N-CD	-8.44	102.04	120.60
1	B	832	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	B	287	ASP	CB-CG-OD1	8.40	125.86	118.30
1	C	224	ASP	CB-CG-OD1	8.40	125.86	118.30
1	B	594	ASP	CB-CG-OD1	8.39	125.85	118.30
1	B	178	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	431	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	C	178	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	233	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	A	917	ARG	NE-CZ-NH1	-8.33	116.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	859	ASP	CB-CG-OD2	-8.33	110.81	118.30
1	A	579	ASP	CB-CG-OD1	8.32	125.79	118.30
1	B	469	ASP	CB-CG-OD1	8.32	125.79	118.30
1	D	591	ASP	CB-CG-OD1	8.31	125.78	118.30
1	D	987	ASP	CB-CG-OD1	8.31	125.78	118.30
1	B	648	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	D	144	ASP	CB-CG-OD1	8.25	125.72	118.30
1	C	561	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	D	224	ASP	CB-CG-OD1	8.20	125.68	118.30
1	B	428	ASP	CB-CG-OD1	8.19	125.67	118.30
1	D	469	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	D	172	ASP	CB-CG-OD1	8.17	125.65	118.30
1	C	997	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	996	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	B	224	ASP	CB-CG-OD1	8.15	125.64	118.30
1	A	251	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	D	233	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	A	909	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	572	ASP	CB-CG-OD2	-8.14	110.98	118.30
1	C	288	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	D	15	ASP	CB-CG-OD1	8.13	125.62	118.30
1	D	859	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	A	46	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	45	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	A	579	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	828	ASP	CB-CG-OD1	8.09	125.58	118.30
1	B	809	ARG	CD-NE-CZ	8.08	134.91	123.60
1	B	368	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	D	859	ASP	CB-CG-OD1	8.06	125.56	118.30
1	D	411	ASP	CB-CG-OD1	8.05	125.54	118.30
1	D	442	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	D	130	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	A	442	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	429	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	B	190	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	973	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	B	859	ASP	CB-CG-OD1	7.99	125.49	118.30
1	A	996	ASP	CB-CG-OD1	7.98	125.48	118.30
1	D	659	ASP	CB-CG-OD1	7.97	125.47	118.30
1	B	746	ASP	CB-CG-OD2	-7.96	111.13	118.30
1	D	403	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	894	ARG	NE-CZ-NH2	7.95	124.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	507	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	439	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	C	15	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	C	204	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	D	572	ASP	CB-CG-OD2	-7.87	111.21	118.30
1	B	973	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	A	610	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	C	802	ASP	CB-CG-OD1	7.80	125.32	118.30
1	C	579	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	C	859	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	B	233	ASP	CB-CG-OD1	7.75	125.27	118.30
1	A	829	THR	CA-CB-CG2	7.75	123.24	112.40
1	B	280	ASP	CB-CG-OD2	-7.74	111.33	118.30
1	A	230	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	C	685	LEU	N-CA-CB	7.73	125.87	110.40
1	A	96	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	B	792	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	A	130	ASP	CB-CG-OD2	-7.73	111.35	118.30
1	B	569	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	B	388	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	C	961	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	D	997	ASP	N-CA-CB	7.71	124.48	110.60
1	A	185	ALA	N-CA-CB	7.70	120.88	110.10
1	B	233	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	594	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	469	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	C	996	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	C	856	TYR	CB-CG-CD2	-7.64	116.42	121.00
1	D	997	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	C	77	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	699	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	557	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	13	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	919	ASP	CB-CG-OD2	-7.57	111.48	118.30
1	B	802	ASP	CB-CG-OD1	7.56	125.10	118.30
1	D	356	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	C	77	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	509	ASP	CB-CG-OD1	7.53	125.08	118.30
1	B	425	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	D	869	ASP	CB-CG-OD1	7.53	125.07	118.30
1	A	630	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	45	ASP	CB-CG-OD1	7.51	125.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	C	735	HIS	CA-CB-CG	7.50	126.35	113.60
1	A	802	ASP	CB-CG-OD1	7.48	125.03	118.30
1	C	234	ASP	CB-CG-OD1	7.46	125.02	118.30
1	B	329	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	D	610	ASP	CB-CG-OD1	7.46	125.02	118.30
1	D	648	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	B	319	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	B	319	ASP	CB-CG-OD1	7.44	124.99	118.30
1	B	178	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	B	469	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	C	699	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	B	579	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	772	ASP	CB-CG-OD1	7.40	124.96	118.30
1	B	411	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	C	439	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	C	329	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	A	13	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	15	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	B	869	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	482	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	746	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	D	997	ASP	CB-CG-OD1	7.24	124.82	118.30
1	B	473	ARG	CD-NE-CZ	7.24	133.73	123.60
1	D	507	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C	183	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	144	ASP	CB-CG-OD1	7.20	124.78	118.30
1	B	579	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	287	ASP	CB-CG-OD1	7.18	124.76	118.30
1	C	958	ASN	N-CA-CB	7.17	123.50	110.60
1	D	287	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	987	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	140	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	D	509	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	632	SER	N-CA-CB	7.13	121.20	110.50
1	D	416	GLU	CG-CD-OE1	7.13	132.57	118.30
1	A	924	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	D	439	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	909	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	178	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	B	721	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	C	909	ARG	NE-CZ-NH1	7.09	123.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	D	855	THR	N-CA-CB	7.07	123.74	110.30
1	D	1013	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	287	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	987	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	569	ASP	CB-CG-OD1	7.04	124.63	118.30
1	A	924	ASP	CB-CG-OD1	7.03	124.63	118.30
1	D	538	TYR	CB-CG-CD2	7.02	125.21	121.00
1	A	285	TYR	CD1-CE1-CZ	-7.01	113.49	119.80
1	C	267	VAL	CA-CB-CG2	-7.00	100.40	110.90
1	D	403	ASP	CB-CG-OD1	7.00	124.60	118.30
1	D	404	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	721	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	671	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	B	611	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	1018	LEU	CB-CA-C	-6.98	96.95	110.20
1	D	428	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	C	287	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	D	233	ASP	CB-CG-OD1	6.97	124.57	118.30
1	B	648	ASP	CB-CG-OD1	6.97	124.57	118.30
1	C	917	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	D	447	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	557	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	C	230	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	C	579	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	792	ASP	CB-CG-OD1	6.88	124.49	118.30
1	D	482	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	C	13	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	442	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	45	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	648	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	D	230	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	B	919	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	319	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	D	663	LEU	CB-CA-C	-6.79	97.30	110.20
1	B	172	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	D	919	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	802	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	A	832	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	B	442	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	428	ASP	CB-CG-OD1	6.76	124.38	118.30
