



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2020 – 12:04 PM BST

PDB ID : 1JZ7  
Title : E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH GALACTOSE  
Authors : Juers, D.H.; Matthews, B.W.  
Deposited on : 2001-09-13  
Resolution : 1.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

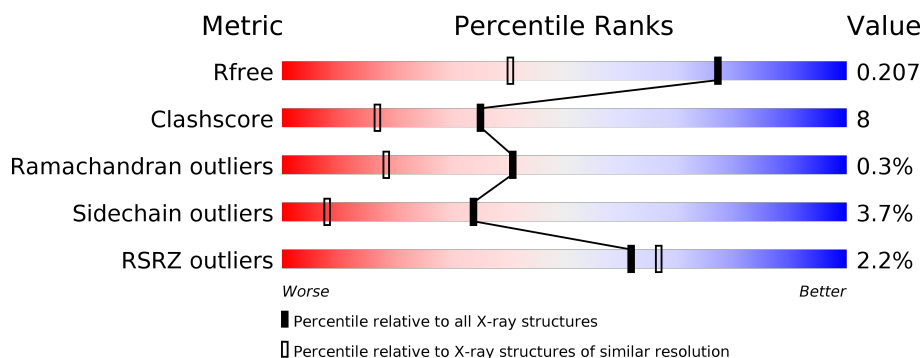
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>.</div> <div>.</div> </div> </div>
1	B	1023	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>.</div> <div>.</div> <div>.</div> </div> </div>
1	C	1023	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>5%</div> <div>.</div> </div> </div>
1	D	1023	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>5%</div> <div>.</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	A	8413	-	X	-	-
5	DMS	B	8407	-	X	-	-
5	DMS	D	8425	-	-	X	-
5	DMS	D	8703	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37213 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	1	0
			8127	5138	1440	1511	38			
1	B	1011	Total	C	N	O	S	0	1	0
			8127	5138	1440	1511	38			
1	C	1011	Total	C	N	O	S	0	1	0
			8127	5138	1440	1511	38			
1	D	1011	Total	C	N	O	S	0	1	0
			8127	5138	1440	1511	38			

There are 36 discrepancies between the modelled and reference sequences:

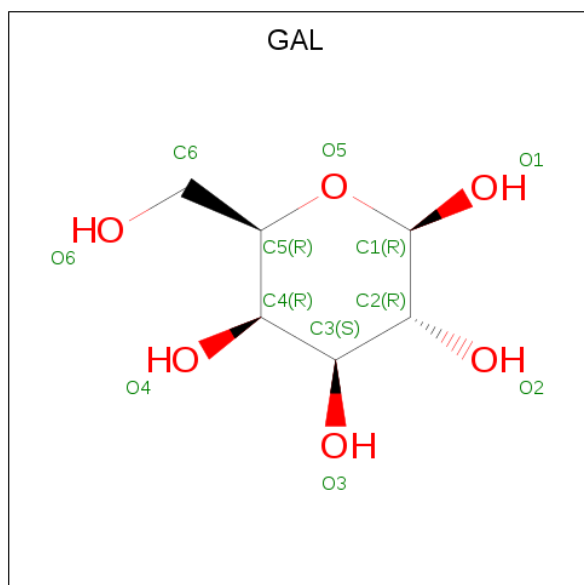
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact	? P00722
A	8	PRO	ALA	cloning artifact	? P00722
A	247	CSO	CYS	modified residue	? P00722
B	1	GLY	THR	cloning artifact	? P00722
B	2	SER	MET	cloning artifact	? P00722
B	3	HIS	ILE	cloning artifact	? P00722
B	4	MET	THR	cloning artifact	? P00722
B	5	LEU	ASP	cloning artifact	? P00722
B	6	GLU	SER	cloning artifact	? P00722
B	7	ASP	LEU	cloning artifact	? P00722
B	8	PRO	ALA	cloning artifact	? P00722
B	247	CSO	CYS	modified residue	? P00722
C	1	GLY	THR	cloning artifact	? P00722
C	2	SER	MET	cloning artifact	? P00722
C	3	HIS	ILE	cloning artifact	? P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	cloning artifact	? P00722
C	5	LEU	ASP	cloning artifact	? P00722
C	6	GLU	SER	cloning artifact	? P00722
C	7	ASP	LEU	cloning artifact	? P00722
C	8	PRO	ALA	cloning artifact	? P00722
C	247	CSO	CYS	modified residue	? P00722
D	1	GLY	THR	cloning artifact	? P00722
D	2	SER	MET	cloning artifact	? P00722
D	3	HIS	ILE	cloning artifact	? P00722
D	4	MET	THR	cloning artifact	? P00722
D	5	LEU	ASP	cloning artifact	? P00722
D	6	GLU	SER	cloning artifact	? P00722
D	7	ASP	LEU	cloning artifact	? P00722
D	8	PRO	ALA	cloning artifact	? P00722
D	247	CSO	CYS	modified residue	? P00722

- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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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	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	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	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	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

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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	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	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	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

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

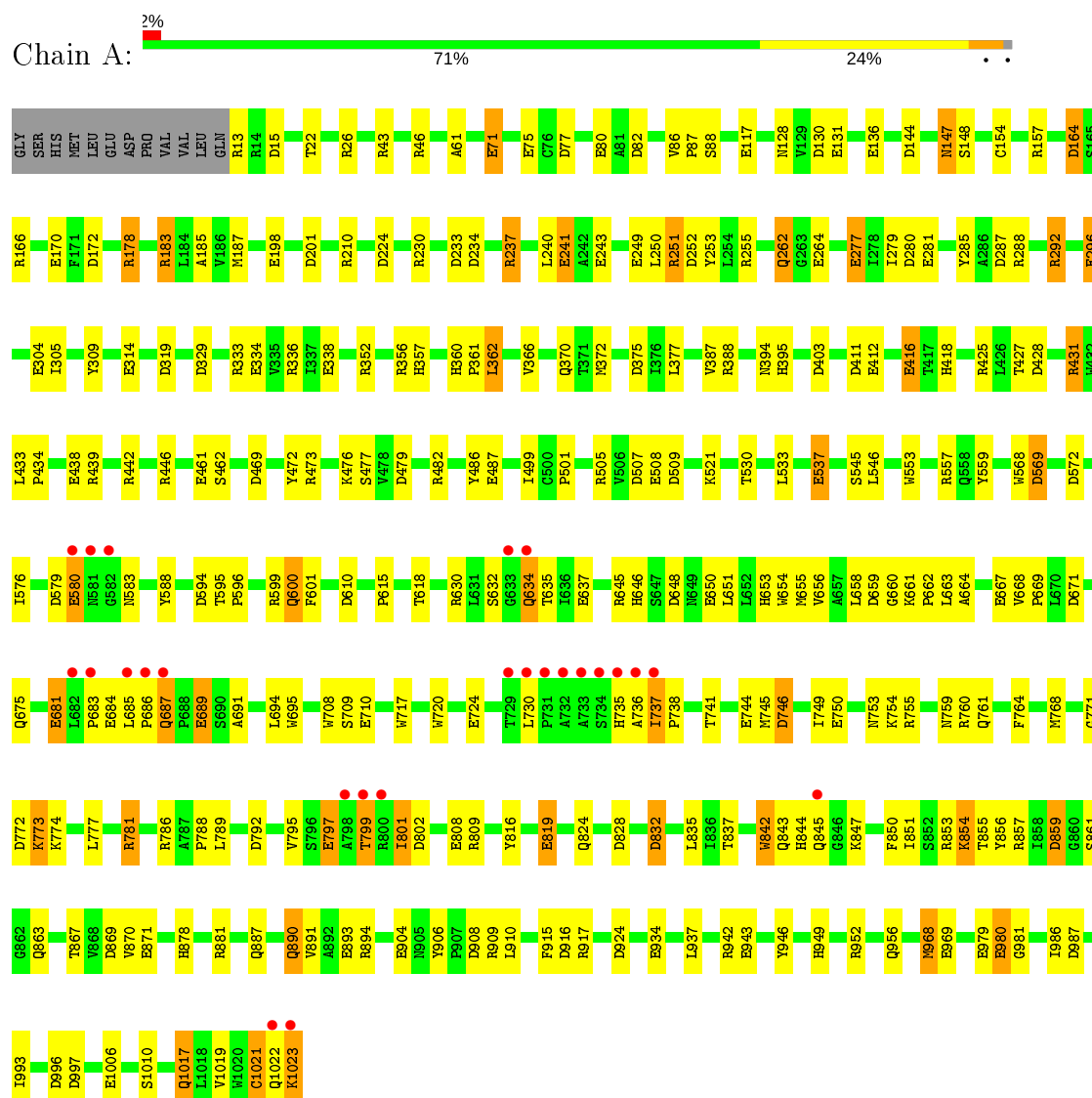
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1054	Total 1054	O 1054	0	0
6	B	1073	Total 1073	O 1073	0	0
6	C	1019	Total 1019	O 1019	0	0
6	D	1068	Total 1068	O 1068	0	0

### 3 Residue-property plots

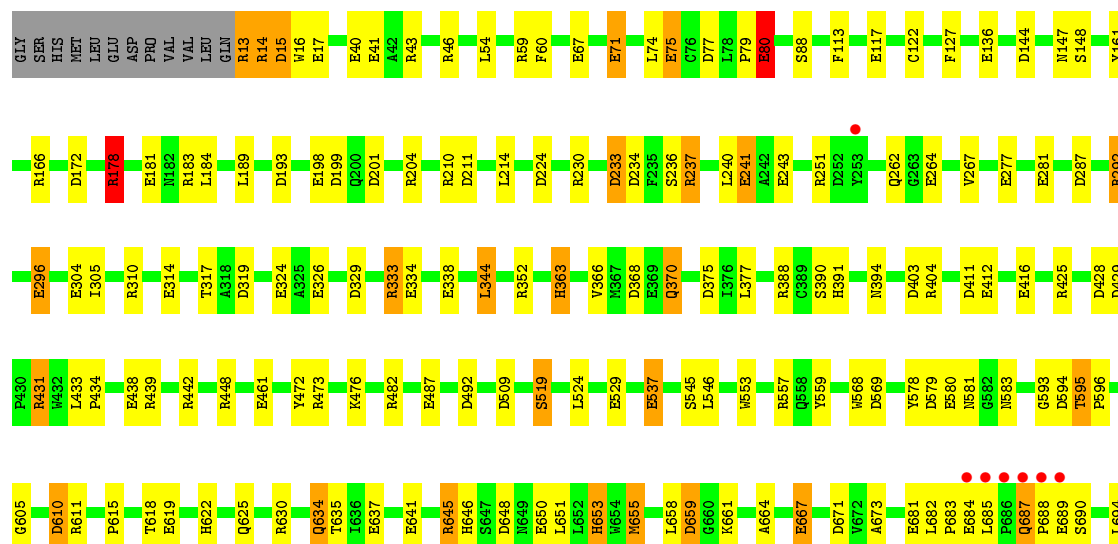
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

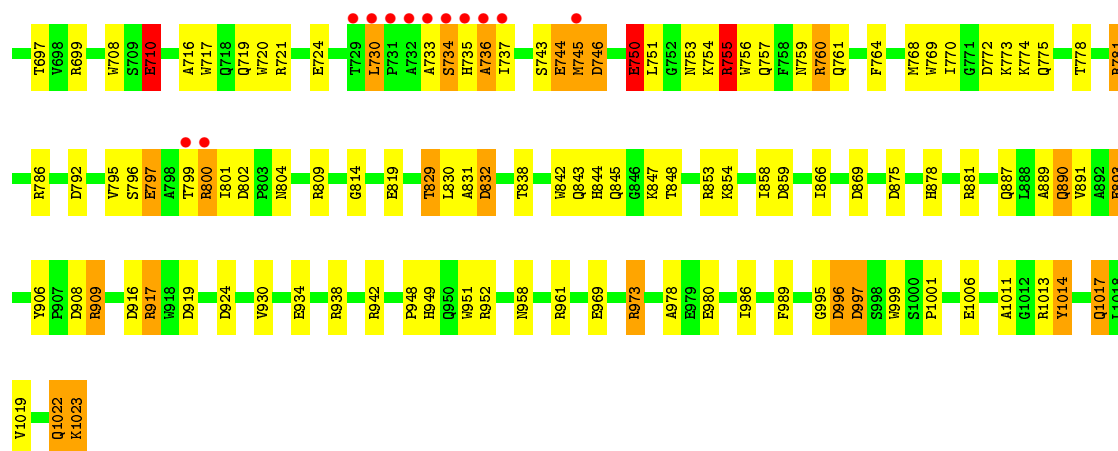
#### • Molecule 1: Beta-Galactosidase



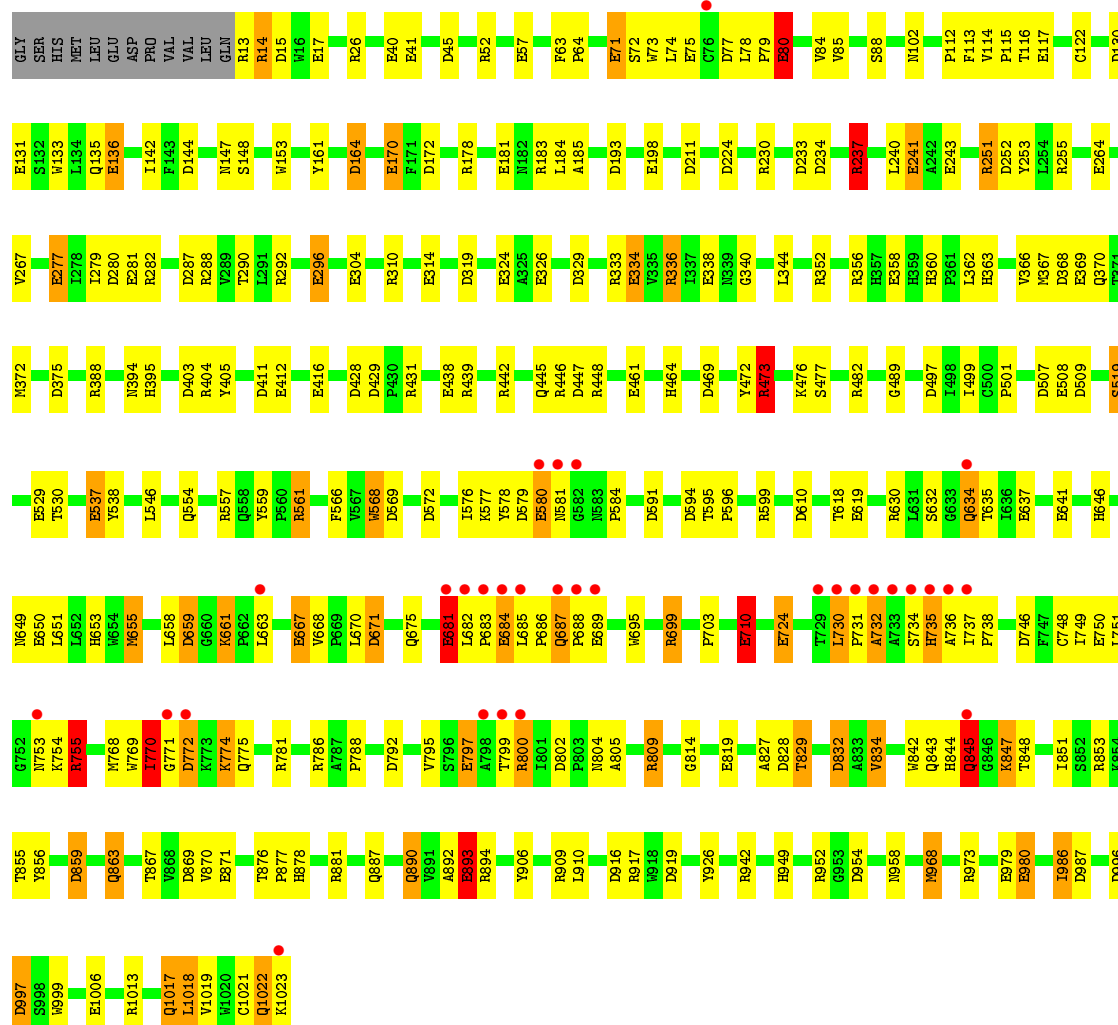
#### • Molecule 1: Beta-Galactosidase







• Molecule 1: Beta-Galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.59Å 168.53Å 200.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.50 35.20 – 1.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (40.00-1.50) 90.9 (35.20-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.50Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.176 , 0.219 0.169 , 0.207	Depositor DCC
$R_{free}$ test set	10970 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 85.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	37213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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 33.85 % 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 7.4923e-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: GAL, NA, CSO, DMS, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.24	48/8360 (0.6%)	1.72	186/11404 (1.6%)
1	B	1.25	44/8360 (0.5%)	1.73	195/11404 (1.7%)
1	C	1.25	52/8360 (0.6%)	1.72	177/11404 (1.6%)
1	D	1.27	58/8360 (0.7%)	1.73	209/11404 (1.8%)
All	All	1.25	202/33440 (0.6%)	1.73	767/45616 (1.7%)

