



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:37 PM UTC

PDB ID : 1JZ7 / pdb_00001jz7
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

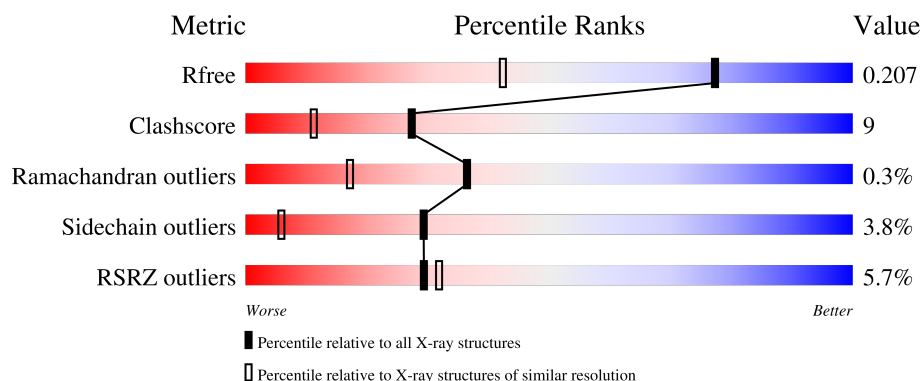
1 Overall quality at a glance

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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	5% 74% 19% 5% .
1	B	1023	6% 76% 19% . ..
1	C	1023	6% 74% 20% 5% ..
1	D	1023	6% 72% 22% . ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	A	8413	-	X	-	-
5	DMS	A	8415	-	-	X	-
5	DMS	A	8506	-	-	X	-
5	DMS	B	8407	-	X	-	-
5	DMS	D	8415	-	-	X	-
5	DMS	D	8425	-	-	X	-
5	DMS	D	8506	-	-	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:

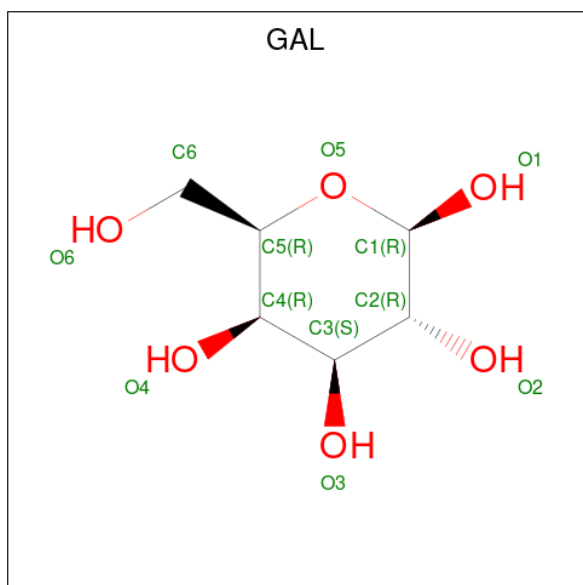
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact	? 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 (CCD ID: GAL) (formula: $C_6H_{12}O_6$).



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 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0

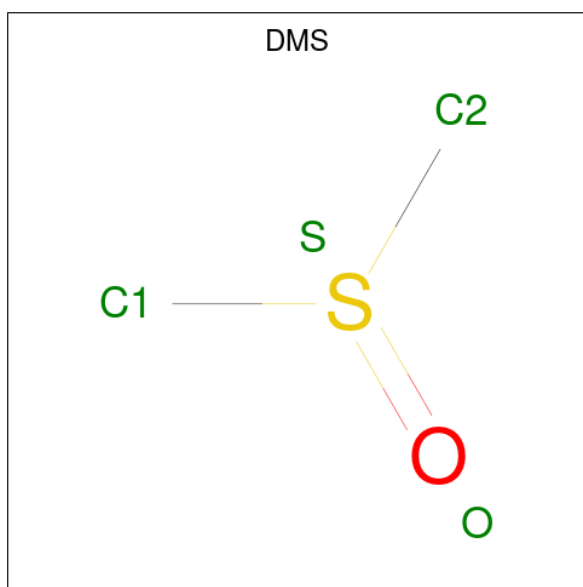
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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 C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0

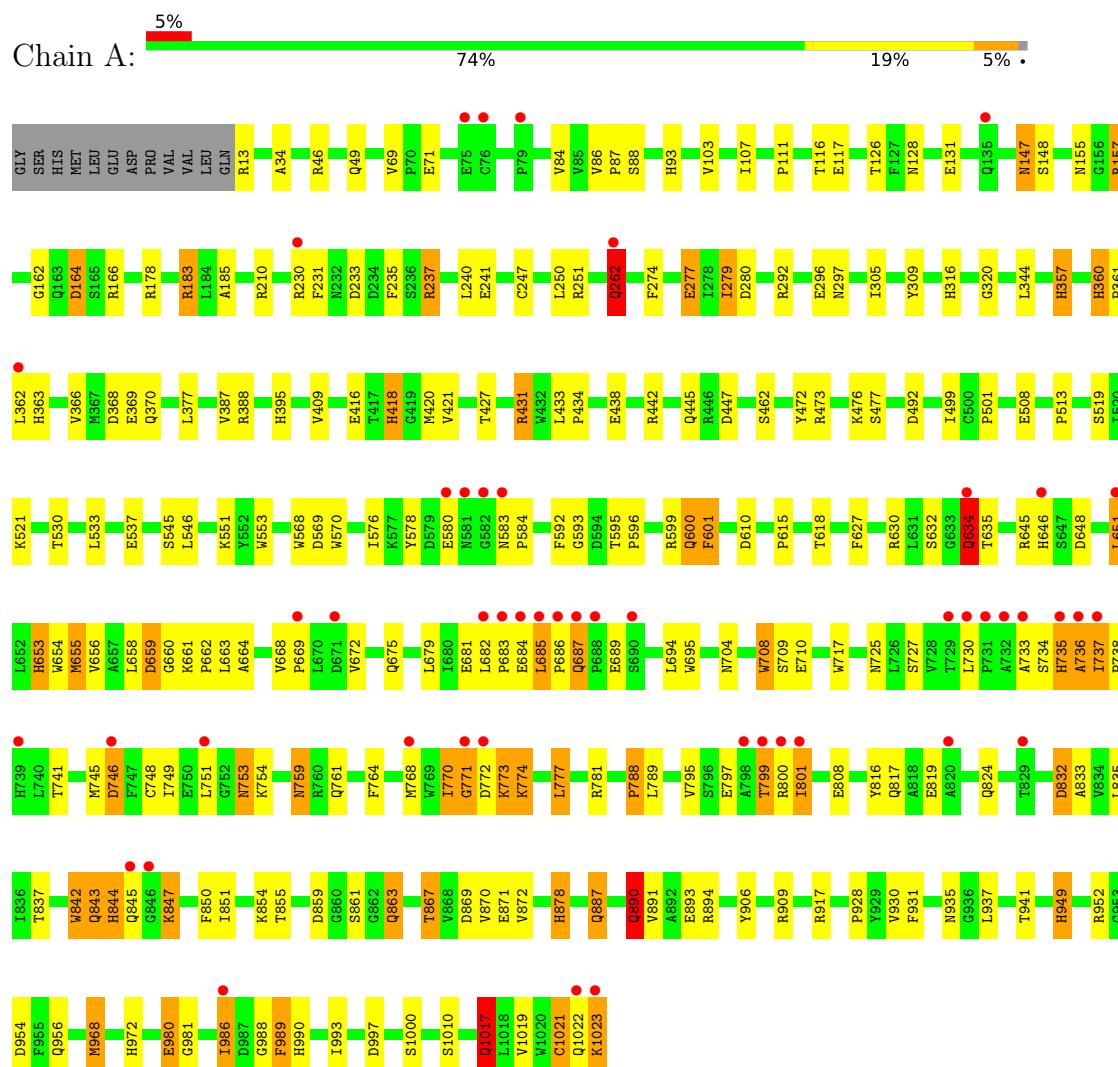
- Molecule 6 is water.

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

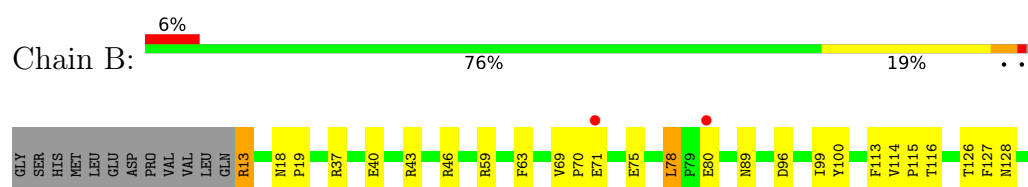
3 Residue-property plots

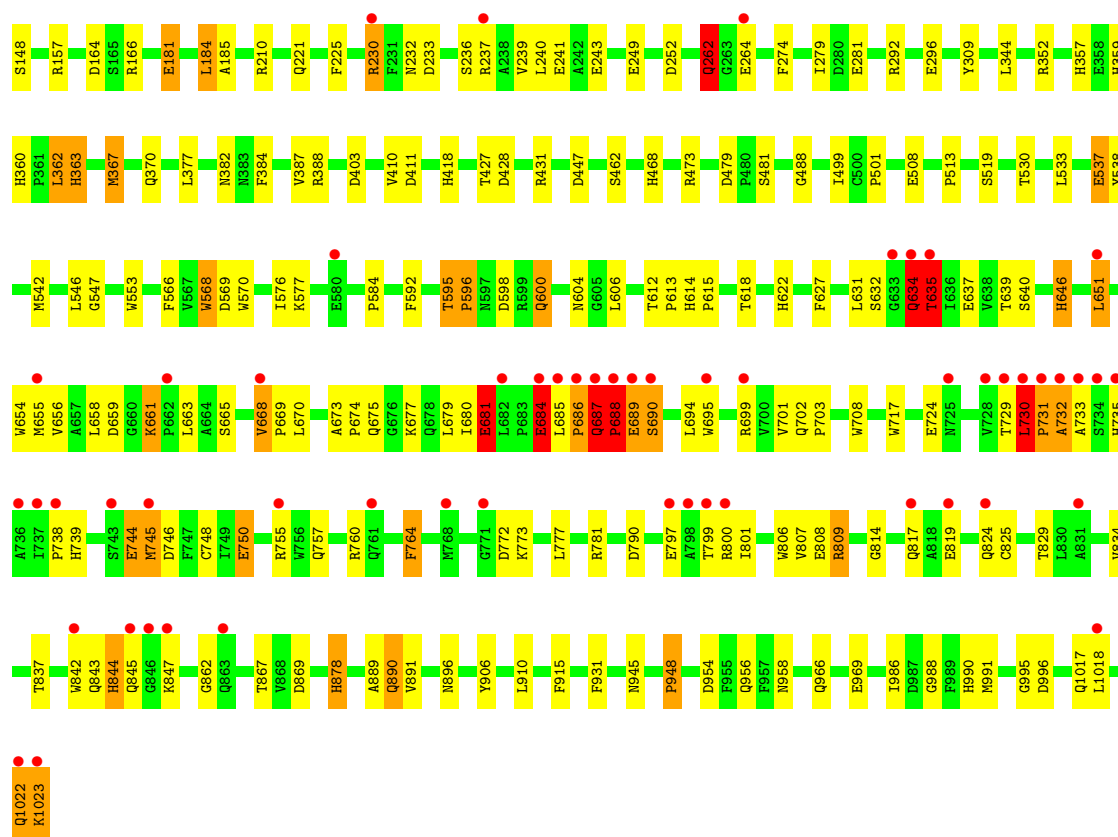
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

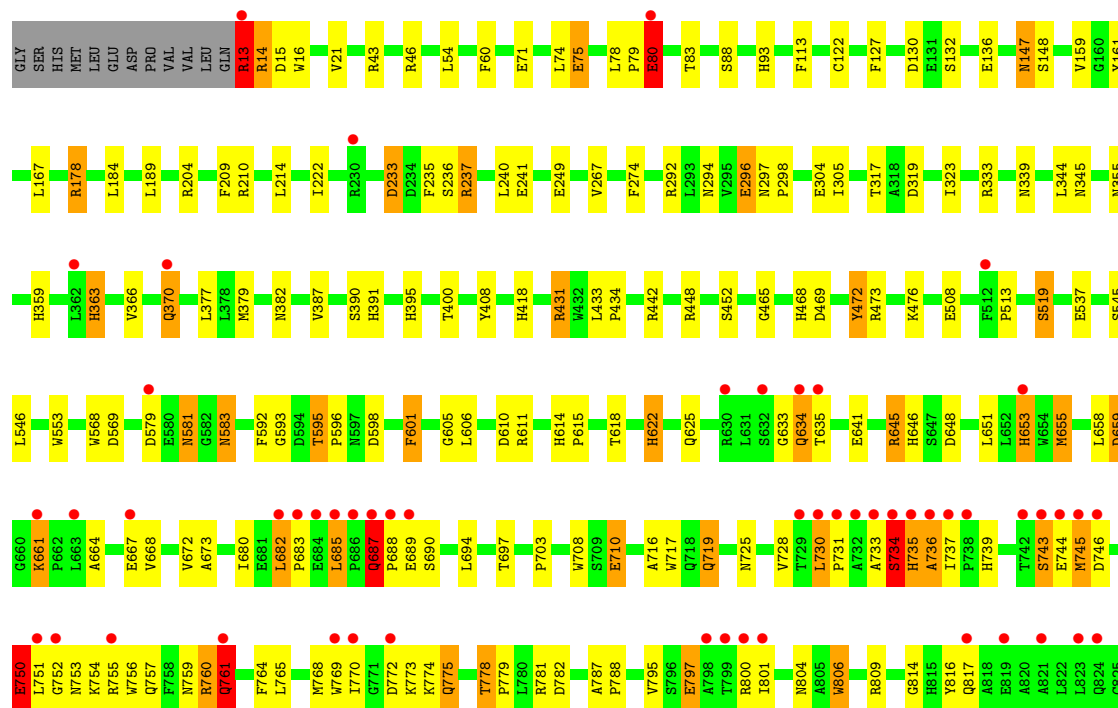
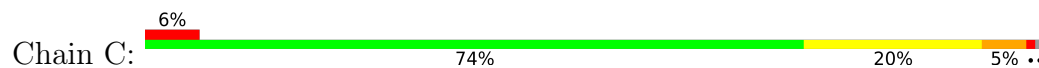