1	D	405	TYR	CB-CG-CD1	-6.76	116.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	809	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	790	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	336	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	C	961	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	C	356	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	82	ASP	CB-CG-OD1	6.70	124.33	118.30
1	C	448	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	987	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	234	ASP	CB-CG-OD1	6.69	124.32	118.30
1	C	721	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	610	ASP	CB-CG-OD1	6.67	124.31	118.30
1	D	909	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	B	224	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	559	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	B	429	ASP	CB-CG-OD1	6.65	124.28	118.30
1	D	116	THR	CA-CB-CG2	-6.65	103.09	112.40
1	B	280	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	509	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	C	144	ASP	CB-CG-OD1	6.62	124.26	118.30
1	D	802	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	234	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	610	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	D	45	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	388	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	D	958	ASN	N-CA-CB	6.57	122.42	110.60
1	B	832	ASP	CB-CG-OD1	6.56	124.20	118.30
1	D	746	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	447	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	130	ASP	CB-CG-OD1	6.55	124.20	118.30
1	C	1016	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	B	640	SER	CB-CA-C	-6.54	97.67	110.10
1	B	668	VAL	CB-CA-C	-6.54	98.98	111.40
1	D	667	GLU	CB-CA-C	6.52	123.45	110.40
1	A	594	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	C	252	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	B	15	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	14	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	D	792	ASP	CB-CG-OD1	6.50	124.15	118.30
1	C	557	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	126	THR	CA-CB-CG2	-6.49	103.31	112.40
1	D	671	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	572	ASP	CB-CG-OD1	6.47	124.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	832	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	659	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	310	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	507	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	C	630	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	D	324	GLU	N-CA-CB	6.43	122.17	110.60
1	C	210	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	388	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	85	VAL	CA-CB-CG2	-6.39	101.32	110.90
1	B	598	ASP	CB-CG-OD1	6.38	124.05	118.30
1	C	531	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	96	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	D	772	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	997	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	B	997	ASP	N-CA-CB	6.36	122.05	110.60
1	A	144	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	D	46	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	356	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	909	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	172	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	224	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	507	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	746	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	821	ALA	N-CA-CB	6.29	118.91	110.10
1	D	140	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	869	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	C	645	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	C	869	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	C	917	ARG	CD-NE-CZ	-6.25	114.86	123.60
1	D	43	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	875	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	699	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	929	TYR	CB-CG-CD1	6.22	124.73	121.00
1	A	1013	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	664	ALA	CB-CA-C	-6.22	100.77	110.10
1	B	329	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	996	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	428	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	482	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	288	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	172	ASP	CB-CG-OD1	6.18	123.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	816	TYR	CB-CG-CD2	6.17	124.70	121.00
1	B	630	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	201	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	771	GLY	N-CA-C	-6.15	97.72	113.10
1	C	404	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	D	772	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	997	ASP	N-CA-CB	6.14	121.65	110.60
1	A	442	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	225	PHE	N-CA-CB	6.12	121.62	110.60
1	D	193	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	D	802	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	553	TRP	CA-CB-CG	-6.09	102.13	113.70
1	C	997	ASP	N-CA-CB	6.09	121.56	110.60
1	B	507	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	26	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	A	591	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	996	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	184	LEU	CB-CA-C	-6.06	98.69	110.20
1	C	599	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	832	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	D	908	ASP	CB-CG-OD1	6.06	123.75	118.30
1	D	472	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	C	924	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	C	183	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	26	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	D	909	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	375	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	B	559	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	B	473	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	572	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	958	ASN	N-CA-CB	5.99	121.38	110.60
1	C	201	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	59	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	183	ARG	CD-NE-CZ	-5.98	115.22	123.60
1	B	829	THR	CA-CB-CG2	-5.97	104.04	112.40
1	B	591	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	C	507	ASP	CB-CG-OD1	5.96	123.66	118.30
1	D	333	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	800	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	569	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	D	193	ASP	CB-CG-OD1	5.94	123.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	247	CYS	CA-CB-SG	-5.94	103.31	114.00
1	A	760	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	786	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	329	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	C	43	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	C	730	LEU	CA-CB-CG	-5.90	101.72	115.30
1	B	800	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	594	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	403	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	446	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	721	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	395	HIS	N-CA-CB	-5.89	100.00	110.60
1	D	591	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	233	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	356	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	700	VAL	CA-CB-CG2	-5.88	102.08	110.90
1	D	482	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	230	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	128	ASN	N-CA-CB	5.87	121.17	110.60
1	A	252	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	755	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	D	140	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	431	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	430	PRO	N-CA-CB	5.84	110.31	103.30
1	C	234	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	B	828	ASP	CB-CG-OD1	5.84	123.55	118.30
1	C	741	THR	CA-CB-CG2	-5.82	104.25	112.40
1	A	201	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	746	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	800	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	D	234	ASP	CB-CG-OD1	5.80	123.53	118.30
1	B	598	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	447	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	199	ASP	CB-CG-OD1	5.79	123.51	118.30
1	D	850	PHE	CB-CA-C	-5.78	98.85	110.40
1	B	568	TRP	CA-CB-CG	-5.77	102.73	113.70
1	A	572	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	656	VAL	CA-CB-CG2	-5.74	102.29	110.90
1	A	768	MET	CA-CB-CG	5.74	123.06	113.30
1	C	473	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	772	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	906	TYR	CB-CG-CD2	-5.70	117.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	790	ASP	CB-CG-OD2	-5.69	113.17	118.30