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

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

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	537	GLU	CD-OE2	9.82	1.36	1.25
1	D	893	GLU	CD-OE2	9.78	1.36	1.25
1	D	979	GLU	CD-OE2	9.26	1.35	1.25
1	B	71	GLU	CD-OE2	9.17	1.35	1.25
1	D	136	GLU	CD-OE2	9.16	1.35	1.25
1	C	80	GLU	CD-OE2	8.97	1.35	1.25
1	B	537	GLU	CD-OE2	8.73	1.35	1.25
1	C	304	GLU	CD-OE2	8.69	1.35	1.25
1	B	181	GLU	CD-OE2	8.60	1.35	1.25
1	C	797	GLU	CD-OE2	8.42	1.34	1.25
1	B	281	GLU	CD-OE2	8.40	1.34	1.25
1	D	650	GLU	CD-OE2	8.39	1.34	1.25
1	B	243	GLU	CD-OE2	8.30	1.34	1.25
1	A	537	GLU	CD-OE2	8.23	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	819	GLU	CD-OE2	8.11	1.34	1.25
1	D	619	GLU	CD-OE2	8.11	1.34	1.25
1	B	684	GLU	CD-OE2	8.03	1.34	1.25
1	C	281	GLU	CD-OE2	7.94	1.34	1.25
1	A	281	GLU	CD-OE2	7.83	1.34	1.25
1	B	980	GLU	CD-OE2	7.81	1.34	1.25
1	B	1006	GLU	CD-OE2	7.80	1.34	1.25
1	B	819	GLU	CD-OE2	7.77	1.34	1.25
1	B	650	GLU	CD-OE2	7.72	1.34	1.25
1	B	641	GLU	CD-OE1	-7.69	1.17	1.25
1	D	461	GLU	CD-OE2	7.68	1.34	1.25
1	D	281	GLU	CD-OE2	7.57	1.33	1.25
1	C	71	GLU	CD-OE2	7.56	1.33	1.25
1	B	264	GLU	CD-OE2	7.55	1.33	1.25
1	D	243	GLU	CD-OE2	7.55	1.33	1.25
1	A	71	GLU	CD-OE2	7.53	1.33	1.25
1	C	324	GLU	CD-OE2	7.53	1.33	1.25
1	A	650	GLU	CD-OE2	7.52	1.33	1.25
1	A	117	GLU	CD-OE2	7.51	1.33	1.25
1	C	416	GLU	CD-OE2	7.48	1.33	1.25
1	C	684	GLU	CD-OE2	7.46	1.33	1.25
1	A	170	GLU	CD-OE2	7.46	1.33	1.25
1	A	249	GLU	CD-OE2	7.40	1.33	1.25
1	C	689	GLU	CD-OE2	7.40	1.33	1.25
1	D	412	GLU	CD-OE2	7.38	1.33	1.25
1	B	979	GLU	CD-OE2	7.34	1.33	1.25
1	A	1006	GLU	CD-OE2	7.30	1.33	1.25
1	C	264	GLU	CD-OE2	7.30	1.33	1.25
1	D	117	GLU	CD-OE2	7.29	1.33	1.25
1	A	296	GLU	CD-OE2	7.22	1.33	1.25
1	C	334	GLU	CD-OE2	7.19	1.33	1.25
1	D	681	GLU	CD-OE2	7.17	1.33	1.25
1	A	979	GLU	CD-OE2	7.16	1.33	1.25
1	A	681	GLU	CD-OE2	7.12	1.33	1.25
1	A	724	GLU	CD-OE2	7.11	1.33	1.25
1	B	296	GLU	CD-OE2	7.06	1.33	1.25
1	D	277	GLU	CD-OE2	7.05	1.33	1.25
1	C	980	GLU	CD-OE2	7.05	1.33	1.25
1	D	326	GLU	CD-OE2	7.04	1.33	1.25
1	C	710	GLU	CD-OE2	7.03	1.33	1.25
1	B	969	GLU	CD-OE2	7.00	1.33	1.25
1	C	537	GLU	CD-OE2	6.97	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	641	GLU	CD-OE1	-6.95	1.18	1.25
1	D	684	GLU	CD-OE2	6.94	1.33	1.25
1	D	71	GLU	CD-OE2	6.92	1.33	1.25
1	A	277	GLU	CD-OE2	6.91	1.33	1.25
1	B	667	GLU	CD-OE2	6.88	1.33	1.25
1	D	131	GLU	CD-OE2	6.87	1.33	1.25
1	C	277	GLU	CD-OE2	6.87	1.33	1.25
1	D	580	GLU	CD-OE2	6.86	1.33	1.25
1	D	980	GLU	CD-OE2	6.84	1.33	1.25
1	A	969	GLU	CD-OE2	6.83	1.33	1.25
1	C	893	GLU	CD-OE2	6.83	1.33	1.25
1	D	296	GLU	CD-OE2	6.83	1.33	1.25
1	D	641	GLU	CD-OE1	-6.81	1.18	1.25
1	C	529	GLU	CD-OE2	6.80	1.33	1.25
1	C	181	GLU	CD-OE2	6.79	1.33	1.25
1	B	681	GLU	CD-OE2	6.78	1.33	1.25
1	A	667	GLU	CD-OE2	6.77	1.33	1.25
1	A	904	GLU	CD-OE2	6.74	1.33	1.25
1	B	580	GLU	CD-OE2	6.70	1.33	1.25
1	D	75	GLU	CD-OE2	6.63	1.32	1.25
1	C	1006	GLU	CD-OE2	6.62	1.32	1.25
1	D	264	GLU	CD-OE2	6.60	1.32	1.25
1	D	797	GLU	CD-OE2	6.60	1.32	1.25
1	C	934	GLU	CD-OE2	6.56	1.32	1.25
1	C	241	GLU	CD-OE2	6.53	1.32	1.25
1	A	893	GLU	CD-OE2	6.53	1.32	1.25
1	D	57	GLU	CD-OE2	6.52	1.32	1.25
1	B	117	GLU	CD-OE2	6.50	1.32	1.25
1	A	487	GLU	CD-OE2	6.50	1.32	1.25
1	B	17	GLU	CD-OE2	6.49	1.32	1.25
1	B	277	GLU	CD-OE2	6.49	1.32	1.25
1	D	819	GLU	CD-OE2	6.48	1.32	1.25
1	D	338	GLU	CD-OE2	6.46	1.32	1.25
1	C	296	GLU	CD-OE2	6.44	1.32	1.25
1	D	170	GLU	CD-OE2	6.42	1.32	1.25
1	D	241	GLU	CD-OE2	6.42	1.32	1.25
1	D	416	GLU	CD-OE2	6.41	1.32	1.25
1	D	324	GLU	CD-OE2	6.39	1.32	1.25
1	A	314	GLU	CD-OE2	6.33	1.32	1.25
1	D	198	GLU	CD-OE2	6.31	1.32	1.25
1	D	529	GLU	CD-OE2	6.31	1.32	1.25
1	D	40	GLU	CD-OE2	6.30	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	637	GLU	CD-OE2	6.29	1.32	1.25
1	A	580	GLU	CD-OE2	6.29	1.32	1.25
1	B	710	GLU	CD-OE2	6.27	1.32	1.25
1	C	681	GLU	CD-OE2	6.23	1.32	1.25
1	A	131	GLU	CD-OE2	6.22	1.32	1.25
1	D	710	GLU	CD-OE2	6.21	1.32	1.25
1	D	667	GLU	CD-OE2	6.18	1.32	1.25
1	B	744	GLU	CD-OE2	6.16	1.32	1.25
1	B	136	GLU	CD-OE2	6.15	1.32	1.25
1	A	797	GLU	CD-OE2	6.12	1.32	1.25
1	D	750	GLU	CD-OE2	6.11	1.32	1.25
1	B	487	GLU	CD-OE2	6.10	1.32	1.25
1	A	338	GLU	CD-OE2	6.04	1.32	1.25
1	B	75	GLU	CD-OE2	6.03	1.32	1.25
1	A	264	GLU	CD-OE2	6.02	1.32	1.25
1	B	170	GLU	CD-OE2	6.01	1.32	1.25
1	D	181	GLU	CD-OE2	6.01	1.32	1.25
1	C	75	GLU	CD-OE2	6.01	1.32	1.25
1	C	198	GLU	CD-OE2	6.01	1.32	1.25
1	C	17	GLU	CD-OE2	5.98	1.32	1.25
1	A	412	GLU	CD-OE2	5.97	1.32	1.25
1	C	67	GLU	CD-OE2	5.97	1.32	1.25
1	A	198	GLU	CD-OE2	5.97	1.32	1.25
1	B	438	GLU	CD-OE2	5.96	1.32	1.25
1	B	326	GLU	CD-OE2	5.95	1.32	1.25
1	B	689	GLU	CD-OE2	5.95	1.32	1.25
1	C	667	GLU	CD-OE2	5.93	1.32	1.25
1	A	75	GLU	CD-OE2	5.92	1.32	1.25
1	D	314	GLU	CD-OE2	5.91	1.32	1.25
1	A	304	GLU	CD-OE2	5.90	1.32	1.25
1	A	243	GLU	CD-OE2	5.88	1.32	1.25
1	C	136	GLU	CD-OE2	5.87	1.32	1.25
1	B	893	GLU	CD-OE2	5.85	1.32	1.25
1	B	461	GLU	CD-OE1	-5.84	1.19	1.25
1	C	744	GLU	CD-OE2	5.84	1.32	1.25
1	D	17	GLU	CD-OE2	5.81	1.32	1.25
1	C	750	GLU	CD-OE2	5.80	1.32	1.25
1	B	198	GLU	CD-OE2	5.78	1.32	1.25
1	D	80	GLU	CD-OE2	5.78	1.32	1.25
1	C	243	GLU	CD-OE2	5.77	1.31	1.25
1	B	358	GLU	CD-OE2	5.76	1.31	1.25
1	D	369	GLU	CD-OE1	-5.76	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1006	GLU	CD-OE2	5.72	1.31	1.25
1	D	438	GLU	CD-OE2	5.71	1.31	1.25
1	C	969	GLU	CD-OE1	-5.71	1.19	1.25
1	A	684	GLU	CD-OE2	5.70	1.31	1.25
1	D	689	GLU	CD-OE2	5.69	1.31	1.25
1	C	619	GLU	CD-OE2	5.68	1.31	1.25
1	A	334	GLU	CD-OE2	5.67	1.31	1.25
1	A	241	GLU	CD-OE2	5.66	1.31	1.25
1	A	744	GLU	CD-OE2	5.65	1.31	1.25
1	D	508	GLU	CD-OE2	5.64	1.31	1.25
1	A	689	GLU	CD-OE2	5.64	1.31	1.25
1	A	819	GLU	CD-OE2	5.64	1.31	1.25
1	A	438	GLU	CD-OE2	5.64	1.31	1.25
1	A	80	GLU	CD-OE2	5.62	1.31	1.25
1	D	334	GLU	CD-OE2	5.60	1.31	1.25
1	B	249	GLU	CD-OE2	5.57	1.31	1.25
1	B	41	GLU	CD-OE2	5.55	1.31	1.25
1	C	326	GLU	CD-OE2	5.54	1.31	1.25
1	C	580	GLU	CD-OE2	5.53	1.31	1.25
1	A	710	GLU	CD-OE2	5.52	1.31	1.25
1	B	808	GLU	CD-OE2	5.51	1.31	1.25
1	D	41	GLU	CD-OE2	5.48	1.31	1.25
1	B	80	GLU	CD-OE2	5.47	1.31	1.25
1	D	724	GLU	CD-OE2	5.45	1.31	1.25
1	C	461	GLU	CD-OE2	5.43	1.31	1.25
1	A	934	GLU	CD-OE2	5.43	1.31	1.25
1	C	41	GLU	CD-OE2	5.41	1.31	1.25
1	B	338	GLU	CD-OE2	5.39	1.31	1.25
1	C	637	GLU	CD-OE2	5.39	1.31	1.25
1	B	842	TRP	CD2-CE3	-5.38	1.32	1.40
1	C	724	GLU	CD-OE2	5.35	1.31	1.25
1	A	980	GLU	CD-OE2	5.30	1.31	1.25
1	C	117	GLU	CD-OE2	5.30	1.31	1.25
1	D	568	TRP	CD2-CE2	5.30	1.47	1.41
1	B	304	GLU	CD-OE2	5.29	1.31	1.25
1	A	637	GLU	CD-OE2	5.29	1.31	1.25
1	A	136	GLU	CD-OE2	5.28	1.31	1.25
1	A	508	GLU	CD-OE2	5.27	1.31	1.25
1	D	233	ASP	CG-OD2	5.24	1.37	1.25
1	A	210	ARG	NE-CZ	5.21	1.39	1.33
1	C	650	GLU	CD-OE2	5.19	1.31	1.25
1	A	461	GLU	CD-OE2	5.18	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	GLU	CD-OE2	5.16	1.31	1.25
1	C	40	GLU	CD-OE2	5.14	1.31	1.25
1	D	893	GLU	CB-CG	5.13	1.61	1.52
1	C	314	GLU	CD-OE2	5.12	1.31	1.25
1	C	338	GLU	CD-OE1	-5.12	1.20	1.25
1	D	358	GLU	CD-OE1	-5.12	1.20	1.25
1	C	412	GLU	CD-OE2	5.11	1.31	1.25
1	A	750	GLU	CD-OE1	-5.09	1.20	1.25
1	D	211	ASP	CG-OD2	5.08	1.37	1.25
1	C	461	GLU	CD-OE1	-5.08	1.20	1.25
1	C	487	GLU	CD-OE2	5.07	1.31	1.25
1	B	416	GLU	CD-OE2	5.07	1.31	1.25
1	A	280	ASP	CG-OD2	5.04	1.36	1.25
1	D	871	GLU	CD-OE1	-5.04	1.20	1.25
1	C	210	ARG	NE-CZ	5.03	1.39	1.33
1	C	438	GLU	CD-OE2	5.03	1.31	1.25
1	B	314	GLU	CD-OE2	5.02	1.31	1.25
1	A	461	GLU	CD-OE1	-5.01	1.20	1.25
1	D	304	GLU	CD-OE2	5.01	1.31	1.25
1	D	280	ASP	CG-OD2	5.00	1.36	1.25