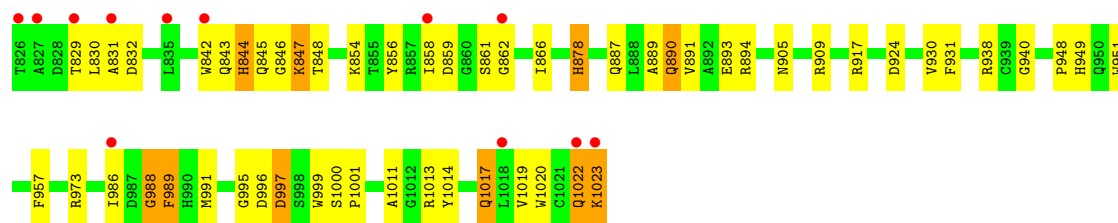
• Molecule 1: Beta-Galactosidase



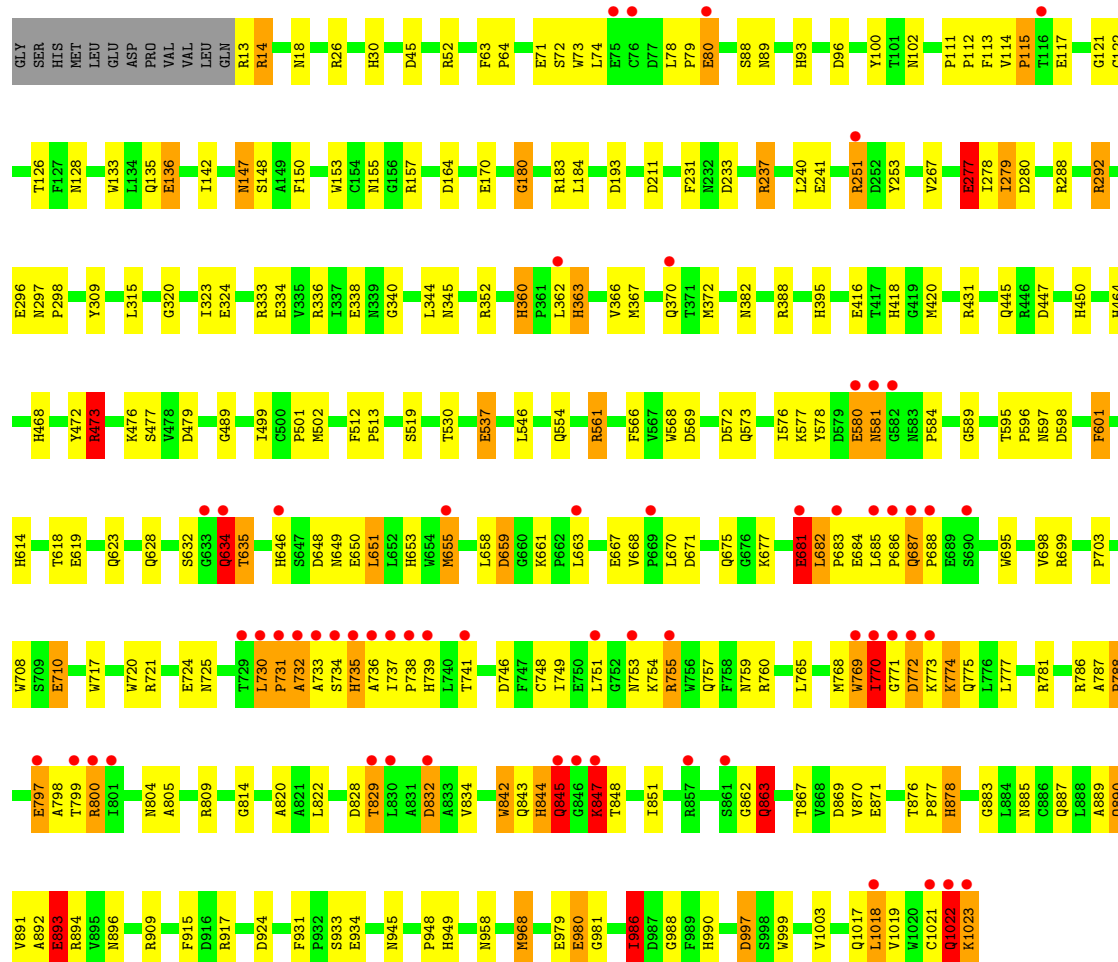


• Molecule 1: Beta-Galactosidase





• Molecule 1: Beta-Galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.59Å 168.53Å 200.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.50 40.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (40.00-1.50) 90.9 (40.00-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	12.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 83.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37213	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, CSO, NA, GAL, DMS

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	1.50	19/8360 (0.2%)	1.84	149/11404 (1.3%)
1	B	1.50	21/8360 (0.3%)	1.83	124/11404 (1.1%)
1	C	1.49	26/8360 (0.3%)	1.82	144/11404 (1.3%)
1	D	1.51	30/8360 (0.4%)	1.85	165/11404 (1.4%)
All	All	1.50	96/33440 (0.3%)	1.83	582/45616 (1.3%)

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 (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	ASN	C-O	-10.82	1.18	1.23
1	B	468	HIS	CE1-NE2	7.62	1.40	1.32
1	C	465	GLY	N-CA	7.13	1.51	1.44
1	C	468	HIS	CE1-NE2	6.87	1.39	1.32
1	B	906	TYR	N-CA	-6.68	1.41	1.46
1	D	418	HIS	CE1-NE2	6.55	1.39	1.32
1	B	990	HIS	CE1-NE2	6.45	1.39	1.32
1	D	479	ASP	C-N	-6.44	1.27	1.33
1	D	233	ASP	CG-OD2	6.34	1.37	1.25
1	A	1017	GLN	CA-C	-6.31	1.44	1.52
1	A	357	HIS	CE1-NE2	6.28	1.38	1.32
1	B	547	GLY	C-O	6.26	1.30	1.24
1	C	622	HIS	CG-CD2	6.25	1.42	1.35
1	A	418	HIS	CE1-NE2	6.22	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	972	HIS	CG-CD2	6.22	1.42	1.35
1	A	421	VAL	CA-CB	6.21	1.59	1.54
1	B	668	VAL	C-N	-6.20	1.25	1.33
1	A	210	ARG	NE-CZ	6.16	1.39	1.33
1	D	211	ASP	CG-OD2	6.15	1.37	1.25
1	B	418	HIS	CE1-NE2	6.12	1.38	1.32
1	A	280	ASP	CG-OD2	6.11	1.36	1.25
1	D	614	HIS	CE1-NE2	-6.10	1.26	1.32
1	D	468	HIS	CE1-NE2	6.10	1.38	1.32
1	D	280	ASP	CG-OD2	6.05	1.36	1.25
1	A	162	GLY	CA-C	6.01	1.58	1.51
1	A	492	ASP	CG-OD2	5.97	1.36	1.25
1	B	481	SER	C-O	5.95	1.31	1.24
1	C	210	ARG	NE-CZ	5.95	1.39	1.33
1	B	418	HIS	CG-CD2	5.89	1.42	1.35
1	B	410	VAL	CA-C	5.89	1.60	1.52
1	D	537	GLU	CD-OE2	5.84	1.36	1.25
1	D	561	ARG	NE-CZ	5.83	1.39	1.33
1	D	893	GLU	CD-OE2	5.82	1.36	1.25
1	D	519	SER	CA-C	5.79	1.59	1.52
1	C	297	ASN	CA-C	-5.78	1.50	1.53
1	B	488	GLY	CA-C	-5.75	1.47	1.52
1	A	409	VAL	CA-CB	5.75	1.62	1.54
1	C	519	SER	C-O	5.74	1.30	1.23
1	C	21	VAL	CA-C	5.69	1.59	1.52
1	D	502	MET	CA-C	5.67	1.59	1.52
1	D	13	ARG	C-N	-5.67	1.26	1.33
1	C	878	HIS	ND1-CE1	5.63	1.38	1.32
1	A	316	HIS	CG-CD2	5.61	1.42	1.35
1	D	30	HIS	CE1-NE2	5.61	1.38	1.32
1	B	210	ARG	NE-CZ	5.57	1.39	1.33
1	A	708	TRP	CA-CB	5.56	1.62	1.53
1	A	930	VAL	C-O	5.54	1.30	1.24
1	D	979	GLU	CD-OE2	5.52	1.35	1.25
1	C	167	LEU	CA-CB	5.50	1.60	1.54
1	B	71	GLU	CD-OE2	5.47	1.35	1.25
1	D	136	GLU	CD-OE2	5.46	1.35	1.25
1	D	150	PHE	C-N	5.42	1.40	1.33
1	C	806	TRP	NE1-CE2	5.41	1.43	1.37
1	A	551	LYS	CA-C	5.39	1.59	1.52
1	D	614	HIS	CG-ND1	-5.39	1.32	1.38
1	D	292	ARG	N-CA	5.39	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	989	PHE	N-CA	5.38	1.52	1.45
1	C	204	ARG	NE-CZ	5.37	1.39	1.33
1	B	418	HIS	CG-ND1	5.36	1.44	1.38
1	D	360	HIS	CE1-NE2	5.36	1.38	1.32
1	B	878	HIS	ND1-CE1	5.35	1.38	1.32
1	C	80	GLU	CD-OE2	5.35	1.35	1.25
1	D	844	HIS	N-CA	-5.33	1.39	1.46
1	D	800	ARG	NE-CZ	5.30	1.38	1.33
1	C	940	GLY	C-O	5.27	1.30	1.24
1	C	355	ASN	C-O	5.27	1.30	1.23
1	D	333	ARG	CD-NE	5.25	1.53	1.46
1	D	990	HIS	CE1-NE2	5.23	1.37	1.32
1	C	894	ARG	C-N	5.22	1.40	1.33
1	C	418	HIS	CE1-NE2	5.22	1.37	1.32
1	B	537	GLU	CD-OE2	5.21	1.35	1.25
1	C	304	GLU	CD-OE2	5.19	1.35	1.25
1	D	468	HIS	CG-ND1	5.17	1.44	1.38
1	A	447	ASP	CG-OD2	5.17	1.35	1.25
1	D	883	GLY	N-CA	5.17	1.50	1.44
1	C	687	GLN	CA-C	-5.16	1.47	1.53
1	D	1003	VAL	C-O	5.15	1.30	1.24
1	A	126	THR	CA-C	-5.14	1.46	1.52
1	B	181	GLU	CD-OE2	5.14	1.35	1.25
1	C	889	ALA	C-N	-5.12	1.26	1.33
1	B	133	TRP	N-CA	5.11	1.52	1.46
1	D	573	GLN	CA-CB	5.11	1.59	1.52
1	A	990	HIS	CD2-NE2	5.10	1.43	1.37
1	B	688	PRO	N-CA	-5.09	1.40	1.47
1	A	421	VAL	C-O	5.08	1.29	1.23
1	B	670	LEU	CA-C	-5.04	1.46	1.52
1	C	797	GLU	CD-OE2	5.04	1.34	1.25
1	B	185	ALA	N-CA	5.02	1.52	1.46
1	B	281	GLU	CD-OE2	5.02	1.34	1.25
1	D	885	ASN	C-N	-5.02	1.27	1.33
1	C	113	PHE	C-N	-5.02	1.27	1.33
1	C	359	HIS	CG-CD2	5.01	1.41	1.35
1	C	940	GLY	CA-C	5.01	1.56	1.51
1	D	650	GLU	CD-OE2	5.01	1.34	1.25
1	C	787	ALA	CA-C	5.01	1.58	1.52
1	A	111	PRO	CA-C	-5.00	1.47	1.52