1	D	751	LEU	CB-CA-C	5.69	121.01	110.20
1	B	1014	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	A	211	ASP	CB-CG-OD1	5.68	123.42	118.30
1	B	247	CYS	CA-CB-SG	-5.68	103.77	114.00
1	D	857	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	978	ALA	CB-CA-C	-5.66	101.61	110.10
1	D	280	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	869	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	685	LEU	C-N-CD	-5.65	108.17	120.60
1	D	497	ASP	CB-CG-OD1	5.65	123.38	118.30
1	D	288	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	161	TYR	CB-CG-CD1	-5.64	117.61	121.00
1	C	828	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	796	SER	N-CA-CB	5.64	118.96	110.50
1	C	411	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	201	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	685	LEU	C-N-CD	-5.63	108.21	120.60
1	D	497	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	C	746	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	C	199	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	C	809	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	35	SER	N-CA-CB	5.62	118.93	110.50
1	D	829	THR	N-CA-CB	5.62	120.98	110.30
1	D	980	GLU	C-N-CA	-5.62	110.51	122.30
1	A	344	LEU	CA-CB-CG	-5.60	102.42	115.30
1	B	781	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	875	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	842	TRP	CE2-CD2-CE3	5.59	125.41	118.70
1	A	77	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	329	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	519	SER	N-CA-CB	-5.59	102.12	110.50
1	C	842	TRP	N-CA-CB	5.59	120.66	110.60
1	C	15	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	736	ALA	CB-CA-C	-5.59	101.72	110.10
1	A	249	GLU	CG-CD-OE2	-5.58	107.14	118.30
1	C	856	TYR	CB-CG-CD1	5.58	124.35	121.00
1	A	700	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	C	428	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	908	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	431	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	287	ASP	CB-CG-OD2	-5.56	113.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	838	THR	CA-CB-CG2	-5.56	104.61	112.40
1	D	509	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	832	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	469	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	781	ARG	CD-NE-CZ	5.54	131.35	123.60
1	A	746	ASP	CB-CA-C	-5.53	99.33	110.40
1	C	288	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	375	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	C	630	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	166	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	45	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	497	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	448	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	D	924	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	630	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	729	THR	N-CA-CB	5.46	120.67	110.30
1	C	659	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	926	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	D	598	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	D	279	ILE	CA-CB-CG2	5.44	121.78	110.90
1	B	559	TYR	CB-CG-CD1	5.44	124.26	121.00
1	A	179	ALA	N-CA-CB	5.43	117.70	110.10
1	C	710	GLU	CB-CA-C	-5.42	99.55	110.40
1	D	908	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	917	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	C	113	PHE	CB-CG-CD2	-5.42	117.01	120.80
1	B	431	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	277	GLU	N-CA-CB	-5.41	100.87	110.60
1	D	210	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	D	416	GLU	CG-CD-OE2	-5.40	107.50	118.30
1	D	96	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	809	ARG	CG-CD-NE	5.40	123.14	111.80
1	C	942	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	285	TYR	CB-CG-CD1	5.40	124.24	121.00
1	D	924	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	A	591	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	505	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	610	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	438	GLU	CG-CD-OE2	-5.38	107.55	118.30
1	A	439	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	840	HIS	CB-CA-C	-5.38	99.65	110.40
1	A	403	ASP	CB-CG-OD2	-5.36	113.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	PHE	CB-CA-C	-5.36	99.68	110.40
1	D	396	PRO	N-CA-CB	5.34	109.71	103.30
1	B	234	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	C	919	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	D	336	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	553	TRP	CA-CB-CG	-5.33	103.58	113.70
1	D	130	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	781	ARG	CD-NE-CZ	5.32	131.04	123.60
1	D	882	ILE	CA-CB-CG1	-5.32	100.90	111.00
1	C	310	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	802	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	D	479	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	280	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	100	TYR	CA-CB-CG	-5.30	103.33	113.40
1	A	252	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	942	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	A	833	ALA	N-CA-CB	-5.28	102.70	110.10
1	A	1003	VAL	CA-CB-CG2	-5.28	102.99	110.90
1	B	161	TYR	CG-CD1-CE1	-5.28	117.08	121.30
1	C	319	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	507	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	D	388	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	561	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	719	GLN	CB-CA-C	-5.26	99.87	110.40
1	C	802	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	D	770	ILE	N-CA-C	-5.26	96.81	111.00
1	D	234	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	309	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	D	252	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	D	610	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	161	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	557	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	954	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	549	PHE	CB-CG-CD1	-5.23	117.14	120.80
1	D	251	ARG	CD-NE-CZ	5.23	130.93	123.60
1	A	492	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	C	611	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	611	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	559	TYR	CB-CG-CD2	-5.22	117.86	121.00
1	A	319	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	572	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	569	ASP	CB-CG-OD1	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	719	GLN	CB-CA-C	-5.20	100.00	110.40
1	D	224	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	D	561	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	282	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	962	TYR	CD1-CE1-CZ	-5.16	115.16	119.80
1	C	772	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	392	TYR	CG-CD2-CE2	5.15	125.42	121.30
1	A	599	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	417	THR	CA-CB-CG2	-5.15	105.19	112.40
1	A	333	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	13	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	D	96	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	164	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	721	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	126	THR	CA-CB-CG2	-5.14	105.21	112.40
1	C	136	GLU	CB-CA-C	-5.13	100.13	110.40
1	C	446	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	477	SER	CB-CA-C	-5.13	100.36	110.10
1	D	569	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	C	919	ASP	CB-CG-OD1	5.12	122.90	118.30
1	C	855	THR	N-CA-CB	5.11	120.01	110.30
1	B	447	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	231	PHE	CB-CG-CD2	-5.09	117.23	120.80
1	B	392	TYR	CB-CG-CD2	5.09	124.06	121.00
1	D	671	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	820	ALA	CB-CA-C	-5.08	102.47	110.10
1	C	214	LEU	CB-CG-CD1	5.08	119.64	111.00
1	D	255	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	166	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	395	HIS	N-CA-CB	-5.08	101.46	110.60
1	D	549	PHE	CB-CG-CD1	-5.08	117.25	120.80
1	D	221	GLN	N-CA-CB	-5.08	101.46	110.60
1	A	100	TYR	N-CA-CB	5.07	119.73	110.60
1	C	26	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	952	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	857	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	411	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	D	731	PRO	N-CA-CB	5.06	109.37	103.30
1	D	772	ASP	CB-CA-C	-5.06	100.28	110.40
1	B	509	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	859	ASP	CB-CG-OD1	5.05	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	598	ASP	CB-CG-OD1	5.05	122.85	118.30
1	C	552	TYR	CZ-CE2-CD2	-5.04	115.26	119.80
1	D	755	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	519	SER	N-CA-CB	-5.04	102.94	110.50
1	A	237	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	161	TYR	CZ-CE2-CD2	-5.04	115.27	119.80
1	D	952	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	161	TYR	N-CA-CB	-5.03	101.54	110.60
1	B	251	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	D	663	LEU	CA-CB-CG	5.03	126.87	115.30
