



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:18 AM UTC

PDB ID : 4TTG / pdb_00004ttg
Title : Beta-galactosidase (E. coli) in the presence of potassium chloride.
Authors : Juers, D.H.
Deposited on : 2014-06-20
Resolution : 1.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

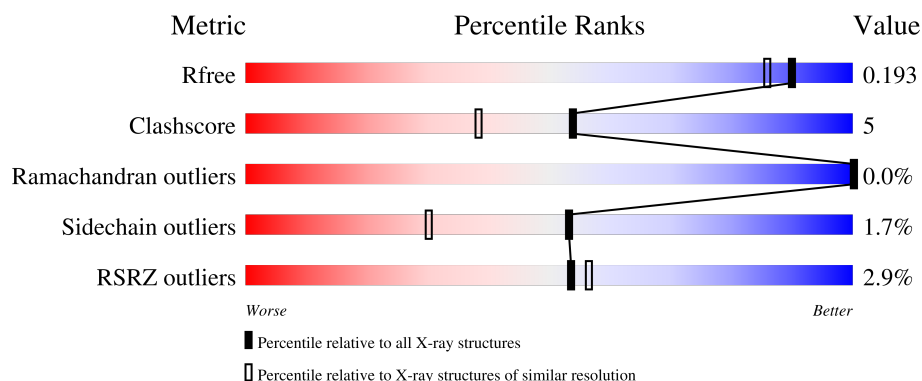
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

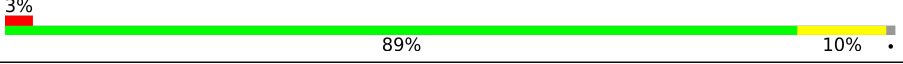
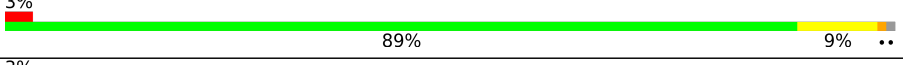
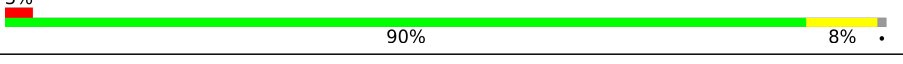
The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	B	1023	
1	C	1023	
1	D	1023	

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	3023	-	-	X	-
5	DMS	A	3024	-	-	X	-
5	DMS	A	3025	-	-	X	-
5	DMS	A	3028	-	-	X	-
5	DMS	B	1119	-	-	X	-
5	DMS	B	1122	-	-	X	-
5	DMS	B	1127	-	-	X	-
5	DMS	C	3019	-	-	X	-
5	DMS	C	3029	-	-	X	-
5	DMS	C	3034	-	-	X	-
5	DMS	D	1122	-	-	X	-
5	DMS	D	1129	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38364 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	1015	Total	C	N	O	S	0	35	0
			8365	5304	1475	1542	44			
1	B	1015	Total	C	N	O	S	0	29	0
			8315	5272	1463	1537	43			
1	C	1015	Total	C	N	O	S	0	31	0
			8342	5286	1471	1542	43			
1	D	1015	Total	C	N	O	S	0	33	0
			8328	5284	1462	1538	44			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8VNN2
A	2	SER	-	expression tag	UNP Q8VNN2
A	3	HIS	-	expression tag	UNP Q8VNN2
A	4	MET	-	expression tag	UNP Q8VNN2
A	5	LEU	-	expression tag	UNP Q8VNN2
A	6	GLU	-	expression tag	UNP Q8VNN2
A	7	ASP	-	expression tag	UNP Q8VNN2
A	8	PRO	-	expression tag	UNP Q8VNN2
B	1	GLY	-	expression tag	UNP Q8VNN2
B	2	SER	-	expression tag	UNP Q8VNN2
B	3	HIS	-	expression tag	UNP Q8VNN2
B	4	MET	-	expression tag	UNP Q8VNN2
B	5	LEU	-	expression tag	UNP Q8VNN2
B	6	GLU	-	expression tag	UNP Q8VNN2
B	7	ASP	-	expression tag	UNP Q8VNN2
B	8	PRO	-	expression tag	UNP Q8VNN2
C	1	GLY	-	expression tag	UNP Q8VNN2
C	2	SER	-	expression tag	UNP Q8VNN2
C	3	HIS	-	expression tag	UNP Q8VNN2
C	4	MET	-	expression tag	UNP Q8VNN2
C	5	LEU	-	expression tag	UNP Q8VNN2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	-	expression tag	UNP Q8VNN2
C	7	ASP	-	expression tag	UNP Q8VNN2
C	8	PRO	-	expression tag	UNP Q8VNN2
D	1	GLY	-	expression tag	UNP Q8VNN2
D	2	SER	-	expression tag	UNP Q8VNN2
D	3	HIS	-	expression tag	UNP Q8VNN2
D	4	MET	-	expression tag	UNP Q8VNN2
D	5	LEU	-	expression tag	UNP Q8VNN2
D	6	GLU	-	expression tag	UNP Q8VNN2
D	7	ASP	-	expression tag	UNP Q8VNN2
D	8	PRO	-	expression tag	UNP Q8VNN2