All (582) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ASP	CA-CB-CG	-16.51	96.09	112.60
1	B	687	GLN	C-N-CD	-13.67	68.96	125.00
1	D	980	GLU	CA-C-N	-13.18	101.16	121.45
1	D	980	GLU	C-N-CA	-13.18	101.16	121.45
1	A	583	ASN	CA-CB-CG	-12.37	100.23	112.60
1	D	733	ALA	N-CA-C	11.94	124.03	111.14
1	C	363	HIS	CA-CB-CG	-11.54	102.27	113.80
1	D	893	GLU	CB-CG-CD	10.72	130.83	112.60
1	C	659	ASP	CA-CB-CG	-10.60	102.00	112.60
1	A	477	SER	N-CA-CB	10.05	124.65	110.07
1	C	581	ASN	CA-CB-CG	-9.84	102.76	112.60
1	A	659	ASP	CA-CB-CG	-9.59	103.02	112.60
1	B	78	LEU	CA-C-O	9.23	127.98	119.76
1	A	771	GLY	CA-C-N	-8.87	108.33	122.79
1	A	771	GLY	C-N-CA	-8.87	108.33	122.79
1	C	294	ASN	CA-CB-CG	-8.87	103.73	112.60
1	C	809	ARG	NE-CZ-NH1	8.79	130.29	121.50
1	B	733	ALA	CB-CA-C	8.73	121.84	109.71
1	D	770	ILE	N-CA-C	-8.55	93.68	107.28
1	C	725	ASN	CA-CB-CG	-8.48	104.12	112.60
1	A	13	ARG	N-CA-CB	8.46	124.88	110.50
1	B	363	HIS	CA-CB-CG	-8.41	105.39	113.80
1	C	845	GLN	CA-C-N	-8.28	110.37	122.46
1	C	845	GLN	C-N-CA	-8.28	110.37	122.46
1	B	986	ILE	CB-CA-C	8.10	122.27	110.77
1	D	277	GLU	CB-CG-CD	8.08	126.33	112.60
1	B	790	ASP	CA-CB-CG	-8.04	104.56	112.60
1	D	121	GLY	O-C-N	-8.03	118.29	123.35
1	D	251	ARG	CD-NE-CZ	8.02	135.63	124.40
1	C	473	ARG	CD-NE-CZ	7.97	135.56	124.40
1	C	989	PHE	CA-CB-CG	-7.96	105.84	113.80
1	C	733	ALA	N-CA-C	7.75	120.98	109.59
1	B	252	ASP	CA-CB-CG	-7.73	104.87	112.60
1	A	832	ASP	CA-CB-CG	-7.71	104.89	112.60
1	B	239	VAL	N-CA-CB	7.69	121.63	111.64
1	C	809	ARG	CD-NE-CZ	7.65	135.11	124.40
1	D	931	PHE	CA-CB-CG	-7.64	106.16	113.80
1	D	578	TYR	CA-C-O	-7.64	112.45	120.70
1	A	771	GLY	N-CA-C	-7.62	96.86	111.02
1	D	734	SER	CA-C-O	7.59	131.37	120.51
1	D	519	SER	N-CA-C	-7.58	99.55	110.24
1	A	235	PHE	CA-CB-CG	-7.53	106.27	113.80
1	D	948	PRO	CB-CA-C	-7.52	100.28	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	768	MET	CA-CB-CG	7.52	129.14	114.10
1	A	736	ALA	N-CA-C	7.48	119.77	107.73
1	C	370	GLN	CB-CG-CD	7.44	125.25	112.60
1	C	733	ALA	CA-C-N	7.41	135.70	121.54
1	C	733	ALA	C-N-CA	7.41	135.70	121.54
1	B	958	ASN	N-CA-CB	7.40	124.56	111.69
1	D	889	ALA	CA-C-O	7.38	128.46	119.97
1	A	817	GLN	CB-CG-CD	-7.37	100.08	112.60
1	C	249	GLU	N-CA-C	7.32	120.60	108.96
1	C	130	ASP	CA-CB-CG	-7.31	105.29	112.60
1	D	844	HIS	CA-CB-CG	-7.26	106.54	113.80
1	A	893	GLU	CA-CB-CG	-7.25	99.59	114.10
1	D	13	ARG	CA-C-N	-7.24	112.20	122.41
1	D	13	ARG	C-N-CA	-7.24	112.20	122.41
1	C	339	ASN	CA-CB-CG	-7.22	105.38	112.60
1	D	869	ASP	CA-CB-CG	-7.21	105.39	112.60
1	A	601	PHE	CA-CB-CG	-7.20	106.60	113.80
1	C	809	ARG	NE-CZ-NH2	-7.16	112.76	119.20
1	D	681	GLU	N-CA-CB	7.12	121.33	109.94
1	D	890	GLN	N-CA-CB	-7.09	99.96	110.17
1	C	237	ARG	CA-CB-CG	-7.07	99.97	114.10
1	A	847	LYS	CA-C-O	7.04	128.11	120.43
1	C	648	ASP	CA-CB-CG	-7.04	105.56	112.60
1	A	420	MET	CA-C-N	-7.04	116.72	122.85
1	A	420	MET	C-N-CA	-7.04	116.72	122.85
1	D	431	ARG	NE-CZ-NH2	-7.04	112.87	119.20
1	B	688	PRO	N-CA-CB	7.01	110.61	103.25
1	A	770	ILE	N-CA-CB	7.00	121.74	111.52
1	D	781	ARG	NE-CZ-NH1	6.96	128.46	121.50
1	C	739	HIS	CA-CB-CG	-6.96	106.84	113.80
1	A	131	GLU	N-CA-CB	-6.93	99.54	110.22
1	D	14	ARG	N-CA-CB	-6.89	100.36	110.49
1	C	345	ASN	CA-CB-CG	-6.89	105.71	112.60
1	A	685	LEU	O-C-N	6.88	129.23	121.32
1	D	980	GLU	O-C-N	-6.86	114.53	122.89
1	D	945	ASN	CA-CB-CG	-6.86	105.75	112.60
1	B	519	SER	N-CA-C	-6.85	100.58	110.24
1	A	513	PRO	CB-CA-C	-6.84	102.64	111.46
1	C	71	GLU	CB-CG-CD	6.83	124.21	112.60
1	A	277	GLU	N-CA-CB	-6.82	100.50	110.26
1	C	685	LEU	CA-C-N	6.82	126.85	119.89
1	C	685	LEU	C-N-CA	6.82	126.85	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	954	ASP	CA-CB-CG	-6.81	105.79	112.60
1	D	863	GLN	CB-CG-CD	-6.80	101.03	112.60
1	A	684	GLU	N-CA-C	-6.80	100.09	110.30
1	C	653	HIS	CA-CB-CG	6.79	120.59	113.80
1	D	360	HIS	CA-CB-CG	-6.79	107.01	113.80
1	A	844	HIS	CA-CB-CG	-6.79	107.01	113.80
1	B	382	ASN	CA-CB-CG	-6.78	105.82	112.60
1	D	735	HIS	N-CA-CB	-6.76	100.18	109.98
1	B	128	ASN	CB-CA-C	-6.74	97.99	109.51
1	A	869	ASP	CA-CB-CG	-6.73	105.87	112.60
1	D	363	HIS	CA-CB-CG	-6.70	107.11	113.80
1	A	997	ASP	CA-CB-CG	-6.68	105.92	112.60
1	B	473	ARG	CD-NE-CZ	6.67	133.74	124.40
1	C	472	TYR	N-CA-C	-6.64	103.97	111.07
1	D	420	MET	CA-C-N	-6.63	117.08	122.85
1	D	420	MET	C-N-CA	-6.63	117.08	122.85
1	B	126	THR	CA-CB-OG1	-6.62	99.66	109.60
1	C	735	HIS	CA-CB-CG	6.62	120.42	113.80
1	D	447	ASP	N-CA-C	6.61	121.50	113.17
1	D	878	HIS	CA-CB-CG	-6.60	107.20	113.80
1	B	772	ASP	N-CA-CB	6.59	120.19	110.56
1	A	360	HIS	CA-CB-CG	-6.58	107.22	113.80
1	A	147	ASN	N-CA-CB	-6.57	100.39	110.65
1	C	734	SER	N-CA-C	6.57	124.80	110.80
1	A	675	GLN	OE1-CD-NE2	6.56	129.16	122.60
1	D	822	LEU	O-C-N	-6.56	114.95	123.02
1	C	579	ASP	CB-CG-OD2	-6.54	103.35	118.40
1	B	680	ILE	CA-C-N	-6.53	113.70	122.72
1	B	680	ILE	C-N-CA	-6.53	113.70	122.72
1	B	878	HIS	CA-CB-CG	-6.51	107.29	113.80
1	D	659	ASP	CA-CB-CG	-6.51	106.09	112.60
1	A	989	PHE	CA-CB-CG	-6.47	107.33	113.80
1	B	842	TRP	CA-CB-CG	-6.47	101.30	113.60
1	B	513	PRO	CB-CA-C	-6.46	103.12	111.46
1	B	689	GLU	CA-C-O	-6.45	114.11	121.66
1	D	477	SER	N-CA-CB	6.45	119.42	110.07
1	B	931	PHE	CA-CB-CG	-6.42	107.38	113.80
1	A	777	LEU	N-CA-C	-6.41	105.77	113.97
1	B	777	LEU	N-CA-CB	6.40	119.10	110.59
1	A	832	ASP	N-CA-CB	-6.39	102.27	111.54
1	C	809	ARG	N-CA-C	-6.39	104.40	111.36
1	D	277	GLU	N-CA-CB	-6.38	101.23	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	924	ASP	CA-CB-CG	-6.38	106.22	112.60
1	B	388	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	B	262	GLN	CB-CA-C	6.37	120.98	111.17
1	A	867	THR	CA-CB-OG1	-6.36	100.06	109.60
1	B	1022	GLN	CA-CB-CG	-6.36	101.38	114.10
1	C	323	ILE	N-CA-C	-6.35	105.54	111.45
1	D	770	ILE	N-CA-CB	6.35	119.90	111.90
1	D	759	ASN	CA-CB-CG	-6.33	106.27	112.60
1	A	735	HIS	CA-CB-CG	-6.32	107.48	113.80
1	B	1018	LEU	CB-CA-C	-6.31	96.19	110.07
1	A	917	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	B	18	ASN	CA-CB-CG	-6.31	106.29	112.60
1	B	688	PRO	O-C-N	6.31	131.16	122.64
1	C	889	ALA	CA-C-O	6.30	127.21	119.97
1	C	782	ASP	CA-CB-CG	-6.30	106.30	112.60
1	B	612	THR	CA-C-N	-6.27	113.49	120.14
1	B	612	THR	C-N-CA	-6.27	113.49	120.14
1	A	878	HIS	CA-CB-CG	-6.27	107.53	113.80
1	A	1021	CYS	CA-CB-SG	-6.27	99.97	114.40
1	C	473	ARG	NE-CZ-NH1	6.27	127.77	121.50
1	A	103	VAL	N-CA-C	6.26	117.28	111.45
1	D	52	ARG	CB-CA-C	-6.26	97.40	109.37
1	B	166	ARG	NE-CZ-NH2	-6.26	113.57	119.20
1	A	890	GLN	N-CA-CB	-6.25	100.79	110.29
1	D	917	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	B	359	HIS	ND1-CG-CD2	6.25	112.34	106.10
1	C	204	ARG	NE-CZ-NH1	6.24	127.74	121.50
1	C	949	HIS	CB-CA-C	-6.23	98.97	109.50
1	A	816	TYR	CA-C-N	-6.23	112.78	122.37
1	A	816	TYR	C-N-CA	-6.23	112.78	122.37
1	A	887	GLN	OE1-CD-NE2	6.21	128.81	122.60
1	B	13	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	D	682	LEU	CA-C-N	6.21	126.18	120.03
1	D	682	LEU	C-N-CA	6.21	126.18	120.03
1	B	568	TRP	CA-CB-CG	-6.21	101.81	113.60
1	D	725	ASN	CA-CB-CG	-6.21	106.39	112.60
1	D	267	VAL	N-CA-CB	-6.18	98.63	111.24
1	D	623	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	A	431	ARG	NE-CZ-NH2	6.16	124.75	119.20
1	C	931	PHE	CA-CB-CG	-6.14	107.66	113.80
1	C	382	ASN	CA-CB-CG	-6.14	106.46	112.60
1	B	733	ALA	N-CA-CB	6.11	118.69	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	GLU	CB-CG-CD	-6.11	102.22	112.60
1	B	519	SER	N-CA-CB	-6.11	99.98	109.69
1	C	1000	SER	CA-CB-OG	-6.11	98.89	111.10
1	B	670	LEU	CB-CA-C	-6.10	99.68	109.75
1	A	477	SER	CB-CA-C	-6.10	101.27	110.90
1	A	368	ASP	CA-CB-CG	-6.09	106.51	112.60
1	C	645	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	230	ARG	CD-NE-CZ	6.08	132.91	124.40
1	C	917	ARG	CD-NE-CZ	-6.07	115.91	124.40
1	D	231	PHE	CA-CB-CG	-6.06	107.74	113.80
1	C	761	GLN	N-CA-CB	6.06	119.41	110.33
1	C	842	TRP	CE2-CD2-CE3	6.06	124.86	118.80
1	C	136	GLU	CB-CA-C	-6.05	96.75	110.07
1	B	748	CYS	N-CA-CB	6.05	120.53	110.85
1	C	606	LEU	N-CA-C	-6.03	105.41	112.89
1	A	369	GLU	CB-CG-CD	-6.02	102.36	112.60
1	C	689	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	274	PHE	CA-CB-CG	-6.01	107.79	113.80
1	A	675	GLN	CA-CB-CG	-6.00	102.09	114.10
1	A	842	TRP	CE2-CD2-CE3	5.99	124.79	118.80
1	D	184	LEU	CB-CA-C	-5.99	99.37	109.50
1	A	277	GLU	CB-CG-CD	5.99	122.78	112.60
1	B	686	PRO	N-CA-CB	5.99	108.58	103.19
1	C	431	ARG	CA-CB-CG	-5.99	102.13	114.10
1	D	781	ARG	CD-NE-CZ	5.97	132.76	124.40
1	B	468	HIS	ND1-CG-CD2	5.97	112.07	106.10
1	C	592	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	93	HIS	ND1-CE1-NE2	5.97	114.37	108.40
1	B	988	GLY	N-CA-C	-5.96	105.14	112.77
1	D	797	GLU	CB-CG-CD	-5.96	102.46	112.60
1	D	1018	LEU	CB-CA-C	-5.96	96.33	109.56
1	B	842	TRP	CE2-CD2-CE3	5.96	124.76	118.80
1	D	891	VAL	CB-CA-C	5.95	117.19	110.41
1	A	872	VAL	N-CA-CB	-5.94	103.92	111.64
1	D	382	ASN	CA-CB-CG	-5.94	106.66	112.60
1	C	395	HIS	ND1-CE1-NE2	5.93	114.33	108.40
1	C	890	GLN	N-CA-CB	-5.92	101.29	110.29
1	B	221	GLN	N-CA-CB	-5.92	101.40	111.69
1	B	634	GLN	N-CA-C	-5.91	105.65	112.92
1	C	682	LEU	CA-C-N	5.91	126.24	119.92
1	C	682	LEU	C-N-CA	5.91	126.24	119.92
1	B	729	THR	N-CA-CB	5.90	119.38	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ASN	N-CA-CB	-5.90	101.29	110.55
1	D	800	ARG	N-CA-CB	5.90	120.46	110.49
1	A	128	ASN	CA-CB-CG	-5.89	106.70	112.60
1	A	725	ASN	CA-CB-CG	-5.89	106.71	112.60
1	C	75	GLU	N-CA-CB	-5.89	101.87	110.47
1	C	209	PHE	CA-CB-CG	-5.89	107.91	113.80
1	D	949	HIS	CB-CA-C	-5.89	100.09	109.80
1	A	710	GLU	CB-CA-C	-5.88	99.40	110.51
1	A	442	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	A	116	THR	CA-CB-OG1	-5.87	100.80	109.60
1	B	431	ARG	CA-CB-CG	-5.86	102.38	114.10
1	D	847	LYS	CA-C-O	5.86	127.66	120.92
1	D	842	TRP	CB-CA-C	-5.86	100.09	109.75
1	A	166	ARG	NE-CZ-NH2	-5.85	113.93	119.20
1	A	746	ASP	CA-CB-CG	-5.84	106.75	112.60
1	A	49	GLN	CB-CG-CD	-5.84	102.67	112.60
1	A	759	ASN	CA-CB-CG	-5.84	106.76	112.60
1	A	592	PHE	CA-CB-CG	-5.83	107.97	113.80
1	A	833	ALA	CA-C-N	-5.83	115.01	123.06
1	A	833	ALA	C-N-CA	-5.83	115.01	123.06
1	A	949	HIS	ND1-CG-CD2	5.83	111.93	106.10
1	C	685	LEU	CA-C-O	5.82	124.95	119.59
1	C	601	PHE	CA-CB-CG	-5.82	107.98	113.80
1	D	352	ARG	CA-C-N	-5.82	116.40	122.69
1	D	352	ARG	C-N-CA	-5.82	116.40	122.69
1	A	1000	SER	CA-CB-OG	-5.81	99.48	111.10
1	A	34	ALA	N-CA-C	-5.80	105.82	114.64
1	D	958	ASN	N-CA-CB	5.80	122.32	111.53
1	D	786	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	C	267	VAL	CA-CB-CG2	-5.79	100.56	110.40
1	C	760	ARG	CG-CD-NE	-5.79	99.26	112.00
1	C	452	SER	CA-C-N	-5.79	113.70	121.80
1	C	452	SER	C-N-CA	-5.79	113.70	121.80
1	D	997	ASP	N-CA-CB	5.78	120.36	111.46
1	D	968	MET	N-CA-CB	-5.78	100.80	110.39
1	D	320	GLY	N-CA-C	5.78	123.41	115.27
1	D	597	ASN	CA-CB-CG	-5.77	106.83	112.60
1	A	675	GLN	O-C-N	5.77	127.93	121.87
1	C	779	PRO	N-CA-CB	5.77	108.81	103.39
1	C	817	GLN	N-CA-CB	-5.76	101.90	110.61
1	C	733	ALA	CB-CA-C	5.76	118.90	110.26
1	D	924	ASP	CA-CB-CG	-5.76	106.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	949	HIS	ND1-CE1-NE2	5.75	114.15	108.40
1	C	680	ILE	CA-C-N	-5.75	114.78	122.72
1	C	680	ILE	C-N-CA	-5.75	114.78	122.72
1	C	161	TYR	N-CA-CB	-5.75	100.83	111.52
1	A	128	ASN	CB-CA-C	-5.75	99.69	109.51
1	B	598	ASP	CA-CB-CG	-5.75	106.86	112.60
1	B	100	TYR	CA-CB-CG	-5.74	103.57	113.90
1	D	772	ASP	CA-CB-CG	-5.74	106.86	112.60
1	A	682	LEU	CA-C-N	5.73	126.05	119.92
1	A	682	LEU	C-N-CA	5.73	126.05	119.92
1	A	69	VAL	N-CA-CB	-5.73	104.10	110.23
1	B	969	GLU	CA-CB-CG	-5.73	102.64	114.10
1	A	388	ARG	NE-CZ-NH2	-5.73	114.05	119.20
1	C	878	HIS	CA-CB-CG	-5.72	108.08	113.80
1	A	445	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	D	832	ASP	CA-CB-CG	-5.71	106.89	112.60
1	B	948	PRO	CB-CA-C	-5.71	102.91	110.27
1	A	968	MET	CA-CB-CG	5.70	125.51	114.10
1	C	917	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	B	596	PRO	CA-N-CD	5.70	119.48	111.50
1	B	735	HIS	CA-CB-CG	5.70	119.50	113.80
1	A	297	ASN	CA-C-O	5.69	124.86	120.48
1	B	538	TYR	O-C-N	5.69	129.24	123.26
1	A	155	ASN	CA-CB-CG	-5.69	106.91	112.60
1	B	370	GLN	CB-CG-CD	5.68	122.27	112.60
1	C	43	ARG	NE-CZ-NH1	5.68	127.19	121.50
1	D	155	ASN	CA-CB-CG	-5.68	106.92	112.60
1	C	862	GLY	CA-C-O	5.68	125.42	119.06
1	A	584	PRO	N-CA-CB	5.68	108.61	103.33
1	D	338	GLU	CA-C-N	-5.68	114.17	122.40
1	D	338	GLU	C-N-CA	-5.68	114.17	122.40
1	A	231	PHE	CA-CB-CG	-5.67	108.13	113.80
1	D	768	MET	CG-SD-CE	5.67	113.38	100.90
1	C	469	ASP	O-C-N	5.67	128.13	122.12
1	D	619	GLU	N-CA-C	-5.67	105.19	111.36
1	C	513	PRO	CB-CA-C	-5.66	104.15	111.46
1	D	126	THR	CA-CB-OG1	-5.66	101.11	109.60
1	B	473	ARG	NE-CZ-NH1	5.66	127.16	121.50