1	A	792	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	280	ASP	CB-CG-OD1	5.03	122.82	118.30
1	B	986	ILE	CB-CA-C	5.02	121.64	111.60
1	D	670	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	D	746	ASP	CB-CA-C	-5.00	100.40	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	685	LEU	CA

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8126	0	7718	148	0
1	B	8126	0	7718	121	0
1	C	8126	0	7718	161	0
1	D	8126	0	7718	131	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	15	0	17	1	0
4	B	15	0	17	0	0
4	C	15	0	17	0	0
4	D	15	0	17	1	0
5	A	96	0	144	16	0
5	B	88	0	132	10	0
5	C	100	0	150	7	0
5	D	92	0	138	13	0
6	A	950	0	0	12	0
6	B	971	0	0	12	0
6	C	943	0	0	14	0
6	D	949	0	0	17	0
All	All	36785	0	31504	562	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (562) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.36	1.06
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.01	0.95
1:A:600:GLN:H	1:A:600:GLN:HE21	1.18	0.89
1:D:773:LYS:HG2	1:D:775:GLN:HE22	1.39	0.88
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.58	0.85
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.10	0.85
1:A:277:GLU:H	1:A:277:GLU:CD	1.77	0.85
1:B:600:GLN:H	1:B:600:GLN:HE21	1.22	0.84
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.93	0.84
1:C:651:LEU:HD11	1:C:653:HIS:ND1	1.93	0.83
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.58	0.83
1:D:687:GLN:HG3	1:D:688:PRO:HD2	1.62	0.81
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.63	0.80
1:B:634:GLN:HG2	1:B:682:LEU:O	1.82	0.80
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.12	0.80
5:D:8413:DMS:H12	6:D:9297:HOH:O	1.81	0.79
1:D:773:LYS:HG2	1:D:775:GLN:NE2	1.96	0.79
1:C:54:LEU:HD21	1:C:214:LEU:CD2	2.13	0.78
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:GLU:O	1:C:760:ARG:HD3	1.83	0.78
1:D:685:LEU:HD23	1:D:686:PRO:HD2	1.64	0.77
1:A:797:GLU:O	1:A:801:ILE:HD13	1.84	0.76
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.16	0.76
1:D:651:LEU:HD12	1:D:651:LEU:C	2.07	0.75
1:B:748:CYS:C	1:B:749:ILE:HD12	2.06	0.75
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.69	0.75
1:B:473:ARG:NH2	1:B:477:SER:HB2	2.02	0.75
1:A:251:ARG:HH11	5:A:8416:DMS:C2	2.00	0.75
1:D:128:ASN:HB3	1:D:180:GLY:O	1.87	0.75
1:B:658:LEU:O	1:B:661:LYS:HG3	1.86	0.74
1:C:634:GLN:OE1	1:C:681:GLU:HG3	1.87	0.74
1:C:734:SER:CB	1:C:860:GLY:HA3	2.18	0.74
1:B:102:ASN:HD22	5:B:8506:DMS:C2	1.99	0.74
1:B:655:MET:HE2	1:B:656:VAL:N	2.03	0.74
1:C:797:GLU:O	1:C:801:ILE:HD13	1.88	0.74
1:B:651:LEU:O	1:B:651:LEU:HD23	1.87	0.73
1:C:690:SER:HB2	6:C:9322:HOH:O	1.88	0.73
1:A:887:GLN:NE2	1:A:980:GLU:O	2.21	0.73
1:C:687:GLN:CG	1:C:688:PRO:HD2	2.14	0.72
1:C:54:LEU:HD21	1:C:214:LEU:HD22	1.71	0.72
1:D:135:GLN:C	1:D:136:GLU:HG2	2.09	0.72
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.71	0.72
1:D:299:LYS:NZ	6:D:9381:HOH:O	2.22	0.71
1:D:660:GLY:O	1:D:662:PRO:HD3	1.90	0.71
1:D:663:LEU:HD11	1:D:688:PRO:HG3	1.72	0.71
1:B:13:ARG:HG3	1:C:13:ARG:NH2	2.05	0.71
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.73	0.70
1:D:629:PHE:O	1:D:630:ARG:HD3	1.91	0.70
1:A:749:ILE:N	1:A:749:ILE:HD12	2.07	0.70
1:A:686:PRO:C	1:A:688:PRO:HD3	2.12	0.70
1:C:745:MET:HE3	1:C:745:MET:HA	1.73	0.70
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.74	0.69
1:D:201:ASP:OD2	4:D:2001:IPT:H62	1.93	0.69
1:A:251:ARG:HH11	5:A:8416:DMS:H23	1.57	0.69
1:D:795:VAL:HG12	5:D:8506:DMS:H22	1.73	0.68
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.23	0.68
1:C:601:PHE:CE1	5:C:8506:DMS:H21	2.28	0.68
1:D:738:PRO:HG3	1:D:751:LEU:HD22	1.75	0.68
1:C:595:THR:HA	1:C:596:PRO:C	2.14	0.67
1:B:231:PHE:O	5:B:8417:DMS:H22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:ARG:NH2	6:C:9411:HOH:O	2.26	0.67
1:D:801:ILE:HD12	1:D:808:GLU:OE2	1.95	0.67
1:A:878:HIS:HD2	6:A:8675:HOH:O	1.78	0.67
1:D:847:LYS:HD3	1:D:848:THR:N	2.10	0.67
1:A:231:PHE:O	5:A:8417:DMS:H22	1.95	0.66
1:D:844:HIS:CE1	1:D:845:GLN:HG2	2.31	0.66
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.28	0.66
1:D:102:ASN:HB3	5:D:8506:DMS:H11	1.79	0.65
1:A:650:GLU:N	5:A:8425:DMS:O	2.27	0.65
1:C:178:ARG:O	1:C:178:ARG:HG2	1.90	0.65
1:C:843:GLN:NE2	1:C:848:THR:OG1	2.30	0.65
1:D:579:ASP:O	1:D:581:ASN:N	2.29	0.64
1:B:878:HIS:HD2	6:B:8689:HOH:O	1.79	0.64
1:C:655:MET:HE2	1:C:664:ALA:O	1.98	0.64
1:D:579:ASP:O	1:D:580:GLU:C	2.36	0.64
1:A:634:GLN:HB2	1:A:682:LEU:HB2	1.80	0.64
1:A:93:HIS:O	5:A:8421:DMS:H23	1.97	0.63
1:B:797:GLU:O	1:B:800:ARG:N	2.30	0.63
1:D:878:HIS:HD2	6:D:8811:HOH:O	1.80	0.63
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.80	0.63
1:B:797:GLU:O	1:B:800:ARG:C	2.37	0.63
1:A:84:VAL:HA	5:A:8414:DMS:O	1.99	0.63
1:B:749:ILE:N	1:B:749:ILE:HD12	2.14	0.63
1:C:658:LEU:HG	1:C:661:LYS:NZ	2.12	0.63
1:A:32:PRO:HB2	5:A:8404:DMS:H12	1.79	0.63
1:A:753:ASN:OD1	1:A:753:ASN:N	2.29	0.63
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.11	0.63
1:A:830:LEU:HD23	1:A:830:LEU:N	2.13	0.63
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.64	0.62
1:C:878:HIS:HD2	6:C:8699:HOH:O	1.80	0.62
1:A:948:PRO:C	1:A:1023:LYS:HE3	2.20	0.62
1:B:600:GLN:N	1:B:600:GLN:HE21	1.96	0.62
1:C:853:ARG:NH1	1:C:871:GLU:OE2	2.24	0.61
1:A:863:GLN:HE22	1:A:952:ARG:HH22	1.48	0.61
1:A:832:ASP:OD1	1:A:832:ASP:N	2.34	0.61
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.82	0.61
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.19	0.61
1:B:826:THR:OG1	1:B:837:THR:HB	2.00	0.61
1:A:370:GLN:HG3	6:A:9095:HOH:O	2.00	0.61
1:A:595:THR:HA	1:A:596:PRO:C	2.20	0.61
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:802:ASP:OD1	1:D:803:PRO:HD2	2.00	0.61
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.82	0.60
1:C:658:LEU:O	1:C:661:LYS:HG3	2.00	0.60
1:D:622:HIS:O	1:D:625:GLN:HG3	2.01	0.60
1:D:685:LEU:CD2	1:D:686:PRO:HD2	2.31	0.60
1:B:684:GLU:O	1:B:686:PRO:HD3	2.02	0.60
1:D:615:PRO:O	1:D:618:THR:HG22	2.02	0.60
1:D:858:ILE:CD1	1:D:864:MET:HB2	2.32	0.60
1:D:887:GLN:NE2	1:D:980:GLU:O	2.34	0.60
1:A:32:PRO:HB2	5:A:8404:DMS:C1	2.31	0.60
1:A:730:LEU:HD21	1:B:823:LEU:HB3	1.82	0.60
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.84	0.59
1:D:595:THR:HA	1:D:596:PRO:C	2.22	0.59
1:B:601:PHE:CD2	5:B:8506:DMS:H22	2.37	0.59
1:A:178:ARG:HD2	6:A:9398:HOH:O	2.02	0.59
1:C:745:MET:CE	1:C:745:MET:HA	2.32	0.59
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.84	0.59
1:B:102:ASN:HD22	5:B:8506:DMS:H21	1.66	0.59
1:C:734:SER:HB3	1:C:860:GLY:CA	2.32	0.59
1:C:634:GLN:H	1:C:634:GLN:NE2	2.01	0.59
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.03	0.59
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.86	0.58
1:C:734:SER:HB3	1:C:860:GLY:C	2.24	0.58
1:C:833:ALA:HB1	1:C:858:ILE:O	2.04	0.58
1:C:78:LEU:HB3	1:C:80:GLU:HG3	1.85	0.58
1:D:684:GLU:HG2	1:D:685:LEU:N	2.14	0.58
1:A:801:ILE:HD12	1:A:808:GLU:OE2	2.04	0.58
5:A:8413:DMS:H22	6:A:9517:HOH:O	2.04	0.58
1:D:649:ASN:HB2	6:D:9342:HOH:O	2.03	0.58
1:C:824:GLN:HG3	1:C:825:CYS:N	2.19	0.57
1:A:252:ASP:H	5:A:8416:DMS:C1	2.17	0.57
1:C:240:LEU:HD23	1:C:240:LEU:C	2.24	0.57
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.69	0.57
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.39	0.57
1:C:387:VAL:HG22	6:C:9481:HOH:O	2.04	0.57
1:A:336:ARG:NH2	1:A:338:GLU:OE1	2.29	0.57
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.87	0.57
1:A:593:GLY:O	1:A:595:THR:HG22	2.05	0.57
1:A:768:MET:HE3	1:A:1020:TRP:CZ2	2.40	0.57
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.39	0.57
1:D:756:TRP:CE2	1:D:858:ILE:HD12	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:MET:HE2	1:A:662:PRO:HA	1.86	0.56
1:C:688:PRO:HG3	1:C:694:LEU:HD11	1.87	0.56
1:A:580:GLU:O	1:A:580:GLU:OE1	2.22	0.56
1:D:579:ASP:O	1:D:579:ASP:OD1	2.24	0.56
1:D:251:ARG:NH2	1:D:253:TYR:OH	2.39	0.56
1:D:277:GLU:H	1:D:277:GLU:CD	1.99	0.56
1:A:135:GLN:NE2	6:A:9464:HOH:O	2.39	0.56
1:A:157:ARG:HB2	6:A:9380:HOH:O	2.06	0.56
1:C:945:ASN:OD1	1:C:1023:LYS:HD2	2.06	0.56
1:C:737:ILE:HG13	1:C:737:ILE:O	2.02	0.56
1:C:275:GLY:O	5:C:8412:DMS:H12	2.05	0.56
1:C:607:VAL:HG12	1:C:613:PRO:HA	1.88	0.56
1:A:648:ASP:OD2	6:A:9426:HOH:O	2.18	0.56
1:C:687:GLN:HG3	1:C:688:PRO:CD	2.23	0.55
1:D:651:LEU:HD11	1:D:653:HIS:ND1	2.21	0.55
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.87	0.55
5:B:8425:DMS:H21	6:B:9366:HOH:O	2.04	0.55
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.27	0.55
1:A:262:GLN:HG3	1:A:309:TYR:CE2	2.41	0.55
1:A:653:HIS:CD2	1:A:667:GLU:HG2	2.42	0.55
1:B:655:MET:HE2	1:B:655:MET:C	2.27	0.55
1:A:634:GLN:HG2	1:A:682:LEU:O	2.05	0.55
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.89	0.55
5:D:8406:DMS:O	6:D:9571:HOH:O	2.17	0.55
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.20	0.55
1:B:595:THR:HA	1:B:596:PRO:C	2.26	0.55
1:C:654:TRP:O	1:C:665:SER:HB2	2.06	0.55
1:A:600:GLN:N	1:A:600:GLN:HE21	1.95	0.55
1:B:473:ARG:HH21	1:B:477:SER:HB2	1.70	0.55
1:B:615:PRO:O	1:B:618:THR:HG22	2.06	0.55
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.88	0.55
1:C:655:MET:HG3	1:C:655:MET:O	2.07	0.55
1:C:577:LYS:HD3	1:C:587:ALA:HB2	1.88	0.54
1:D:651:LEU:HD12	1:D:651:LEU:O	2.08	0.54
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.89	0.54
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.26	0.54
1:B:634:GLN:HG2	1:B:682:LEU:HB2	1.89	0.54
1:A:737:ILE:O	1:A:737:ILE:HD13	2.07	0.54
1:D:795:VAL:HB	6:D:9340:HOH:O	2.07	0.54
1:B:683:PRO:O	1:B:685:LEU:HG	2.07	0.53
1:C:655:MET:SD	1:C:657:ALA:HB2	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:LEU:HD23	1:D:240:LEU:C	2.28	0.53