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

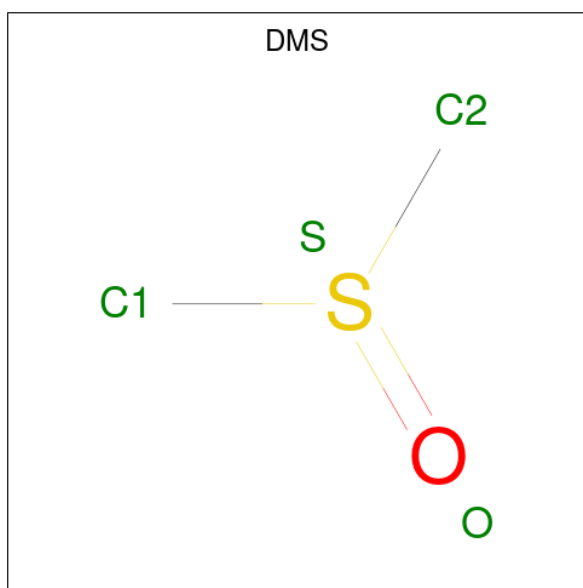
- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



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

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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	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	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

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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	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

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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	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 8	C 4	O 2	S 2	0	1
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

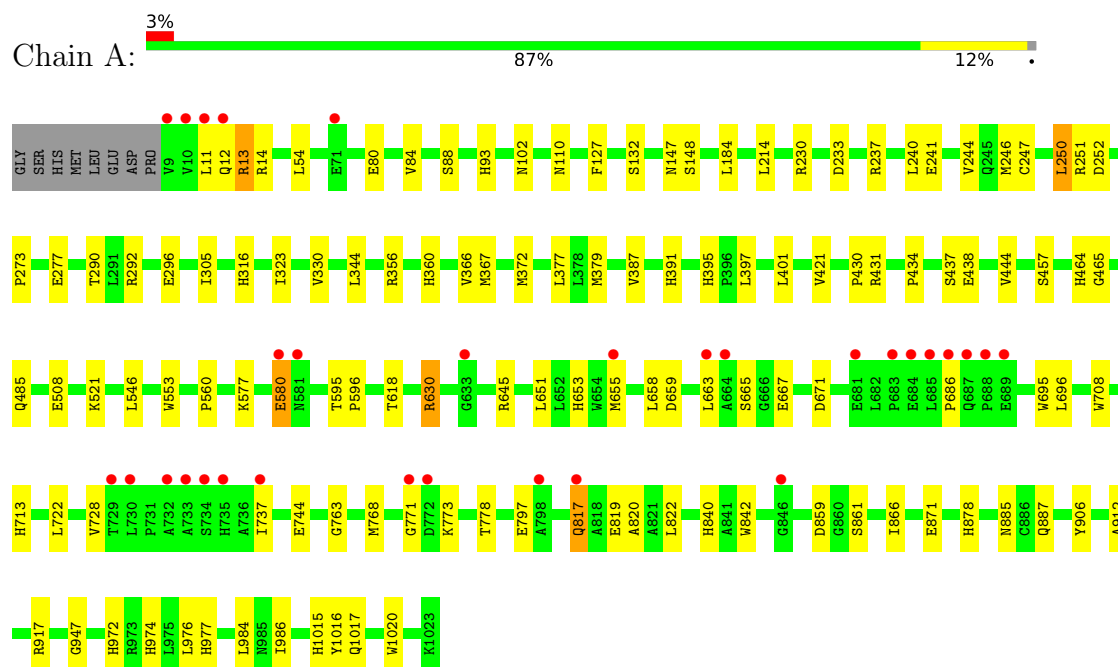
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1130	Total O 1130 1130	0	0
6	B	1114	Total O 1114 1114	0	0
6	C	1094	Total O 1094 1094	0	0
6	D	1113	Total O 1113 1113	0	0