1	D	829	THR	N-CA-CB	5.66	119.86	110.52
1	A	519	SER	N-CA-C	-5.65	102.27	110.24
1	B	834	VAL	N-CA-C	-5.65	100.34	108.48
1	B	862	GLY	CA-C-O	5.64	125.28	119.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	395	HIS	ND1-CG-CD2	5.63	111.73	106.10
1	C	750	GLU	CB-CG-CD	-5.63	103.03	112.60
1	B	896	ASN	CA-C-O	5.62	126.56	120.32
1	D	681	GLU	CB-CG-CD	5.62	122.16	112.60
1	D	820	ALA	CA-C-O	5.62	128.55	120.51
1	D	896	ASN	CA-C-O	5.62	126.56	120.32
1	D	769	TRP	CA-C-N	-5.62	115.61	123.13
1	D	769	TRP	C-N-CA	-5.62	115.61	123.13
1	D	572	ASP	CB-CA-C	-5.61	101.15	109.90
1	B	367	MET	CA-C-O	-5.61	114.77	120.71
1	A	788	PRO	N-CA-CB	5.60	108.31	103.27
1	C	775	GLN	CA-C-N	-5.60	114.02	122.81
1	C	775	GLN	C-N-CA	-5.60	114.02	122.81
1	A	935	ASN	CA-CB-CG	-5.59	107.01	112.60
1	D	648	ASP	CA-C-O	5.59	126.46	119.59
1	B	184	LEU	CB-CA-C	-5.58	100.06	109.50
1	A	893	GLU	N-CA-C	5.58	117.44	111.36
1	C	598	ASP	CA-CB-CG	-5.58	107.02	112.60
1	C	856	TYR	N-CA-C	-5.58	99.33	108.76
1	C	147	ASN	N-CA-CB	-5.58	101.95	110.65
1	D	931	PHE	CA-C-O	5.58	124.04	119.36
1	D	820	ALA	N-CA-C	5.57	122.67	110.80
1	B	702	GLN	CA-C-O	5.57	124.04	119.36
1	D	601	PHE	CA-CB-CG	-5.57	108.23	113.80
1	A	610	ASP	CA-C-O	5.56	126.16	119.43
1	A	431	ARG	CB-CG-CD	5.56	124.08	111.30
1	D	765	LEU	N-CA-C	-5.56	101.15	109.15
1	C	614	HIS	N-CA-C	-5.55	102.92	110.36
1	B	59	ARG	CD-NE-CZ	-5.54	116.65	124.40
1	B	279	ILE	N-CA-C	-5.54	106.80	111.56
1	B	755	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	D	746	ASP	N-CA-C	5.53	117.47	109.07
1	B	384	PHE	CA-CB-CG	-5.52	108.28	113.80
1	C	728	VAL	CA-C-N	-5.52	113.92	122.09
1	C	728	VAL	C-N-CA	-5.52	113.92	122.09
1	C	298	PRO	CB-CA-C	-5.52	104.16	111.23
1	D	297	ASN	CA-CB-CG	-5.52	107.08	112.60
1	B	730	LEU	CA-C-N	5.52	126.74	119.84
1	B	730	LEU	C-N-CA	5.52	126.74	119.84
1	D	981	GLY	N-CA-C	5.52	122.51	112.58
1	D	183	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	A	772	ASP	N-CA-C	-5.51	104.10	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	703	PRO	CB-CA-C	-5.51	103.64	111.68
1	B	889	ALA	CA-C-N	-5.50	111.01	122.07
1	B	889	ALA	C-N-CA	-5.50	111.01	122.07
1	A	741	THR	CA-CB-OG1	-5.49	101.36	109.60
1	C	333	ARG	CG-CD-NE	5.49	124.09	112.00
1	A	980	GLU	N-CA-CB	-5.49	101.91	109.97
1	B	570	TRP	N-CA-C	5.49	117.12	111.03
1	C	159	VAL	N-CA-CB	-5.49	105.38	111.41
1	D	828	ASP	CA-C-N	-5.48	114.48	122.65
1	D	828	ASP	C-N-CA	-5.48	114.48	122.65
1	C	788	PRO	N-CA-CB	5.47	108.19	103.27
1	B	640	SER	CB-CA-C	-5.47	100.83	109.80
1	B	829	THR	CA-CB-OG1	-5.47	101.40	109.60
1	D	115	PRO	N-CA-CB	5.46	108.11	103.35
1	D	628	GLN	CG-CD-NE2	-5.46	108.20	116.40
1	A	653	HIS	CA-CB-CG	5.46	119.26	113.80
1	C	940	GLY	CA-C-N	-5.46	114.49	122.19
1	C	940	GLY	C-N-CA	-5.46	114.49	122.19
1	A	986	ILE	CB-CG1-CD1	-5.45	102.35	113.80
1	D	757	GLN	N-CA-C	5.45	117.30	108.41
1	C	816	TYR	CA-C-N	-5.45	114.05	122.49
1	C	816	TYR	C-N-CA	-5.45	114.05	122.49
1	A	185	ALA	N-CA-CB	5.45	119.32	110.77
1	C	844	HIS	ND1-CG-CD2	5.45	111.55	106.10
1	B	89	ASN	N-CA-C	-5.44	100.31	109.07
1	D	820	ALA	O-C-N	-5.44	115.35	122.59
1	D	589	GLY	O-C-N	5.44	128.31	122.93
1	D	635	THR	CA-CB-OG1	-5.44	101.44	109.60
1	C	997	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	164	ASP	N-CA-CB	5.43	119.67	110.49
1	A	727	SER	CA-CB-OG	-5.43	100.24	111.10
1	C	938	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	D	949	HIS	ND1-CG-CD2	5.42	111.52	106.10
1	D	988	GLY	N-CA-C	-5.42	105.84	112.77
1	B	576	ILE	CB-CA-C	-5.42	103.65	111.34
1	D	634	GLN	CA-C-N	-5.41	115.53	123.00
1	D	634	GLN	C-N-CA	-5.41	115.53	123.00
1	A	679	LEU	O-C-N	5.41	129.52	123.19
1	D	473	ARG	CD-NE-CZ	5.41	131.97	124.40
1	D	788	PRO	N-CA-CB	5.41	108.01	103.25
1	D	889	ALA	O-C-N	-5.41	115.62	122.27
1	B	46	ARG	NE-CZ-NH2	-5.40	114.34	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	388	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	B	63	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	599	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	A	634	GLN	CB-CA-C	5.39	119.75	111.02
1	A	751	LEU	CB-CA-C	-5.39	104.36	111.42
1	A	672	VAL	CB-CA-C	-5.38	102.67	110.63
1	A	438	GLU	CG-CD-OE2	-5.37	106.05	118.40
1	D	721	ARG	CB-CA-C	-5.37	100.46	109.53
1	B	646	HIS	CA-CB-CG	-5.36	108.44	113.80
1	A	117	GLU	CB-CG-CD	5.36	121.71	112.60
1	C	442	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	D	909	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	B	679	LEU	N-CA-CB	5.36	118.98	110.57
1	C	46	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	B	479	ASP	CA-CB-CG	-5.36	107.25	112.60
1	A	262	GLN	N-CA-C	-5.35	98.65	108.02
1	B	931	PHE	CA-C-O	5.35	122.77	119.29
1	D	479	ASP	CA-C-O	5.35	126.25	121.06
1	A	695	TRP	CB-CA-C	-5.35	97.69	109.56
1	C	448	ARG	NE-CZ-NH2	-5.35	114.39	119.20
1	B	738	PRO	CB-CA-C	-5.34	103.95	110.95
1	D	1022	GLN	N-CA-CB	5.34	119.49	110.46
1	B	627	PHE	CA-CB-CG	-5.34	108.46	113.80
1	A	279	ILE	CB-CG1-CD1	-5.34	102.59	113.80
1	C	519	SER	N-CA-CB	-5.33	101.21	109.69
1	C	988	GLY	N-CA-C	-5.33	106.23	113.37
1	B	684	GLU	CA-C-N	-5.33	113.92	123.08
1	B	684	GLU	C-N-CA	-5.33	113.92	123.08
1	B	915	PHE	CA-CB-CG	-5.33	108.47	113.80
1	C	846	GLY	CA-C-N	-5.33	114.71	122.65
1	C	846	GLY	C-N-CA	-5.33	114.71	122.65
1	A	553	TRP	CA-CB-CG	-5.33	103.48	113.60
1	D	986	ILE	CB-CG1-CD1	-5.33	102.61	113.80
1	B	764	PHE	CA-C-O	5.32	127.12	121.11
1	D	324	GLU	N-CA-CB	5.32	119.65	111.56
1	B	403	ASP	CB-CA-C	-5.32	101.96	110.79
1	B	724	GLU	CA-C-N	-5.32	115.56	123.11
1	B	724	GLU	C-N-CA	-5.32	115.56	123.11
1	D	147	ASN	OD1-CG-ND2	5.31	127.91	122.60
1	B	869	ASP	CA-CB-CG	-5.31	107.29	112.60
1	A	843	GLN	O-C-N	5.30	130.04	123.15
1	B	639	THR	CA-CB-OG1	-5.30	101.64	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	831	ALA	CB-CA-C	-5.30	100.82	110.63
1	A	733	ALA	CA-C-N	-5.30	113.62	122.64
1	A	733	ALA	C-N-CA	-5.30	113.62	122.64
1	A	418	HIS	ND1-CG-CD2	5.30	111.40	106.10
1	A	735	HIS	CB-CA-C	5.30	118.34	111.50
1	B	646	HIS	ND1-CG-CD2	5.30	111.40	106.10
1	B	843	GLN	CB-CG-CD	-5.30	103.59	112.60
1	A	774	LYS	CA-CB-CG	-5.29	103.51	114.10
1	C	222	ILE	N-CA-C	-5.28	100.72	108.54
1	A	941	THR	O-C-N	5.28	129.23	123.22
1	B	99	ILE	CA-C-N	-5.28	115.33	123.14
1	B	99	ILE	C-N-CA	-5.28	115.33	123.14
1	C	93	HIS	N-CA-C	-5.28	106.52	113.17
1	A	107	ILE	O-C-N	-5.27	117.19	123.04
1	B	760	ARG	N-CA-C	5.27	117.77	111.71
1	D	739	HIS	CA-CB-CG	-5.27	108.53	113.80
1	C	519	SER	N-CA-C	-5.26	102.82	110.24
1	B	729	THR	N-CA-C	5.26	116.82	108.67
1	A	93	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	C	641	GLU	N-CA-CB	5.25	118.27	110.49
1	A	570	TRP	N-CA-C	5.25	116.86	111.03
1	D	147	ASN	N-CA-CB	-5.25	102.45	110.65
1	D	309	TYR	N-CA-C	-5.25	102.42	110.14
1	A	363	HIS	ND1-CG-CD2	5.25	111.35	106.10
1	A	772	ASP	CA-C-N	-5.25	115.48	122.72
1	A	772	ASP	C-N-CA	-5.25	115.48	122.72
1	B	274	PHE	CA-CB-CG	-5.25	108.55	113.80
1	C	274	PHE	CA-CB-CG	-5.25	108.56	113.80
1	B	69	VAL	CA-C-O	-5.24	115.17	119.47
1	D	512	PHE	CA-CB-CG	-5.24	108.56	113.80
1	A	753	ASN	CA-C-N	-5.23	114.45	122.87
1	A	753	ASN	C-N-CA	-5.23	114.45	122.87
1	C	473	ARG	CG-CD-NE	-5.23	100.49	112.00
1	C	847	LYS	CA-C-N	-5.23	115.47	122.42
1	C	847	LYS	C-N-CA	-5.23	115.47	122.42
1	D	598	ASP	CA-CB-CG	-5.22	107.38	112.60
1	D	180	GLY	O-C-N	-5.22	117.80	122.86
1	A	395	HIS	ND1-CG-CD2	5.22	111.32	106.10
1	B	116	THR	CA-CB-OG1	-5.22	101.78	109.60
1	B	606	LEU	N-CA-C	-5.21	106.42	112.89
1	D	735	HIS	CA-CB-CG	-5.21	108.59	113.80
1	C	731	PRO	CB-CA-C	-5.20	104.57	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	GLU	N-CA-C	5.20	117.21	109.25
1	D	416	GLU	CG-CD-OE1	5.20	130.36	118.40
1	C	13	ARG	CG-CD-NE	-5.20	100.56	112.00
1	B	19	PRO	N-CA-CB	5.20	108.29	103.41
1	D	315	LEU	N-CA-C	-5.19	100.26	108.73
1	A	233	ASP	CA-C-N	-5.19	114.42	122.67
1	A	233	ASP	C-N-CA	-5.19	114.42	122.67
1	A	297	ASN	CB-CA-C	-5.19	106.49	111.00
1	D	323	ILE	N-CA-C	-5.19	106.62	111.45
1	D	100	TYR	CA-CB-CG	-5.19	104.57	113.90
1	D	695	TRP	CB-CA-C	-5.19	98.05	109.56
1	A	46	ARG	CA-C-O	5.18	126.69	120.88
1	A	431	ARG	CA-CB-CG	-5.18	103.74	114.10
1	D	871	GLU	CB-CG-CD	-5.18	103.80	112.60
1	A	627	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	1019	VAL	CA-CB-CG2	-5.17	101.61	110.40
1	A	632	SER	N-CA-CB	5.17	118.97	110.90
1	A	126	THR	N-CA-C	-5.17	100.75	109.07
1	D	93	HIS	N-CA-C	-5.17	106.66	113.17
1	D	288	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	B	635	THR	N-CA-C	5.17	117.15	108.73
1	A	894	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	894	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	A	863	GLN	OE1-CD-NE2	5.16	127.76	122.60
1	B	681	GLU	CA-CB-CG	-5.16	103.78	114.10
1	D	45	ASP	CA-CB-CG	-5.16	107.44	112.60
1	D	345	ASN	CA-CB-CG	-5.16	107.44	112.60
1	C	553	TRP	CA-CB-CG	-5.15	103.81	113.60
1	D	96	ASP	N-CA-CB	5.15	119.38	111.24
1	C	743	SER	O-C-N	-5.15	116.45	123.15
1	B	96	ASP	CA-CB-CG	-5.14	107.45	112.60
1	B	113	PHE	CA-CB-CG	-5.14	108.66	113.80
1	C	1013	ARG	CA-CB-CG	-5.14	103.82	114.10
1	D	581	ASN	CA-C-O	5.14	125.69	119.11
1	D	298	PRO	CB-CA-C	-5.14	104.83	111.46
1	D	798	ALA	CA-C-N	5.13	131.59	121.58
1	D	798	ALA	C-N-CA	5.13	131.59	121.58
1	D	26	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	B	634	GLN	O-C-N	5.13	128.49	122.34
1	B	844	HIS	CA-CB-CG	-5.13	108.67	113.80
1	C	74	LEU	CA-C-O	5.13	125.89	120.10
1	B	592	PHE	CA-CB-CG	-5.12	108.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	LEU	N-CA-C	-5.12	103.19	109.65
1	A	704	ASN	CA-CB-CG	-5.12	107.48	112.60
1	B	614	HIS	N-CA-CB	5.12	116.85	109.78
1	B	689	GLU	O-C-N	5.12	129.48	122.41
1	D	915	PHE	CA-CB-CG	-5.12	108.68	113.80
1	D	720	TRP	CA-C-N	-5.12	114.10	121.42
1	D	720	TRP	C-N-CA	-5.12	114.10	121.42
1	C	235	PHE	CA-CB-CG	-5.11	108.69	113.80
1	D	760	ARG	N-CA-CB	5.11	119.00	110.41
1	A	917	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	C	210	ARG	N-CA-CB	5.11	118.71	111.05
1	A	800	ARG	N-CA-CB	-5.10	101.87	110.49
1	C	854	LYS	CB-CA-C	-5.10	98.84	110.07
1	D	632	SER	N-CA-CB	5.10	118.86	110.90
1	D	659	ASP	N-CA-C	5.10	118.36	111.17
1	D	845	GLN	CA-C-N	-5.10	111.41	121.41
1	D	845	GLN	C-N-CA	-5.10	111.41	121.41
1	D	513	PRO	CA-C-O	5.10	127.15	121.34
1	C	735	HIS	CB-CA-C	5.10	118.97	111.17
1	C	400	THR	CA-CB-OG1	-5.09	101.96	109.60
1	B	966	GLN	CB-CG-CD	5.09	121.25	112.60
1	C	233	ASP	CA-C-N	-5.09	114.66	122.60
1	C	233	ASP	C-N-CA	-5.09	114.66	122.60
1	C	736	ALA	CB-CA-C	-5.09	101.16	110.62
1	D	698	VAL	N-CA-CB	5.09	120.24	111.39
1	D	759	ASN	CB-CA-C	5.08	118.63	110.29
1	D	89	ASN	OD1-CG-ND2	5.08	127.68	122.60
1	D	450	HIS	CA-CB-CG	-5.08	108.72	113.80
1	A	578	TYR	N-CA-CB	-5.08	102.15	110.68
1	A	157	ARG	CG-CD-NE	5.08	123.17	112.00
1	D	278	ILE	CA-C-N	-5.08	115.62	121.71
1	D	278	ILE	C-N-CA	-5.08	115.62	121.71
1	A	297	ASN	CA-C-N	-5.07	114.72	119.85
1	A	297	ASN	C-N-CA	-5.07	114.72	119.85
1	D	580	GLU	N-CA-C	5.07	118.94	112.34
1	C	689	GLU	CB-CA-C	5.07	119.26	110.84
1	D	561	ARG	CA-C-N	-5.07	115.68	122.42
1	D	561	ARG	C-N-CA	-5.07	115.68	122.42
1	A	734	SER	CA-C-O	5.06	127.26	121.28
1	D	18	ASN	CA-CB-CG	-5.06	107.54	112.60
1	C	682	LEU	O-C-N	5.06	127.10	121.53
1	A	986	ILE	N-CA-CB	5.06	118.22	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	777	LEU	N-CA-C	-5.06	107.66	113.88
1	C	579	ASP	CB-CG-OD1	5.05	130.03	118.40
1	D	862	GLY	CA-C-N	-5.05	113.43	122.07
1	D	862	GLY	C-N-CA	-5.05	113.43	122.07
1	C	633	GLY	CA-C-N	5.05	130.42	122.49
1	C	633	GLY	C-N-CA	5.05	130.42	122.49
1	C	668	VAL	N-CA-CB	-5.05	104.14	111.21
1	A	928	PRO	CB-CA-C	-5.04	106.28	112.89
1	B	75	GLU	CA-CB-CG	-5.04	104.01	114.10
1	A	931	PHE	CA-CB-CG	-5.04	108.76	113.80
1	B	138	GLN	N-CA-CB	-5.03	102.23	110.68
1	D	193	ASP	N-CA-C	-5.03	106.25	112.38
1	D	731	PRO	N-CA-C	5.03	118.26	111.22
1	C	408	TYR	CA-C-N	-5.03	115.95	122.94
1	C	408	TYR	C-N-CA	-5.03	115.95	122.94
1	C	957	PHE	CA-CB-CG	-5.03	108.77	113.80
1	C	778	THR	O-C-N	5.03	127.22	121.94
1	B	954	ASP	N-CA-C	-5.02	99.03	107.32
1	C	83	THR	CA-CB-OG1	-5.02	102.07	109.60
1	B	595	THR	CA-C-O	5.02	124.15	119.13
1	A	183	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	B	1022	GLN	OE1-CD-NE2	5.02	127.62	122.60
1	C	583	ASN	CA-C-O	-5.02	115.97	120.19
1	D	111	PRO	N-CA-CB	5.02	107.95	103.08
1	A	320	GLY	CA-C-N	-5.01	115.53	122.30
1	A	320	GLY	C-N-CA	-5.01	115.53	122.30
1	C	931	PHE	CB-CA-C	5.01	115.13	110.17
1	D	777	LEU	N-CA-CB	5.01	117.85	110.33
1	B	1022	GLN	N-CA-CB	5.01	118.59	110.43
1	C	296	GLU	CA-C-N	-5.01	118.29	123.10
1	C	296	GLU	C-N-CA	-5.01	118.29	123.10
1	D	279	ILE	CA-CB-CG2	5.01	119.01	110.50
1	C	905	ASN	OD1-CG-ND2	5.00	127.61	122.60
1	A	593	GLY	CA-C-O	5.00	124.57	119.02
1	D	773	LYS	N-CA-C	5.00	116.91	108.96