1:A:58:TRP:CE2	1:A:125:LEU:HD22	2.44	0.53
1:B:651:LEU:C	1:B:651:LEU:HD23	2.29	0.53
1:C:54:LEU:CD2	1:C:214:LEU:HD22	2.35	0.53
1:D:749:ILE:N	1:D:749:ILE:HD12	2.24	0.53
1:D:805:ALA:O	1:D:809:ARG:HG3	2.08	0.53
1:D:858:ILE:HD13	1:D:864:MET:HB2	1.90	0.53
1:D:804:ASN:O	1:D:809:ARG:NH1	2.42	0.53
1:A:473:ARG:HH12	1:A:477:SER:N	2.07	0.53
1:B:659:ASP:OD2	1:B:692:GLY:HA3	2.09	0.53
1:B:651:LEU:HD22	1:B:701:VAL:O	2.09	0.53
1:D:808:GLU:OE1	1:D:811:LYS:NZ	2.36	0.53
1:C:178:ARG:HD3	6:C:9418:HOH:O	2.08	0.53
1:D:765:LEU:HD21	1:D:768:MET:SD	2.48	0.53
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.39	0.52
1:B:16:TRP:CG	1:B:189:LEU:HD13	2.44	0.52
1:B:859:ASP:OD1	1:B:861:SER:OG	2.23	0.52
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.91	0.52
1:A:829:THR:C	1:A:830:LEU:HD23	2.30	0.52
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.24	0.52
1:A:890:GLN:HG3	1:A:891:VAL:N	2.24	0.52
1:B:128:ASN:HA	1:B:180:GLY:O	2.09	0.52
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.09	0.52
1:A:88:SER:HA	1:A:366:VAL:HG21	1.91	0.52
1:D:685:LEU:CG	1:D:686:PRO:HD2	2.39	0.52
1:D:71:GLU:HG2	6:D:9463:HOH:O	2.09	0.52
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.25	0.52
1:D:952:ARG:O	1:D:1018:LEU:HD22	2.09	0.52
1:D:134:LEU:HA	5:D:8705:DMS:H22	1.90	0.52
1:A:634:GLN:N	1:A:634:GLN:OE1	2.43	0.52
1:A:737:ILE:HD13	1:A:737:ILE:C	2.30	0.52
1:D:687:GLN:CG	1:D:688:PRO:HD2	2.36	0.52
1:D:251:ARG:NE	1:D:253:TYR:OH	2.40	0.52
1:A:237:ARG:HG2	1:A:296:GLU:OE1	2.09	0.52
1:B:250:LEU:O	1:B:251:ARG:HG2	2.09	0.52
1:D:513:PRO:O	1:D:514:ALA:HB3	2.10	0.52
1:A:66:PRO:HG3	1:A:189:LEU:CD2	2.40	0.51
1:B:262:GLN:HG3	6:B:9543:HOH:O	2.08	0.51
1:C:54:LEU:CG	1:C:214:LEU:HD22	2.40	0.51
1:C:806:TRP:CD1	1:C:809:ARG:NH2	2.78	0.51
1:C:785:THR:O	1:C:881:ARG:HD2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.79	0.51
1:D:577:LYS:O	1:D:584:PRO:HA	2.10	0.51
1:A:735:HIS:CD2	1:A:735:HIS:N	2.78	0.51
1:D:651:LEU:C	1:D:651:LEU:CD1	2.78	0.51
1:D:797:GLU:O	1:D:801:ILE:HD13	2.10	0.51
1:C:610:ASP:O	1:C:611:ARG:HB2	2.11	0.51
1:C:806:TRP:CE2	1:C:809:ARG:NH2	2.79	0.51
1:B:806:TRP:CE2	1:B:809:ARG:NH2	2.78	0.51
1:A:608:PHE:CE1	1:A:614:HIS:CD2	2.99	0.51
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.38	0.51
1:A:863:GLN:NE2	1:A:952:ARG:HH22	2.08	0.51
1:B:319:ASP:OD1	1:B:320:GLY:N	2.44	0.51
1:B:292:ARG:HH12	5:B:8412:DMS:C2	2.24	0.51
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.92	0.51
1:C:157:ARG:HD3	6:C:9513:HOH:O	2.10	0.51
1:A:655:MET:CE	1:A:662:PRO:HB3	2.41	0.50
1:D:102:ASN:ND2	5:D:8506:DMS:H13	2.26	0.50
1:D:773:LYS:HG3	1:D:774:LYS:N	2.19	0.50
1:A:357:HIS:HD2	6:A:9482:HOH:O	1.94	0.50
1:C:278:ILE:HD13	1:C:278:ILE:N	2.25	0.50
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.79	0.50
1:C:1001:PRO:HD3	6:C:8939:HOH:O	2.11	0.50
1:C:569:ASP:HB2	6:C:9359:HOH:O	2.10	0.50
1:B:797:GLU:O	1:B:801:ILE:N	2.43	0.50
1:B:78:LEU:HD23	6:B:9094:HOH:O	2.11	0.50
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.95	0.50
1:C:608:PHE:CE1	1:C:614:HIS:CD2	2.99	0.50
1:C:806:TRP:HA	1:C:809:ARG:HE	1.75	0.50
1:D:853:ARG:NH1	1:D:871:GLU:OE2	2.38	0.50
1:A:357:HIS:CD2	6:A:9482:HOH:O	2.65	0.50
1:B:910:LEU:C	1:B:910:LEU:HD12	2.32	0.50
1:B:685:LEU:O	1:B:686:PRO:C	2.50	0.49
1:D:646:HIS:CD2	1:D:647:SER:N	2.80	0.49
1:B:601:PHE:CG	5:B:8506:DMS:H22	2.47	0.49
1:A:890:GLN:CG	1:A:891:VAL:N	2.75	0.49
1:A:1022:GLN:O	1:A:1023:LYS:HG3	2.13	0.49
1:A:252:ASP:H	5:A:8416:DMS:H11	1.76	0.49
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.46	0.49
1:B:890:GLN:OE1	1:B:948:PRO:HD2	2.11	0.49
1:C:615:PRO:O	1:C:618:THR:HG22	2.13	0.49
1:C:843:GLN:HG2	1:C:848:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLN:N	1:A:688:PRO:HD3	2.26	0.49
1:A:819:GLU:HA	1:A:819:GLU:OE1	2.12	0.49
1:B:178:ARG:HG2	1:B:178:ARG:O	1.96	0.49
1:C:878:HIS:HE1	6:C:9521:HOH:O	1.94	0.49
1:A:296:GLU:HA	1:A:296:GLU:OE1	2.12	0.49
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.48	0.49
1:D:135:GLN:O	1:D:136:GLU:HG2	2.12	0.49
1:D:847:LYS:HD2	1:D:848:THR:O	2.11	0.49
1:A:268:ALA:HA	5:A:8602:DMS:H22	1.95	0.49
1:B:240:LEU:HD23	1:B:240:LEU:C	2.33	0.49
1:C:847:LYS:HG3	1:C:849:LEU:HD23	1.94	0.49
1:A:433:LEU:N	1:A:434:PRO:CD	2.76	0.49
1:D:961:ARG:NH2	1:D:979:GLU:O	2.45	0.49
1:C:890:GLN:HG2	1:C:891:VAL:N	2.27	0.48
1:D:68:ALA:O	1:D:70:PRO:HD3	2.12	0.48
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.94	0.48
1:D:102:ASN:HD22	5:D:8506:DMS:C1	2.26	0.48
1:A:674:PRO:C	1:A:675:GLN:HG2	2.33	0.48
1:A:835:LEU:HD11	1:A:855:THR:HB	1.95	0.48
1:B:387:VAL:HG22	6:B:9491:HOH:O	2.12	0.48
1:C:601:PHE:CE1	5:C:8506:DMS:C2	2.96	0.48
1:D:102:ASN:ND2	5:D:8506:DMS:C1	2.77	0.48
1:C:847:LYS:HE2	6:C:9340:HOH:O	2.12	0.48
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.43	0.48
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.49	0.48
1:C:743:SER:O	1:C:744:GLU:C	2.44	0.48
1:C:963:SER:HB3	1:C:983:TRP:CE2	2.49	0.48
1:B:367:MET:HE2	1:B:367:MET:HB3	1.56	0.48
5:B:8413:DMS:O	6:B:8959:HOH:O	2.20	0.48
1:C:356:ARG:HD2	1:C:379:MET:CE	2.43	0.48
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.48	0.48
1:B:1017:GLN:HB2	6:B:9469:HOH:O	2.14	0.48
1:D:634:GLN:HB2	1:D:682:LEU:HB2	1.96	0.48
1:B:102:ASN:ND2	5:B:8506:DMS:H21	2.26	0.48
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.96	0.48
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.95	0.47
1:B:596:PRO:HB3	6:B:9359:HOH:O	2.15	0.47
1:B:601:PHE:CG	5:B:8506:DMS:C2	2.97	0.47
1:C:658:LEU:O	1:C:659:ASP:C	2.52	0.47
1:D:675:GLN:HG3	6:D:9495:HOH:O	2.14	0.47
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:MET:HB2	1:C:768:MET:HE2	1.80	0.47
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.97	0.47
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.49	0.47
1:A:608:PHE:CD1	1:A:614:HIS:HD2	2.33	0.47
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.96	0.47
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.49	0.47
1:C:16:TRP:CG	1:C:189:LEU:CD1	2.98	0.47
1:C:802:ASP:O	1:C:808:GLU:HG3	2.14	0.47
1:D:1022:GLN:HG3	1:D:1022:GLN:O	2.00	0.47
1:B:655:MET:CA	1:B:655:MET:HE2	2.44	0.47
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.50	0.47
1:C:577:LYS:HE3	1:C:577:LYS:HB3	1.69	0.47
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.50	0.47
1:A:756:TRP:CD1	1:A:768:MET:HG2	2.49	0.47
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.47
1:B:251:ARG:CZ	1:B:253:TYR:HE2	2.27	0.47
1:B:473:ARG:HE	1:C:469:ASP:HB3	1.80	0.47
1:C:54:LEU:HD11	1:C:214:LEU:HD22	1.96	0.47
1:C:577:LYS:HD3	1:C:587:ALA:CB	2.45	0.47
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.50	0.47
1:B:832:ASP:O	1:B:833:ALA:HB2	2.14	0.47
1:A:742:THR:HG22	1:A:743:SER:N	2.29	0.46
1:A:890:GLN:HG3	1:A:891:VAL:H	1.80	0.46
1:B:583:ASN:HA	1:B:584:PRO:HD3	1.74	0.46
1:C:796:SER:OG	1:C:802:ASP:N	2.36	0.46
1:C:829:THR:C	1:C:830:LEU:HD23	2.36	0.46
1:D:843:GLN:HA	1:D:847:LYS:O	2.16	0.46
1:A:241:GLU:OE1	1:A:292:ARG:NH2	2.48	0.46
1:A:948:PRO:O	1:A:1023:LYS:HE3	2.15	0.46
1:D:251:ARG:NE	1:D:253:TYR:CE2	2.82	0.46
1:B:634:GLN:HG2	1:B:682:LEU:C	2.36	0.46
1:C:687:GLN:HA	1:C:688:PRO:HD3	1.72	0.46
1:C:601:PHE:CE2	5:C:8506:DMS:H22	2.51	0.46
1:B:907:PRO:HG2	1:B:990:HIS:O	2.15	0.46
1:C:830:LEU:N	1:C:830:LEU:HD23	2.31	0.46
1:D:824:GLN:NE2	1:D:837:THR:HG22	2.31	0.46
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.97	0.46
1:C:804:ASN:ND2	1:C:1001:PRO:CD	2.79	0.46
1:C:178:ARG:HG3	6:C:9373:HOH:O	2.15	0.46
1:D:961:ARG:NE	1:D:981:GLY:O	2.45	0.46
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ARG:HD3	6:D:9324:HOH:O	2.15	0.46
1:B:961:ARG:NH1	6:B:9170:HOH:O	2.30	0.46
1:A:662:PRO:O	1:A:663:LEU:HD23	2.16	0.46
1:C:804:ASN:HD21	1:C:1001:PRO:CD	2.28	0.46
1:D:628:GLN:NE2	6:D:9277:HOH:O	2.48	0.46
1:D:777:LEU:HG	1:D:889:ALA:HA	1.97	0.46
1:A:1022:GLN:CD	1:A:1023:LYS:H	2.19	0.46
1:A:554:GLN:OE1	6:A:9027:HOH:O	2.21	0.46
1:B:682:LEU:HA	1:B:682:LEU:HD23	1.80	0.46
1:C:88:SER:HA	1:C:366:VAL:HG21	1.98	0.46
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.98	0.46
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.16	0.46
1:D:893:GLU:HG3	1:D:893:GLU:O	2.12	0.46
1:D:858:ILE:HD11	1:D:864:MET:HB2	1.96	0.45
1:A:250:LEU:C	1:A:251:ARG:HG2	2.35	0.45
1:A:521:LYS:HE2	6:A:9027:HOH:O	2.15	0.45
1:C:835:LEU:HD11	1:C:855:THR:HB	1.98	0.45
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.96	0.45
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.97	0.45
1:D:340:GLY:O	1:D:561:ARG:HG2	2.16	0.45
1:D:787:ALA:HA	1:D:968:MET:HE2	1.97	0.45
1:B:658:LEU:HD11	1:B:692:GLY:HA3	1.99	0.45
1:A:431:ARG:HG3	6:A:9321:HOH:O	2.16	0.45
1:C:254:LEU:C	1:C:255:ARG:HG2	2.36	0.45
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.99	0.45
1:D:829:THR:HG21	6:D:9621:HOH:O	2.16	0.45
1:A:851:ILE:O	1:A:870:VAL:HA	2.17	0.45
1:B:730:LEU:H	1:B:730:LEU:HG	1.28	0.45
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.26	0.45
1:D:845:GLN:OE1	1:D:845:GLN:N	2.50	0.45
1:B:49:GLN:HG2	6:B:9283:HOH:O	2.17	0.44
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.51	0.44
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.98	0.44
1:C:147:ASN:HA	1:C:148:SER:HA	1.66	0.44
1:C:569:ASP:O	1:C:605:GLY:HA2	2.18	0.44
1:C:942:ARG:HA	1:C:953:GLY:O	2.17	0.44
1:B:13:ARG:CB	1:C:13:ARG:HH22	2.30	0.44
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.18	0.44
1:D:685:LEU:HG	1:D:686:PRO:CD	2.48	0.44
1:B:600:GLN:H	1:B:600:GLN:NE2	2.03	0.44