All (767) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	687	GLN	C-N-CD	-23.47	68.96	120.60
1	C	809	ARG	NE-CZ-NH1	19.98	130.29	120.30
1	C	579	ASP	CB-CG-OD2	-16.61	103.35	118.30
1	D	781	ARG	NE-CZ-NH1	16.32	128.46	120.30
1	C	809	ARG	NE-CZ-NH2	-15.09	112.76	120.30
1	C	473	ARG	NE-CZ-NH1	14.93	127.77	120.30
1	C	204	ARG	NE-CZ-NH1	14.89	127.74	120.30
1	D	431	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	D	786	ARG	NE-CZ-NH1	13.98	127.29	120.30
1	C	43	ARG	NE-CZ-NH1	13.77	127.19	120.30
1	B	473	ARG	NE-CZ-NH1	13.72	127.16	120.30
1	B	388	ARG	NE-CZ-NH2	-13.68	113.46	120.30
1	B	166	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	B	13	ARG	NE-CZ-NH2	-13.39	113.61	120.30
1	C	645	ARG	NE-CZ-NH2	-13.16	113.72	120.30
1	C	579	ASP	CB-CG-OD1	13.03	130.03	118.30
1	A	233	ASP	CB-CG-OD1	12.84	129.85	118.30
1	A	442	ARG	NE-CZ-NH2	-12.76	113.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH2	-12.74	113.93	120.30
1	C	224	ASP	CB-CG-OD1	12.69	129.72	118.30
1	B	368	ASP	CB-CG-OD1	12.51	129.56	118.30
1	A	388	ARG	NE-CZ-NH2	-12.51	114.05	120.30
1	B	611	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	A	233	ASP	CB-CG-OD2	-12.18	107.34	118.30
1	B	579	ASP	CB-CG-OD1	12.03	129.12	118.30
1	B	233	ASP	CB-CG-OD1	12.02	129.12	118.30
1	B	46	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	D	388	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	D	909	ARG	NE-CZ-NH2	-11.85	114.38	120.30
1	C	442	ARG	NE-CZ-NH2	-11.85	114.38	120.30
1	C	448	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	251	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	224	ASP	CB-CG-OD1	11.54	128.69	118.30
1	A	746	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	B	368	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	D	288	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	A	881	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	B	336	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	C	233	ASP	CB-CG-OD1	11.35	128.52	118.30
1	A	671	ASP	CB-CG-OD2	-11.35	108.09	118.30
1	A	336	ARG	NE-CZ-NH1	11.33	125.97	120.30
1	D	172	ASP	CB-CG-OD2	-11.30	108.13	118.30
1	D	952	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	B	431	ARG	NE-CZ-NH2	-11.19	114.71	120.30
1	C	431	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	A	505	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	C	204	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	D	630	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	B	473	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	C	909	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	A	755	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	D	579	ASP	CB-CG-OD2	-10.74	108.64	118.30
1	B	224	ASP	CB-CG-OD1	10.73	127.96	118.30
1	C	492	ASP	CB-CG-OD2	-10.70	108.67	118.30
1	B	425	ARG	NE-CZ-NH2	-10.69	114.95	120.30
1	D	237	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	D	336	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	130	ASP	CB-CG-OD2	-10.43	108.91	118.30
1	C	183	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	B	356	ARG	NE-CZ-NH1	10.32	125.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	429	ASP	CB-CG-OD1	10.25	127.53	118.30
1	A	428	ASP	CB-CG-OD1	10.24	127.52	118.30
1	A	917	ARG	NE-CZ-NH1	-10.22	115.19	120.30
1	D	699	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	D	917	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	A	442	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	D	980	GLU	C-N-CA	-10.07	101.16	122.30
1	D	786	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	B	671	ASP	CB-CG-OD2	-10.02	109.28	118.30
1	A	336	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	809	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	C	43	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	B	288	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	C	473	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	A	292	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	B	557	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	C	442	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	D	578	TYR	CB-CG-CD2	-9.89	115.07	121.00
1	A	509	ASP	CB-CG-OD1	9.85	127.17	118.30
1	D	439	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	D	428	ASP	CB-CG-OD1	9.83	127.15	118.30
1	D	755	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	C	428	ASP	CB-CG-OD1	9.79	127.11	118.30
1	C	996	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	B	557	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	699	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	B	252	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	A	859	ASP	CB-CG-OD1	9.64	126.98	118.30
1	D	800	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	C	388	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	D	429	ASP	CB-CG-OD2	-9.58	109.67	118.30
1	B	492	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	A	859	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	C	832	ASP	CB-CG-OD2	-9.51	109.74	118.30
1	A	579	ASP	CB-CG-OD1	9.49	126.84	118.30
1	D	942	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	559	TYR	CB-CG-CD2	-9.45	115.33	121.00
1	B	802	ASP	CB-CG-OD1	9.45	126.81	118.30
1	A	477	SER	N-CA-CB	9.43	124.65	110.50
1	B	611	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	D	828	ASP	CB-CG-OD2	-9.41	109.83	118.30
1	B	319	ASP	CB-CG-OD1	9.39	126.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	579	ASP	CB-CG-OD1	9.39	126.75	118.30
1	C	166	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	C	352	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	130	ASP	CB-CG-OD1	9.36	126.73	118.30
1	A	768	MET	CA-CB-CG	9.32	129.14	113.30
1	D	431	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	C	425	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	D	746	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	C	699	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	B	630	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	252	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	C	659	ASP	CB-CG-OD1	9.11	126.50	118.30
1	C	425	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	234	ASP	CB-CG-OD1	9.04	126.44	118.30
1	D	469	ASP	CB-CG-OD1	9.04	126.43	118.30
1	C	352	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	B	579	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	D	446	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	D	996	ASP	CB-CG-OD2	-9.02	110.19	118.30
1	D	987	ASP	CB-CG-OD1	9.01	126.41	118.30
1	D	469	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	C	909	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	C	952	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	D	45	ASP	CB-CG-OD1	8.91	126.32	118.30
1	A	431	ARG	NE-CZ-NH2	8.89	124.75	120.30
1	D	375	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	C	942	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	D	356	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	B	428	ASP	CB-CG-OD1	8.88	126.29	118.30
1	D	255	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	B	172	ASP	CB-CG-OD1	8.86	126.27	118.30
1	B	919	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	C	648	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	B	469	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	A	482	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	924	ASP	CB-CG-OD1	8.79	126.21	118.30
1	A	230	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	26	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	832	ASP	CB-CG-OD2	-8.75	110.42	118.30
1	B	746	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	B	442	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	C	428	ASP	CB-CG-OD2	-8.69	110.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	610	ASP	CB-CG-OD1	8.67	126.11	118.30
1	B	755	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	D	183	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	D	802	ASP	CB-CG-OD2	-8.61	110.56	118.30
1	D	251	ARG	CD-NE-CZ	8.59	135.63	123.60
1	A	469	ASP	CB-CG-OD1	8.57	126.01	118.30
1	D	144	ASP	CB-CG-OD1	8.56	126.01	118.30
1	B	469	ASP	CB-CG-OD1	8.56	126.01	118.30
1	A	610	ASP	CB-CG-OD1	8.55	126.00	118.30
1	C	404	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	C	473	ARG	CD-NE-CZ	8.54	135.56	123.60
1	C	557	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	288	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	D	561	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	A	579	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	D	329	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	D	439	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	C	961	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	772	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	C	938	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	A	987	ASP	CB-CG-OD1	8.43	125.89	118.30
1	B	648	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	599	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	B	648	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	C	201	ASP	CB-CG-OD2	-8.37	110.76	118.30
1	D	404	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	D	942	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	439	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	875	ASP	CB-CG-OD1	8.34	125.81	118.30
1	C	578	TYR	CB-CG-CD1	-8.33	116.00	121.00
1	C	908	ASP	CB-CG-OD1	8.33	125.80	118.30
1	C	368	ASP	CB-CG-OD1	8.32	125.79	118.30
1	C	46	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	D	497	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	428	ASP	CB-CG-OD2	-8.31	110.83	118.30
1	B	559	TYR	CB-CG-CD1	8.29	125.97	121.00
1	B	671	ASP	CB-CG-OD1	8.27	125.75	118.30
1	C	786	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	B	319	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	D	768	MET	CG-SD-CE	8.23	113.38	100.20
1	C	996	ASP	CB-CG-OD1	8.22	125.70	118.30
1	C	809	ARG	CD-NE-CZ	8.22	135.11	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	469	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	A	288	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	D	230	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	D	802	ASP	CB-CG-OD1	8.13	125.61	118.30
1	B	802	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	A	916	ASP	CB-CG-OD1	8.10	125.59	118.30
1	B	594	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	659	ASP	CB-CG-OD1	8.07	125.57	118.30
1	B	251	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	C	917	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	A	509	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	C	659	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	D	411	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	C	233	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	A	172	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	D	755	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	B	924	ASP	CB-CG-OD1	7.99	125.49	118.30
1	B	832	ASP	CB-CG-OD1	7.97	125.47	118.30
1	B	996	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	A	13	ARG	N-CA-CB	7.93	124.88	110.60
1	A	894	ARG	NE-CZ-NH1	-7.93	116.34	120.30
1	D	164	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	46	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	D	671	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	B	559	TYR	CB-CG-CD2	-7.89	116.27	121.00
1	B	204	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	B	659	ASP	CA-CB-CG	-7.87	96.09	113.40
1	C	439	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	D	26	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	B	919	ASP	CB-CG-OD1	7.84	125.36	118.30
1	D	699	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	D	869	ASP	CB-CG-OD1	7.83	125.35	118.30
1	B	733	ALA	CB-CA-C	7.83	121.84	110.10
1	B	908	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	997	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	1021	CYS	CA-CB-SG	-7.79	99.97	114.00
1	C	721	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	C	881	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	D	442	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	958	ASN	N-CA-CB	7.76	124.56	110.60
1	C	310	ARG	NE-CZ-NH1	7.75	124.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ASP	CB-CG-OD2	-7.75	111.33	118.30
1	D	919	ASP	CB-CG-OD2	-7.75	111.33	118.30
1	A	319	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	C	509	ASP	CB-CG-OD1	7.71	125.24	118.30
1	D	881	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	43	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	699	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	B	908	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	C	906	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	D	368	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	234	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	594	ASP	CB-CG-OD1	7.59	125.13	118.30
1	D	1013	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	C	509	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	D	15	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	C	645	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	507	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	B	792	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	D	352	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	D	853	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	287	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	C	13	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	C	916	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	828	ASP	CB-CG-OD1	7.47	125.03	118.30
1	D	442	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	C	859	ASP	CB-CG-OD1	7.46	125.01	118.30
1	D	859	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	D	252	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	D	172	ASP	CB-CG-OD1	7.41	124.97	118.30
1	B	792	ASP	CB-CG-OD1	7.41	124.97	118.30
1	D	234	ASP	CB-CG-OD1	7.39	124.95	118.30
1	C	224	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	B	1018	LEU	CB-CA-C	-7.38	96.19	110.20
1	B	479	ASP	CB-CG-OD1	7.37	124.94	118.30
1	C	230	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	201	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	C	59	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	B	356	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	D	909	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	B	425	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	486	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	D	282	ARG	NE-CZ-NH2	-7.32	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	D	1018	LEU	CB-CA-C	-7.30	96.33	110.20
1	C	875	ASP	CB-CG-OD1	7.29	124.86	118.30
1	D	987	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	D	193	ASP	CB-CG-OD1	7.28	124.85	118.30
1	D	403	ASP	CB-CG-OD1	7.28	124.85	118.30
1	D	507	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	B	1013	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	C	172	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	781	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	230	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	C	802	ASP	CB-CG-OD1	7.25	124.83	118.30
1	B	473	ARG	CD-NE-CZ	7.24	133.74	123.60
1	A	329	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	C	832	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	171	PHE	CB-CG-CD2	-7.22	115.75	120.80
1	A	13	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	B	234	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	77	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	D	224	ASP	CB-CG-OD1	7.18	124.77	118.30
1	B	59	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	C	924	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	968	MET	CA-CB-CG	7.18	125.51	113.30
1	A	439	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	C	557	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	15	ASP	CB-CG-OD1	7.16	124.74	118.30
1	C	800	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	572	ASP	CB-CG-OD1	7.15	124.73	118.30
1	B	15	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	411	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	741	THR	CA-CB-CG2	-7.14	102.41	112.40
1	A	755	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	C	403	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	D	164	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	164	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	B	77	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	429	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	569	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	894	ARG	NE-CZ-NH2	7.09	123.85	120.30
1	B	429	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	D	996	ASP	CB-CG-OD1	7.06	124.66	118.30
1	C	144	ASP	CB-CG-OD1	7.06	124.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	973	ARG	NE-CZ-NH1	-7.05	116.77	120.30
1	A	164	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	352	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	287	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	377	LEU	CB-CG-CD2	7.03	122.96	111.00
1	A	996	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	C	310	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	B	509	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	519	SER	N-CA-CB	-7.01	99.98	110.50
1	D	130	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	786	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	721	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	D	14	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	671	ASP	CB-CG-OD1	6.94	124.55	118.30
1	A	411	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	B	367	MET	CG-SD-CE	6.92	111.27	100.20
1	B	105	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	C	267	VAL	CA-CB-CG2	-6.90	100.56	110.90
1	A	916	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	D	772	ASP	CB-CG-OD2	-6.88	112.10	118.30
1	A	786	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	781	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	630	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	D	411	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	329	ASP	CB-CG-OD1	6.83	124.45	118.30
1	B	375	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	D	1018	LEU	CB-CG-CD1	-6.83	99.39	111.00
1	C	136	GLU	CB-CA-C	-6.82	96.75	110.40
1	D	578	TYR	CB-CG-CD1	6.82	125.09	121.00
1	A	505	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	D	403	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	22	THR	CA-CB-CG2	-6.81	102.87	112.40
1	C	853	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	336	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	996	ASP	CB-CG-OD1	6.79	124.41	118.30
1	D	572	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	362	LEU	CA-CB-CG	-6.75	99.77	115.30
1	C	746	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	D	288	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	524	LEU	CB-CG-CD1	-6.73	99.56	111.00
1	D	792	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	924	ASP	CB-CG-OD2	-6.72	112.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ASP	CB-CG-OD1	6.71	124.33	118.30
1	A	828	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	D	610	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	96	ASP	CB-CG-OD2	-6.68	112.28	118.30
1	D	233	ASP	CB-CG-OD1	6.67	124.30	118.30
1	D	832	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	C	363	HIS	CA-CB-CG	-6.67	102.27	113.60
1	B	224	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	D	13	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	557	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	B	869	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	230	ARG	CD-NE-CZ	6.65	132.91	123.60
1	B	894	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	D	997	ASP	CB-CG-OD1	6.64	124.28	118.30
1	D	161	TYR	CZ-CE2-CD2	-6.63	113.83	119.80
1	D	448	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	285	TYR	CB-CG-CD2	-6.59	117.04	121.00
1	A	185	ALA	N-CA-CB	6.58	119.32	110.10
1	A	772	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	B	13	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	C	13	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	569	ASP	CB-CG-OD1	6.55	124.19	118.30
1	D	781	ARG	CD-NE-CZ	6.55	132.76	123.60
1	B	842	TRP	CA-CB-CG	-6.53	101.30	113.70
1	D	14	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	D	77	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	538	TYR	CG-CD2-CE2	6.52	126.51	121.30
1	D	958	ASN	N-CA-CB	6.51	122.32	110.60
1	D	926	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	C	183	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	771	GLY	N-CA-C	-6.50	96.86	113.10
1	D	52	ARG	CB-CA-C	-6.50	97.40	110.40
1	D	15	ASP	CB-CG-OD1	6.49	124.14	118.30
1	C	368	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	D	193	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	760	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	15	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	561	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	746	ASP	CB-CG-OD1	6.47	124.13	118.30
1	C	938	ARG	NE-CZ-NH2	6.47	123.54	120.30
1	D	594	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	287	ASP	CB-CG-OD2	-6.46	112.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	482	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	D	671	ASP	CB-CG-OD1	6.44	124.09	118.30
1	D	116	THR	CA-CB-CG2	-6.44	103.39	112.40
1	A	942	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	987	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	C	973	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	D	559	TYR	CB-CG-CD1	6.42	124.85	121.00
1	C	746	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	859	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	D	770	ILE	N-CA-C	-6.41	93.68	111.00