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	143	0
1	B	8127	0	7713	123	0
1	C	8127	0	7713	141	0
1	D	8127	0	7713	161	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	19	0
5	B	88	0	132	13	0
5	C	92	0	138	13	0
5	D	92	0	138	25	0
6	A	1054	0	0	21	2
6	B	1073	0	0	20	1
6	C	1019	0	0	20	0
6	D	1068	0	0	24	1
All	All	37213	0	31490	587	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 9.

All (587) 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:C2	5:A:8415:DMS:S	2.02	1.46
5:B:8601:DMS:C2	5:B:8601:DMS:S	2.04	1.44
5:D:8415:DMS:S	5:D:8415:DMS:C1	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:B:655:MET:HE2	1:B:665:SER:HB3	1.18	1.16
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:HH11	1:D:237:ARG:HG2	1.25	0.99
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.31	0.95
1:B:233:ASP:HA	5:B:8417:DMS:H13	1.49	0.93
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:HA	1:C:687:GLN:NE2	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:A:795:VAL:CG1	5:A:8506:DMS:H22	2.06	0.85
1:B:824:GLN:HG2	1:B:825:CYS:N	1.92	0.84
1:A:795:VAL:HG12	5:A:8506:DMS:H22	1.60	0.84
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:NE2	1:C:634:GLN:N	2.29	0.80
1:B:655:MET:HE2	1:B:665:SER:CB	2.08	0.80
1:B:824:GLN:HE22	1:B:837:THR:CG2	1.94	0.80
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:C:13:ARG:O	1:C:14:ARG:C	2.27	0.78
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:C:745:MET:HE3	1:C:745:MET:O	1.83	0.78
5:D:8703:DMS:H21	6:D:9648:HOH:O	1.82	0.78
1:B:655:MET:CE	1:B:665:SER:HB3	2.09	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:893:GLU:HG2	1:D:894:ARG:HG2	1.66	0.77
1:A:251:ARG:HH11	5:A:8416:DMS:H23	1.50	0.77
1:A:277:GLU:H	1:A:277:GLU:CD	1.90	0.76
1:B:890:GLN:HG3	1:B:891:VAL:N	2.01	0.74
1:D:703:PRO:HG2	5:D:8425:DMS:C1	2.18	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:A:717:TRP:CZ3	5:A:8415:DMS:H12	2.23	0.73
1:C:745:MET:HE2	1:C:759:ASN:HD21	1.51	0.73
1:D:651:LEU:C	1:D:651:LEU:HD12	2.14	0.73
1:A:737:ILE:O	1:A:737:ILE:HD13	1.87	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:508:GLU:OE2	5:A:8407:DMS:H11	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:133:TRP:NE1	5:D:8703:DMS:H23	2.06	0.71
1:D:749:ILE:HD12	1:D:749:ILE:N	2.05	0.71
1:D:649:ASN:HA	5:D:8425:DMS:H13	1.73	0.71
1:A:717:TRP:CH2	5:A:8415:DMS:H12	2.26	0.70
5:B:8410:DMS:H22	6:B:8876:HOH:O	1.90	0.70
1:A:651:LEU:HD11	1:A:653:HIS:CD2	2.26	0.70
1:D:655:MET:HE1	1:D:699:ARG:HE	1.56	0.70
1:D:890:GLN:HE21	1:D:892:ALA:HB2	1.57	0.70
1:B:809:ARG:HG2	1:B:809:ARG:NH1	2.06	0.70
1:B:744:GLU:HA	1:B:744:GLU:OE2	1.90	0.69
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
1:B:878:HIS:HD2	6:B:8690:HOH:O	1.74	0.69
1:D:863:GLN:CG	1:D:1021:CYS:HB3	2.18	0.69
5:C:8410:DMS:H11	6:C:8974:HOH:O	1.91	0.69
1:B:686:PRO:O	1:B:688:PRO:HD3	1.91	0.69
1:D:277:GLU:CD	1:D:277:GLU:H	1.92	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:135:GLN:C	1:D:136:GLU:HG2	2.18	0.68
1:D:717:TRP:CH2	5:D:8415:DMS:H12	2.29	0.68
1:D:476:LYS:NZ	6:D:8797:HOH:O	2.27	0.68
1:D:770:ILE:HD13	1:D:775:GLN:CG	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:B:9377:HOH:O	5:C:8420:DMS:H22	1.94	0.67
1:D:1022:GLN:HE21	1:D:1022:GLN:C	2.02	0.67
1:B:508:GLU:OE2	5:B:8407:DMS:H11	1.94	0.67
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
1:C:1023:LYS:HA	1:C:1023:LYS:HZ3	1.59	0.67
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.30	0.67
5:D:8421:DMS:H12	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:703:PRO:HG2	5:D:8425:DMS:H11	1.75	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
5:A:8420:DMS:H22	6:D:9502:HOH:O	1.95	0.66
1:B:689:GLU:O	1:B:690:SER:HB3	1.94	0.66
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.21	0.66
5:A:8421:DMS:H12	6:A:9110:HOH:O	1.95	0.66
1:C:651:LEU:HD12	1:C:651:LEU:C	2.21	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:N	1:C:761:GLN:OE1	2.30	0.65
1:D:847:LYS:NZ	6:D:9483:HOH:O	2.29	0.65
1:A:749:ILE:HD12	1:A:749:ILE:N	2.11	0.65
5:C:8415:DMS:H11	6:C:9565:HOH:O	1.95	0.65
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.10	0.64
1:D:71:GLU:HG2	6:D:9512:HOH:O	1.97	0.64
1:A:878:HIS:HD2	6:A:8578:HOH:O	1.81	0.64
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:B:236:SER:C	1:B:237:ARG:HG2	2.23	0.63
1:D:863:GLN:HG2	1:D:1019:VAL:CG1	2.29	0.63
1:D:634:GLN:CG	1:D:682:LEU:HB2	2.09	0.62
1:A:651:LEU:C	1:A:651:LEU:HD12	2.25	0.62
1:A:664:ALA:HB2	1:A:686:PRO:HG3	1.81	0.62
1:D:102:ASN:HD22	5:D:8506:DMS:H21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:240:LEU:C	1:C:240:LEU:HD23	2.26	0.61
1:A:745:MET:HE1	1:A:761:GLN:HB2	1.82	0.61
1:A:832:ASP:OD1	1:A:832:ASP:N	2.34	0.61
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.15	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:C:13:ARG:O	1:C:15:ASP:N	2.33	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:B:595:THR:HA	1:B:596:PRO:C	2.26	0.60
1:D:240:LEU:HD23	1:D:240:LEU:C	2.27	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:78:LEU:HB3	1:D:80:GLU:OE2	2.02	0.59
1:D:686:PRO:C	1:D:688:PRO:HD3	2.27	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
5:A:8410:DMS:H22	6:A:8766:HOH:O	2.02	0.59
6:A:9336:HOH:O	2:B:2002:GAL:H2	2.02	0.59
1:D:595:THR:HA	1:D:596:PRO:C	2.26	0.59
1:C:615:PRO:O	1:C:618:THR:HG22	2.03	0.59
1:A:240:LEU:C	1:A:240:LEU:HD23	2.28	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:H	1:B:730:LEU:HD12	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:D:769:TRP:C	1:D:770:ILE:HD12	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.18	0.58
1:A:595:THR:HA	1:A:596:PRO:C	2.27	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:D:292:ARG:NH1	5:D:8412:DMS:H23	2.13	0.58
1:B:824:GLN:HE22	1:B:837:THR:CB	2.16	0.57
1:C:80:GLU:H	1:C:80:GLU:CD	2.11	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
5:C:8410:DMS:H22	6:C:8891:HOH:O	2.04	0.57
1:D:601:PHE:CG	5:D:8506:DMS:H23	2.40	0.57
1:D:754:LYS:C	1:D:755:ARG:HG2	2.20	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:A:241:GLU:CD	1:A:292:ARG:HE	2.13	0.57
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.20	0.57
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.69	0.57
1:C:237:ARG:HG2	1:C:296:GLU:OE1	2.04	0.57
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.86	0.57
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.35	0.57
1:D:133:TRP:HE1	5:D:8703:DMS:C2	2.18	0.57
1:D:649:ASN:HA	5:D:8425:DMS:C1	2.34	0.57
1:D:133:TRP:HE1	5:D:8703:DMS:H23	1.69	0.56
1:D:887:GLN:NE2	1:D:980:GLU:O	2.38	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:292:ARG:HH12	5:B:8412:DMS:C2	2.19	0.56
1:B:428:ASP:O	5:B:8420:DMS:H11	2.05	0.56
1:D:890:GLN:NE2	1:D:892:ALA:HB2	2.20	0.56
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.88	0.56
1:C:132:SER:HB2	5:C:8504:DMS:H11	1.86	0.55
1:C:658:LEU:HD23	1:C:661:LYS:HZ3	1.71	0.55
1:D:703:PRO:HG2	5:D:8425:DMS:H12	1.87	0.55
1:D:237:ARG:HG2	1:D:237:ARG:NH1	1.99	0.55
1:C:710:GLU:HG2	6:C:8978:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LEU:HD23	1:B:651:LEU:C	2.32	0.55
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.89	0.55
1:D:655:MET:HE1	1:D:699:ARG:NE	2.21	0.55
1:C:317:THR:OG1	1:C:319:ASP:OD1	2.25	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:B:806:TRP:CD2	1:B:991:MET:HE1	2.42	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:C:770:ILE:HD12	1:C:775:GLN:CD	2.32	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:360:HIS:HE1	1:D:362:LEU:HD12	1.73	0.54
1:A:178:ARG:HD2	6:A:9334:HOH:O	2.08	0.54
1:A:737:ILE:HD13	1:A:737:ILE:C	2.33	0.54
1:C:866:ILE:O	1:C:1017:GLN:HG2	2.07	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:595:THR:HA	1:C:596:PRO:C	2.32	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
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.07	0.54
1:A:601:PHE:CE1	5:A:8506:DMS:H13	2.43	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
5:B:8406:DMS:H21	6:B:9247:HOH:O	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: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: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
1:A:370:GLN:HG3	6:A:9004:HOH:O	2.08	0.53
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.91	0.53
1:B:240:LEU:C	1:B:240:LEU:HD23	2.34	0.53
1:D:736:ALA:HB1	1:D:751:LEU:HD11	1.90	0.53
1:A:84:VAL:HG12	5:A:8414:DMS:H12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:VAL:HG11	5:A:8506:DMS:H22	1.88	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:651:LEU:C	1:D:651:LEU:CD1	2.82	0.53
1:A:296:GLU:OE1	1:A:296:GLU:HA	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:651:LEU:HD11	1:A:653:HIS:HD2	1.74	0.52
1:D:667:GLU:C	1:D:668:VAL:HG23	2.33	0.52
1:A:1022:GLN:CD	1:A:1023:LYS:H	2.16	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:C:795:VAL:HG12	5:C:8506:DMS:H22	1.90	0.52
1:B:824:GLN:NE2	1:B:837:THR:O	2.42	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:OD1	1:C:832:ASP:N	2.42	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:D:1022:GLN:O	1:D:1022:GLN:HG3	2.09	0.51
1:B:632:SER:N	1:B:635:THR:O	2.30	0.51
1:C:601:PHE:CZ	5:C:8506:DMS:H23	2.46	0.51
1:B:800:ARG:NH1	6:B:9556:HOH:O	2.43	0.51
1:C:745:MET:HE2	1:C:759:ASN:ND2	2.24	0.51
1:B:684:GLU:O	1:B:686:PRO:HD3	2.10	0.51
1:C:236:SER:C	1:C:237:ARG:HG3	2.35	0.51
1:A:781:ARG:NH1	6:A:9214:HOH:O	2.44	0.51
1:A:533:LEU:C	1:A:533:LEU:HD23	2.35	0.51
1:B:600:GLN:HE21	1:B:600:GLN:N	1.98	0.51
5:D:8410:DMS:H22	6:D:9006:HOH:O	2.10	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
5:C:8417:DMS:H22	6:C:9224:HOH:O	2.11	0.50
1:B:910:LEU:C	1:B:910:LEU:HD12	2.36	0.50
1:C:847:LYS:HG3	1:C:848:THR:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:CD1	1:D:653:HIS:CE1	2.93	0.50
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.47	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
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: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: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:D:717:TRP:CZ2	5:D:8415:DMS:H12	2.48	0.49
1:A:361:PRO:HB2	1:A:576:ILE:HG12	1.93	0.49
1:C:634:GLN:HE21	1:C:634:GLN:N	1.98	0.49
1:A:655:MET:HE2	1:A:656:VAL:O	2.12	0.49
1:D:748:CYS:C	1:D:749:ILE:HD12	2.37	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:C:717:TRP:CH2	5:C:8415:DMS:H12	2.48	0.48
1:D:618:THR:HG21	6:D:9060:HOH:O	2.12	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:D:717:TRP:CZ3	5:D:8415:DMS:H12	2.49	0.48
1:A:863:GLN:NE2	1:A:1021:CYS:CB	2.76	0.48
1:C:890:GLN:HG3	1:C:891:VAL:N	2.28	0.48
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.14	0.48
1:D:658:LEU:O	1:D:659:ASP:C	2.57	0.48
1:A:600:GLN:HE21	1:A:600:GLN:N	2.04	0.48
1:A:773:LYS:HB2	1:A:773:LYS:HE2	1.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.95	0.48
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.96	0.48
1:A:433:LEU:N	1:A:434:PRO:CD	2.76	0.47
1:A:717:TRP:CZ2	5:A:8415:DMS:H12	2.48	0.47
1:D:79:PRO:HD2	6:D:9733:HOH:O	2.13	0.47
1:D:237:ARG:CG	1:D:237:ARG:NH1	2.75	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:C:241:GLU:CD	1:C:292:ARG:HE	2.23	0.47
1:C:745:MET:HE1	1:C:761:GLN:OE1	2.14	0.47
1:D:893:GLU:O	1:D:893:GLU:HG3	2.08	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:A:736:ALA:C	1:A:737:ILE:HG22	2.40	0.47
1:B:668:VAL:HA	1:B:669:PRO:HD3	1.66	0.47
1:B:533:LEU:HD23	1:B:533:LEU:C	2.40	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:88:SER:HA	1:D:366:VAL:HG21	1.97	0.47
1:D:473:ARG:HD3	6:D:9456:HOH:O	2.13	0.47
1:D:805:ALA:O	1:D:809:ARG:HG3	2.15	0.47
1:D:845:GLN:OE1	1:D:845:GLN:N	2.47	0.47
1:D:655:MET:HE3	6:D:9565:HOH:O	2.14	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:HD12	1:D:730:LEU:H	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:C:655:MET:HE2	1:C:664:ALA:O	2.15	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:B:292:ARG:NH1	5:B:8412:DMS:H23	2.31	0.46
1:A:251:ARG:HH11	5:A:8416:DMS:C2	2.26	0.46
1:A:651:LEU:CD1	1:A:653:HIS:HD2	2.27	0.46
1:A:735:HIS:O	1:A:736:ALA:HB2	2.14	0.46
1:B:292:ARG:HH12	5:B:8412:DMS:H23	1.80	0.46
1:D:71:GLU:O	1:D:72:SER:C	2.57	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:770:ILE:CD1	1:D:770:ILE:N	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:C:806:TRP:CD2	1:C:991:MET:HE1	2.50	0.46
1:D:670:LEU:HA	1:D:670:LEU:HD23	1.58	0.46
1:B:806:TRP:CE2	1:B:991:MET:HE1	2.51	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:D:133:TRP:CD1	5:D:8703:DMS:H23	2.51	0.46
1:D:703:PRO:CG	5:D:8425:DMS:H12	2.46	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: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
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:601:PHE:CE2	5:C:8506:DMS:H23	2.51	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:768:MET:HE1	1:C:1020:TRP:CZ2	2.51	0.45
1:D:708:TRP:CZ2	5:D:8403:DMS:H13	2.50	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: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:HB3	1:B:577:LYS:HE3	1.86	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
5:D:8506:DMS:H12	6:D:9527:HOH:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:995:GLY:O	1:C:996:ASP:C	2.58	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:D:367:MET:HB3	1:D:372:MET:HE3	1.98	0.45
1:C:508:GLU:OE2	5:C:8407:DMS:H11	2.16	0.45
1:C:730:LEU:H	1:C:730:LEU:HG	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: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:C:734:SER:C	1:C:736:ALA:H	2.26	0.44
5:C:8412:DMS:H22	6:C:9438:HOH:O	2.18	0.44
1:D:74:LEU:HD22	1:D:153:TRP:CG	2.53	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:HD23	1:D:682:LEU:HA	1.80	0.44
1:D:863:GLN:HE21	1:D:1021:CYS:CB	2.27	0.44
1:A:788:PRO:CD	1:A:968:MET:HG3	2.48	0.44
1:A:859:ASP:OD1	1:A:861:SER:OG	2.29	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:HA	1:B:773:LYS:HD3	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:D:634:GLN:CG	1:D:634:GLN:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD12	1:C:651:LEU:O	2.17	0.43
1:D:731:PRO:C	1:D:732:ALA:O	2.60	0.43
1:A:717:TRP:CE3	5:A:8415:DMS:H12	2.53	0.43
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:A:708:TRP:CZ2	5:A:8403:DMS:H13	2.53	0.43
1:B:637:GLU:CD	1:B:677:LYS:HE3	2.43	0.43
1:B:824:GLN:HE22	1:B:837:THR:HB	1.81	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:842:TRP:C	1:D:843:GLN:HG3	2.43	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: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:D:933:SER:O	1:D:934:GLU:C	2.61	0.43
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.00	0.43
1:C:751:LEU:O	1:C:752:GLY:C	2.60	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:634:GLN:NE2	1:B:685:LEU:HB2	2.34	0.43
1:B:663:LEU:HD23	1:B:663:LEU:HA	1.85	0.43
1:C:745:MET:CE	1:C:759:ASN:HD21	2.23	0.43
1:C:768:MET:HE1	1:C:1020:TRP:CZ3	2.54	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:HG2	1:C:710:GLU:H	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: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:634:GLN:CD	1:C:634:GLN:C	2.87	0.42
1:C:847:LYS:HD2	6:C:9365:HOH:O	2.18	0.42
1:C:1023:LYS:HA	1:C:1023:LYS:NZ	2.32	0.42
1:D:537:GLU:HA	1:D:566:PHE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:LEU:HD11	1:A:993:ILE:HG22	2.00	0.42
1:B:13:ARG:HB2	1:C:13:ARG:HH22	1.84	0.42
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.76	0.42
1:D:279:ILE:HD13	1:D:279:ILE:HG21	1.84	0.42
1:B:70:PRO:HG2	1:B:78:LEU:HD21	2.00	0.42
1:B:674:PRO:O	1:B:675:GLN:HB2	2.20	0.42
5:B:8406:DMS:H21	6:B:9289:HOH:O	2.19	0.42
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: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:B:824:GLN:NE2	1:B:837:THR:C	2.78	0.42
1:C:379:MET:HE1	1:C:387:VAL:HB	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: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:B:428:ASP:CG	5:B:8420:DMS:H11	2.45	0.41
1:D:128:ASN:HD22	1:D:180:GLY:C	2.28	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:A:615:PRO:O	1:A:618:THR:HG22	2.21	0.41
1:A:634:GLN:N	1:A:634:GLN:CD	2.78	0.41
5:A:8504:DMS:H23	6:A:9343:HOH:O	2.20	0.41
1:B:995:GLY:O	1:B:996:ASP:C	2.64	0.41
1:C:569:ASP:O	1:C:605:GLY:HA2	2.21	0.41
1:C:951:TRP:HA	1:C:1019:VAL:O	2.20	0.41
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.55	0.41
1:A:770:ILE:O	1:A:771:GLY:C	2.64	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:835:LEU:HD11	1:A:855:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ILE:HD11	1:C:645:ARG:HB3	2.01	0.41
1:C:847:LYS:NZ	6:C:9365:HOH:O	2.44	0.41
1:D:787:ALA:HA	1:D:968:MET:HE2	2.02	0.41
1:B:537:GLU:HA	1:B:566:PHE:O	2.21	0.41
1:C:859:ASP:OD1	1:C:861:SER:OG	2.36	0.41
1:D:804:ASN:ND2	1:D:809:ARG:HH21	2.10	0.41
1:A:279:ILE:HD13	1:A:279:ILE:HG21	1.68	0.41
1:A:748:CYS:C	1:A:749:ILE:HD12	2.46	0.41
1:A:988:GLY:C	1:A:989:PHE:CD1	2.98	0.41
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.35	0.41
1:B:37:ARG:NH1	5:B:8504:DMS:H21	2.36	0.41
1:C:610:ASP:O	1:C:611:ARG:HB2	2.21	0.41
1:C:687:GLN:HA	1:C:687:GLN:HE21	1.76	0.41
1:D:753:ASN:O	1:D:771:GLY:N	2.37	0.41
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.56	0.41
1:A:576:ILE:HD13	1:A:576:ILE:HA	1.88	0.41
1:A:687:GLN:NE2	1:A:687:GLN:HA	2.34	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:C:988:GLY:C	1:C:989:PHE:CD1	3.00	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:659:ASP:C	2.64	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
5:B:8410:DMS:H11	6:B:8960:HOH:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.56	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: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: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
6:A:9370:HOH:O	6:B:9592:HOH:O[2_454]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1008/1023 (98%)	972 (96%)	35 (4%)	1 (0%)	48 24
1	B	1008/1023 (98%)	972 (96%)	30 (3%)	6 (1%)	21 6
1	C	1008/1023 (98%)	966 (96%)	39 (4%)	3 (0%)	36 17
1	D	1008/1023 (98%)	969 (96%)	37 (4%)	2 (0%)	43 22
All	All	4032/4092 (98%)	3879 (96%)	141 (4%)	12 (0%)	36 17