1:C:580:GLU:HG3	1:C:580:GLU:H	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LEU:CB	1:A:686:PRO:CD	2.95	0.44
1:A:730:LEU:HA	1:A:731:PRO:HD3	1.93	0.44
1:A:826:THR:OG1	1:A:837:THR:HB	2.18	0.44
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.52	0.44
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.42	0.44
1:C:1023:LYS:HE2	1:C:1023:LYS:HB3	1.67	0.44
1:C:843:GLN:CG	1:C:848:THR:HA	2.46	0.44
1:D:363:HIS:HD2	6:D:9295:HOH:O	1.99	0.44
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.00	0.44
1:D:233:ASP:HA	5:D:8417:DMS:C1	2.47	0.44
1:A:251:ARG:HA	5:A:8416:DMS:H12	1.99	0.44
1:B:655:MET:HE3	1:B:655:MET:HB2	1.70	0.44
1:B:749:ILE:N	1:B:749:ILE:CD1	2.80	0.44
1:C:13:ARG:NH1	6:C:8624:HOH:O	2.30	0.44
1:D:794:ALA:CB	6:D:8984:HOH:O	2.66	0.44
1:A:608:PHE:CE1	1:A:614:HIS:HD2	2.36	0.44
1:A:843:GLN:HA	1:A:847:LYS:O	2.18	0.44
1:A:950:GLN:OE1	1:A:952:ARG:NE	2.51	0.44
1:C:757:GLN:OE1	1:C:769:TRP:HH2	2.01	0.44
1:C:601:PHE:CZ	5:C:8506:DMS:C2	3.01	0.44
1:C:930:VAL:O	1:C:932:PRO:HD3	2.17	0.44
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.83	0.44
1:A:952:ARG:NH2	1:A:1021:CYS:SG	2.85	0.44
1:B:88:SER:HA	1:B:366:VAL:HG21	2.00	0.44
1:C:795:VAL:HG22	6:C:8872:HOH:O	2.17	0.44
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.18	0.44
1:A:201:ASP:OD2	4:A:2001:IPT:H62	2.18	0.43
1:A:32:PRO:CB	5:A:8404:DMS:C1	2.97	0.43
1:A:683:PRO:O	1:A:685:LEU:HG	2.17	0.43
1:C:770:ILE:HD12	1:C:775:GLN:CD	2.38	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.01	0.43
1:A:608:PHE:CD1	1:A:614:HIS:CD2	3.06	0.43
1:A:738:PRO:HD3	1:A:860:GLY:HA2	2.01	0.43
1:A:773:LYS:HB2	1:A:773:LYS:HE2	1.84	0.43
1:C:232:ASN:ND2	1:C:237:ARG:HG3	2.32	0.43
1:C:619:GLU:HG2	1:C:909:ARG:HG3	1.99	0.43
1:C:837:THR:O	1:C:837:THR:HG22	2.13	0.43
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.36	0.43
1:D:933:SER:O	1:D:934:GLU:C	2.57	0.43
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.54	0.43
1:C:272:ALA:HB1	1:C:273:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.54	0.43
1:A:910:LEU:C	1:A:910:LEU:HD12	2.38	0.43
1:B:807:VAL:CG1	1:B:808:GLU:N	2.81	0.43
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.52	0.43
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.18	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.53	0.43
1:C:754:LYS:HZ3	1:C:754:LYS:HG3	1.57	0.43
1:C:781:ARG:NH1	1:C:781:ARG:HG2	2.34	0.43
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.84	0.43
1:A:506:VAL:CG1	1:A:521:LYS:HE3	2.48	0.43
1:C:634:GLN:H	1:C:634:GLN:HE21	1.66	0.43
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.79	0.43
1:D:1022:GLN:HG3	1:D:1023:LYS:HG2	2.01	0.43
1:D:472:TYR:OH	1:D:476:LYS:HE2	2.18	0.43
5:D:8705:DMS:H21	6:D:9643:HOH:O	2.18	0.43
1:A:615:PRO:O	1:A:618:THR:HG22	2.19	0.43
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.74	0.43
1:A:737:ILE:HD13	1:A:738:PRO:O	2.18	0.43
1:A:986:ILE:HD13	1:A:986:ILE:HG23	1.57	0.43
1:C:292:ARG:HG3	1:C:292:ARG:NH1	2.33	0.43
1:D:685:LEU:CG	1:D:686:PRO:CD	2.96	0.43
1:B:200:GLN:HG2	1:B:391:HIS:HB2	2.01	0.43
1:C:336:ARG:NH2	1:C:338:GLU:OE1	2.39	0.43
1:B:699:ARG:NH1	6:B:9545:HOH:O	2.45	0.43
1:C:655:MET:HE2	1:C:656:VAL:N	2.34	0.43
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.82	0.43
1:C:748:CYS:SG	1:C:755:ARG:NH2	2.92	0.43
1:C:822:LEU:HD11	1:C:824:GLN:O	2.19	0.43
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.84	0.42
1:B:178:ARG:HG2	1:B:179:ALA:O	2.19	0.42
1:B:763:GLY:HA3	1:B:822:LEU:HD13	2.01	0.42
1:C:639:THR:OG1	1:C:677:LYS:HG2	2.19	0.42
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.54	0.42
1:B:279:ILE:HG23	1:B:279:ILE:HD12	1.69	0.42
1:C:637:GLU:OE2	1:C:677:LYS:HD3	2.19	0.42
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.55	0.42
1:D:756:TRP:CE2	1:D:858:ILE:CD1	3.02	0.42
1:B:661:LYS:HG3	1:B:661:LYS:H	1.64	0.42
1:C:750:GLU:HG3	1:C:754:LYS:O	2.19	0.42
1:A:658:LEU:O	1:A:659:ASP:C	2.56	0.42
1:D:147:ASN:HA	1:D:148:SER:HA	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:SER:HA	1:D:366:VAL:HG21	2.01	0.42
1:A:473:ARG:O	1:A:473:ARG:NH1	2.52	0.42
1:B:807:VAL:HG13	1:B:808:GLU:N	2.34	0.42
1:C:699:ARG:HH12	5:C:8415:DMS:C1	2.33	0.42
1:C:806:TRP:NE1	1:C:809:ARG:NH2	2.68	0.42
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.00	0.42
1:B:183:ARG:HD3	6:B:8920:HOH:O	2.19	0.42
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.20	0.42
1:D:219:THR:HG21	6:D:9600:HOH:O	2.19	0.42
1:D:833:ALA:HB1	1:D:858:ILE:O	2.20	0.42
1:B:802:ASP:OD1	1:B:804:ASN:HB3	2.20	0.42
1:C:824:GLN:O	1:C:838:THR:HA	2.19	0.42
1:B:367:MET:CE	1:B:372:MET:HG3	2.50	0.42
1:B:578:TYR:HA	1:B:583:ASN:O	2.20	0.42
1:C:637:GLU:CD	1:C:677:LYS:HD3	2.40	0.42
1:C:622:HIS:HB2	1:C:717:TRP:CZ2	2.55	0.42
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.55	0.42
1:D:753:ASN:OD1	1:D:753:ASN:N	2.45	0.42
1:D:795:VAL:CG1	5:D:8506:DMS:H22	2.48	0.42
1:D:682:LEU:C	1:D:683:PRO:O	2.57	0.42
1:C:895:VAL:O	1:C:919:ASP:HA	2.19	0.42
1:D:829:THR:HG23	1:D:834:VAL:HG22	2.02	0.42
1:B:85:VAL:HG12	1:B:86:VAL:N	2.34	0.41
1:C:54:LEU:HD11	1:C:214:LEU:CD2	2.50	0.41
1:D:685:LEU:HG	1:D:686:PRO:HD3	2.01	0.41
1:A:789:LEU:HD11	1:A:993:ILE:HG22	2.00	0.41
1:B:965:GLN:O	1:B:969:GLU:HG3	2.20	0.41
1:C:989:PHE:CD1	1:C:989:PHE:N	2.88	0.41
1:D:708:TRP:CZ3	1:D:709:SER:HB3	2.54	0.41
1:D:869:ASP:OD1	1:D:1015:HIS:ND1	2.53	0.41
1:A:58:TRP:CZ2	1:A:125:LEU:HD22	2.55	0.41
1:B:634:GLN:HG2	1:B:682:LEU:CB	2.51	0.41
1:A:472:TYR:O	1:A:476:LYS:HG2	2.21	0.41
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.20	0.41
1:A:861:SER:OG	1:A:863:GLN:HG3	2.21	0.41
1:C:542:MET:HA	1:C:604:ASN:HA	2.02	0.41
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.55	0.41
1:C:601:PHE:CZ	5:C:8506:DMS:H21	2.55	0.41
1:D:573:GLN:HB2	1:D:602:CYS:O	2.20	0.41
1:D:847:LYS:HD3	1:D:848:THR:H	1.84	0.41
1:B:577:LYS:O	1:B:584:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:VAL:HG12	1:B:669:PRO:O	2.20	0.41
1:A:252:ASP:H	5:A:8416:DMS:H12	1.83	0.41
1:A:533:LEU:C	1:A:533:LEU:HD23	2.41	0.41
1:A:696:LEU:HD23	1:A:720:TRP:CE3	2.56	0.41
1:B:340:GLY:O	1:B:561:ARG:HG2	2.21	0.41
1:D:373:VAL:O	1:D:377:LEU:HG	2.21	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.94	0.41
1:A:147:ASN:HA	1:A:148:SER:HA	1.54	0.41
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.37	0.41
1:A:738:PRO:CD	1:A:751:LEU:HD13	2.51	0.41
1:A:32:PRO:CB	5:A:8404:DMS:H11	2.50	0.41
1:C:114:VAL:HB	1:C:115:PRO:CD	2.51	0.41
1:D:794:ALA:HB1	6:D:8984:HOH:O	2.20	0.41
1:D:986:ILE:HD13	1:D:986:ILE:HG23	1.87	0.41
1:A:636:ILE:HD11	1:A:682:LEU:HD11	2.02	0.41
1:A:836:ILE:HD12	1:A:836:ILE:HG23	1.80	0.41
1:A:787:ALA:HA	1:A:968:MET:HG3	2.03	0.41
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.56	0.41
1:B:731:PRO:HB2	1:B:732:ALA:H	1.64	0.41
1:B:806:TRP:CD2	1:B:809:ARG:NH2	2.89	0.41
1:C:977:HIS:O	1:C:977:HIS:CD2	2.74	0.41
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.56	0.41
1:A:660:GLY:O	1:A:662:PRO:HD3	2.21	0.41
1:B:441:THR:O	1:B:445:GLN:HG3	2.20	0.41
1:B:473:ARG:NH2	1:B:477:SER:CB	2.79	0.41
1:B:634:GLN:NE2	1:B:685:LEU:HD12	2.36	0.41
1:C:60:PHE:HA	1:C:122:CYS:O	2.21	0.41
1:A:869:ASP:OD1	1:A:1015:HIS:ND1	2.54	0.41
1:B:668:VAL:HG11	1:B:680:ILE:HG12	2.02	0.41
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.82	0.41
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.56	0.41
1:A:843:GLN:HG3	1:A:847:LYS:O	2.21	0.40
1:A:986:ILE:HD12	1:A:986:ILE:HG21	1.61	0.40
1:C:1000:SER:HA	6:C:8939:HOH:O	2.22	0.40
1:D:658:LEU:O	1:D:659:ASP:C	2.59	0.40
1:D:770:ILE:HD12	6:D:9560:HOH:O	2.21	0.40
1:A:35:SER:HB2	1:A:217:LYS:HD3	2.02	0.40
1:B:145:GLY:HA3	1:B:210:ARG:HB2	2.03	0.40
1:C:687:GLN:CB	1:C:688:PRO:HD2	2.52	0.40
1:C:984:LEU:HD12	1:C:985:ASN:N	2.37	0.40
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ASP:O	1:A:580:GLU:C	2.58	0.40
1:A:742:THR:CG2	1:A:743:SER:N	2.85	0.40
1:B:513:PRO:O	1:B:514:ALA:HB3	2.22	0.40
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.51	0.40
1:A:390:SER:HA	1:A:391:HIS:HA	1.90	0.40
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.57	0.40
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.40	0.40
1:C:625:GLN:HG2	1:C:716:ALA:HA	2.03	0.40
1:D:847:LYS:O	1:D:847:LYS:HG3	2.13	0.40
1:D:847:LYS:CD	1:D:848:THR:N	2.82	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	971 (96%)	37 (4%)	1 (0%)	55	30
1	B	1009/1023 (99%)	967 (96%)	35 (4%)	7 (1%)	25	7
1	C	1009/1023 (99%)	962 (95%)	46 (5%)	1 (0%)	55	30
1	D	1009/1023 (99%)	969 (96%)	36 (4%)	4 (0%)	38	16
All	All	4036/4092 (99%)	3869 (96%)	154 (4%)	13 (0%)	44	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	690	SER
1	B	731	PRO
1	C	1022	GLN
1	D	580	GLU

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Mol	Chain	Res	Type
1	D	688	PRO
1	B	685	LEU
1	B	687	GLN
1	B	800	ARG
1	D	164	ASP
1	A	164	ASP
1	D	683	PRO
1	B	684	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	831 (96%)	33 (4%)	38	12
1	B	864/875 (99%)	827 (96%)	37 (4%)	33	10
1	C	864/875 (99%)	820 (95%)	44 (5%)	28	7
1	D	864/875 (99%)	828 (96%)	36 (4%)	34	11
All	All	3456/3500 (99%)	3306 (96%)	150 (4%)	33	10

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	71	GLU
1	A	213	SER
1	A	250	LEU
1	A	262	GLN
1	A	277	GLU
1	A	333	ARG
1	A	394	ASN
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	634	GLN
1	A	651	LEU
1	A	655	MET
1	A	667	GLU
1	A	675	GLN
1	A	689	GLU
1	A	730	LEU
1	A	734	SER
1	A	735	HIS
1	A	737	ILE
1	A	796	SER
1	A	799	THR
1	A	801	ILE
1	A	817	GLN
1	A	829	THR
1	A	843	GLN
1	A	910	LEU
1	A	956	GLN
1	A	986	ILE
1	A	1023	LYS