1	A	942	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	916	ASP	CB-CG-OD1	6.40	124.06	118.30
1	C	77	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	610	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	329	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	193	ASP	CB-CG-OD1	6.36	124.03	118.30
1	C	648	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	695	TRP	CB-CA-C	-6.35	97.69	110.40
1	A	292	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	183	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	B	33	PHE	CB-CG-CD1	-6.33	116.37	120.80
1	D	497	ASP	CB-CG-OD1	6.32	123.99	118.30
1	D	352	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	224	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	D	916	ASP	CB-CG-OD1	6.31	123.98	118.30
1	C	482	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	144	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	C	961	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	557	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	893	GLU	CA-CB-CG	-6.28	99.59	113.40
1	C	829	THR	CA-CB-CG2	-6.28	103.61	112.40
1	B	987	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	507	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	B	568	TRP	CA-CB-CG	-6.26	101.81	113.70
1	B	691	ALA	CB-CA-C	-6.24	100.74	110.10
1	C	578	TYR	CB-CG-CD2	6.24	124.74	121.00
1	C	172	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	204	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	356	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	D	77	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	B	610	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	B	128	ASN	CB-CA-C	-6.20	97.99	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	45	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	B	909	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	1019	VAL	CA-CB-CG2	-6.20	101.61	110.90
1	C	519	SER	N-CA-CB	-6.19	101.21	110.50
1	A	802	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	831	ALA	CB-CA-C	-6.19	100.82	110.10
1	D	746	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	74	LEU	CB-CG-CD1	-6.18	100.49	111.00
1	D	695	TRP	CB-CA-C	-6.18	98.05	110.40
1	B	252	ASP	CB-CG-OD1	6.17	123.85	118.30
1	D	893	GLU	CB-CG-CD	6.16	130.83	114.20
1	C	15	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	D	859	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	82	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	772	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	131	GLU	N-CA-CB	-6.14	99.54	110.60
1	D	405	TYR	CB-CG-CD1	-6.14	117.31	121.00
1	B	497	ASP	CB-CG-OD1	6.14	123.83	118.30
1	C	113	PHE	CB-CG-CD2	-6.14	116.50	120.80
1	A	425	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	997	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	733	ALA	N-CA-CB	6.13	118.69	110.10
1	C	411	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	438	GLU	CG-CD-OE2	-6.13	106.05	118.30
1	D	230	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	559	TYR	CG-CD2-CE2	-6.12	116.41	121.30
1	D	233	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	C	237	ARG	CA-CB-CG	-6.11	99.97	113.40
1	D	856	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	A	908	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	688	PRO	N-CA-CB	6.09	110.61	103.30
1	A	691	ALA	CB-CA-C	-6.09	100.97	110.10
1	C	199	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	45	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	45	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	688	PRO	CA-C-N	-6.07	103.84	117.20
1	A	13	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	997	ASP	CB-CG-OD1	6.05	123.74	118.30
1	D	234	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	D	591	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	1014	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	C	760	ARG	NE-CZ-NH2	-6.03	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	GLU	CG-CD-OE1	6.03	130.36	118.30
1	A	166	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	429	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	D	178	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	237	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	287	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	252	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	943	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	D	986	ILE	CG1-CB-CG2	-5.99	98.22	111.40
1	C	375	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	583	ASN	CA-CB-CG	-5.99	100.23	113.40
1	B	1013	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	659	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	362	LEU	CA-CB-CG	-5.98	101.55	115.30
1	D	473	ARG	CD-NE-CZ	5.98	131.97	123.60
1	A	588	TYR	CD1-CE1-CZ	-5.97	114.42	119.80
1	C	781	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	C	760	ARG	CG-CD-NE	-5.97	99.26	111.80
1	C	736	ALA	CB-CA-C	-5.96	101.16	110.10
1	D	681	GLU	N-CA-CB	5.96	121.33	110.60
1	C	869	ASP	CB-CG-OD1	5.95	123.66	118.30
1	C	755	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	D	477	SER	N-CA-CB	5.95	119.42	110.50
1	B	996	ASP	CB-CG-OD1	5.95	123.65	118.30
1	D	919	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	890	GLN	N-CA-CB	-5.91	99.96	110.60
1	A	853	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	178	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	264	GLU	OE1-CD-OE2	5.90	130.38	123.30
1	B	172	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	856	TYR	CG-CD2-CE2	-5.89	116.59	121.30
1	D	224	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	486	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	C	178	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	926	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	C	733	ALA	CB-CA-C	5.87	118.90	110.10
1	B	225	PHE	CB-CG-CD1	-5.85	116.70	120.80
1	A	869	ASP	CB-CG-OD1	5.85	123.57	118.30
1	C	333	ARG	CG-CD-NE	5.85	124.09	111.80
1	D	267	VAL	N-CA-CB	-5.85	98.63	111.50
1	A	230	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	C	287	ASP	CB-CG-OD1	5.84	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	280	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	D	473	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	559	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	A	986	ILE	CG1-CB-CG2	-5.83	98.56	111.40
1	C	333	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	77	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	772	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	997	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	446	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	130	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	D	735	HIS	N-CA-CB	-5.79	100.18	110.60
1	C	854	LYS	CB-CA-C	-5.78	98.84	110.40
1	D	559	TYR	CZ-CE2-CD2	5.77	124.99	119.80
1	B	431	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	344	LEU	CA-CB-CG	-5.75	102.07	115.30
1	C	287	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	C	431	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	255	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	161	TYR	CG-CD1-CE1	-5.73	116.72	121.30
1	C	949	HIS	CB-CA-C	-5.71	98.97	110.40
1	D	853	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	659	ASP	CB-CG-OD2	-5.71	113.17	118.30
1	C	403	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	594	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	184	LEU	CB-CA-C	-5.70	99.37	110.20
1	D	144	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	519	SER	N-CA-CB	-5.69	101.96	110.50
1	D	14	ARG	N-CA-CB	-5.69	100.36	110.60
1	B	1014	TYR	CG-CD2-CE2	-5.69	116.75	121.30
1	C	845	GLN	C-N-CA	-5.68	110.37	122.30
1	D	827	ALA	N-CA-CB	5.68	118.05	110.10
1	C	924	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	D	856	TYR	CG-CD2-CE2	-5.68	116.76	121.30
1	C	1014	TYR	CG-CD2-CE2	-5.67	116.76	121.30
1	B	853	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	D	416	GLU	CG-CD-OE2	-5.67	106.96	118.30
1	A	147	ASN	N-CA-CB	-5.67	100.39	110.60
1	A	178	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	572	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	356	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	557	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	869	ASP	CB-CG-OD2	-5.65	113.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	SER	N-CA-CB	5.64	118.97	110.50
1	B	800	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	832	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	786	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	333	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	816	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	D	559	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	D	594	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	277	GLU	N-CA-CB	-5.61	100.50	110.60
1	C	720	TRP	CB-CA-C	-5.60	99.19	110.40
1	C	733	ALA	C-N-CA	5.60	135.70	121.70
1	D	161	TYR	CG-CD2-CE2	5.58	125.77	121.30
1	B	748	CYS	CA-CB-SG	-5.58	103.95	114.00
1	D	632	SER	N-CA-CB	5.57	118.86	110.50
1	B	596	PRO	CA-N-CD	5.56	119.48	111.70
1	B	881	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	795	VAL	CG1-CB-CG2	-5.56	102.01	110.90
1	D	310	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	610	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	670	LEU	CB-CA-C	-5.54	99.68	110.20
1	B	338	GLU	CG-CD-OE2	-5.53	107.24	118.30
1	D	809	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	746	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	832	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	438	GLU	CG-CD-OE2	-5.52	107.26	118.30
1	B	748	CYS	N-CA-CB	5.51	120.53	110.60
1	C	594	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	926	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	710	GLU	CB-CA-C	-5.50	99.40	110.40
1	C	772	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	781	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	352	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	917	ARG	CD-NE-CZ	-5.50	115.91	123.60
1	A	802	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	D	447	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C	201	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C	251	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	800	ARG	N-CA-CB	5.48	120.46	110.60
1	A	856	TYR	CD1-CE1-CZ	-5.48	114.87	119.80
1	A	403	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	A	416	GLU	CG-CD-OE2	-5.46	107.37	118.30
1	B	1022	GLN	CA-CB-CG	-5.46	101.38	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ALA	N-CA-CB	-5.46	102.46	110.10
1	A	890	GLN	N-CA-CB	-5.45	100.79	110.60
1	B	942	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	781	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	968	MET	N-CA-CB	-5.44	100.80	110.60
1	A	853	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	161	TYR	N-CA-CB	-5.43	100.83	110.60
1	C	292	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	997	ASP	N-CA-CB	5.42	120.36	110.60
1	A	479	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	251	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	329	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	157	ARG	CG-CD-NE	5.41	123.17	111.80
1	B	403	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	908	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	61	ALA	N-CA-CB	5.40	117.66	110.10
1	C	482	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	388	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	538	TYR	CB-CG-CD2	5.39	124.24	121.00
1	B	161	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	C	671	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	C	473	ARG	CG-CD-NE	-5.38	100.49	111.80
1	D	185	ALA	N-CA-CB	5.38	117.64	110.10
1	D	85	VAL	CA-CB-CG2	-5.38	102.83	110.90
1	A	553	TRP	CA-CB-CG	-5.38	103.48	113.70
1	B	388	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	746	ASP	CB-CA-C	-5.38	99.65	110.40
1	D	367	MET	CG-SD-CE	5.37	108.80	100.20
1	D	375	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	734	SER	CA-C-O	5.37	131.37	120.10
1	A	128	ASN	CB-CA-C	-5.36	99.69	110.40
1	C	13	ARG	CG-CD-NE	-5.35	100.56	111.80
1	A	771	GLY	C-N-CA	-5.35	108.33	121.70
1	C	958	ASN	N-CA-CB	5.35	120.22	110.60
1	D	388	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	184	LEU	CB-CA-C	-5.34	100.06	110.20
1	B	986	ILE	CB-CA-C	5.33	122.27	111.60
1	C	842	TRP	CH2-CZ2-CE2	-5.33	112.07	117.40
1	A	746	ASP	CB-CA-C	-5.33	99.74	110.40
1	C	193	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	183	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	C	211	ASP	CB-CG-OD2	-5.33	113.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	280	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	772	ASP	N-CA-CB	5.33	120.19	110.60
1	A	832	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	869	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	C	792	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	889	ALA	N-CA-CB	-5.32	102.66	110.10
1	D	319	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	507	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	290	THR	CA-CB-CG2	-5.30	104.98	112.40
1	B	262	GLN	CB-CA-C	5.29	120.98	110.40
1	B	720	TRP	CB-CA-C	-5.29	99.82	110.40
1	B	875	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	D	952	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	688	PRO	O-C-N	5.28	131.16	122.70
1	A	720	TRP	CB-CA-C	-5.28	99.85	110.40
1	B	987	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	201	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	842	TRP	CG-CD2-CE3	-5.27	129.16	133.90
1	B	96	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	77	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	695	TRP	CB-CA-C	-5.26	99.87	110.40
1	B	797	GLU	CG-CD-OE2	-5.26	107.77	118.30
1	C	768	MET	N-CA-CB	5.26	120.07	110.60
1	D	599	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	370	GLN	CB-CG-CD	5.25	125.25	111.60
1	A	154	CYS	CA-CB-SG	-5.25	104.56	114.00
1	D	772	ASP	CB-CG-OD1	5.24	123.01	118.30
1	B	538	TYR	CZ-CE2-CD2	-5.23	115.09	119.80
1	A	546	LEU	N-CA-CB	5.22	120.85	110.40
1	B	429	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	842	TRP	CD1-NE1-CE2	-5.22	104.30	109.00
1	C	329	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	161	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	D	405	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	D	538	TYR	CB-CG-CD2	5.21	124.13	121.00
1	C	553	TRP	CA-CB-CG	-5.21	103.81	113.70
1	D	277	GLU	N-CA-CB	-5.20	101.23	110.60
1	D	280	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	416	GLU	CG-CD-OE1	5.20	128.69	118.30
1	B	379	MET	CA-CB-CG	-5.20	104.47	113.30
1	D	845	GLN	C-N-CA	-5.19	111.41	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	659	ASP	CA-CB-CG	-5.18	102.00	113.40
1	B	100	TYR	CA-CB-CG	-5.17	103.57	113.40
1	B	147	ASN	N-CA-CB	-5.17	101.29	110.60
1	B	572	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	C	890	GLN	N-CA-CB	-5.17	101.29	110.60
1	D	178	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	924	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	A	599	ARG	NH1-CZ-NH2	5.16	125.07	119.40
1	A	768	MET	N-CA-CB	5.16	119.88	110.60
1	B	507	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	842	TRP	CB-CA-C	-5.16	100.09	110.40
1	D	949	HIS	CB-CA-C	-5.16	100.09	110.40
1	B	509	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	405	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	C	786	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	164	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	997	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	630	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	699	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	675	GLN	CA-CB-CG	-5.14	102.09	113.40
1	C	375	ASP	CB-CG-OD1	5.14	122.92	118.30
1	C	842	TRP	CE2-CD2-CE3	5.13	124.86	118.70
1	C	431	ARG	CA-CB-CG	-5.12	102.13	113.40
1	C	724	GLU	CB-CA-C	-5.12	100.15	110.40
1	D	287	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	221	GLN	N-CA-CB	-5.11	101.40	110.60
1	C	734	SER	N-CA-C	5.11	124.80	111.00
1	A	792	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	906	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	C	838	THR	CA-CB-CG2	-5.11	105.25	112.40
1	D	428	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	980	GLU	O-C-N	-5.10	114.53	123.20
1	C	230	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	857	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	131	GLU	CG-CD-OE1	5.09	128.49	118.30
1	B	859	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	978	ALA	CB-CA-C	-5.09	102.47	110.10
1	B	1014	TYR	CD1-CG-CD2	5.08	123.49	117.90
1	C	799	THR	CA-CB-CG2	-5.08	105.28	112.40
1	A	842	TRP	CE2-CD2-CE3	5.08	124.79	118.70
1	B	280	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	781	ARG	CD-NE-CZ	5.08	130.71	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	855	THR	N-CA-CB	5.08	119.94	110.30
1	B	161	TYR	CZ-CE2-CD2	-5.07	115.24	119.80
1	B	855	THR	N-CA-CB	5.07	119.93	110.30
1	D	509	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	187	MET	CA-CB-CG	-5.07	104.69	113.30
1	C	919	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	253	TYR	CG-CD2-CE2	5.06	125.35	121.30
1	A	375	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	C	797	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	D	734	SER	CB-CA-C	5.05	119.70	110.10
1	A	46	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	329	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	A	915	PHE	CG-CD2-CE2	-5.05	115.25	120.80
1	B	842	TRP	CE2-CD2-CE3	5.05	124.76	118.70
1	A	946	TYR	CG-CD1-CE1	-5.04	117.27	121.30
1	B	472	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	A	164	ASP	N-CA-CB	5.04	119.67	110.60
1	D	509	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	508	GLU	CG-CD-OE1	5.03	128.36	118.30
1	D	829	THR	N-CA-CB	5.03	119.86	110.30
1	B	492	ASP	CB-CG-OD1	5.03	122.82	118.30
1	D	255	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
1	D	324	GLU	N-CA-CB	5.03	119.65	110.60
1	A	183	ARG	NH1-CZ-NH2	5.02	124.92	119.40
1	D	834	VAL	CA-CB-CG2	-5.02	103.37	110.90
1	A	816	TYR	CB-CG-CD2	5.02	124.01	121.00
1	B	736	ALA	CB-CA-C	-5.02	102.58	110.10
1	C	1013	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	285	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
1	A	854	LYS	CB-CA-C	-5.01	100.38	110.40
1	C	524	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	D	84	VAL	CG1-CB-CG2	-5.01	102.89	110.90
1	B	166	ARG	NH1-CZ-NH2	5.01	124.91	119.40
1	B	431	ARG	CA-CB-CG	-5.01	102.38	113.40
1	D	954	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	759	ASN	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8127	0	7713	131	0
1	B	8127	0	7713	116	0
1	C	8127	0	7713	124	0
1	D	8127	0	7713	147	0
2	A	24	0	23	1	0
2	B	24	0	23	3	0
2	C	24	0	23	1	0
2	D	24	0	23	1	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	92	0	138	12	0
5	B	88	0	132	8	0
5	C	92	0	138	4	0
5	D	92	0	138	17	0
6	A	1054	0	0	20	2
6	B	1073	0	0	19	1
6	C	1019	0	0	15	0
6	D	1068	0	0	22	1
All	All	37213	0	31490	530	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (530) 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)
5:A:8415:DMS:S	5:A:8415:DMS:C2	2.02	1.46
5:B:8601:DMS:C2	5:B:8601:DMS:S	2.04	1.44
5:D:8415:DMS:C1	5:D:8415:DMS:S	2.05	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:8407:DMS:C2	5:A:8407:DMS:S	2.06	1.43
1:C:634:GLN:H	1:C:634:GLN:NE2	1.45	1.14
1:D:634:GLN:HG3	1:D:682:LEU:HB2	1.15	1.07
1:D:863:GLN:HG3	1:D:1021:CYS:HB3	1.38	1.05
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.26	1.01
1:D:237:ARG:HG2	1:D:237:ARG:HH11	1.25	0.99
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.50	0.92
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.51	0.91
1:A:863:GLN:HE22	1:A:952:ARG:HH22	1.10	0.91
1:B:600:GLN:H	1:B:600:GLN:HE21	1.17	0.90
1:C:687:GLN:NE2	1:C:687:GLN:HA	1.87	0.90
6:C:9523:HOH:O	1:D:530:THR:HG22	1.72	0.88
1:D:634:GLN:HG3	1:D:682:LEU:CB	2.03	0.87
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.38	0.87
1:C:634:GLN:H	1:C:634:GLN:HE21	1.18	0.86
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.57	0.86
1:B:824:GLN:HG2	1:B:825:CYS:N	1.92	0.84
1:B:655:MET:HE2	1:B:665:SER:HB3	1.58	0.84
1:B:655:MET:CE	1:B:665:SER:HB3	2.09	0.83
1:A:600:GLN:H	1:A:600:GLN:HE21	1.27	0.82
1:A:530:THR:HG22	6:B:8614:HOH:O	1.79	0.80
1:B:824:GLN:HE22	1:B:837:THR:HG22	1.44	0.80
1:C:634:GLN:N	1:C:634:GLN:NE2	2.29	0.80
1:B:824:GLN:HE22	1:B:837:THR:CG2	1.94	0.80
1:D:703:PRO:HG2	5:D:8425:DMS:H13	1.62	0.79
1:A:237:ARG:HB3	1:A:237:ARG:NH1	1.97	0.79
1:C:690:SER:HB2	6:C:9345:HOH:O	1.82	0.79
1:A:237:ARG:HG2	1:A:296:GLU:OE1	1.81	0.79
1:A:648:ASP:OD2	6:A:9374:HOH:O	2.00	0.79
1:A:797:GLU:O	1:A:801:ILE:HD13	1.83	0.78
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.13	0.78
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.66	0.77
1:A:237:ARG:HH11	1:A:237:ARG:CB	1.97	0.77
1:C:178:ARG:HD2	6:C:9497:HOH:O	1.85	0.77
1:D:893:GLU:HG2	1:D:894:ARG:HG2	1.66	0.77
1:B:890:GLN:HG3	1:B:891:VAL:N	2.01	0.74
5:B:8410:DMS:H21	6:B:8876:HOH:O	1.88	0.74
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.23	0.74
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.52	0.74
1:C:13:ARG:O	1:C:14:ARG:C	2.27	0.73
5:D:8703:DMS:H23	6:D:9648:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:O	1:A:737:ILE:HD13	1.87	0.73
1:D:703:PRO:HG2	5:D:8425:DMS:C1	2.18	0.73
1:C:797:GLU:O	1:C:801:ILE:HD13	1.88	0.72
1:D:804:ASN:HD22	1:D:809:ARG:HH21	1.35	0.72
1:B:651:LEU:O	1:B:651:LEU:HD23	1.87	0.72
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.01	0.72
1:A:277:GLU:H	1:A:277:GLU:CD	1.90	0.72
1:B:744:GLU:HA	1:B:744:GLU:OE2	1.90	0.71
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.25	0.71
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.73	0.71
1:D:749:ILE:N	1:D:749:ILE:HD12	2.05	0.71
1:A:651:LEU:HD11	1:A:653:HIS:CD2	2.26	0.70
1:D:890:GLN:HE21	1:D:892:ALA:HB2	1.57	0.70
1:B:809:ARG:NH1	1:B:809:ARG:HG2	2.06	0.70