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%)	835 (97%)	28 (3%)	34	8
1	B	863/874 (99%)	832 (96%)	31 (4%)	31	6
1	C	863/874 (99%)	830 (96%)	33 (4%)	29	6
1	D	863/874 (99%)	825 (96%)	38 (4%)	25	4
All	All	3452/3496 (99%)	3322 (96%)	130 (4%)	29	6

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	157	ARG
1	A	237	ARG
1	A	250	LEU
1	A	262	GLN
1	A	344	LEU
1	A	377	LEU
1	A	546	LEU
1	A	580	GLU
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	630	ARG
1	A	634	GLN
1	A	651	LEU
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	890	GLN
1	A	956	GLN
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	80	GLU
1	B	230	ARG
1	B	262	GLN
1	B	264	GLU
1	B	344	LEU
1	B	362	LEU
1	B	367	MET
1	B	546	LEU
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	797	GLU
1	B	799	THR
1	B	801	ILE
1	B	809	ARG

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Mol	Chain	Res	Type
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	13	ARG
1	C	75	GLU
1	C	80	GLU
1	C	178	ARG
1	C	344	LEU
1	C	370	GLN
1	C	519	SER
1	C	546	LEU
1	C	595	THR
1	C	634	GLN
1	C	635	THR
1	C	655	MET
1	C	661	LYS
1	C	667	GLU
1	C	672	VAL
1	C	687	GLN
1	C	710	GLU
1	C	719	GLN
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	761	GLN
1	C	772	ASP
1	C	773	LYS
1	C	800	ARG
1	C	829	THR
1	C	893	GLU
1	C	986	ILE
1	C	1017	GLN
1	C	1023	LYS
1	D	80	GLU
1	D	117	GLU

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Mol	Chain	Res	Type
1	D	157	ARG
1	D	237	ARG
1	D	277	GLU
1	D	344	LEU
1	D	370	GLN
1	D	473	ARG
1	D	546	LEU
1	D	580	GLU
1	D	581	ASN
1	D	634	GLN
1	D	651	LEU
1	D	655	MET
1	D	677	LYS
1	D	681	GLU
1	D	684	GLU
1	D	687	GLN
1	D	710	GLU
1	D	730	LEU
1	D	735	HIS
1	D	737	ILE
1	D	741	THR
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	863	GLN
1	D	893	GLU
1	D	986	ILE
1	D	1018	LEU
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	GLN
1	A	485	GLN

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Mol	Chain	Res	Type
1	A	600	GLN
1	A	624	GLN
1	A	653	HIS
1	A	687	GLN
1	A	757	GLN
1	A	817	GLN
1	A	824	GLN
1	A	843	GLN
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	A	903	GLN
1	A	1017	GLN
1	B	50	GLN
1	B	163	GLN
1	B	262	GLN
1	B	266	GLN
1	B	363	HIS
1	B	365	GLN
1	B	485	GLN
1	B	554	GLN
1	B	600	GLN
1	B	624	GLN
1	B	646	HIS
1	B	687	GLN
1	B	757	GLN
1	B	817	GLN
1	B	824	GLN
1	B	843	GLN
1	B	878	HIS
1	B	945	ASN
1	B	950	GLN
1	B	977	HIS
1	C	163	GLN
1	C	363	HIS
1	C	374	GLN
1	C	485	GLN
1	C	634	GLN
1	C	646	HIS
1	C	687	GLN
1	C	704	ASN
1	C	775	GLN

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Mol	Chain	Res	Type
1	C	804	ASN
1	C	824	GLN
1	C	878	HIS
1	D	128	ASN
1	D	163	GLN
1	D	262	GLN
1	D	363	HIS
1	D	365	GLN
1	D	394	ASN
1	D	445	GLN
1	D	485	GLN
1	D	583	ASN
1	D	624	GLN
1	D	628	GLN
1	D	739	HIS
1	D	804	ASN
1	D	843	GLN
1	D	844	HIS
1	D	863	GLN
1	D	878	HIS
1	D	890	GLN
1	D	903	GLN
1	D	950	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	D	247[B]	-	3,6,7	0.97	0	1,6,8	0.43	0
1	CSO	A	247[A]	-	3,6,7	0.99	0	1,6,8	2.56	1 (100%)
1	CSO	C	247[A]	-	3,6,7	1.07	0	1,6,8	1.27	0
1	CSO	A	247[B]	-	3,6,7	0.99	0	1,6,8	2.56	1 (100%)
1	CSO	C	247[B]	-	3,6,7	1.07	0	1,6,8	1.27	0
1	CSO	D	247[A]	-	3,6,7	0.97	0	1,6,8	0.43	0
1	CSO	B	247[A]	-	3,6,7	0.96	0	1,6,8	1.75	0
1	CSO	B	247[B]	-	3,6,7	0.96	0	1,6,8	1.75	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
1	CSO	D	247[B]	-	-	0/1/5/7	-
1	CSO	A	247[A]	-	-	0/1/5/7	-
1	CSO	C	247[A]	-	-	0/1/5/7	-
1	CSO	A	247[B]	-	-	0/1/5/7	-
1	CSO	C	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	B	247[B]	-	-	0/1/5/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247[A]	CSO	CB-CA-C	-2.56	103.84	110.80
1	A	247[B]	CSO	CB-CA-C	-2.56	103.84	110.80

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 [i](#)

There are no oligosaccharides 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	8401	-	3,3,3	1.18	0	3,3,3	0.67	0
5	DMS	A	8411	-	3,3,3	0.75	0	3,3,3	0.30	0
5	DMS	A	8406	-	3,3,3	1.64	1 (33%)	3,3,3	0.80	0
5	DMS	C	8425	4	3,3,3	1.28	1 (33%)	3,3,3	0.98	0
5	DMS	A	8405	-	3,3,3	1.70	1 (33%)	3,3,3	0.77	0
5	DMS	C	8415	-	3,3,3	2.08	1 (33%)	3,3,3	1.18	0
5	DMS	C	8421	-	3,3,3	1.35	0	3,3,3	0.69	0
5	DMS	B	8401	-	3,3,3	0.71	0	3,3,3	0.24	0
5	DMS	A	8404	-	3,3,3	1.49	0	3,3,3	0.35	0
5	DMS	B	8425	4	3,3,3	1.93	1 (33%)	3,3,3	0.63	0
5	DMS	B	8406	-	3,3,3	1.78	1 (33%)	3,3,3	0.31	0
5	DMS	C	8401	-	3,3,3	1.08	0	3,3,3	0.61	0
5	DMS	B	8412	-	3,3,3	1.39	0	3,3,3	0.62	0
5	DMS	C	8416	-	3,3,3	0.89	0	3,3,3	0.11	0
5	DMS	B	8501	-	3,3,3	0.80	0	3,3,3	0.60	0
5	DMS	A	8402	-	3,3,3	1.55	1 (33%)	3,3,3	0.33	0
5	DMS	B	8410	-	3,3,3	1.24	0	3,3,3	0.32	0
5	DMS	A	8420	-	3,3,3	1.01	0	3,3,3	0.91	0
5	DMS	C	8410	-	3,3,3	0.77	0	3,3,3	0.67	0
5	DMS	A	8414	-	3,3,3	1.05	0	3,3,3	0.64	0
5	DMS	B	8502	-	3,3,3	1.38	0	3,3,3	1.68	1 (33%)
2	GAL	A	2002	-	12,12,12	0.41	0	17,17,17	1.24	2 (11%)
5	DMS	C	8501	-	3,3,3	1.11	0	3,3,3	1.22	1 (33%)
5	DMS	A	8415	-	3,3,3	2.71	2 (66%)	3,3,3	1.14	0
5	DMS	C	8404	-	3,3,3	1.47	0	3,3,3	1.28	1 (33%)
5	DMS	B	8414	-	3,3,3	0.61	0	3,3,3	1.06	0
5	DMS	D	8414	-	3,3,3	0.69	0	3,3,3	0.91	0
5	DMS	D	8411	-	3,3,3	1.16	0	3,3,3	0.68	0
5	DMS	A	8425	4	3,3,3	1.96	2 (66%)	3,3,3	1.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8501	-	3,3,3	0.84	0	3,3,3	0.48	0
5	DMS	B	8404	-	3,3,3	1.00	0	3,3,3	0.93	0
5	DMS	A	8421	-	3,3,3	1.64	1 (33%)	3,3,3	0.11	0
5	DMS	B	8402	-	3,3,3	1.39	1 (33%)	3,3,3	0.24	0
5	DMS	D	8410	-	3,3,3	1.07	0	3,3,3	0.61	0
5	DMS	D	8703	-	3,3,3	1.18	0	3,3,3	0.53	0
5	DMS	C	8409	-	3,3,3	2.26	1 (33%)	3,3,3	0.53	0
5	DMS	D	8405	-	3,3,3	1.52	1 (33%)	3,3,3	0.30	0
5	DMS	D	8701	-	3,3,3	2.44	2 (66%)	3,3,3	0.70	0
5	DMS	C	8402	-	3,3,3	2.01	1 (33%)	3,3,3	0.40	0
5	DMS	A	8410	-	3,3,3	0.36	0	3,3,3	0.90	0
5	DMS	A	8403	-	3,3,3	1.58	1 (33%)	3,3,3	0.83	0
5	DMS	B	8408	-	3,3,3	0.91	0	3,3,3	0.21	0
5	DMS	D	8402	-	3,3,3	2.15	2 (66%)	3,3,3	0.28	0
5	DMS	D	8409	-	3,3,3	3.47	2 (66%)	3,3,3	0.92	0
5	DMS	B	8421	-	3,3,3	0.33	0	3,3,3	0.90	0
2	GAL	D	2002	-	12,12,12	0.86	0	17,17,17	1.73	5 (29%)
5	DMS	C	8407	-	3,3,3	2.25	2 (66%)	3,3,3	0.06	0
5	DMS	C	8405	-	3,3,3	1.98	2 (66%)	3,3,3	0.63	0
5	DMS	C	8504	-	3,3,3	1.48	0	3,3,3	0.34	0
5	DMS	A	8502	-	3,3,3	2.14	1 (33%)	3,3,3	1.69	1 (33%)
5	DMS	D	8408	-	3,3,3	1.28	0	3,3,3	0.34	0
5	DMS	A	8409	-	3,3,3	2.76	2 (66%)	3,3,3	0.14	0
5	DMS	B	8504	-	3,3,3	1.00	0	3,3,3	0.21	0
5	DMS	B	8409	-	3,3,3	3.00	1 (33%)	3,3,3	0.29	0
5	DMS	C	8411	-	3,3,3	0.83	0	3,3,3	0.29	0
5	DMS	D	8406	-	3,3,3	1.51	0	3,3,3	0.66	0
5	DMS	C	8506	-	3,3,3	1.44	0	3,3,3	0.57	0
5	DMS	A	8506	-	3,3,3	1.49	1 (33%)	3,3,3	0.45	0
5	DMS	D	8508	-	3,3,3	1.78	1 (33%)	3,3,3	0.57	0
5	DMS	B	8601	-	3,3,3	2.43	1 (33%)	3,3,3	0.94	0
5	DMS	D	8413	-	3,3,3	1.62	0	3,3,3	0.67	0
5	DMS	B	8416	-	3,3,3	0.95	0	3,3,3	0.19	0
2	GAL	A	2001	4	12,12,12	1.61	3 (25%)	17,17,17	1.67	5 (29%)
5	DMS	A	8413	-	3,3,3	2.81	3 (100%)	3,3,3	0.19	0
5	DMS	C	8417	-	3,3,3	1.09	0	3,3,3	0.31	0
5	DMS	C	8408	-	3,3,3	0.96	0	3,3,3	0.85	0
5	DMS	D	8506	-	3,3,3	0.67	0	3,3,3	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8504	-	3,3,3	3.21	1 (33%)	3,3,3	0.28	0
5	DMS	B	8420	-	3,3,3	1.56	1 (33%)	3,3,3	0.28	0
5	DMS	B	8407	-	3,3,3	2.16	2 (66%)	3,3,3	1.33	1 (33%)
5	DMS	D	8416	-	3,3,3	0.59	0	3,3,3	0.33	0
5	DMS	A	8501	-	3,3,3	0.78	0	3,3,3	0.65	0
2	GAL	D	2001	4	12,12,12	1.36	2 (16%)	17,17,17	1.96	5 (29%)
5	DMS	D	8403	-	3,3,3	1.49	0	3,3,3	0.45	0
5	DMS	C	8602	-	3,3,3	1.36	1 (33%)	3,3,3	0.68	0
5	DMS	C	8412	-	3,3,3	0.79	0	3,3,3	0.40	0
5	DMS	A	8412	-	3,3,3	2.09	2 (66%)	3,3,3	0.33	0
5	DMS	B	8411	-	3,3,3	0.53	0	3,3,3	0.68	0
5	DMS	D	8404	-	3,3,3	1.46	1 (33%)	3,3,3	0.56	0
5	DMS	C	8413	-	3,3,3	1.98	1 (33%)	3,3,3	0.18	0
5	DMS	C	8403	-	3,3,3	0.62	0	3,3,3	0.49	0
5	DMS	A	8408	-	3,3,3	0.74	0	3,3,3	0.42	0
5	DMS	B	8417	-	3,3,3	1.30	0	3,3,3	0.41	0
2	GAL	B	2001	4	12,12,12	1.29	1 (8%)	17,17,17	1.85	5 (29%)
5	DMS	D	8412	-	3,3,3	0.71	0	3,3,3	0.79	0
5	DMS	B	8403	-	3,3,3	1.79	1 (33%)	3,3,3	0.67	0
5	DMS	A	8407	-	3,3,3	3.78	2 (66%)	3,3,3	0.31	0
5	DMS	D	8401	-	3,3,3	1.67	0	3,3,3	0.55	0
5	DMS	A	8416	-	3,3,3	1.17	0	3,3,3	0.30	0
5	DMS	D	8425	4	3,3,3	0.55	0	3,3,3	0.38	0
2	GAL	C	2002	-	12,12,12	0.84	0	17,17,17	1.87	7 (41%)
5	DMS	D	8421	-	3,3,3	0.40	0	3,3,3	0.14	0
2	GAL	C	2001	4	12,12,12	1.30	2 (16%)	17,17,17	1.88	3 (17%)
5	DMS	B	8405	-	3,3,3	1.71	1 (33%)	3,3,3	0.89	0
5	DMS	D	8705	-	3,3,3	1.99	1 (33%)	3,3,3	0.52	0
5	DMS	D	8415	-	3,3,3	2.60	1 (33%)	3,3,3	0.88	0
5	DMS	C	8420	-	3,3,3	1.93	1 (33%)	3,3,3	0.55	0
5	DMS	C	8414	-	3,3,3	1.12	0	3,3,3	1.35	1 (33%)
2	GAL	B	2002	-	12,12,12	0.67	0	17,17,17	1.49	4 (23%)