1	B	71	GLU
1	B	76	CYS
1	B	80	GLU
1	B	178	ARG
1	B	262	GLN
1	B	264	GLU
1	B	333	ARG
1	B	344	LEU
1	B	370	GLN
1	B	394	ASN
1	B	473	ARG
1	B	546	LEU
1	B	554	GLN
1	B	581	ASN
1	B	594	ASP
1	B	600	GLN
1	B	630	ARG
1	B	634	GLN
1	B	646	HIS
1	B	651	LEU
1	B	652	LEU
1	B	655	MET

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Mol	Chain	Res	Type
1	B	661	LYS
1	B	663	LEU
1	B	681	GLU
1	B	689	GLU
1	B	730	LEU
1	B	745	MET
1	B	748	CYS
1	B	754	LYS
1	B	799	THR
1	B	800	ARG
1	B	819	GLU
1	B	847	LYS
1	B	917	ARG
1	B	1022	GLN
1	B	1023	LYS
1	C	19	PRO
1	C	71	GLU
1	C	75	GLU
1	C	76	CYS
1	C	80	GLU
1	C	117	GLU
1	C	135	GLN
1	C	178	ARG
1	C	214	LEU
1	C	262	GLN
1	C	264	GLU
1	C	278	ILE
1	C	333	ARG
1	C	344	LEU
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	630	ARG
1	C	634	GLN
1	C	651	LEU
1	C	653	HIS
1	C	655	MET
1	C	663	LEU
1	C	667	GLU
1	C	672	VAL
1	C	684	GLU

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Mol	Chain	Res	Type
1	C	685	LEU
1	C	687	GLN
1	C	688	PRO
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	750	GLU
1	C	768	MET
1	C	799	THR
1	C	800	ARG
1	C	845	GLN
1	C	847	LYS
1	C	859	ASP
1	C	934	GLU
1	C	956	GLN
1	C	1023	LYS
1	D	75	GLU
1	D	90	TRP
1	D	117	GLU
1	D	333	ARG
1	D	370	GLN
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	684	GLU
1	D	685	LEU
1	D	689	GLU
1	D	710	GLU
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	797	GLU
1	D	799	THR
1	D	801	ILE

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Mol	Chain	Res	Type
1	D	845	GLN
1	D	861	SER
1	D	863	GLN
1	D	893	GLU
1	D	910	LEU
1	D	956	GLN
1	D	980	GLU
1	D	1017	GLN
1	D	1018	LEU
1	D	1022	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	363	HIS
1	A	370	GLN
1	A	600	GLN
1	A	624	GLN
1	A	675	GLN
1	A	702	GLN
1	A	735	HIS
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	A	1017	GLN
1	B	102	ASN
1	B	262	GLN
1	B	363	HIS
1	B	554	GLN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	687	GLN
1	B	878	HIS
1	C	163	GLN
1	C	262	GLN
1	C	363	HIS
1	C	614	HIS
1	C	624	GLN
1	C	646	HIS

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Mol	Chain	Res	Type
1	C	804	ASN
1	C	878	HIS
1	D	102	ASN
1	D	135	GLN
1	D	163	GLN
1	D	363	HIS
1	D	628	GLN
1	D	704	ASN
1	D	761	GLN
1	D	804	ASN
1	D	824	GLN
1	D	878	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 32 are monoatomic - leaving 98 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	IPT	A	2001	3	15,15,15	0.60	0	19,21,21	1.55	3 (15%)
5	DMS	A	8401	-	3,3,3	0.87	0	3,3,3	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	A	8402	-	3,3,3	1.52	0	3,3,3	0.34	0
5	DMS	A	8403	-	3,3,3	1.58	0	3,3,3	0.61	0
5	DMS	A	8404	-	3,3,3	1.28	0	3,3,3	0.40	0
5	DMS	A	8405	-	3,3,3	1.38	1 (33%)	3,3,3	0.35	0
5	DMS	A	8406	-	3,3,3	1.33	0	3,3,3	0.43	0
5	DMS	A	8407	-	3,3,3	1.28	0	3,3,3	0.32	0
5	DMS	A	8408	-	3,3,3	0.88	0	3,3,3	0.50	0
5	DMS	A	8409	-	3,3,3	2.06	1 (33%)	3,3,3	0.23	0
5	DMS	A	8410	-	3,3,3	0.74	0	3,3,3	0.65	0
5	DMS	A	8411	-	3,3,3	0.44	0	3,3,3	0.38	0
5	DMS	A	8412	-	3,3,3	1.11	0	3,3,3	0.38	0
5	DMS	A	8413	-	3,3,3	1.95	2 (66%)	3,3,3	0.39	0
5	DMS	A	8414	-	3,3,3	0.94	0	3,3,3	0.16	0
5	DMS	A	8416	-	3,3,3	3.00	1 (33%)	3,3,3	0.45	0
5	DMS	A	8417	-	3,3,3	0.71	0	3,3,3	0.65	0
5	DMS	A	8420	-	3,3,3	0.67	0	3,3,3	0.26	0
5	DMS	A	8421	-	3,3,3	1.12	0	3,3,3	0.13	0
5	DMS	A	8425	3	3,3,3	1.19	0	3,3,3	0.58	0
5	DMS	A	8501	-	3,3,3	1.28	0	3,3,3	0.43	0
5	DMS	A	8502	-	3,3,3	1.86	1 (33%)	3,3,3	1.06	0
5	DMS	A	8503	-	3,3,3	1.67	1 (33%)	3,3,3	0.41	0
5	DMS	A	8504	-	3,3,3	0.96	0	3,3,3	0.85	0
5	DMS	A	8602	-	3,3,3	0.87	0	3,3,3	0.18	0
4	IPT	B	2001	3	15,15,15	0.59	0	19,21,21	1.57	2 (10%)
5	DMS	B	8401	-	3,3,3	0.61	0	3,3,3	0.39	0
5	DMS	B	8402	-	3,3,3	1.67	1 (33%)	3,3,3	0.52	0
5	DMS	B	8403	-	3,3,3	0.68	0	3,3,3	0.54	0
5	DMS	B	8404	-	3,3,3	0.89	0	3,3,3	0.40	0
5	DMS	B	8405	-	3,3,3	2.01	2 (66%)	3,3,3	0.47	0
5	DMS	B	8408	-	3,3,3	1.47	1 (33%)	3,3,3	0.28	0
5	DMS	B	8409	-	3,3,3	2.49	1 (33%)	3,3,3	0.47	0
5	DMS	B	8410	-	3,3,3	1.04	0	3,3,3	0.77	0
5	DMS	B	8411	-	3,3,3	1.31	0	3,3,3	0.51	0
5	DMS	B	8412	-	3,3,3	1.05	0	3,3,3	0.23	0
5	DMS	B	8413	-	3,3,3	0.95	0	3,3,3	0.29	0
5	DMS	B	8414	-	3,3,3	0.60	0	3,3,3	0.58	0
5	DMS	B	8416	-	3,3,3	0.60	0	3,3,3	0.33	0
5	DMS	B	8417	-	3,3,3	0.43	0	3,3,3	0.63	0
5	DMS	B	8421	-	3,3,3	1.13	0	3,3,3	0.62	0
5	DMS	B	8423	-	3,3,3	0.34	0	3,3,3	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	B	8425	3	3,3,3	1.23	0	3,3,3	0.40	0
5	DMS	B	8502	-	3,3,3	1.29	0	3,3,3	0.98	0
5	DMS	B	8504	-	3,3,3	1.00	0	3,3,3	0.04	0
5	DMS	B	8506	-	3,3,3	0.98	0	3,3,3	1.19	1 (33%)
5	DMS	B	8508	-	3,3,3	1.81	1 (33%)	3,3,3	0.52	0
5	DMS	B	8601	-	3,3,3	1.41	0	3,3,3	0.89	0
4	IPT	C	2001	3	15,15,15	0.59	0	19,21,21	1.33	3 (15%)
5	DMS	C	8401	-	3,3,3	1.56	0	3,3,3	0.72	0
5	DMS	C	8402	-	3,3,3	1.85	1 (33%)	3,3,3	0.38	0
5	DMS	C	8403	-	3,3,3	0.70	0	3,3,3	0.75	0
5	DMS	C	8404	-	3,3,3	1.39	0	3,3,3	1.61	1 (33%)
5	DMS	C	8405	-	3,3,3	1.59	1 (33%)	3,3,3	0.89	0
5	DMS	C	8407	-	3,3,3	0.86	0	3,3,3	0.12	0
5	DMS	C	8408	-	3,3,3	0.43	0	3,3,3	1.40	1 (33%)
5	DMS	C	8409	-	3,3,3	2.13	1 (33%)	3,3,3	0.25	0
5	DMS	C	8410	-	3,3,3	0.51	0	3,3,3	0.31	0
5	DMS	C	8411	-	3,3,3	0.48	0	3,3,3	0.26	0
5	DMS	C	8412	-	3,3,3	1.17	0	3,3,3	0.10	0
5	DMS	C	8413	-	3,3,3	1.10	0	3,3,3	0.61	0
5	DMS	C	8414	-	3,3,3	1.05	0	3,3,3	0.65	0
5	DMS	C	8415	-	3,3,3	1.83	1 (33%)	3,3,3	0.40	0
5	DMS	C	8417	-	3,3,3	0.39	0	3,3,3	0.76	0
5	DMS	C	8420	-	3,3,3	0.67	0	3,3,3	0.20	0
5	DMS	C	8421	-	3,3,3	0.44	0	3,3,3	0.96	0
5	DMS	C	8423	-	3,3,3	0.48	0	3,3,3	0.36	0
5	DMS	C	8425	3	3,3,3	1.08	0	3,3,3	0.52	0
5	DMS	C	8501	-	3,3,3	1.66	1 (33%)	3,3,3	0.65	0
5	DMS	C	8503	-	3,3,3	0.32	0	3,3,3	0.78	0
5	DMS	C	8504	-	3,3,3	0.66	0	3,3,3	0.73	0
5	DMS	C	8506	-	3,3,3	1.45	1 (33%)	3,3,3	0.66	0
5	DMS	C	8601	-	3,3,3	1.27	1 (33%)	3,3,3	0.61	0
5	DMS	C	8602	-	3,3,3	0.88	0	3,3,3	0.55	0
4	IPT	D	2001	3	15,15,15	0.82	0	19,21,21	1.83	6 (31%)
5	DMS	D	8401	-	3,3,3	1.75	0	3,3,3	0.36	0
5	DMS	D	8402	-	3,3,3	1.79	1 (33%)	3,3,3	0.26	0
5	DMS	D	8403	-	3,3,3	1.40	0	3,3,3	0.84	0
5	DMS	D	8404	-	3,3,3	0.64	0	3,3,3	0.71	0
5	DMS	D	8405	-	3,3,3	1.14	0	3,3,3	0.94	0
5	DMS	D	8406	-	3,3,3	0.94	0	3,3,3	0.49	0
5	DMS	D	8408	-	3,3,3	1.14	0	3,3,3	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	D	8409	-	3,3,3	1.85	1 (33%)	3,3,3	0.73	0
5	DMS	D	8410	-	3,3,3	1.11	0	3,3,3	0.52	0
5	DMS	D	8411	-	3,3,3	0.99	0	3,3,3	0.24	0
5	DMS	D	8412	-	3,3,3	1.36	0	3,3,3	0.72	0
5	DMS	D	8413	-	3,3,3	1.24	1 (33%)	3,3,3	0.41	0
5	DMS	D	8414	-	3,3,3	0.19	0	3,3,3	0.41	0
5	DMS	D	8416	-	3,3,3	0.96	0	3,3,3	0.21	0
5	DMS	D	8417	-	3,3,3	0.43	0	3,3,3	1.18	1 (33%)
5	DMS	D	8421	-	3,3,3	0.63	0	3,3,3	0.93	0
5	DMS	D	8501	-	3,3,3	0.92	0	3,3,3	0.59	0
5	DMS	D	8503	-	3,3,3	0.94	0	3,3,3	0.38	0
5	DMS	D	8506	-	3,3,3	0.58	0	3,3,3	0.34	0
5	DMS	D	8508	-	3,3,3	1.88	2 (66%)	3,3,3	0.37	0
5	DMS	D	8701	-	3,3,3	2.23	2 (66%)	3,3,3	0.79	0
5	DMS	D	8703	-	3,3,3	0.97	0	3,3,3	0.38	0
5	DMS	D	8705	-	3,3,3	2.07	1 (33%)	3,3,3	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IPT	A	2001	3	-	0/6/26/26	0/1/1/1
5	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8420	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8425	3	-	0/0/0/0	0/0/0/0
5	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8602	-	-	0/0/0/0	0/0/0/0
4	IPT	B	2001	3	-	0/6/26/26	0/1/1/1
5	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	3	-	0/0/0/0	0/0/0/0
5	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
4	IPT	C	2001	3	-	0/6/26/26	0/1/1/1
5	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8412	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	C	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8425	3	-	0/0/0/0	0/0/0/0
5	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
4	IPT	D	2001	3	-	0/6/26/26	0/1/1/1
5	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

All (28) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8416	DMS	C1-S	-4.91	1.38	1.75
5	C	8501	DMS	C1-S	-2.35	1.58	1.75
5	D	8508	DMS	C1-S	2.07	1.91	1.75
5	C	8405	DMS	O-S	2.07	1.64	1.50
5	B	8405	DMS	O-S	2.11	1.64	1.50
5	A	8413	DMS	C2-S	2.11	1.91	1.75
5	D	8413	DMS	O-S	2.13	1.64	1.50
5	A	8413	DMS	O-S	2.14	1.64	1.50
5	B	8408	DMS	C1-S	2.17	1.92	1.75
5	A	8405	DMS	O-S	2.17	1.64	1.50
5	C	8601	DMS	C2-S	2.17	1.92	1.75
5	C	8506	DMS	C1-S	2.20	1.92	1.75
5	B	8405	DMS	C2-S	2.37	1.93	1.75
5	D	8508	DMS	O-S	2.50	1.67	1.50
5	D	8402	DMS	C2-S	2.50	1.94	1.75
5	B	8508	DMS	C1-S	2.51	1.94	1.75
5	D	8701	DMS	C2-S	2.57	1.95	1.75
5	D	8409	DMS	O-S	2.71	1.68	1.50
5	B	8402	DMS	C2-S	2.72	1.96	1.75
5	D	8701	DMS	O-S	2.75	1.68	1.50
5	A	8503	DMS	C2-S	2.84	1.97	1.75
5	A	8502	DMS	C1-S	2.86	1.97	1.75
5	C	8415	DMS	C1-S	2.90	1.97	1.75
5	C	8402	DMS	C2-S	3.08	1.99	1.75
5	D	8705	DMS	O-S	3.32	1.72	1.50
5	A	8409	DMS	O-S	3.42	1.73	1.50
5	C	8409	DMS	O-S	3.50	1.74	1.50
5	B	8409	DMS	O-S	3.95	1.77	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	IPT	O5-C5-C6	-4.44	95.77	106.41
4	D	2001	IPT	O5-C5-C6	-4.42	95.81	106.41
4	C	2001	IPT	O5-C1-S1	-3.10	102.17	110.21
4	D	2001	IPT	C1-O5-C5	-3.00	106.92	112.69
4	D	2001	IPT	O6-C6-C5	-2.93	101.48	111.34
4	A	2001	IPT	C3-C4-C5	-2.67	105.52	110.22
4	B	2001	IPT	O3-C3-C2	-2.58	104.74	110.36
4	A	2001	IPT	O6-C6-C5	-2.47	103.04	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2001	IPT	O2-C2-C1	-2.40	105.48	110.27
4	D	2001	IPT	C6-C5-C4	-2.29	107.65	113.00
4	D	2001	IPT	C3-C4-C5	-2.21	106.32	110.22
4	D	2001	IPT	C3'-C1'-C2'	-2.06	103.92	111.71
5	D	8417	DMS	C2-S-C1	2.01	108.89	98.44
5	B	8506	DMS	C2-S-C1	2.06	109.14	98.44