1:C:658:LEU:O	1:C:661:LYS:HG3	1.91	0.69
1:C:745:MET:HB3	1:C:746:ASP:OD1	1.92	0.69
5:C:8410:DMS:H13	6:C:8974:HOH:O	1.91	0.69
1:D:863:GLN:CG	1:D:1021:CYS:HB3	2.18	0.69
1:B:878:HIS:HD2	6:B:8690:HOH:O	1.74	0.69
1:B:686:PRO:O	1:B:688:PRO:HD3	1.91	0.69
1:A:887:GLN:NE2	1:A:980:GLU:O	2.26	0.68
1:D:675:GLN:HG3	6:D:9547:HOH:O	1.93	0.68
1:D:651:LEU:HD12	1:D:651:LEU:C	2.14	0.68
1:D:770:ILE:HD13	1:D:775:GLN:CG	2.24	0.68
1:A:799:THR:HG22	6:A:9504:HOH:O	1.92	0.68
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.26	0.68
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.74	0.68
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.28	0.67
1:B:781:ARG:NH1	6:B:9589:HOH:O	2.28	0.67
5:D:8421:DMS:H11	6:D:9353:HOH:O	1.93	0.67
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.77	0.66
1:D:863:GLN:HE21	1:D:1021:CYS:HB2	1.59	0.66
1:D:878:HIS:HD2	6:D:8820:HOH:O	1.78	0.66
5:D:8406:DMS:O	6:D:9646:HOH:O	2.11	0.66
1:A:863:GLN:HE22	1:A:952:ARG:NH2	1.90	0.66
1:B:689:GLU:O	1:B:690:SER:HB3	1.94	0.66
1:B:230:ARG:NH1	1:B:241:GLU:OE1	2.28	0.65
1:C:878:HIS:HD2	6:C:8704:HOH:O	1.78	0.65
1:A:949:HIS:O	1:A:1023:LYS:NZ	2.29	0.65
1:C:761:GLN:OE1	1:C:761:GLN:N	2.30	0.65
1:A:749:ILE:N	1:A:749:ILE:HD12	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ARG:CB	1:C:237:ARG:HH11	2.10	0.64
1:D:71:GLU:HG2	6:D:9512:HOH:O	1.97	0.64
5:A:8420:DMS:H21	6:D:9502:HOH:O	1.98	0.64
1:A:878:HIS:HD2	6:A:8578:HOH:O	1.81	0.64
1:D:135:GLN:C	1:D:136:GLU:HG2	2.18	0.63
1:A:863:GLN:HE21	1:A:1021:CYS:CB	2.12	0.63
1:C:241:GLU:HG3	1:C:292:ARG:HG2	1.80	0.63
1:D:80:GLU:HG3	6:D:9733:HOH:O	1.98	0.63
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.64	0.63
1:D:863:GLN:HG2	1:D:1019:VAL:CG1	2.29	0.63
1:D:1022:GLN:HE21	1:D:1022:GLN:C	2.02	0.62
1:D:634:GLN:CG	1:D:682:LEU:HB2	2.09	0.62
1:A:664:ALA:HB2	1:A:686:PRO:HG3	1.81	0.62
1:A:237:ARG:NH1	6:A:9030:HOH:O	2.29	0.62
1:A:262:GLN:HG3	1:A:309:TYR:CE2	2.35	0.61
1:A:387:VAL:HG22	6:A:9469:HOH:O	1.98	0.61
1:D:634:GLN:OE1	1:D:683:PRO:O	2.18	0.61
1:D:277:GLU:H	1:D:277:GLU:CD	1.92	0.61
1:A:832:ASP:OD1	1:A:832:ASP:N	2.34	0.61
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.21	0.61
1:C:13:ARG:O	1:C:15:ASP:N	2.33	0.61
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.15	0.61
1:C:651:LEU:HD12	1:C:651:LEU:C	2.21	0.61
1:D:651:LEU:HD12	1:D:651:LEU:O	2.01	0.61
1:C:682:LEU:HD13	1:C:685:LEU:HD11	1.83	0.61
1:D:685:LEU:HB3	1:D:686:PRO:CD	2.30	0.60
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.82	0.60
1:B:730:LEU:H	1:B:730:LEU:CD1	2.13	0.60
1:A:431:ARG:HH21	1:D:445:GLN:HE22	1.49	0.60
1:D:663:LEU:CD1	1:D:688:PRO:HG3	2.32	0.60
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.37	0.59
1:B:296:GLU:OE1	1:B:296:GLU:HA	2.00	0.59
1:B:675:GLN:NE2	6:B:9434:HOH:O	2.35	0.59
1:D:14:ARG:NH1	6:D:9647:HOH:O	2.21	0.59
1:D:102:ASN:HD22	5:D:8506:DMS:H21	1.67	0.59
6:B:9377:HOH:O	5:C:8420:DMS:H21	2.03	0.59
1:D:655:MET:HE3	1:D:699:ARG:HE	1.66	0.59
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.02	0.59
1:A:1022:GLN:NE2	1:A:1023:LYS:O	2.36	0.59
1:C:753:ASN:OD1	1:C:754:LYS:NZ	2.30	0.59
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9336:HOH:O	2:B:2002:GAL:H2	2.02	0.59
1:C:615:PRO:O	1:C:618:THR:HG22	2.03	0.59
1:C:581:ASN:HB2	1:C:583:ASN:ND2	2.17	0.59
1:C:756:TRP:CD2	1:C:858:ILE:HD13	2.37	0.59
1:D:554:GLN:NE2	6:D:9623:HOH:O	2.27	0.59
1:D:893:GLU:HG2	1:D:894:ARG:CG	2.32	0.59
1:B:730:LEU:HD12	1:B:730:LEU:H	1.68	0.58
1:C:878:HIS:HE1	6:C:9260:HOH:O	1.86	0.58
1:A:863:GLN:NE2	1:A:952:ARG:HH22	1.91	0.58
1:A:357:HIS:HB3	6:A:9093:HOH:O	2.02	0.58
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.18	0.58
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.85	0.58
1:B:800:ARG:NH2	6:B:9556:HOH:O	2.35	0.58
1:B:824:GLN:HE22	1:B:837:THR:CB	2.16	0.57
1:C:431:ARG:HB3	6:C:9504:HOH:O	2.04	0.57
1:C:688:PRO:HG3	1:C:694:LEU:HD11	1.85	0.57
1:A:651:LEU:HD12	1:A:651:LEU:C	2.25	0.57
1:B:236:SER:C	1:B:237:ARG:HG2	2.23	0.57
1:A:890:GLN:HG3	1:A:891:VAL:N	2.17	0.57
1:B:730:LEU:HD12	1:B:730:LEU:N	2.19	0.57
1:B:745:MET:SD	1:B:745:MET:N	2.77	0.57
1:D:649:ASN:HA	5:D:8425:DMS:C1	2.34	0.57
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.20	0.57
1:C:237:ARG:HB3	1:C:237:ARG:HH11	1.69	0.57
1:C:237:ARG:HG2	1:C:296:GLU:OE1	2.04	0.57
1:D:847:LYS:NZ	6:D:9483:HOH:O	2.29	0.57
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.35	0.57
1:C:1023:LYS:HZ3	1:C:1023:LYS:HA	1.70	0.57
1:D:133:TRP:HE1	5:D:8703:DMS:C2	2.18	0.57
1:D:887:GLN:NE2	1:D:980:GLU:O	2.38	0.56
1:C:240:LEU:HD23	1:C:240:LEU:C	2.26	0.56
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.20	0.56
1:C:233:ASP:HA	5:C:8417:DMS:S	2.46	0.56
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.10	0.56
1:B:181:GLU:HG3	6:B:9546:HOH:O	2.05	0.56
1:B:237:ARG:HD2	1:B:296:GLU:OE1	2.05	0.56
1:D:577:LYS:O	1:D:584:PRO:HA	2.06	0.56
1:B:632:SER:O	1:B:635:THR:N	2.37	0.56
1:B:595:THR:HA	1:B:596:PRO:C	2.26	0.56
1:B:292:ARG:HH12	5:B:8412:DMS:C2	2.19	0.56
1:D:890:GLN:NE2	1:D:892:ALA:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.88	0.56
1:D:133:TRP:HE1	5:D:8703:DMS:H23	1.70	0.56
1:D:240:LEU:HD23	1:D:240:LEU:C	2.27	0.55
1:D:237:ARG:NH1	1:D:237:ARG:HG2	1.99	0.55
1:D:595:THR:HA	1:D:596:PRO:C	2.26	0.55
1:C:710:GLU:HG2	6:C:8978:HOH:O	2.06	0.55
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.89	0.55
1:D:655:MET:CE	1:D:699:ARG:HE	2.19	0.55
1:D:682:LEU:HB3	1:D:683:PRO:HD2	1.87	0.55
1:A:664:ALA:CB	1:A:686:PRO:HG3	2.37	0.55
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.06	0.55
1:D:893:GLU:HG2	1:D:894:ARG:CD	2.36	0.55
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.69	0.54
1:C:843:GLN:HG2	1:C:848:THR:HA	1.87	0.54
1:A:656:VAL:CG1	1:A:694:LEU:HD22	2.36	0.54
1:D:847:LYS:HG3	1:D:848:THR:N	2.22	0.54
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.75	0.54
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.07	0.54
1:D:360:HIS:HE1	1:D:362:LEU:HD12	1.73	0.54
1:D:686:PRO:C	1:D:688:PRO:HD3	2.27	0.54
1:A:178:ARG:HD2	6:A:9334:HOH:O	2.08	0.54
1:C:866:ILE:O	1:C:1017:GLN:HG2	2.07	0.54
1:A:240:LEU:C	1:A:240:LEU:HD23	2.28	0.54
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.37	0.54
1:A:980:GLU:HA	6:A:9246:HOH:O	2.08	0.54
1:C:658:LEU:HG	1:C:661:LYS:NZ	2.23	0.54
1:D:102:ASN:HD22	5:D:8506:DMS:C2	2.21	0.54
5:D:8506:DMS:H11	6:D:9527:HOH:O	2.08	0.54
1:A:843:GLN:HA	1:A:847:LYS:O	2.08	0.54
1:B:157:ARG:HD3	6:B:9446:HOH:O	2.08	0.54
1:D:893:GLU:O	1:D:893:GLU:HG3	2.08	0.54
1:A:521:LYS:HE2	6:A:8929:HOH:O	2.08	0.54
1:D:682:LEU:CB	1:D:683:PRO:HD2	2.38	0.54
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.20	0.54
1:C:658:LEU:HD23	1:C:661:LYS:HZ3	1.73	0.53
1:A:1017:GLN:HG3	1:A:1017:GLN:O	2.07	0.53
1:B:615:PRO:O	1:B:618:THR:HG22	2.07	0.53
1:D:769:TRP:C	1:D:770:ILE:HD12	2.28	0.53
1:A:753:ASN:OD1	1:A:754:LYS:HG3	2.08	0.53
1:B:622:HIS:HB2	1:B:717:TRP:CZ2	2.44	0.53
5:B:8406:DMS:H21	6:B:9289:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLN:HG3	6:A:9004:HOH:O	2.08	0.53
1:C:80:GLU:H	1:C:80:GLU:CD	2.11	0.53
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.91	0.53
1:A:595:THR:HA	1:A:596:PRO:C	2.27	0.53
1:D:736:ALA:HB1	1:D:751:LEU:HD11	1.90	0.53
1:C:658:LEU:HD23	1:C:661:LYS:NZ	2.24	0.53
1:D:241:GLU:HG3	1:D:292:ARG:HG2	1.90	0.53
1:D:649:ASN:HA	5:D:8425:DMS:H12	1.91	0.53
1:A:296:GLU:HA	1:A:296:GLU:OE1	2.09	0.52
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.77	0.52
1:A:241:GLU:OE2	1:A:292:ARG:NE	2.34	0.52
1:A:241:GLU:CD	1:A:292:ARG:HE	2.13	0.52
1:A:651:LEU:HD11	1:A:653:HIS:HD2	1.74	0.52
1:D:843:GLN:HA	1:D:847:LYS:O	2.09	0.52
1:D:363:HIS:HD2	6:D:9318:HOH:O	1.93	0.52
1:A:88:SER:HA	1:A:366:VAL:HG21	1.91	0.52
1:A:431:ARG:NH2	1:D:445:GLN:HE22	2.07	0.52
1:B:655:MET:HE1	1:B:665:SER:HB3	1.90	0.52
1:B:824:GLN:NE2	1:B:837:THR:O	2.42	0.52
1:C:745:MET:CE	1:C:759:ASN:HD21	2.23	0.52
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.92	0.52
1:A:651:LEU:CD1	1:A:653:HIS:CD2	2.92	0.52
1:A:981:GLY:N	6:A:9246:HOH:O	2.26	0.52
1:D:251:ARG:CZ	1:D:253:TYR:HE2	2.23	0.52
1:C:832:ASP:N	1:C:832:ASP:OD1	2.42	0.51
1:D:1022:GLN:O	1:D:1022:GLN:HG3	2.09	0.51
1:D:251:ARG:NH1	1:D:253:TYR:HE2	2.07	0.51
1:D:731:PRO:O	1:D:732:ALA:O	2.29	0.51
1:B:632:SER:N	1:B:635:THR:O	2.30	0.51
1:B:800:ARG:NH1	6:B:9556:HOH:O	2.43	0.51
1:B:684:GLU:O	1:B:686:PRO:HD3	2.10	0.51
1:A:781:ARG:NH1	6:A:9214:HOH:O	2.44	0.51
1:B:600:GLN:N	1:B:600:GLN:HE21	1.98	0.51
1:C:16:TRP:CG	1:C:189:LEU:HD13	2.46	0.51
1:C:774:LYS:HE2	6:C:9158:HOH:O	2.11	0.51
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.46	0.51
1:D:769:TRP:CD1	1:D:774:LYS:HG3	2.45	0.51
1:C:847:LYS:HG3	1:C:848:THR:N	2.27	0.50
1:D:651:LEU:CD1	1:D:653:HIS:CE1	2.93	0.50
1:B:651:LEU:C	1:B:651:LEU:HD23	2.32	0.50
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:VAL:HG12	5:C:8506:DMS:H22	1.92	0.50
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.91	0.50
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.46	0.50
1:A:183:ARG:HG2	6:A:8809:HOH:O	2.11	0.50
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.32	0.50
5:A:8421:DMS:H11	6:A:9110:HOH:O	2.11	0.50
1:C:54:LEU:HD11	1:C:214:LEU:HG	1.93	0.50
1:C:847:LYS:NZ	1:D:724:GLU:O	2.44	0.50
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.74	0.50
1:C:743:SER:HB3	6:C:9284:HOH:O	2.10	0.50
1:D:687:GLN:N	1:D:688:PRO:HD3	2.27	0.50
1:C:770:ILE:HD12	1:C:775:GLN:CD	2.32	0.50
1:C:814:GLY:HA3	1:C:844:HIS:CG	2.47	0.49
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.94	0.49
1:A:737:ILE:HD13	1:A:737:ILE:C	2.33	0.49
1:C:595:THR:HA	1:C:596:PRO:C	2.32	0.49
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.94	0.49
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.77	0.49
1:B:945:ASN:HB3	1:B:1023:LYS:NZ	2.28	0.49
1:A:361:PRO:HB2	1:A:576:ILE:HG12	1.93	0.49
1:B:428:ASP:OD2	5:B:8420:DMS:H13	2.12	0.49
1:C:634:GLN:N	1:C:634:GLN:HE21	1.98	0.49
1:B:240:LEU:HD23	1:B:240:LEU:C	2.34	0.49
1:D:251:ARG:CZ	1:D:253:TYR:CE2	2.96	0.49
1:D:618:THR:HG23	6:D:9077:HOH:O	2.12	0.49
1:A:851:ILE:O	1:A:870:VAL:HA	2.12	0.49
1:C:363:HIS:HD2	6:C:9191:HOH:O	1.96	0.49
1:C:622:HIS:HB2	1:C:717:TRP:CZ2	2.48	0.49
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.78	0.48
1:B:537:GLU:OE2	2:B:2001:GAL:H1	2.13	0.48
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.13	0.48
1:D:136:GLU:HB3	6:D:9680:HOH:O	2.13	0.48
1:A:646:HIS:ND1	6:A:9304:HOH:O	2.35	0.48
1:D:618:THR:HG21	6:D:9060:HOH:O	2.12	0.48
1:A:251:ARG:HH11	5:A:8416:DMS:C2	2.26	0.48
1:D:770:ILE:CD1	1:D:775:GLN:HG3	2.44	0.48
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.49	0.48
1:C:745:MET:HE3	1:C:745:MET:O	2.12	0.48
1:A:863:GLN:NE2	1:A:1021:CYS:CB	2.76	0.48
1:A:859:ASP:OD1	1:A:861:SER:OG	2.29	0.48
1:C:890:GLN:HG3	1:C:891:VAL:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.14	0.48
1:A:735:HIS:O	1:A:736:ALA:HB2	2.14	0.48
1:A:600:GLN:N	1:A:600:GLN:HE21	2.04	0.48
1:A:773:LYS:HB2	1:A:773:LYS:HE2	1.43	0.48
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.95	0.48
1:C:655:MET:HG3	1:C:655:MET:O	2.04	0.48
1:D:667:GLU:C	1:D:668:VAL:HG23	2.33	0.48
1:A:433:LEU:N	1:A:434:PRO:CD	2.76	0.47
1:A:1022:GLN:CD	1:A:1023:LYS:H	2.16	0.47
1:B:233:ASP:HA	5:B:8417:DMS:C1	2.44	0.47
1:D:237:ARG:NH1	1:D:237:ARG:CG	2.75	0.47
1:D:79:PRO:HD2	6:D:9733:HOH:O	2.13	0.47
1:D:832:ASP:OD1	1:D:832:ASP:N	2.47	0.47
1:A:861:SER:OG	1:A:863:GLN:HG3	2.13	0.47
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.47
1:C:659:ASP:HB2	6:C:9522:HOH:O	2.15	0.47
1:D:655:MET:HE3	6:D:9565:HOH:O	2.14	0.47
1:B:632:SER:O	1:B:635:THR:OG1	2.29	0.47
1:D:863:GLN:HG2	1:D:1019:VAL:HG11	1.97	0.47
1:B:668:VAL:HA	1:B:669:PRO:HD3	1.66	0.47
1:C:317:THR:OG1	1:C:319:ASP:OD1	2.25	0.47
1:B:613:PRO:HG2	6:B:9242:HOH:O	2.14	0.47
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.13	0.47
1:D:473:ARG:HD3	6:D:9456:HOH:O	2.13	0.47
1:D:845:GLN:N	1:D:845:GLN:OE1	2.47	0.47
1:D:88:SER:HA	1:D:366:VAL:HG21	1.97	0.47
1:D:754:LYS:C	1:D:755:ARG:HG2	2.20	0.47
1:D:805:ALA:O	1:D:809:ARG:HG3	2.15	0.47
1:A:601:PHE:CE1	5:A:8506:DMS:H12	2.50	0.47
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.50	0.47
1:C:625:GLN:HG2	1:C:716:ALA:HA	1.96	0.47
1:D:112:PRO:HD2	1:D:113:PHE:CE1	2.50	0.47
1:D:730:LEU:H	1:D:730:LEU:HD12	1.80	0.47
1:A:854:LYS:HA	1:A:867:THR:O	2.15	0.47
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.96	0.47
1:D:537:GLU:OE2	2:D:2001:GAL:H1	2.13	0.47
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.45	0.46
1:B:655:MET:SD	1:B:656:VAL:N	2.88	0.46
1:A:533:LEU:C	1:A:533:LEU:HD23	2.35	0.46
1:D:133:TRP:NE1	5:D:8703:DMS:C2	2.79	0.46
1:A:651:LEU:CD1	1:A:653:HIS:HD2	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ASN:HA	1:D:148:SER:HA	1.63	0.46
1:D:651:LEU:C	1:D:651:LEU:CD1	2.82	0.46
1:D:770:ILE:N	1:D:770:ILE:CD1	2.78	0.46
1:A:799:THR:O	1:A:799:THR:OG1	2.32	0.46
1:B:688:PRO:HG2	1:B:694:LEU:HD21	1.97	0.46
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.14	0.46
1:C:593:GLY:O	1:C:595:THR:HG22	2.15	0.46
1:D:670:LEU:HD23	1:D:670:LEU:HA	1.58	0.46
1:D:770:ILE:HD13	1:D:775:GLN:HG3	1.96	0.46
1:B:147:ASN:HA	1:B:148:SER:HA	1.60	0.46
1:B:357:HIS:HB3	6:B:9208:HOH:O	2.16	0.46
1:C:537:GLU:OE2	2:C:2001:GAL:H1	2.16	0.46
1:A:660:GLY:O	1:A:662:PRO:HD3	2.15	0.46
1:B:695:TRP:HZ2	2:B:2002:GAL:H4	1.81	0.46
1:B:806:TRP:CD2	1:B:991:MET:HE1	2.50	0.46
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.98	0.46
1:B:764:PHE:CE1	1:B:781:ARG:NH1	2.84	0.46
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.46	0.45
5:A:8502:DMS:H12	6:A:9224:HOH:O	2.14	0.45
1:B:731:PRO:O	1:B:732:ALA:HB2	2.17	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.62	0.45
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.96	0.45
1:C:658:LEU:CG	1:C:661:LYS:NZ	2.79	0.45
1:C:745:MET:HE3	1:C:761:GLN:OE1	2.15	0.45
1:B:867:THR:HA	1:B:1017:GLN:HG2	1.98	0.45
1:C:16:TRP:CG	1:C:189:LEU:CD1	2.99	0.45
1:C:655:MET:HE2	1:C:664:ALA:O	2.16	0.45
1:C:745:MET:SD	1:C:761:GLN:NE2	2.89	0.45
1:D:829:THR:HG23	1:D:834:VAL:HG22	1.97	0.45
1:B:577:LYS:HE3	1:B:577:LYS:HB3	1.86	0.45
1:B:910:LEU:HD12	1:B:910:LEU:C	2.36	0.45
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.30	0.45
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.98	0.45
1:C:745:MET:CE	1:C:759:ASN:ND2	2.80	0.45
1:A:801:ILE:HD12	1:A:808:GLU:OE2	2.16	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.53	0.45
1:B:824:GLN:NE2	1:B:837:THR:HG22	2.21	0.45
1:C:88:SER:HA	1:C:366:VAL:HG21	1.97	0.45
1:C:683:PRO:O	1:C:685:LEU:HG	2.17	0.45
1:C:750:GLU:OE2	1:C:755:ARG:HD2	2.17	0.45
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:MET:HE1	1:A:761:GLN:HB2	1.98	0.45
1:B:530:THR:OG1	6:B:9338:HOH:O	2.21	0.45
1:C:756:TRP:CD2	1:C:858:ILE:CD1	2.99	0.45
1:B:577:LYS:O	1:B:584:PRO:HA	2.16	0.45
1:B:668:VAL:HG12	1:B:669:PRO:N	2.32	0.45
1:C:730:LEU:HG	1:C:730:LEU:H	0.95	0.45
1:D:986:ILE:HD13	1:D:986:ILE:HG21	1.33	0.45
1:A:431:ARG:HB3	6:A:9511:HOH:O	2.16	0.44
1:B:387:VAL:HG13	6:B:9574:HOH:O	2.16	0.44
1:C:658:LEU:CD2	1:C:661:LYS:NZ	2.80	0.44
1:D:893:GLU:CG	1:D:894:ARG:CD	2.95	0.44
1:A:717:TRP:CH2	5:A:8415:DMS:H12	2.52	0.44
1:B:739:HIS:HB3	1:B:750:GLU:OE1	2.16	0.44
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.99	0.44
1:B:890:GLN:OE1	1:B:948:PRO:HD3	2.17	0.44
1:C:241:GLU:OE1	1:C:292:ARG:NE	2.50	0.44
1:C:697:THR:OG1	1:C:719:GLN:HG2	2.16	0.44
1:D:748:CYS:C	1:D:749:ILE:HD12	2.37	0.44
1:B:292:ARG:HH12	5:B:8412:DMS:H21	1.82	0.44
1:D:74:LEU:HD22	1:D:153:TRP:CG	2.53	0.44
1:D:863:GLN:HE21	1:D:1021:CYS:CB	2.27	0.44
1:D:635:THR:HG23	1:D:681:GLU:OE1	2.18	0.44
1:D:658:LEU:O	1:D:661:LYS:HG3	2.17	0.44
1:D:682:LEU:HA	1:D:682:LEU:HD23	1.80	0.44
1:A:788:PRO:CD	1:A:968:MET:HG3	2.48	0.44
1:C:757:GLN:OE1	1:C:769:TRP:HH2	2.01	0.44
1:C:781:ARG:HD2	6:C:9559:HOH:O	2.17	0.44
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.52	0.44
1:B:773:LYS:HD3	1:B:773:LYS:HA	1.61	0.44
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.53	0.44
1:B:658:LEU:O	1:B:661:LYS:HG3	2.18	0.44
1:D:851:ILE:O	1:D:870:VAL:HA	2.18	0.44
1:A:427:THR:HG21	1:A:462:SER:HB3	2.00	0.44
1:A:844:HIS:HD2	6:A:9302:HOH:O	2.01	0.44
1:A:601:PHE:CD1	5:A:8506:DMS:H11	2.53	0.44
1:D:634:GLN:O	1:D:634:GLN:CG	2.65	0.44
1:A:416:GLU:OE2	1:A:418:HIS:HB2	2.18	0.43
1:B:878:HIS:HE1	6:B:9262:HOH:O	1.99	0.43
1:C:236:SER:C	1:C:237:ARG:HG3	2.35	0.43
1:C:651:LEU:HD12	1:C:651:LEU:O	2.17	0.43
1:B:859:ASP:OD1	1:B:861:SER:OG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:HD22	1:B:708:TRP:HA	2.00	0.43
1:A:472:TYR:O	1:A:476:LYS:HG2	2.19	0.43
1:B:824:GLN:HE22	1:B:837:THR:HB	1.81	0.43
1:C:1023:LYS:HA	1:C:1023:LYS:NZ	2.32	0.43
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.54	0.43
1:C:736:ALA:HB1	1:C:751:LEU:HD11	2.00	0.43
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.53	0.43
1:B:262:GLN:HB2	1:B:309:TYR:CD2	2.54	0.43
1:D:658:LEU:O	1:D:659:ASP:C	2.57	0.43
1:A:662:PRO:O	1:A:663:LEU:HD23	2.19	0.43
1:B:687:GLN:NE2	1:B:687:GLN:N	2.66	0.43
1:C:545:SER:O	1:C:909:ARG:HD3	2.18	0.43
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.54	0.43
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.18	0.43
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.00	0.43
1:A:537:GLU:OE2	2:A:2001:GAL:H1	2.19	0.43
1:B:387:VAL:HG22	6:B:9574:HOH:O	2.18	0.43
1:B:663:LEU:HA	1:B:663:LEU:HD23	1.85	0.43
1:B:634:GLN:NE2	1:B:685:LEU:HB2	2.34	0.43
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.54	0.43
1:A:842:TRP:N	1:A:842:TRP:CE3	2.87	0.43
1:B:40:GLU:OE2	1:B:43:ARG:NH2	2.49	0.43
1:C:710:GLU:H	1:C:710:GLU:HG2	1.51	0.43
1:D:867:THR:HA	1:D:1017:GLN:HG2	2.00	0.43
1:A:774:LYS:HB2	1:A:774:LYS:HE2	1.89	0.42
1:B:824:GLN:NE2	1:B:837:THR:HB	2.34	0.42
1:C:241:GLU:CD	1:C:292:ARG:HE	2.23	0.42
1:C:687:GLN:HE21	1:C:688:PRO:HD2	1.84	0.42
1:A:686:PRO:O	1:A:687:GLN:NE2	2.52	0.42
1:A:824:GLN:NE2	6:A:9248:HOH:O	2.52	0.42
1:C:847:LYS:HD2	6:C:9365:HOH:O	2.18	0.42
1:D:537:GLU:HA	1:D:566:PHE:O	2.19	0.42
1:A:736:ALA:C	1:A:737:ILE:HG22	2.40	0.42
5:B:8421:DMS:H22	6:B:9128:HOH:O	2.19	0.42
1:A:789:LEU:HD11	1:A:993:ILE:HG22	2.00	0.42
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.76	0.42
1:B:13:ARG:HB2	1:C:13:ARG:HH22	1.84	0.42
1:B:533:LEU:C	1:B:533:LEU:HD23	2.40	0.42
1:D:279:ILE:HG21	1:D:279:ILE:HD13	1.84	0.42
1:B:674:PRO:O	1:B:675:GLN:HB2	2.20	0.42
1:B:70:PRO:HG2	1:B:78:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:ASP:OD2	6:C:9522:HOH:O	2.22	0.42
1:A:634:GLN:OE1	1:A:634:GLN:N	2.53	0.42
1:A:795:VAL:CG1	5:A:8506:DMS:C2	2.97	0.42
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.54	0.42
1:B:427:THR:HG21	1:B:462:SER:HB3	2.02	0.42
1:D:340:GLY:O	1:D:561:ARG:HG2	2.20	0.42
1:B:262:GLN:HB2	1:B:309:TYR:CE2	2.54	0.42
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.54	0.42
1:C:830:LEU:HD23	1:C:830:LEU:HA	1.75	0.42
1:A:687:GLN:NE2	1:A:687:GLN:HA	2.34	0.42
1:C:997:ASP:HB2	1:C:999:TRP:CE2	2.55	0.42
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.52	0.42
1:D:863:GLN:HG3	1:D:1021:CYS:CB	2.28	0.42
1:C:989:PHE:CD1	1:C:989:PHE:N	2.88	0.41
1:D:584:PRO:HD2	6:D:9441:HOH:O	2.19	0.41
1:D:71:GLU:O	1:D:72:SER:C	2.57	0.41
1:A:717:TRP:CE3	5:A:8415:DMS:H11	2.55	0.41
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.38	0.41
1:B:655:MET:SD	1:B:656:VAL:O	2.78	0.41
1:C:847:LYS:CG	1:C:848:THR:N	2.83	0.41
1:A:615:PRO:O	1:A:618:THR:HG22	2.21	0.41
1:C:951:TRP:HA	1:C:1019:VAL:O	2.20	0.41
1:C:569:ASP:O	1:C:605:GLY:HA2	2.21	0.41
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.55	0.41
1:B:631:LEU:HA	1:B:635:THR:O	2.21	0.41
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.76	0.41
1:C:687:GLN:HE21	1:C:688:PRO:CD	2.33	0.41
1:A:654:TRP:CZ2	1:A:683:PRO:HG2	2.55	0.41
1:B:114:VAL:HB	1:B:115:PRO:HD2	2.02	0.41
1:C:743:SER:O	1:C:760:ARG:NH1	2.43	0.41
1:A:372:MET:HE1	1:A:395:HIS:HB3	2.02	0.41
1:A:835:LEU:HD11	1:A:855:THR:HB	2.03	0.41
1:C:305:ILE:HD11	1:C:645:ARG:HB3	2.01	0.41
1:B:537:GLU:HA	1:B:566:PHE:O	2.21	0.41
1:D:804:ASN:ND2	1:D:809:ARG:HH21	2.10	0.41
1:D:133:TRP:NE1	5:D:8703:DMS:H23	2.36	0.41
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.76	0.41
1:D:753:ASN:O	1:D:771:GLY:N	2.37	0.41
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.35	0.41
1:A:279:ILE:HD13	1:A:279:ILE:HG21	1.68	0.41
1:C:610:ASP:O	1:C:611:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.56	0.41
1:A:576:ILE:HA	1:A:576:ILE:HD13	1.88	0.41
1:B:225:PHE:HA	1:B:243:GLU:O	2.21	0.41
1:B:681:GLU:H	1:B:681:GLU:HG2	1.18	0.41
1:B:807:VAL:HG13	1:B:808:GLU:N	2.36	0.41
1:C:804:ASN:ND2	1:C:1001:PRO:CD	2.84	0.41
1:D:754:LYS:HD3	6:D:9752:HOH:O	2.20	0.41
1:D:845:GLN:OE1	1:D:845:GLN:CA	2.69	0.41
1:D:893:GLU:CG	1:D:894:ARG:HD2	2.50	0.41
1:A:86:VAL:HG13	1:A:87:PRO:HA	2.02	0.40
1:C:60:PHE:HA	1:C:122:CYS:O	2.21	0.40
1:D:576:ILE:HD13	1:D:576:ILE:HA	1.81	0.40
1:A:433:LEU:N	1:A:434:PRO:HD2	2.36	0.40
1:A:545:SER:O	1:A:909:ARG:HD3	2.22	0.40
1:A:658:LEU:O	1:A:661:LYS:HE3	2.21	0.40
1:A:850:PHE:HA	1:A:871:GLU:O	2.20	0.40
1:B:363:HIS:HD2	6:B:9189:HOH:O	2.04	0.40
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.54	0.40
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.55	0.40
1:D:464:HIS:HB2	1:D:489:GLY:HA3	2.02	0.40
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.55	0.40
1:A:906:TYR:CZ	1:A:937:LEU:HB2	2.57	0.40
1:B:668:VAL:CG1	1:B:669:PRO:CD	2.99	0.40
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.56	0.40
1:C:1022:GLN:HB3	1:C:1023:LYS:H	1.50	0.40
1:D:472:TYR:O	1:D:476:LYS:HG2	2.21	0.40
1:A:251:ARG:HH11	5:A:8416:DMS:H22	1.86	0.40
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.92	0.40
1:B:542:MET:HA	1:B:604:ASN:HA	2.03	0.40
1:B:701:VAL:O	1:B:703:PRO:HD3	2.21	0.40
1:C:390:SER:HA	1:C:391:HIS:HA	1.94	0.40
1:C:995:GLY:O	1:C:996:ASP:C	2.58	0.40
1:D:710:GLU:HG2	6:D:8928:HOH:O	2.20	0.40
1:D:738:PRO:HG3	1:D:751:LEU:HD13	2.02	0.40
1:D:770:ILE:HD12	1:D:770:ILE:N	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9505:HOH:O	6:D:9542:HOH:O[4_545]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9370:HOH:O	6:B:9592:HOH:O[2_454]	2.18	0.02