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	C	2001	4	-	1/2/22/22	0/1/1/1
2	GAL	C	2002	-	-	1/2/22/22	0/1/1/1
2	GAL	D	2002	-	-	0/2/22/22	0/1/1/1
2	GAL	A	2001	4	-	1/2/22/22	0/1/1/1
2	GAL	B	2001	4	-	1/2/22/22	0/1/1/1
2	GAL	D	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

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8504	DMS	C1-S	-5.33	1.37	1.76
5	D	8409	DMS	O-S	5.21	1.84	1.50
5	A	8407	DMS	O-S	4.85	1.82	1.50
5	B	8409	DMS	O-S	4.70	1.81	1.50
5	A	8407	DMS	C2-S	4.23	2.06	1.76
5	D	8415	DMS	C1-S	4.11	2.05	1.76
5	B	8601	DMS	C2-S	4.03	2.04	1.76
5	A	8409	DMS	O-S	3.88	1.75	1.50
5	A	8415	DMS	C2-S	3.71	2.02	1.76
5	C	8409	DMS	O-S	3.65	1.74	1.50
5	A	8413	DMS	C1-S	3.38	2.00	1.76
5	C	8402	DMS	C2-S	3.34	1.99	1.76
2	A	2001	GAL	O2-C2	3.34	1.51	1.43
5	A	8502	DMS	C1-S	3.21	1.99	1.76
5	C	8407	DMS	C2-S	3.20	1.98	1.76
5	C	8415	DMS	C2-S	3.15	1.98	1.76
5	C	8420	DMS	O-S	3.09	1.70	1.50
5	D	8705	DMS	O-S	3.07	1.70	1.50
5	B	8425	DMS	O-S	3.02	1.70	1.50
5	D	8701	DMS	O-S	2.95	1.69	1.50
5	C	8413	DMS	O-S	2.91	1.69	1.50
5	D	8409	DMS	C1-S	2.84	1.96	1.76
5	D	8402	DMS	O-S	2.73	1.68	1.50
2	B	2001	GAL	O2-C2	2.73	1.49	1.43
5	B	8407	DMS	C2-S	2.72	1.95	1.76
5	A	8412	DMS	O-S	2.68	1.67	1.50
5	A	8409	DMS	C1-S	2.67	1.95	1.76
5	A	8405	DMS	O-S	2.65	1.67	1.50
5	A	8413	DMS	C2-S	2.60	1.94	1.76
5	A	8421	DMS	C1-S	2.56	1.94	1.76
2	D	2001	GAL	O2-C2	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	GAL	C4-C3	2.56	1.59	1.52
5	B	8407	DMS	C1-S	-2.55	1.57	1.76
5	A	8415	DMS	C1-S	2.54	1.94	1.76
5	D	8508	DMS	O-S	2.45	1.66	1.50
5	C	8405	DMS	O-S	2.45	1.66	1.50
5	B	8406	DMS	C1-S	2.44	1.93	1.76
5	A	8412	DMS	C1-S	2.40	1.93	1.76
5	C	8405	DMS	C1-S	2.38	1.93	1.76
5	B	8403	DMS	C2-S	2.37	1.93	1.76
5	A	8413	DMS	O-S	2.36	1.65	1.50
5	B	8420	DMS	C2-S	2.32	1.92	1.76
5	C	8602	DMS	C2-S	-2.31	1.59	1.76
5	D	8701	DMS	C1-S	2.30	1.92	1.76
5	B	8405	DMS	O-S	2.30	1.65	1.50
5	A	8406	DMS	C1-S	-2.30	1.59	1.76
5	A	8425	DMS	C2-S	2.28	1.92	1.76
5	D	8404	DMS	C2-S	2.28	1.92	1.76
5	D	8405	DMS	C1-S	2.25	1.92	1.76
5	B	8402	DMS	C2-S	2.24	1.92	1.76
2	C	2001	GAL	O2-C2	2.21	1.48	1.43
5	A	8506	DMS	O-S	2.15	1.64	1.50
2	A	2001	GAL	O1-C1	2.13	1.46	1.39
5	D	8402	DMS	C2-S	2.12	1.91	1.76
5	C	8425	DMS	O-S	2.11	1.64	1.50
5	A	8402	DMS	O-S	2.08	1.64	1.50
2	A	2001	GAL	C6-C5	2.08	1.58	1.51
2	D	2001	GAL	C4-C3	2.06	1.57	1.52
5	A	8425	DMS	C1-S	2.03	1.90	1.76
5	C	8407	DMS	O-S	2.01	1.63	1.50
5	A	8403	DMS	O-S	2.01	1.63	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	GAL	O4-C4-C5	-4.99	97.02	109.32
2	B	2001	GAL	O1-C1-O5	-3.95	98.69	110.41
2	C	2001	GAL	O2-C2-C1	3.85	118.13	109.25
2	D	2001	GAL	O2-C2-C1	3.81	118.04	109.25
2	D	2001	GAL	O1-C1-O5	-3.75	99.26	110.41
2	A	2001	GAL	O2-C2-C1	3.75	117.91	109.25
2	D	2002	GAL	C1-C2-C3	3.71	117.91	110.36
2	C	2002	GAL	C3-C4-C5	-3.65	103.62	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	GAL	O4-C4-C5	-3.57	100.53	109.32
2	B	2001	GAL	O4-C4-C5	-3.32	101.14	109.32
2	B	2001	GAL	O2-C2-C1	3.22	116.67	109.25
2	A	2001	GAL	C1-O5-C5	3.10	119.65	113.65
2	C	2002	GAL	O5-C5-C4	2.99	115.09	109.70
5	A	8502	DMS	C2-S-C1	2.91	113.35	98.42
5	B	8502	DMS	C2-S-C1	2.91	113.31	98.42
2	C	2001	GAL	O1-C1-O5	-2.90	101.81	110.41
2	D	2001	GAL	O2-C2-C3	2.79	116.96	110.38
2	D	2002	GAL	O1-C1-O5	-2.77	102.19	110.41
2	C	2002	GAL	O4-C4-C5	2.73	116.04	109.32
2	D	2002	GAL	O2-C2-C1	2.72	115.52	109.25
2	C	2002	GAL	O1-C1-O5	-2.66	102.53	110.41
2	B	2002	GAL	C1-C2-C3	2.62	115.69	110.36
2	A	2001	GAL	O1-C1-O5	-2.51	102.96	110.41
2	D	2002	GAL	C1-O5-C5	-2.45	108.91	113.65
2	B	2001	GAL	O1-C1-C2	2.44	116.07	108.98
2	B	2002	GAL	O4-C4-C5	2.43	115.32	109.32
2	A	2002	GAL	O1-C1-O5	-2.35	103.45	110.41
2	A	2001	GAL	O1-C1-C2	2.34	115.77	108.98
2	D	2002	GAL	C3-C4-C5	-2.31	106.05	110.23
2	B	2001	GAL	C1-O5-C5	2.29	118.08	113.65
2	B	2002	GAL	O1-C1-O5	-2.28	103.63	110.41
2	C	2002	GAL	O2-C2-C3	-2.24	105.10	110.38
2	D	2001	GAL	O1-C1-C2	2.19	115.34	108.98
2	A	2001	GAL	O5-C5-C4	-2.19	105.75	109.70
5	C	8414	DMS	C2-S-C1	2.19	109.63	98.42
2	C	2002	GAL	O5-C5-C6	2.18	111.85	106.44
5	B	8407	DMS	C2-S-C1	2.11	109.23	98.42
5	C	8404	DMS	C2-S-C1	2.11	109.21	98.42
2	C	2002	GAL	O3-C3-C4	-2.05	105.54	110.38
5	C	8501	DMS	C2-S-C1	-2.02	88.05	98.42
2	A	2002	GAL	C1-O5-C5	-2.01	109.75	113.65
2	B	2002	GAL	O5-C5-C4	-2.00	106.09	109.70

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

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

There are no ring outliers.