5	C	8408	DMS	C2-S-C1	2.30	110.39	98.44
4	C	2001	IPT	O3-C3-C4	2.45	115.68	110.36
5	C	8404	DMS	C2-S-C1	2.74	112.64	98.44
4	B	2001	IPT	C6-C5-C4	5.05	124.82	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	IPT	1	0
5	A	8404	DMS	4	0
5	A	8413	DMS	1	0
5	A	8414	DMS	1	0
5	A	8416	DMS	6	0
5	A	8417	DMS	1	0
5	A	8421	DMS	1	0
5	A	8425	DMS	1	0
5	A	8602	DMS	1	0
5	B	8412	DMS	1	0
5	B	8413	DMS	1	0
5	B	8417	DMS	1	0
5	B	8425	DMS	1	0
5	B	8506	DMS	6	0
5	C	8412	DMS	1	0
5	C	8415	DMS	1	0
5	C	8506	DMS	5	0
4	D	2001	IPT	1	0
5	D	8406	DMS	1	0
5	D	8412	DMS	2	0
5	D	8413	DMS	1	0
5	D	8417	DMS	1	0
5	D	8506	DMS	6	0
5	D	8705	DMS	2	0



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.12	32 (3%) 48 46	9, 17, 46, 98	0
1	B	1011/1023 (98%)	0.03	27 (2%) 55 54	8, 17, 43, 100	0
1	C	1011/1023 (98%)	-0.02	25 (2%) 58 57	10, 17, 48, 98	0
1	D	1011/1023 (98%)	0.05	36 (3%) 43 42	9, 17, 49, 98	0
All	All	4044/4092 (98%)	0.05	120 (2%) 51 49	8, 17, 47, 100	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	11.8
1	A	735	HIS	8.7
1	C	732	ALA	8.5
1	B	733	ALA	8.3
1	B	732	ALA	7.7
1	B	685	LEU	7.7
1	A	730	LEU	7.5
1	B	730	LEU	7.4
1	D	734	SER	7.1
1	C	730	LEU	6.9
1	C	733	ALA	6.8
1	B	731	PRO	6.8
1	D	735	HIS	6.4
1	D	686	PRO	6.4
1	C	731	PRO	6.0
1	D	732	ALA	5.6
1	A	689	GLU	5.6
1	C	735	HIS	5.4
1	D	733	ALA	5.4
1	B	689	GLU	5.3
1	D	689	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	686	PRO	5.1
1	D	688	PRO	4.9
1	C	686	PRO	4.9
1	C	689	GLU	4.6
1	A	733	ALA	4.6
1	D	800	ARG	4.2
1	A	737	ILE	4.1
1	B	687	GLN	4.0
1	D	736	ALA	4.0
1	D	799	THR	4.0
1	A	1023	LYS	3.9
1	C	734	SER	3.9
1	A	732	ALA	3.8
1	C	687	GLN	3.7
1	B	735	HIS	3.7
1	A	687	GLN	3.6
1	A	685	LEU	3.6
1	D	580	GLU	3.6
1	D	683	PRO	3.6
1	B	799	THR	3.5
1	A	734	SER	3.5
1	D	581	ASN	3.5
1	B	684	GLU	3.5
1	D	730	LEU	3.4
1	A	798	ALA	3.4
1	C	800	ARG	3.4
1	D	684	GLU	3.4
1	A	736	ALA	3.3
1	B	734	SER	3.3
1	C	685	LEU	3.3
1	D	845	GLN	3.3
1	D	663	LEU	3.3
1	D	687	GLN	3.3
1	A	731	PRO	3.2
1	D	685	LEU	3.2
1	D	582	GLY	3.2
1	C	736	ALA	3.2
1	D	770	ILE	3.1
1	B	580	GLU	3.1
1	A	71	GLU	3.1
1	A	799	THR	3.1
1	A	580	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	831	ALA	3.0
1	D	737	ILE	3.0
1	C	684	GLU	3.0
1	B	798	ALA	3.0
1	A	682	LEU	3.0
1	A	801	ILE	2.9
1	D	666	GLY	2.9
1	D	771	GLY	2.9
1	C	798	ALA	2.9
1	D	798	ALA	2.9
1	A	800	ARG	2.9
1	C	253	TYR	2.9
1	C	745	MET	2.9
1	A	729	THR	2.9
1	A	582	GLY	2.8
1	D	861	SER	2.8
1	C	801	ILE	2.8
1	A	688	PRO	2.7
1	D	634	GLN	2.7
1	D	829	THR	2.7
1	B	581	ASN	2.7
1	D	731	PRO	2.6
1	D	769	TRP	2.6
1	C	729	THR	2.6
1	C	861	SER	2.6
1	A	683	PRO	2.6
1	A	1022	GLN	2.5
1	C	830	LEU	2.5
1	D	830	LEU	2.5
1	B	664	ALA	2.4
1	B	801	ILE	2.4
1	A	845	GLN	2.4
1	B	800	ARG	2.3
1	C	76	CYS	2.3
1	D	1023	LYS	2.3
1	C	799	THR	2.3
1	B	738	PRO	2.3
1	C	634	GLN	2.3
1	A	748	CYS	2.3
1	D	728	VAL	2.2
1	C	772	ASP	2.2
1	B	79	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	668	VAL	2.1
1	D	679	LEU	2.1
1	B	690	SER	2.1
1	A	684	GLU	2.1
1	B	771	GLY	2.1
1	B	845	GLN	2.1
1	A	634	GLN	2.1
1	D	801	ILE	2.1
1	C	580	GLU	2.1
1	B	748	CYS	2.1
1	B	595	THR	2.0
1	A	664	ALA	2.0
1	B	737	ILE	2.0
1	A	771	GLY	2.0
1	B	736	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	DMS	C	8407	4/4	0.82	0.23	10.57	51,100,100,100	0
5	DMS	D	8501	4/4	0.89	0.12	8.69	22,29,41,50	0
5	DMS	B	8506	4/4	0.95	0.16	8.58	44,100,100,100	0
5	DMS	C	8412	4/4	0.97	0.16	7.58	34,37,75,100	0
5	DMS	B	8508	4/4	0.85	0.15	7.25	36,41,54,56	0
5	DMS	A	8407	4/4	0.82	0.19	7.07	29,50,51,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	A	8420	4/4	0.95	0.13	6.68	47,53,82,100	0
3	NA	B	3101	1/1	0.97	0.10	5.33	15,15,15,15	0
5	DMS	D	8404	4/4	0.89	0.13	5.13	26,27,54,57	0
5	DMS	A	8406	4/4	0.89	0.18	5.11	15,52,66,83	0
5	DMS	C	8420	4/4	0.93	0.13	4.87	38,50,61,100	0
5	DMS	B	8417	4/4	0.91	0.17	4.76	24,30,61,69	0
5	DMS	A	8417	4/4	0.88	0.15	4.37	26,29,59,100	0
5	DMS	A	8504	4/4	0.94	0.12	4.32	25,38,42,100	0
5	DMS	A	8404	4/4	0.91	0.12	4.29	17,30,39,41	0
5	DMS	D	8508	4/4	0.93	0.15	4.13	37,42,52,100	0
5	DMS	C	8425	4/4	0.95	0.16	3.68	34,41,43,45	0
5	DMS	B	8425	4/4	0.86	0.13	3.31	23,37,39,46	0
5	DMS	C	8417	4/4	0.90	0.17	3.27	30,31,51,69	0
3	NA	D	3104	1/1	0.84	0.17	3.17	44,44,44,44	0
5	DMS	A	8411	4/4	0.96	0.14	3.11	26,27,30,100	0
5	DMS	A	8416	4/4	0.92	0.18	2.99	13,32,46,66	0
5	DMS	C	8501	4/4	0.93	0.11	2.88	22,25,38,53	0
5	DMS	D	8417	4/4	0.93	0.13	2.81	23,27,70,75	0
5	DMS	C	8423	4/4	0.90	0.14	2.77	32,34,67,76	0
5	DMS	D	8405	4/4	0.97	0.11	2.75	25,26,30,35	0
5	DMS	A	8405	4/4	0.99	0.11	2.70	24,25,25,29	0
5	DMS	C	8404	4/4	0.94	0.09	2.64	20,22,32,35	0
3	NA	A	3103	1/1	0.87	0.14	2.61	32,32,32,32	0
5	DMS	A	8412	4/4	0.96	0.19	2.61	31,36,40,100	0
5	DMS	C	8411	4/4	0.97	0.13	2.52	24,28,32,100	0
5	DMS	B	8502	4/4	0.95	0.12	2.49	26,29,36,42	0
5	DMS	A	8502	4/4	0.92	0.16	2.31	29,29,52,61	0
3	NA	C	3104	1/1	0.93	0.14	2.30	29,29,29,29	0
3	NA	B	3104	1/1	0.84	0.13	2.28	32,32,32,32	0
5	DMS	D	8705	4/4	0.89	0.13	1.97	30,42,42,44	0
5	DMS	D	8401	4/4	0.98	0.08	1.92	13,14,18,19	0
5	DMS	A	8425	4/4	0.84	0.22	1.89	37,55,76,100	0
5	DMS	C	8602	4/4	0.92	0.14	1.73	21,61,62,71	0
5	DMS	D	8402	4/4	0.97	0.10	1.71	17,20,21,22	0
5	DMS	A	8501	4/4	0.92	0.13	1.68	20,25,31,36	0
5	DMS	B	8423	4/4	0.94	0.11	1.57	46,55,57,100	0
5	DMS	C	8410	4/4	0.96	0.13	1.47	24,36,40,80	0
5	DMS	A	8401	4/4	0.99	0.10	1.45	13,14,15,16	0
5	DMS	B	8408	4/4	0.96	0.12	1.41	27,28,35,59	0
5	DMS	A	8403	4/4	0.96	0.11	1.36	22,26,29,32	0
5	DMS	D	8701	4/4	0.97	0.11	1.32	16,18,20,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	C	8402	4/4	0.97	0.10	1.09	18,18,26,30	0
5	DMS	A	8408	4/4	0.94	0.10	1.04	17,35,41,100	0
5	DMS	B	8401	4/4	0.99	0.09	1.01	18,19,20,20	0
5	DMS	B	8405	4/4	0.95	0.09	0.97	23,30,31,32	0
3	NA	A	3104	1/1	0.88	0.12	0.89	30,30,30,30	0
5	DMS	B	8504	4/4	0.96	0.10	0.73	26,38,43,54	0
3	NA	D	3103	1/1	0.92	0.11	0.69	30,30,30,30	0
5	DMS	B	8404	4/4	0.96	0.08	0.59	23,25,35,55	0
5	DMS	B	8402	4/4	0.96	0.10	0.58	14,15,20,21	0
5	DMS	D	8408	4/4	0.96	0.10	0.53	19,29,31,38	0
5	DMS	D	8411	4/4	0.96	0.12	0.52	29,30,34,100	0
5	DMS	C	8405	4/4	0.96	0.08	0.36	21,26,27,28	0
4	IPT	D	2001	15/15	0.96	0.09	0.36	13,17,22,22	0
5	DMS	B	8412	4/4	0.98	0.08	0.36	25,29,33,35	0
5	DMS	D	8406	4/4	0.97	0.09	0.22	22,25,25,30	0
5	DMS	D	8412	4/4	0.98	0.09	0.07	20,20,30,92	0
3	NA	C	3103	1/1	0.95	0.10	0.02	25,25,25,25	0
5	DMS	D	8506	4/4	0.96	0.11	-0.01	42,52,59,100	0
5	DMS	C	8401	4/4	0.98	0.08	-0.15	16,20,20,27	0
5	DMS	B	8411	4/4	0.96	0.09	-0.37	28,32,38,43	0
4	IPT	A	2001	15/15	0.97	0.09	-0.40	11,16,24,28	0
5	DMS	D	8403	4/4	0.98	0.07	-0.43	20,26,28,36	0
3	NA	B	3103	1/1	0.93	0.10	-0.54	25,25,25,25	0
4	IPT	B	2001	15/15	0.97	0.08	-0.66	14,16,23,27	0
2	MG	D	3002	1/1	0.97	0.07	-0.73	14,14,14,14	0
4	IPT	C	2001	15/15	0.97	0.07	-0.89	14,17,28,28	0
2	MG	C	3002	1/1	0.99	0.06	-0.97	14,14,14,14	0
5	DMS	C	8403	4/4	0.98	0.07	-0.99	21,22,26,29	0
3	NA	C	3102	1/1	0.99	0.06	-1.15	14,14,14,14	0
3	NA	A	3102	1/1	0.97	0.06	-1.32	12,12,12,12	0
2	MG	B	3002	1/1	0.97	0.06	-1.32	15,15,15,15	0
2	MG	A	3002	1/1	0.98	0.06	-1.57	16,16,16,16	0
2	MG	B	3001	1/1	0.98	0.06	-1.75	12,12,12,12	0
2	MG	A	3001	1/1	0.97	0.07	-1.76	15,15,15,15	0
3	NA	A	3101	1/1	0.97	0.08	-1.82	16,16,16,16	0
5	DMS	B	8403	4/4	0.98	0.06	-1.99	22,25,28,30	0
5	DMS	A	8402	4/4	0.98	0.09	-2.20	15,18,21,25	0
3	NA	B	3102	1/1	0.99	0.05	-2.31	12,12,12,12	0
3	NA	D	3102	1/1	0.99	0.05	-2.42	12,12,12,12	0
2	MG	C	3001	1/1	0.99	0.05	-2.67	14,14,14,14	0
5	DMS	C	8408	4/4	0.97	0.06	-2.69	26,28,30,33	0
3	NA	D	3101	1/1	0.96	0.08	-2.76	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	C	3101	1/1	0.98	0.07	-2.78	15,15,15,15	0
2	MG	D	3001	1/1	0.98	0.06	-2.79	13,13,13,13	0
5	DMS	B	8409	4/4	0.93	0.11	-	22,26,44,51	0
2	MG	C	3105	1/1	0.95	0.08	-	28,28,28,28	1
5	DMS	C	8421	4/4	0.97	0.09	-	35,46,47,62	0
5	DMS	B	8601	4/4	0.96	0.10	-	34,36,44,49	0
5	DMS	A	8602	4/4	0.97	0.14	-	31,53,100,100	0
5	DMS	D	8413	4/4	0.92	0.16	-	46,49,51,100	0
5	DMS	B	8414	4/4	0.92	0.13	-	29,54,62,88	0
2	MG	B	3105	1/1	0.78	0.18	-	28,28,28,28	1
5	DMS	A	8421	4/4	0.92	0.21	-	45,52,72,81	0
2	MG	A	3005	1/1	0.95	0.07	-	30,30,30,30	0
5	DMS	C	8504	4/4	0.79	0.17	-	39,52,72,76	0
5	DMS	A	8413	4/4	0.93	0.17	-	34,36,42,47	0
5	DMS	D	8410	4/4	0.97	0.10	-	23,33,34,37	0
5	DMS	A	8409	4/4	0.92	0.13	-	27,29,29,54	0
5	DMS	D	8409	4/4	0.94	0.12	-	27,29,31,37	0
5	DMS	C	8506	4/4	0.92	0.17	-	42,45,48,100	0
5	DMS	A	8503	4/4	0.89	0.15	-	36,51,55,100	0
5	DMS	C	8413	4/4	0.85	0.18	-	49,59,61,97	0
5	DMS	C	8503	4/4	0.87	0.15	-	25,32,50,52	0
2	MG	C	3004	1/1	0.84	0.11	-	53,53,53,53	0
5	DMS	B	8413	4/4	0.77	0.20	-	33,40,53,58	0
5	DMS	C	8601	4/4	0.95	0.15	-	34,44,46,100	0
5	DMS	C	8414	4/4	0.95	0.09	-	20,35,36,43	0
5	DMS	B	8421	4/4	0.90	0.14	-	26,42,54,55	0
5	DMS	D	8416	4/4	0.86	0.22	-	32,43,61,100	0
5	DMS	A	8410	4/4	0.97	0.13	-	33,37,47,61	0
5	DMS	D	8421	4/4	0.93	0.17	-	40,48,96,100	0
5	DMS	D	8703	4/4	0.90	0.15	-	37,48,53,98	0
5	DMS	B	8416	4/4	0.94	0.17	-	37,43,47,100	0
2	MG	D	3005	1/1	0.95	0.07	-	25,25,25,25	0
5	DMS	C	8415	4/4	0.91	0.14	-	25,36,60,100	0
2	MG	C	3006	1/1	0.83	0.17	-	53,53,53,53	0
2	MG	D	3105	1/1	0.77	0.18	-	38,38,38,38	1
5	DMS	D	8414	4/4	0.97	0.12	-	26,42,83,100	0
5	DMS	D	8503	4/4	0.93	0.14	-	28,58,59,61	0
5	DMS	B	8410	4/4	0.91	0.20	-	28,33,34,70	0
5	DMS	C	8409	4/4	0.96	0.10	-	26,38,39,40	0
5	DMS	A	8414	4/4	0.95	0.11	-	24,47,55,91	0
2	MG	A	3105	1/1	0.58	0.90	-	97,97,97,97	1



## 6.5 Other polymers [i](#)

There are no such residues in this entry.