## 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	1008/1023 (98%)	972 (96%)	35 (4%)	1 (0%)	51	25
1	B	1008/1023 (98%)	972 (96%)	30 (3%)	6 (1%)	25	7
1	C	1008/1023 (98%)	966 (96%)	39 (4%)	3 (0%)	41	18
1	D	1008/1023 (98%)	969 (96%)	37 (4%)	2 (0%)	47	23
All	All	4032/4092 (98%)	3879 (96%)	141 (4%)	12 (0%)	41	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	690	SER
1	B	731	PRO
1	B	732	ALA
1	D	732	ALA
1	C	14	ARG
1	C	1022	GLN
1	C	734	SER
1	A	164	ASP
1	B	164	ASP
1	D	164	ASP
1	B	687	GLN

### 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	863/874 (99%)	838 (97%)	25 (3%)	42	13
1	B	863/874 (99%)	832 (96%)	31 (4%)	35	8
1	C	863/874 (99%)	828 (96%)	35 (4%)	30	6
1	D	863/874 (99%)	826 (96%)	37 (4%)	29	5
All	All	3452/3496 (99%)	3324 (96%)	128 (4%)	34	8

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	237	ARG
1	A	250	LEU
1	A	262	GLN
1	A	333	ARG
1	A	377	LEU
1	A	394	ASN
1	A	580	GLU
1	A	600	GLN
1	A	630	ARG
1	A	634	GLN
1	A	655	MET
1	A	687	GLN
1	A	689	GLU
1	A	730	LEU
1	A	737	ILE
1	A	746	ASP
1	A	773	LYS
1	A	799	THR
1	A	801	ILE
1	A	819	GLU
1	A	910	LEU
1	A	956	GLN
1	A	1017	GLN

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Mol	Chain	Res	Type
1	A	1023	LYS
1	B	71	GLU
1	B	80	GLU
1	B	230	ARG
1	B	262	GLN
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
1	B	394	ASN
1	B	535	LEU
1	B	546	LEU
1	B	554	GLN
1	B	600	GLN
1	B	634	GLN
1	B	635	THR
1	B	651	LEU
1	B	661	LYS
1	B	681	GLU
1	B	684	GLU
1	B	699	ARG
1	B	730	LEU
1	B	744	GLU
1	B	745	MET
1	B	750	GLU
1	B	799	THR
1	B	817	GLN
1	B	819	GLU
1	B	845	GLN
1	B	847	LYS
1	B	890	GLN
1	B	956	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	75	GLU
1	C	80	GLU
1	C	178	ARG
1	C	262	GLN
1	C	333	ARG
1	C	344	LEU
1	C	370	GLN
1	C	394	ASN
1	C	519	SER

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Mol	Chain	Res	Type
1	C	546	LEU
1	C	595	THR
1	C	634	GLN
1	C	635	THR
1	C	653	HIS
1	C	655	MET
1	C	667	GLU
1	C	687	GLN
1	C	710	GLU
1	C	730	LEU
1	C	735	HIS
1	C	737	ILE
1	C	744	GLU
1	C	745	MET
1	C	750	GLU
1	C	755	ARG
1	C	773	LYS
1	C	796	SER
1	C	800	ARG
1	C	829	THR
1	C	893	GLU
1	C	917	ARG
1	C	986	ILE
1	C	1017	GLN
1	C	1023	LYS
1	D	80	GLU
1	D	237	ARG
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	394	ASN
1	D	473	ARG
1	D	519	SER
1	D	546	LEU
1	D	580	GLU
1	D	581	ASN
1	D	634	GLN
1	D	655	MET
1	D	661	LYS
1	D	681	GLU
1	D	684	GLU
1	D	687	GLN