40 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8415	DMS	2	0
5	B	8406	DMS	2	0
5	B	8412	DMS	3	0
5	B	8410	DMS	2	0
5	A	8420	DMS	1	0
5	C	8410	DMS	2	0
5	A	8414	DMS	1	0
5	A	8415	DMS	5	0
5	A	8421	DMS	1	0
5	D	8410	DMS	1	0
5	D	8703	DMS	5	0
5	A	8410	DMS	1	0
5	A	8403	DMS	1	0
5	C	8407	DMS	1	0
5	C	8504	DMS	1	0
5	B	8504	DMS	1	0
5	D	8406	DMS	1	0
5	C	8506	DMS	3	0
5	A	8506	DMS	4	0
5	B	8601	DMS	1	0
2	A	2001	GAL	1	0
5	C	8417	DMS	2	0
5	D	8506	DMS	4	0
5	A	8504	DMS	1	0
5	B	8420	DMS	2	0
5	B	8407	DMS	1	0
2	D	2001	GAL	1	0
5	D	8403	DMS	1	0
5	C	8412	DMS	1	0
5	B	8417	DMS	1	0
2	B	2001	GAL	1	0
5	D	8412	DMS	2	0
5	A	8407	DMS	2	0
5	A	8416	DMS	2	0
5	D	8425	DMS	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8421	DMS	1	0
2	C	2001	GAL	1	0
5	D	8415	DMS	4	0
5	C	8420	DMS	1	0
2	B	2002	GAL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	1010/1023 (98%)	-0.10	49 (4%)	35	38	8, 15, 43, 97	0
1	B	1010/1023 (98%)	-0.09	57 (5%)	30	33	8, 15, 45, 91	0
1	C	1010/1023 (98%)	-0.03	66 (6%)	25	27	8, 15, 47, 99	0
1	D	1010/1023 (98%)	-0.02	59 (5%)	29	31	8, 16, 47, 97	0
All	All	4040/4092 (98%)	-0.06	231 (5%)	29	32	8, 15, 46, 99	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	730	LEU	7.7
1	B	686	PRO	6.1
1	C	732	ALA	5.6
1	D	1023	LYS	5.5
1	B	685	LEU	5.5
1	B	730	LEU	5.5
1	B	732	ALA	5.3
1	D	733	ALA	5.2
1	C	736	ALA	5.1
1	C	733	ALA	5.1
1	D	730	LEU	5.0
1	D	686	PRO	5.0
1	C	686	PRO	4.9
1	A	737	ILE	4.9
1	A	736	ALA	4.8
1	C	685	LEU	4.7
1	A	1023	LYS	4.7
1	B	733	ALA	4.5
1	B	635	THR	4.5
1	A	732	ALA	4.5
1	D	829	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	663	LEU	4.4
1	C	737	ILE	4.4
1	D	732	ALA	4.4
1	C	730	LEU	4.3
1	B	845	GLN	4.3
1	C	831	ALA	4.3
1	A	686	PRO	4.2
1	A	729	THR	4.2
1	D	737	ILE	4.1
1	A	735	HIS	4.1
1	C	761	GLN	4.0
1	A	634	GLN	4.0
1	A	771	GLY	3.9
1	B	1023	LYS	3.9
1	D	735	HIS	3.9
1	C	1022	GLN	3.9
1	B	745	MET	3.9
1	D	581	ASN	3.9
1	B	690	SER	3.8
1	B	737	ILE	3.7
1	C	689	GLU	3.7
1	B	729	THR	3.7
1	D	690	SER	3.7
1	D	736	ALA	3.7
1	D	634	GLN	3.7
1	B	725	ASN	3.6
1	B	687	GLN	3.6
1	D	687	GLN	3.6
1	B	634	GLN	3.6
1	A	798	ALA	3.6
1	C	634	GLN	3.6
1	B	580	GLU	3.5
1	C	731	PRO	3.5
1	B	817	GLN	3.5
1	A	772	ASP	3.5
1	D	683	PRO	3.5
1	D	116	THR	3.5
1	B	655	MET	3.5
1	D	861	SER	3.5
1	B	731	PRO	3.5
1	D	669	PRO	3.5
1	D	751	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	842	TRP	3.4
1	A	1022	GLN	3.4
1	A	688	PRO	3.4
1	A	646	HIS	3.3
1	D	681	GLU	3.3
1	D	799	THR	3.3
1	B	738	PRO	3.3
1	C	735	HIS	3.3
1	C	687	GLN	3.3
1	C	821	ALA	3.3
1	A	687	GLN	3.3
1	B	846	GLY	3.2
1	B	819	GLU	3.2
1	C	729	THR	3.2
1	B	831	ALA	3.2
1	B	863	GLN	3.2
1	B	735	HIS	3.2
1	B	736	ALA	3.1
1	B	799	THR	3.1
1	A	683	PRO	3.1
1	B	651	LEU	3.1
1	B	1022	GLN	3.1
1	B	768	MET	3.1
1	C	688	PRO	3.0
1	D	731	PRO	3.0
1	D	580	GLU	3.0
1	D	76	CYS	3.0
1	C	801	ILE	3.0
1	C	986	ILE	3.0
1	C	80	GLU	3.0
1	D	846	GLY	3.0
1	A	690	SER	2.9
1	D	773	LYS	2.9
1	C	772	ASP	2.8
1	C	734	SER	2.8
1	A	801	ILE	2.8
1	A	986	ILE	2.8
1	D	75	GLU	2.8
1	B	682	LEU	2.8
1	C	1023	LYS	2.8
1	D	739	HIS	2.8
1	B	761	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	582	GLY	2.7
1	C	743	SER	2.7
1	D	370	GLN	2.7
1	C	800	ARG	2.7
1	C	858	ILE	2.7
1	A	731	PRO	2.7
1	D	734	SER	2.7
1	A	820	ALA	2.7
1	A	362	LEU	2.7
1	C	842	TRP	2.7
1	D	729	THR	2.7
1	A	739	HIS	2.7
1	C	770	ILE	2.7
1	D	741	THR	2.6
1	D	1022	GLN	2.6
1	C	684	GLU	2.6
1	D	646	HIS	2.6
1	C	835	LEU	2.6
1	D	847	LYS	2.6
1	A	669	PRO	2.6
1	A	75	GLU	2.6
1	D	769	TRP	2.6
1	D	655	MET	2.6
1	A	829	THR	2.6
1	C	799	THR	2.6
1	B	1018	LEU	2.6
1	A	684	GLU	2.6
1	C	745	MET	2.6
1	A	751	LEU	2.5
1	C	362	LEU	2.5
1	C	682	LEU	2.5
1	A	800	ARG	2.5
1	B	633	GLY	2.5
1	B	688	PRO	2.5
1	C	635	THR	2.5
1	A	733	ALA	2.5
1	C	370	GLN	2.5
1	C	230	ARG	2.5
1	D	801	ILE	2.5
1	D	771	GLY	2.5
1	B	695	TRP	2.5
1	D	1018	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	738	PRO	2.5
1	B	699	ARG	2.5
1	C	667	GLU	2.4
1	D	770	ILE	2.4
1	D	685	LEU	2.4
1	A	799	THR	2.4
1	A	580	GLU	2.4
1	D	845	GLN	2.4
1	C	752	GLY	2.4
1	A	79	PRO	2.4
1	B	264	GLU	2.4
1	C	751	LEU	2.4
1	D	362	LEU	2.4
1	C	632	SER	2.4
1	C	579	ASP	2.4
1	C	826	THR	2.4
1	A	583	ASN	2.4
1	A	135	GLN	2.3
1	B	662	PRO	2.3
1	B	755	ARG	2.3
1	D	857	ARG	2.3
1	B	728	VAL	2.3
1	C	742	THR	2.3
1	C	862	GLY	2.3
1	D	772	ASP	2.3
1	C	824	GLN	2.3
1	D	800	ARG	2.3
1	C	827	ALA	2.3
1	B	684	GLU	2.3
1	D	688	PRO	2.3
1	A	582	GLY	2.3
1	B	230	ARG	2.3
1	B	824	GLN	2.3
1	C	653	HIS	2.2
1	B	797	GLU	2.2
1	A	651	LEU	2.2
1	D	753	ASN	2.2
1	A	845	GLN	2.2
1	B	798	ALA	2.2
1	C	630	ARG	2.2
1	B	771	GLY	2.2
1	A	682	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	797	GLU	2.2
1	A	76	CYS	2.2
1	D	1021	CYS	2.2
1	A	846	GLY	2.2
1	A	262	GLN	2.2
1	A	581	ASN	2.2
1	D	832	ASP	2.2
1	B	847	LYS	2.2
1	D	663	LEU	2.1
1	C	683	PRO	2.1
1	A	230	ARG	2.1
1	C	817	GLN	2.1
1	C	819	GLU	2.1
1	B	800	ARG	2.1
1	C	798	ALA	2.1
1	B	71	GLU	2.1
1	C	744	GLU	2.1
1	A	768	MET	2.1
1	C	661	LYS	2.1
1	B	237	ARG	2.1
1	C	755	ARG	2.1
1	B	734	SER	2.1
1	B	743	SER	2.1
1	B	689	GLU	2.1
1	D	738	PRO	2.1
1	C	823	LEU	2.1
1	C	13	ARG	2.1
1	D	755	ARG	2.1
1	C	769	TRP	2.1
1	C	512	PHE	2.0
1	B	668	VAL	2.0
1	D	251	ARG	2.0
1	A	685	LEU	2.0
1	D	830	LEU	2.0
1	B	80	GLU	2.0
1	D	80	GLU	2.0
1	A	671	ASP	2.0
1	D	633	GLY	2.0
1	C	829	THR	2.0
1	C	1018	LEU	2.0
1	A	746	ASP	2.0
1	C	746	ASP	2.0

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, 95th 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 ²)	Q<0.9
1	CSO	A	247[A]	7/8	0.97	0.06	9,11,17,23	1
1	CSO	A	247[B]	7/8	0.97	0.06	9,11,19,23	1
1	CSO	B	247[A]	7/8	0.97	0.06	13,14,17,24	1
1	CSO	B	247[B]	7/8	0.97	0.06	13,14,18,24	1
1	CSO	C	247[A]	7/8	0.98	0.05	11,14,18,23	1
1	CSO	C	247[B]	7/8	0.98	0.05	11,14,18,23	1
1	CSO	D	247[A]	7/8	0.98	0.06	12,13,16,22	1
1	CSO	D	247[B]	7/8	0.98	0.06	12,13,22,25	1

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
5	DMS	B	8416	4/4	0.75	0.20	40,43,55,89	0
5	DMS	B	8407	4/4	0.81	0.26	30,33,43,100	0
5	DMS	A	8413	4/4	0.82	0.18	32,37,45,63	0
5	DMS	B	8420	4/4	0.82	0.26	36,61,77,100	0
5	DMS	C	8602	4/4	0.82	0.24	25,60,68,100	0
5	DMS	D	8415	4/4	0.82	0.22	24,41,66,100	0
5	DMS	A	8421	4/4	0.83	0.18	45,47,58,61	0
5	DMS	B	8410	4/4	0.83	0.18	33,33,37,100	0
5	DMS	B	8406	4/4	0.83	0.18	26,45,45,78	0
5	DMS	D	8416	4/4	0.85	0.19	28,50,52,100	0
5	DMS	D	8506	4/4	0.85	0.18	18,46,92,97	0
5	DMS	D	8703	4/4	0.85	0.16	27,53,54,55	0
5	DMS	A	8416	4/4	0.86	0.18	19,38,75,100	0
5	DMS	A	8506	4/4	0.86	0.20	28,72,82,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	D	8425	4/4	0.88	0.25	19,35,36,97	4
5	DMS	C	8421	4/4	0.88	0.20	37,46,56,100	0
5	DMS	B	8601	4/4	0.88	0.19	34,35,47,54	0
5	DMS	A	8407	4/4	0.89	0.15	25,28,44,46	0
5	DMS	C	8407	4/4	0.89	0.19	29,40,44,100	0
3	MG	A	3105	1/1	0.89	0.11	24,24,24,24	1
5	DMS	C	8504	4/4	0.89	0.16	24,33,65,100	0
5	DMS	B	8421	4/4	0.89	0.12	28,37,39,48	0
5	DMS	D	8705	4/4	0.89	0.19	38,41,44,56	0
5	DMS	C	8416	4/4	0.90	0.16	37,44,55,100	0
5	DMS	A	8406	4/4	0.90	0.17	15,36,67,72	0
5	DMS	C	8413	4/4	0.90	0.21	35,37,44,100	0
5	DMS	C	8506	4/4	0.90	0.21	34,44,65,100	0
5	DMS	C	8415	4/4	0.90	0.14	23,30,31,47	0
5	DMS	D	8404	4/4	0.90	0.14	20,25,43,76	0
5	DMS	A	8412	4/4	0.91	0.19	30,40,41,100	0
5	DMS	A	8420	4/4	0.91	0.18	38,38,40,70	0
5	DMS	D	8413	4/4	0.91	0.20	30,42,49,100	0
5	DMS	C	8417	4/4	0.91	0.15	25,29,49,71	0
5	DMS	C	8420	4/4	0.91	0.21	37,46,55,100	0
5	DMS	A	8414	4/4	0.91	0.16	26,32,54,100	0
5	DMS	C	8425	4/4	0.91	0.24	30,31,38,100	0
5	DMS	D	8508	4/4	0.91	0.17	32,42,47,100	0
5	DMS	A	8502	4/4	0.91	0.15	19,27,43,58	0
5	DMS	A	8504	4/4	0.91	0.20	12,38,65,100	0
5	DMS	C	8412	4/4	0.92	0.20	30,41,46,74	0
2	GAL	B	2002	12/12	0.92	0.15	22,32,100,100	0
5	DMS	C	8414	4/4	0.92	0.20	19,34,45,100	0
2	GAL	C	2002	12/12	0.92	0.15	21,31,100,100	0
5	DMS	D	8421	4/4	0.92	0.16	34,55,55,100	0
5	DMS	B	8409	4/4	0.93	0.14	24,25,35,69	0
5	DMS	A	8425	4/4	0.93	0.13	27,32,39,40	0
4	NA	A	3103	1/1	0.93	0.12	28,28,28,28	0
5	DMS	D	8414	4/4	0.93	0.18	23,39,62,78	0
5	DMS	C	8410	4/4	0.93	0.11	24,36,39,41	0
5	DMS	A	8410	4/4	0.93	0.15	28,35,41,100	0
5	DMS	D	8410	4/4	0.94	0.11	32,38,39,62	0
5	DMS	A	8409	4/4	0.94	0.12	26,29,40,47	0
2	GAL	D	2002	12/12	0.94	0.09	17,25,30,37	0
5	DMS	B	8425	4/4	0.94	0.10	27,32,35,40	0
2	GAL	A	2002	12/12	0.94	0.13	20,27,80,86	0
5	DMS	B	8408	4/4	0.94	0.16	27,35,38,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	8409	4/4	0.94	0.11	29,31,36,40	0
5	DMS	D	8501	4/4	0.94	0.10	19,26,44,46	0
3	MG	D	3005	1/1	0.94	0.09	29,29,29,29	0
5	DMS	A	8408	4/4	0.94	0.17	18,31,36,100	0
5	DMS	A	8415	4/4	0.94	0.12	22,41,41,43	0
5	DMS	B	8417	4/4	0.94	0.12	25,36,59,79	0
5	DMS	A	8501	4/4	0.95	0.10	18,22,30,33	0
5	DMS	B	8501	4/4	0.95	0.12	23,28,37,64	0
5	DMS	B	8502	4/4	0.95	0.10	20,26,35,38	0
4	NA	D	3103	1/1	0.95	0.09	30,30,30,30	0
4	NA	D	3104	1/1	0.95	0.12	33,33,33,33	0
5	DMS	B	8414	4/4	0.95	0.12	28,45,56,64	0
3	MG	D	3105	1/1	0.95	0.09	23,23,23,23	1
5	DMS	B	8404	4/4	0.95	0.09	15,20,29,30	0
3	MG	B	3105	1/1	0.95	0.07	21,21,21,21	1
4	NA	C	3104	1/1	0.95	0.13	25,25,25,25	0
5	DMS	D	8406	4/4	0.95	0.13	21,22,24,33	0
5	DMS	D	8409	4/4	0.95	0.10	23,25,30,32	0
2	GAL	B	2001	12/12	0.96	0.08	11,19,31,31	0
5	DMS	B	8504	4/4	0.96	0.08	21,24,27,33	0
5	DMS	D	8411	4/4	0.96	0.14	23,24,28,100	0
4	NA	B	3104	1/1	0.96	0.13	27,27,27,27	0
5	DMS	C	8405	4/4	0.96	0.10	23,30,31,31	0
2	GAL	D	2001	12/12	0.96	0.07	10,16,20,22	0
5	DMS	C	8408	4/4	0.96	0.11	24,31,36,47	0
5	DMS	C	8501	4/4	0.96	0.09	17,29,31,32	0
5	DMS	B	8405	4/4	0.96	0.09	22,25,26,27	0
3	MG	C	3105	1/1	0.96	0.10	20,20,20,20	1
2	GAL	A	2001	12/12	0.96	0.08	10,18,25,31	0
5	DMS	A	8404	4/4	0.96	0.09	16,22,27,28	0
3	MG	A	3005	1/1	0.96	0.11	30,30,30,30	0
5	DMS	D	8408	4/4	0.96	0.08	17,25,30,42	0
5	DMS	A	8403	4/4	0.97	0.08	16,21,22,26	0
5	DMS	B	8412	4/4	0.97	0.09	23,28,29,33	0
5	DMS	C	8402	4/4	0.97	0.09	13,24,25,26	0
5	DMS	D	8403	4/4	0.97	0.07	15,22,25,25	0
5	DMS	B	8402	4/4	0.97	0.08	15,18,21,21	0
5	DMS	D	8701	4/4	0.97	0.12	14,15,20,58	0
4	NA	C	3103	1/1	0.97	0.06	24,24,24,24	0
2	GAL	C	2001	12/12	0.97	0.07	11,17,24,25	0
5	DMS	B	8411	4/4	0.98	0.10	21,21,24,67	0
5	DMS	D	8412	4/4	0.98	0.08	20,26,29,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8402	4/4	0.98	0.08	15,16,20,24	0
5	DMS	C	8411	4/4	0.98	0.09	20,23,25,41	0
4	NA	B	3103	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	D	8402	4/4	0.98	0.07	15,20,22,25	0
5	DMS	A	8405	4/4	0.98	0.06	21,22,22,24	0
5	DMS	C	8403	4/4	0.98	0.07	17,19,22,30	0
5	DMS	D	8405	4/4	0.98	0.07	22,22,28,30	0
5	DMS	C	8404	4/4	0.98	0.06	17,18,21,24	0
5	DMS	A	8411	4/4	0.98	0.08	22,26,26,35	0
4	NA	A	3104	1/1	0.98	0.07	24,24,24,24	0
5	DMS	B	8403	4/4	0.98	0.06	15,19,23,24	0
5	DMS	C	8401	4/4	0.99	0.05	13,14,16,16	0
5	DMS	D	8401	4/4	0.99	0.05	12,13,16,17	0
4	NA	D	3102	1/1	0.99	0.02	11,11,11,11	0
3	MG	D	3001	1/1	0.99	0.02	11,11,11,11	0
3	MG	D	3002	1/1	0.99	0.03	14,14,14,14	0
5	DMS	A	8401	4/4	0.99	0.05	12,13,13,15	0
3	MG	B	3002	1/1	0.99	0.03	14,14,14,14	0
3	MG	A	3002	1/1	0.99	0.04	14,14,14,14	0
4	NA	A	3101	1/1	0.99	0.04	13,13,13,13	0
4	NA	A	3102	1/1	0.99	0.03	12,12,12,12	0
5	DMS	B	8401	4/4	0.99	0.06	13,16,19,20	0
4	NA	D	3101	1/1	0.99	0.04	13,13,13,13	0
3	MG	B	3001	1/1	1.00	0.02	10,10,10,10	0
4	NA	B	3101	1/1	1.00	0.02	11,11,11,11	0
4	NA	B	3102	1/1	1.00	0.04	11,11,11,11	0
3	MG	C	3001	1/1	1.00	0.03	10,10,10,10	0
3	MG	C	3002	1/1	1.00	0.02	13,13,13,13	0
4	NA	C	3101	1/1	1.00	0.02	11,11,11,11	0
4	NA	C	3102	1/1	1.00	0.04	12,12,12,12	0
3	MG	A	3001	1/1	1.00	0.02	11,11,11,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.