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Mol	Chain	Res	Type
1	D	710	GLU
1	D	730	LEU
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	770	ILE
1	D	772	ASP
1	D	774	LYS
1	D	797	GLU
1	D	799	THR
1	D	800	ARG
1	D	845	GLN
1	D	847	LYS
1	D	859	ASP
1	D	863	GLN
1	D	893	GLU
1	D	910	LEU
1	D	1017	GLN
1	D	1018	LEU
1	D	1022	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	370	GLN
1	A	600	GLN
1	A	624	GLN
1	A	653	HIS
1	A	687	GLN
1	A	824	GLN
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	A	1017	GLN
1	B	262	GLN
1	B	266	GLN
1	B	363	HIS
1	B	554	GLN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN

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Mol	Chain	Res	Type
1	B	646	HIS
1	B	687	GLN
1	B	824	GLN
1	B	878	HIS
1	B	977	HIS
1	C	163	GLN
1	C	294	ASN
1	C	363	HIS
1	C	583	ASN
1	C	634	GLN
1	C	646	HIS
1	C	687	GLN
1	C	804	ASN
1	C	824	GLN
1	C	878	HIS
1	D	102	ASN
1	D	128	ASN
1	D	135	GLN
1	D	363	HIS
1	D	445	GLN
1	D	624	GLN
1	D	628	GLN
1	D	704	ASN
1	D	804	ASN
1	D	863	GLN
1	D	878	HIS
1	D	890	GLN
1	D	903	GLN
1	D	1022	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	CSO	A	247[B]	-	3,6,7	1.01	0	0,6,8	0.00	-
1	CSO	C	247[A]	-	3,6,7	1.05	0	0,6,8	0.00	-
1	CSO	B	247[B]	-	3,6,7	0.95	0	0,6,8	0.00	-
1	CSO	D	247[A]	-	3,6,7	0.98	0	0,6,8	0.00	-
1	CSO	B	247[A]	-	3,6,7	0.95	0	0,6,8	0.00	-
1	CSO	D	247[B]	-	3,6,7	0.98	0	0,6,8	0.00	-
1	CSO	C	247[B]	-	3,6,7	1.05	0	0,6,8	0.00	-
1	CSO	A	247[A]	-	3,6,7	1.01	0	0,6,8	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	247[B]	-	-	0/1/5/7	-
1	CSO	C	247[A]	-	-	0/1/5/7	-
1	CSO	B	247[B]	-	-	0/1/5/7	-
1	CSO	D	247[A]	-	-	0/1/5/7	-
1	CSO	B	247[A]	-	-	0/1/5/7	-
1	CSO	D	247[B]	-	-	0/1/5/7	-
1	CSO	C	247[B]	-	-	0/1/5/7	-
1	CSO	A	247[A]	-	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 130 ligands modelled in this entry, 31 are monoatomic - leaving 99 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
5	DMS	A	8412	-	3,3,3	2.04	2 (66%)	3,3,3	0.33	0
5	DMS	C	8405	-	3,3,3	1.93	2 (66%)	3,3,3	0.63	0
5	DMS	A	8405	-	3,3,3	1.67	1 (33%)	3,3,3	0.77	0
5	DMS	B	8412	-	3,3,3	1.36	0	3,3,3	0.62	0
5	DMS	A	8502	-	3,3,3	2.08	1 (33%)	3,3,3	1.68	1 (33%)
2	GAL	D	2002	-	12,12,12	0.88	0	17,17,17	1.73	5 (29%)
5	DMS	D	8501	-	3,3,3	0.80	0	3,3,3	0.47	0
5	DMS	C	8506	-	3,3,3	1.41	0	3,3,3	0.56	0
5	DMS	B	8407	-	3,3,3	2.08	2 (66%)	3,3,3	1.32	1 (33%)
5	DMS	C	8414	-	3,3,3	1.07	0	3,3,3	1.34	1 (33%)
5	DMS	A	8420	-	3,3,3	1.00	0	3,3,3	0.90	0
5	DMS	D	8405	-	3,3,3	1.48	1 (33%)	3,3,3	0.30	0
5	DMS	A	8401	-	3,3,3	1.15	0	3,3,3	0.66	0
5	DMS	B	8402	-	3,3,3	1.36	1 (33%)	3,3,3	0.23	0
5	DMS	A	8506	-	3,3,3	1.45	1 (33%)	3,3,3	0.45	0
2	GAL	B	2002	-	12,12,12	0.69	0	17,17,17	1.49	3 (17%)
5	DMS	A	8407	-	3,3,3	3.68	2 (66%)	3,3,3	0.31	0
5	DMS	A	8504	-	3,3,3	3.10	1 (33%)	3,3,3	0.29	0
5	DMS	B	8409	-	3,3,3	2.93	1 (33%)	3,3,3	0.28	0
5	DMS	D	8705	-	3,3,3	1.95	1 (33%)	3,3,3	0.52	0
5	DMS	B	8601	-	3,3,3	2.36	1 (33%)	3,3,3	0.94	0
5	DMS	A	8410	-	3,3,3	0.36	0	3,3,3	0.89	0
5	DMS	B	8403	-	3,3,3	1.74	1 (33%)	3,3,3	0.67	0
5	DMS	C	8417	-	3,3,3	1.05	0	3,3,3	0.30	0
5	DMS	C	8407	-	3,3,3	2.19	1 (33%)	3,3,3	0.06	0
5	DMS	B	8502	-	3,3,3	1.35	0	3,3,3	1.68	1 (33%)
5	DMS	D	8701	-	3,3,3	2.38	2 (66%)	3,3,3	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	C	8409	-	3,3,3	2.21	1 (33%)	3,3,3	0.52	0
5	DMS	B	8411	-	3,3,3	0.52	0	3,3,3	0.68	0
2	GAL	A	2002	-	12,12,12	0.42	0	17,17,17	1.25	2 (11%)
5	DMS	C	8420	-	3,3,3	1.88	1 (33%)	3,3,3	0.54	0
5	DMS	D	8410	-	3,3,3	1.05	0	3,3,3	0.60	0
5	DMS	C	8504	-	3,3,3	1.43	0	3,3,3	0.34	0
5	DMS	D	8416	-	3,3,3	0.57	0	3,3,3	0.33	0
5	DMS	A	8409	-	3,3,3	2.69	2 (66%)	3,3,3	0.13	0
5	DMS	A	8403	-	3,3,3	1.54	0	3,3,3	0.83	0
5	DMS	D	8414	-	3,3,3	0.65	0	3,3,3	0.91	0
5	DMS	D	8413	-	3,3,3	1.58	0	3,3,3	0.66	0
5	DMS	B	8401	-	3,3,3	0.70	0	3,3,3	0.25	0
5	DMS	A	8408	-	3,3,3	0.71	0	3,3,3	0.42	0
2	GAL	C	2002	-	12,12,12	0.86	0	17,17,17	1.87	7 (41%)
5	DMS	D	8421	-	3,3,3	0.40	0	3,3,3	0.14	0
5	DMS	D	8401	-	3,3,3	1.63	0	3,3,3	0.55	0
5	DMS	A	8413	-	3,3,3	2.74	3 (100%)	3,3,3	0.20	0
5	DMS	D	8402	-	3,3,3	2.10	2 (66%)	3,3,3	0.28	0
5	DMS	C	8413	-	3,3,3	1.93	1 (33%)	3,3,3	0.18	0
5	DMS	D	8703	-	3,3,3	1.15	0	3,3,3	0.52	0
5	DMS	C	8408	-	3,3,3	0.93	0	3,3,3	0.84	0
5	DMS	A	8406	-	3,3,3	1.57	1 (33%)	3,3,3	0.80	0
5	DMS	A	8425	4	3,3,3	1.92	1 (33%)	3,3,3	1.12	0
5	DMS	A	8414	-	3,3,3	1.01	0	3,3,3	0.63	0
5	DMS	D	8408	-	3,3,3	1.24	0	3,3,3	0.33	0
2	GAL	A	2001	4	12,12,12	1.64	3 (25%)	17,17,17	1.68	5 (29%)
5	DMS	D	8409	-	3,3,3	3.38	2 (66%)	3,3,3	0.91	0
5	DMS	D	8425	4	3,3,3	0.54	0	3,3,3	0.38	0
5	DMS	D	8412	-	3,3,3	0.70	0	3,3,3	0.79	0
5	DMS	C	8501	-	3,3,3	1.07	0	3,3,3	1.21	1 (33%)
5	DMS	D	8406	-	3,3,3	1.47	0	3,3,3	0.66	0
5	DMS	C	8425	4	3,3,3	1.26	1 (33%)	3,3,3	0.97	0
5	DMS	B	8405	-	3,3,3	1.67	1 (33%)	3,3,3	0.89	0
5	DMS	D	8411	-	3,3,3	1.14	0	3,3,3	0.68	0
5	DMS	C	8421	-	3,3,3	1.32	0	3,3,3	0.69	0
5	DMS	C	8410	-	3,3,3	0.76	0	3,3,3	0.67	0
5	DMS	D	8404	-	3,3,3	1.42	1 (33%)	3,3,3	0.56	0
5	DMS	C	8415	-	3,3,3	2.02	1 (33%)	3,3,3	1.17	0
5	DMS	A	8402	-	3,3,3	1.52	1 (33%)	3,3,3	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	A	8421	-	3,3,3	1.60	1 (33%)	3,3,3	0.10	0
5	DMS	B	8406	-	3,3,3	1.72	1 (33%)	3,3,3	0.31	0
5	DMS	B	8504	-	3,3,3	0.98	0	3,3,3	0.21	0
5	DMS	D	8403	-	3,3,3	1.46	0	3,3,3	0.44	0
5	DMS	D	8415	-	3,3,3	2.52	1 (33%)	3,3,3	0.87	0
5	DMS	B	8416	-	3,3,3	0.93	0	3,3,3	0.18	0
5	DMS	C	8602	-	3,3,3	1.31	1 (33%)	3,3,3	0.67	0
5	DMS	C	8403	-	3,3,3	0.61	0	3,3,3	0.48	0
5	DMS	B	8414	-	3,3,3	0.60	0	3,3,3	1.06	0
5	DMS	B	8425	4	3,3,3	1.88	1 (33%)	3,3,3	0.63	0
2	GAL	B	2001	4	12,12,12	1.32	1 (8%)	17,17,17	1.85	5 (29%)
5	DMS	B	8420	-	3,3,3	1.52	1 (33%)	3,3,3	0.28	0
5	DMS	C	8411	-	3,3,3	0.81	0	3,3,3	0.29	0
2	GAL	C	2001	4	12,12,12	1.32	2 (16%)	17,17,17	1.88	3 (17%)
5	DMS	B	8421	-	3,3,3	0.33	0	3,3,3	0.90	0
5	DMS	C	8412	-	3,3,3	0.78	0	3,3,3	0.40	0
5	DMS	B	8410	-	3,3,3	1.21	0	3,3,3	0.31	0
5	DMS	C	8404	-	3,3,3	1.44	0	3,3,3	1.27	1 (33%)
5	DMS	D	8508	-	3,3,3	1.74	1 (33%)	3,3,3	0.56	0
5	DMS	B	8404	-	3,3,3	0.98	0	3,3,3	0.92	0
5	DMS	A	8501	-	3,3,3	0.77	0	3,3,3	0.64	0
5	DMS	A	8415	-	3,3,3	2.64	2 (66%)	3,3,3	1.12	0
5	DMS	C	8416	-	3,3,3	0.87	0	3,3,3	0.12	0
5	DMS	A	8416	-	3,3,3	1.14	0	3,3,3	0.30	0
5	DMS	A	8404	-	3,3,3	1.46	0	3,3,3	0.35	0
5	DMS	B	8408	-	3,3,3	0.89	0	3,3,3	0.20	0
5	DMS	C	8402	-	3,3,3	1.95	1 (33%)	3,3,3	0.40	0
5	DMS	D	8506	-	3,3,3	0.67	0	3,3,3	0.67	0
5	DMS	C	8401	-	3,3,3	1.06	0	3,3,3	0.61	0
2	GAL	D	2001	4	12,12,12	1.39	2 (16%)	17,17,17	1.97	5 (29%)
5	DMS	B	8417	-	3,3,3	1.27	0	3,3,3	0.41	0
5	DMS	A	8411	-	3,3,3	0.74	0	3,3,3	0.30	0
5	DMS	B	8501	-	3,3,3	0.78	0	3,3,3	0.60	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
2	GAL	B	2001	4	-	1/2/22/22	0/1/1/1
2	GAL	B	2002	-	-	0/2/22/22	0/1/1/1
2	GAL	A	2002	-	-	0/2/22/22	0/1/1/1
2	GAL	D	2001	4	-	1/2/22/22	0/1/1/1
2	GAL	D	2002	-	-	0/2/22/22	0/1/1/1
2	GAL	C	2002	-	-	1/2/22/22	0/1/1/1
2	GAL	A	2001	4	-	1/2/22/22	0/1/1/1
2	GAL	C	2001	4	-	1/2/22/22	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8504	DMS	C1-S	-5.13	1.37	1.75
5	D	8409	DMS	O-S	5.08	1.84	1.50
5	A	8407	DMS	O-S	4.74	1.82	1.50
5	B	8409	DMS	O-S	4.58	1.81	1.50
5	A	8407	DMS	C2-S	4.10	2.06	1.75
5	D	8415	DMS	C1-S	3.99	2.05	1.75
5	B	8601	DMS	C2-S	3.90	2.04	1.75
5	A	8409	DMS	O-S	3.79	1.75	1.50
5	A	8415	DMS	C2-S	3.60	2.02	1.75
5	C	8409	DMS	O-S	3.56	1.74	1.50
2	A	2001	GAL	O2-C2	3.50	1.51	1.43
5	A	8413	DMS	C1-S	3.28	2.00	1.75
5	C	8402	DMS	C2-S	3.24	1.99	1.75
5	A	8502	DMS	C1-S	3.11	1.99	1.75
5	C	8407	DMS	C2-S	3.11	1.98	1.75
5	C	8415	DMS	C2-S	3.06	1.98	1.75
5	C	8420	DMS	O-S	3.02	1.70	1.50
5	D	8705	DMS	O-S	3.00	1.70	1.50
5	B	8425	DMS	O-S	2.95	1.70	1.50
5	D	8701	DMS	O-S	2.89	1.69	1.50
2	B	2001	GAL	O2-C2	2.86	1.49	1.43
5	C	8413	DMS	O-S	2.84	1.69	1.50
5	D	8409	DMS	C1-S	2.76	1.96	1.75
2	D	2001	GAL	O2-C2	2.68	1.49	1.43
5	D	8402	DMS	O-S	2.67	1.68	1.50
5	B	8407	DMS	C2-S	2.64	1.95	1.75
5	A	8412	DMS	O-S	2.62	1.67	1.50
2	C	2001	GAL	C4-C3	2.61	1.59	1.52
5	A	8405	DMS	O-S	2.59	1.67	1.50
5	A	8409	DMS	C1-S	2.59	1.95	1.75
5	A	8413	DMS	C2-S	2.53	1.94	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8421	DMS	C1-S	2.49	1.94	1.75
5	A	8415	DMS	C1-S	2.47	1.94	1.75
5	B	8407	DMS	C1-S	-2.45	1.57	1.75
5	D	8508	DMS	O-S	2.40	1.66	1.50
5	C	8405	DMS	O-S	2.40	1.66	1.50
5	B	8406	DMS	C1-S	2.37	1.93	1.75
5	A	8412	DMS	C1-S	2.33	1.93	1.75
5	C	8405	DMS	C1-S	2.32	1.93	1.75
2	C	2001	GAL	O2-C2	2.32	1.48	1.43
5	B	8403	DMS	C2-S	2.31	1.93	1.75
5	A	8413	DMS	O-S	2.31	1.65	1.50
5	B	8420	DMS	C2-S	2.25	1.92	1.75
5	B	8405	DMS	O-S	2.25	1.65	1.50
5	D	8701	DMS	C1-S	2.24	1.92	1.75
5	A	8425	DMS	C2-S	2.22	1.92	1.75
5	D	8404	DMS	C2-S	2.22	1.92	1.75
5	C	8602	DMS	C2-S	-2.21	1.59	1.75
5	A	8406	DMS	C1-S	-2.20	1.59	1.75
5	D	8405	DMS	C1-S	2.19	1.92	1.75
5	B	8402	DMS	C2-S	2.18	1.92	1.75
5	A	8506	DMS	O-S	2.11	1.64	1.50
2	D	2001	GAL	C4-C3	2.11	1.57	1.52
2	A	2001	GAL	O1-C1	2.10	1.46	1.39
2	A	2001	GAL	C6-C5	2.07	1.58	1.51
5	C	8425	DMS	O-S	2.07	1.64	1.50
5	D	8402	DMS	C2-S	2.06	1.91	1.75
5	A	8402	DMS	O-S	2.04	1.64	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	GAL	O4-C4-C5	-4.94	97.02	109.30
2	B	2001	GAL	O1-C1-O5	-3.89	98.69	110.38
2	C	2001	GAL	O2-C2-C1	3.87	118.13	109.16
2	D	2001	GAL	O2-C2-C1	3.83	118.04	109.16
2	A	2001	GAL	O2-C2-C1	3.77	117.91	109.16
2	C	2002	GAL	C3-C4-C5	-3.71	103.62	110.24
2	D	2001	GAL	O1-C1-O5	-3.71	99.26	110.38
2	D	2002	GAL	C1-C2-C3	3.66	117.91	110.31
2	D	2001	GAL	O4-C4-C5	-3.53	100.53	109.30
2	B	2001	GAL	O4-C4-C5	-3.28	101.14	109.30
2	B	2001	GAL	O2-C2-C1	3.24	116.67	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	GAL	C1-O5-C5	3.17	119.65	113.66
2	C	2002	GAL	O5-C5-C4	2.97	115.09	109.69
5	A	8502	DMS	C2-S-C1	2.90	113.35	98.44
5	B	8502	DMS	C2-S-C1	2.89	113.31	98.44
2	D	2001	GAL	O2-C2-C3	2.86	116.96	110.35
2	C	2001	GAL	O1-C1-O5	-2.86	101.81	110.38
2	D	2002	GAL	O2-C2-C1	2.74	115.52	109.16
2	D	2002	GAL	O1-C1-O5	-2.73	102.19	110.38
2	C	2002	GAL	O4-C4-C5	2.72	116.04	109.30
2	C	2002	GAL	O1-C1-O5	-2.62	102.53	110.38
2	B	2002	GAL	C1-C2-C3	2.59	115.69	110.31
2	D	2002	GAL	C1-O5-C5	-2.52	108.91	113.66
2	B	2001	GAL	O1-C1-C2	2.50	116.07	109.03
2	A	2001	GAL	O1-C1-O5	-2.47	102.96	110.38
2	B	2002	GAL	O4-C4-C5	2.42	115.32	109.30
2	A	2001	GAL	O1-C1-C2	2.39	115.77	109.03
2	D	2002	GAL	C3-C4-C5	-2.35	106.05	110.24
2	B	2001	GAL	C1-O5-C5	2.34	118.08	113.66
2	A	2002	GAL	O1-C1-O5	-2.31	103.45	110.38
2	C	2002	GAL	O2-C2-C3	-2.27	105.10	110.35
2	B	2002	GAL	O1-C1-O5	-2.25	103.63	110.38
2	D	2001	GAL	O1-C1-C2	2.24	115.34	109.03
2	C	2002	GAL	O5-C5-C6	2.18	111.85	106.44
5	C	8414	DMS	C2-S-C1	2.17	109.63	98.44
2	A	2001	GAL	O5-C5-C4	-2.17	105.75	109.69
5	B	8407	DMS	C2-S-C1	2.10	109.23	98.44
5	C	8404	DMS	C2-S-C1	2.09	109.21	98.44
2	C	2002	GAL	O3-C3-C4	-2.08	105.54	110.35
2	A	2002	GAL	C1-O5-C5	-2.07	109.75	113.66
5	C	8501	DMS	C2-S-C1	-2.02	88.05	98.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2002	GAL	O5-C5-C6-O6
2	C	2001	GAL	O5-C5-C6-O6
2	A	2001	GAL	O5-C5-C6-O6
2	B	2001	GAL	O5-C5-C6-O6
2	D	2001	GAL	O5-C5-C6-O6

There are no ring outliers.

30 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8412	DMS	2	0
5	A	8502	DMS	1	0
5	C	8506	DMS	1	0
5	A	8420	DMS	1	0
5	A	8506	DMS	3	0
2	B	2002	GAL	2	0
5	A	8407	DMS	1	0
5	B	8601	DMS	1	0
5	C	8417	DMS	1	0
5	C	8420	DMS	1	0
5	D	8421	DMS	1	0
5	D	8703	DMS	5	0
2	A	2001	GAL	1	0
5	D	8425	DMS	4	0
5	D	8412	DMS	2	0
5	D	8406	DMS	1	0
5	C	8410	DMS	1	0
5	A	8421	DMS	1	0
5	B	8406	DMS	1	0
5	D	8415	DMS	1	0
2	B	2001	GAL	1	0
5	B	8420	DMS	1	0
2	C	2001	GAL	1	0
5	B	8421	DMS	1	0
5	B	8410	DMS	1	0
5	A	8415	DMS	3	0
5	A	8416	DMS	2	0
5	D	8506	DMS	3	0
2	D	2001	GAL	1	0
5	B	8417	DMS	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	1010/1023 (98%)	-0.34	25 (2%) 57 62	8, 15, 43, 97	0
1	B	1010/1023 (98%)	-0.40	13 (1%) 77 81	8, 15, 45, 91	0
1	C	1010/1023 (98%)	-0.40	19 (1%) 66 71	8, 15, 47, 99	0
1	D	1010/1023 (98%)	-0.31	31 (3%) 49 54	8, 16, 47, 97	0
All	All	4040/4092 (98%)	-0.36	88 (2%) 62 67	8, 15, 46, 99	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	8.4
1	A	730	LEU	8.4
1	C	732	ALA	8.0
1	C	730	LEU	7.9
1	D	735	HIS	7.7
1	B	730	LEU	7.6
1	D	732	ALA	6.9
1	C	685	LEU	6.4
1	A	686	PRO	6.0
1	C	731	PRO	5.9
1	B	687	GLN	5.6
1	D	733	ALA	5.6
1	C	689	GLU	5.6
1	B	685	LEU	5.5
1	B	731	PRO	5.4
1	A	732	ALA	5.1
1	A	1023	LYS	5.0
1	C	735	HIS	4.9
1	D	687	GLN	4.9
1	B	686	PRO	4.5
1	D	736	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	1023	LYS	4.4
1	B	689	GLU	4.3
1	D	581	ASN	4.2
1	D	730	LEU	4.2
1	A	733	ALA	4.1
1	D	734	SER	3.9
1	A	685	LEU	3.8
1	C	736	ALA	3.8
1	A	580	GLU	3.7
1	A	734	SER	3.7
1	A	736	ALA	3.6
1	C	733	ALA	3.5
1	C	687	GLN	3.5
1	B	732	ALA	3.4
1	D	683	PRO	3.4
1	D	845	GLN	3.4
1	A	1022	GLN	3.3
1	A	687	GLN	3.2
1	D	798	ALA	3.2
1	A	581	ASN	3.2
1	A	634	GLN	3.2
1	D	634	GLN	3.2
1	B	684	GLU	3.2
1	B	733	ALA	3.1
1	D	580	GLU	3.1
1	A	737	ILE	3.1
1	A	682	LEU	3.0
1	B	799	THR	3.0
1	C	686	PRO	2.9
1	D	689	GLU	2.8
1	D	800	ARG	2.8
1	D	688	PRO	2.8
1	D	685	LEU	2.7
1	C	684	GLU	2.7
1	A	845	GLN	2.7
1	B	580	GLU	2.7
1	A	582	GLY	2.7
1	D	729	THR	2.6
1	C	737	ILE	2.6
1	A	731	PRO	2.6
1	C	688	PRO	2.6
1	C	253	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	800	ARG	2.6
1	D	582	GLY	2.5
1	D	799	THR	2.5
1	C	745	MET	2.5
1	C	799	THR	2.4
1	A	798	ALA	2.4
1	A	800	ARG	2.4
1	D	731	PRO	2.4
1	D	772	ASP	2.4
1	D	663	LEU	2.4
1	D	737	ILE	2.3
1	D	682	LEU	2.3
1	B	735	HIS	2.3
1	A	799	THR	2.3
1	D	684	GLU	2.3
1	D	753	ASN	2.3
1	D	681	GLU	2.2
1	D	771	GLY	2.2
1	A	729	THR	2.2
1	C	734	SER	2.2
1	A	683	PRO	2.2
1	D	76	CYS	2.2
1	B	690	SER	2.1
1	A	633	GLY	2.1
1	C	729	THR	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	B	247[B]	7/8	0.97	0.06	13,14,18,24	1
1	CSO	B	247[A]	7/8	0.97	0.06	13,14,17,24	1
1	CSO	A	247[B]	7/8	0.98	0.06	9,11,19,23	1
1	CSO	D	247[A]	7/8	0.98	0.06	12,13,16,22	1
1	CSO	C	247[A]	7/8	0.98	0.06	11,14,18,23	1
1	CSO	D	247[B]	7/8	0.98	0.06	12,13,22,25	1
1	CSO	C	247[B]	7/8	0.98	0.06	11,14,18,23	1
1	CSO	A	247[A]	7/8	0.98	0.06	9,11,17,23	1

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	B	8407	4/4	0.78	0.18	30,33,43,100	0
5	DMS	A	8413	4/4	0.81	0.12	32,37,45,63	0
5	DMS	B	8416	4/4	0.81	0.24	40,43,55,89	0
5	DMS	B	8420	4/4	0.84	0.20	36,61,77,100	0
5	DMS	B	8410	4/4	0.84	0.17	33,33,37,100	0
5	DMS	D	8703	4/4	0.87	0.14	27,53,54,55	0
5	DMS	D	8506	4/4	0.88	0.15	18,46,92,97	0
5	DMS	C	8417	4/4	0.89	0.14	25,29,49,71	0
5	DMS	A	8421	4/4	0.89	0.14	45,47,58,61	0
2	GAL	B	2002	12/12	0.90	0.13	22,32,100,100	0
3	MG	A	3105	1/1	0.91	0.13	24,24,24,24	1
5	DMS	D	8404	4/4	0.91	0.11	20,25,43,76	0
2	GAL	C	2002	12/12	0.91	0.11	21,31,100,100	0
5	DMS	B	8406	4/4	0.91	0.15	26,45,45,78	0
5	DMS	D	8415	4/4	0.91	0.15	24,41,66,100	0
3	MG	B	3105	1/1	0.92	0.12	21,21,21,21	1
5	DMS	A	8406	4/4	0.92	0.14	15,36,67,72	0
5	DMS	D	8705	4/4	0.92	0.12	38,41,44,56	0
5	DMS	A	8407	4/4	0.93	0.11	25,28,44,46	0
3	MG	C	3105	1/1	0.94	0.09	20,20,20,20	1
5	DMS	B	8601	4/4	0.94	0.12	34,35,47,54	0
2	GAL	D	2002	12/12	0.94	0.08	17,25,30,37	0
2	GAL	A	2002	12/12	0.94	0.09	20,27,80,86	0
5	DMS	D	8416	4/4	0.94	0.17	28,50,52,100	0
5	DMS	D	8425	4/4	0.94	0.18	19,35,36,97	4
5	DMS	B	8421	4/4	0.94	0.11	28,37,39,48	0
5	DMS	C	8504	4/4	0.94	0.12	24,33,65,100	0
4	NA	D	3104	1/1	0.94	0.11	33,33,33,33	0
5	DMS	C	8415	4/4	0.94	0.10	23,30,31,47	0
5	DMS	A	8502	4/4	0.94	0.10	19,27,43,58	0
4	NA	C	3104	1/1	0.95	0.13	25,25,25,25	0
5	DMS	C	8425	4/4	0.95	0.13	30,31,38,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	C	8602	4/4	0.95	0.11	25,60,68,100	0
5	DMS	B	8425	4/4	0.95	0.15	27,32,35,40	0
5	DMS	A	8506	4/4	0.95	0.12	28,72,82,100	0
4	NA	D	3103	1/1	0.95	0.07	30,30,30,30	0
4	NA	A	3103	1/1	0.95	0.07	28,28,28,28	0
5	DMS	C	8420	4/4	0.95	0.12	37,46,55,100	0
5	DMS	D	8508	4/4	0.95	0.11	32,42,47,100	0
5	DMS	A	8501	4/4	0.95	0.10	18,22,30,33	0
5	DMS	C	8416	4/4	0.95	0.23	37,44,55,100	0
5	DMS	D	8501	4/4	0.95	0.07	19,26,44,46	0
5	DMS	C	8414	4/4	0.95	0.12	19,34,45,100	0
2	GAL	D	2001	12/12	0.95	0.08	10,16,20,22	0
5	DMS	B	8417	4/4	0.95	0.10	25,36,59,79	0
5	DMS	C	8409	4/4	0.96	0.08	29,31,36,40	0
5	DMS	A	8425	4/4	0.96	0.09	27,32,39,40	0
5	DMS	C	8506	4/4	0.96	0.11	34,44,65,100	0
2	GAL	A	2001	12/12	0.96	0.08	10,18,25,31	0
2	GAL	B	2001	12/12	0.96	0.09	11,19,31,31	0
5	DMS	D	8409	4/4	0.96	0.07	23,25,30,32	0
2	GAL	C	2001	12/12	0.96	0.09	11,17,24,25	0
5	DMS	A	8409	4/4	0.96	0.10	26,29,40,47	0
5	DMS	C	8407	4/4	0.96	0.10	29,40,44,100	0
5	DMS	C	8412	4/4	0.96	0.13	30,41,46,74	0
5	DMS	A	8420	4/4	0.96	0.11	38,38,40,70	0
5	DMS	C	8421	4/4	0.96	0.10	37,46,56,100	0
5	DMS	D	8421	4/4	0.96	0.13	34,55,55,100	0
5	DMS	B	8409	4/4	0.96	0.08	24,25,35,69	0
5	DMS	A	8416	4/4	0.96	0.18	19,38,75,100	0
5	DMS	C	8413	4/4	0.96	0.14	35,37,44,100	0
3	MG	A	3005	1/1	0.96	0.07	30,30,30,30	0
5	DMS	A	8412	4/4	0.96	0.11	30,40,41,100	0
5	DMS	C	8408	4/4	0.96	0.08	24,31,36,47	0
5	DMS	C	8405	4/4	0.97	0.07	23,30,31,31	0
5	DMS	A	8414	4/4	0.97	0.10	26,32,54,100	0
3	MG	D	3105	1/1	0.97	0.09	23,23,23,23	1
5	DMS	A	8410	4/4	0.97	0.12	28,35,41,100	0
5	DMS	D	8413	4/4	0.97	0.12	30,42,49,100	0
5	DMS	A	8408	4/4	0.97	0.08	18,31,36,100	0
5	DMS	B	8404	4/4	0.97	0.10	15,20,29,30	0
5	DMS	C	8501	4/4	0.97	0.07	17,29,31,32	0
5	DMS	D	8406	4/4	0.97	0.09	21,22,24,33	0
5	DMS	A	8504	4/4	0.97	0.12	12,38,65,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	B	8414	4/4	0.97	0.11	28,45,56,64	0
5	DMS	B	8408	4/4	0.97	0.11	27,35,38,87	0
3	MG	D	3005	1/1	0.97	0.07	29,29,29,29	0
5	DMS	C	8410	4/4	0.97	0.08	24,36,39,41	0
5	DMS	B	8501	4/4	0.97	0.08	23,28,37,64	0
5	DMS	A	8405	4/4	0.98	0.07	21,22,22,24	0
5	DMS	D	8414	4/4	0.98	0.13	23,39,62,78	0
5	DMS	D	8701	4/4	0.98	0.10	14,15,20,58	0
5	DMS	B	8504	4/4	0.98	0.06	21,24,27,33	0
5	DMS	C	8404	4/4	0.98	0.07	17,18,21,24	0
5	DMS	D	8403	4/4	0.98	0.07	15,22,25,25	0
4	NA	B	3104	1/1	0.98	0.11	27,27,27,27	0
4	NA	B	3103	1/1	0.98	0.08	24,24,24,24	0
5	DMS	B	8405	4/4	0.98	0.08	22,25,26,27	0
5	DMS	A	8415	4/4	0.98	0.07	22,41,41,43	0
5	DMS	D	8411	4/4	0.98	0.07	23,24,28,100	0
5	DMS	D	8408	4/4	0.98	0.08	17,25,30,42	0
5	DMS	A	8404	4/4	0.98	0.06	16,22,27,28	0
5	DMS	D	8410	4/4	0.98	0.08	32,38,39,62	0
5	DMS	C	8402	4/4	0.98	0.07	13,24,25,26	0
4	NA	C	3103	1/1	0.98	0.05	24,24,24,24	0
4	NA	A	3104	1/1	0.98	0.06	24,24,24,24	0
3	MG	C	3006	1/1	0.98	0.12	23,23,23,23	0
5	DMS	B	8402	4/4	0.98	0.07	15,18,21,21	0
5	DMS	B	8502	4/4	0.98	0.10	20,26,35,38	0
5	DMS	B	8403	4/4	0.99	0.06	15,19,23,24	0
4	NA	A	3101	1/1	0.99	0.05	13,13,13,13	0
5	DMS	A	8402	4/4	0.99	0.05	15,16,20,24	0
5	DMS	D	8401	4/4	0.99	0.05	12,13,16,17	0
5	DMS	B	8411	4/4	0.99	0.04	21,21,24,67	0
5	DMS	D	8402	4/4	0.99	0.06	15,20,22,25	0
5	DMS	A	8403	4/4	0.99	0.06	16,21,22,26	0
4	NA	D	3101	1/1	0.99	0.05	13,13,13,13	0
4	NA	B	3101	1/1	0.99	0.06	11,11,11,11	0
3	MG	D	3002	1/1	0.99	0.04	14,14,14,14	0
5	DMS	B	8401	4/4	0.99	0.06	13,16,19,20	0
5	DMS	A	8401	4/4	0.99	0.07	12,13,13,15	0
5	DMS	C	8403	4/4	0.99	0.06	17,19,22,30	0
5	DMS	B	8412	4/4	0.99	0.08	23,28,29,33	0
4	NA	D	3102	1/1	0.99	0.06	11,11,11,11	0
5	DMS	D	8412	4/4	0.99	0.07	20,26,29,39	0
5	DMS	C	8401	4/4	0.99	0.05	13,14,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	3002	1/1	0.99	0.05	14,14,14,14	0
3	MG	B	3002	1/1	0.99	0.05	14,14,14,14	0
5	DMS	C	8411	4/4	0.99	0.07	20,23,25,41	0
5	DMS	A	8411	4/4	0.99	0.07	22,26,26,35	0
5	DMS	D	8405	4/4	0.99	0.06	22,22,28,30	0
4	NA	B	3102	1/1	1.00	0.04	11,11,11,11	0
4	NA	C	3101	1/1	1.00	0.08	11,11,11,11	0
3	MG	D	3001	1/1	1.00	0.04	11,11,11,11	0
4	NA	A	3102	1/1	1.00	0.03	12,12,12,12	0
3	MG	C	3002	1/1	1.00	0.04	13,13,13,13	0
3	MG	B	3001	1/1	1.00	0.03	10,10,10,10	0
3	MG	A	3001	1/1	1.00	0.04	11,11,11,11	0
4	NA	C	3102	1/1	1.00	0.04	12,12,12,12	0
3	MG	C	3001	1/1	1.00	0.04	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.