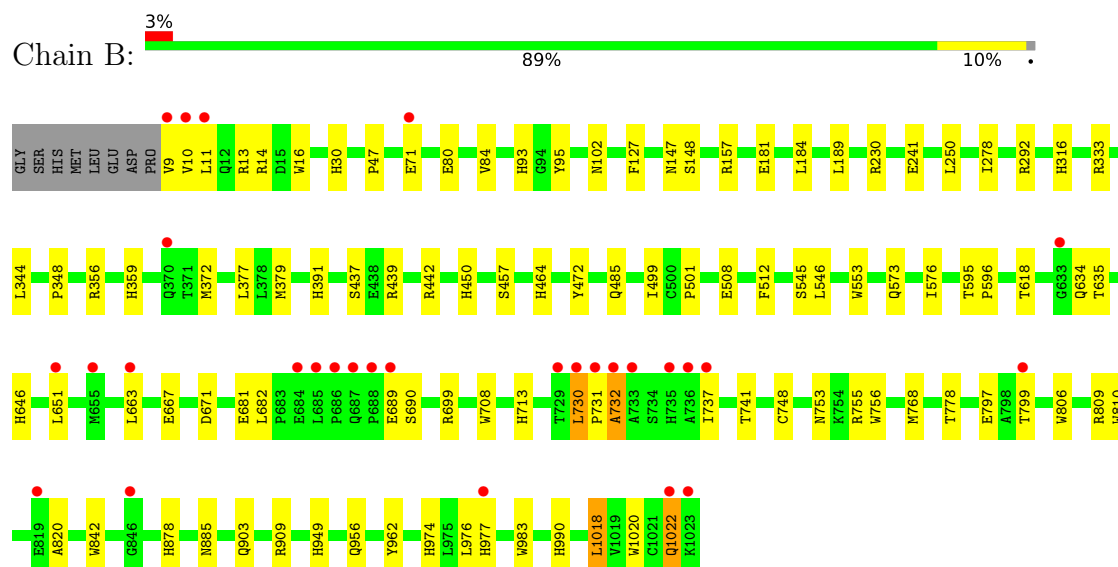
3 Residue-property plots [i](#)

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

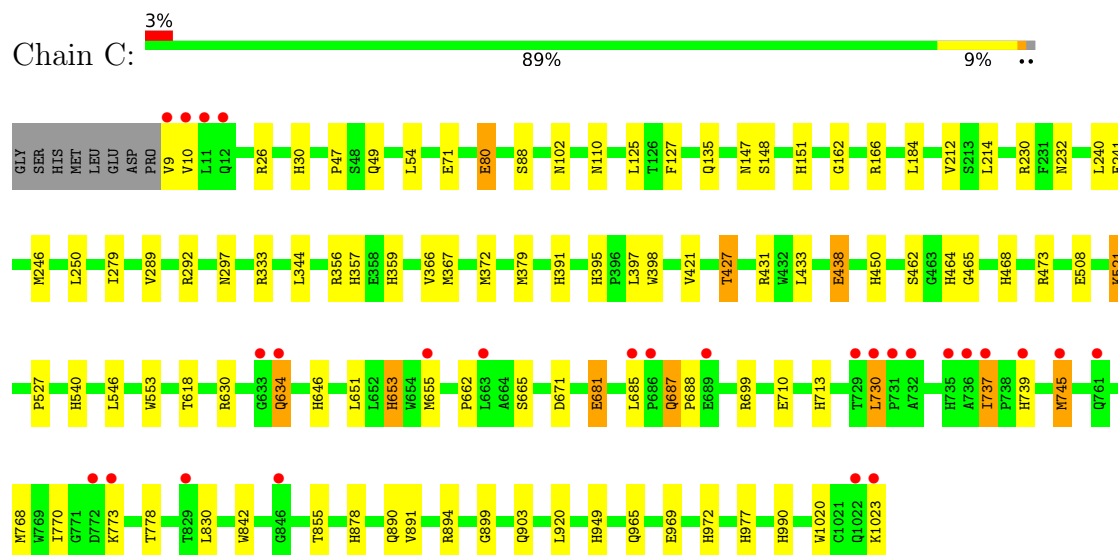
• Molecule 1: Beta-galactosidase



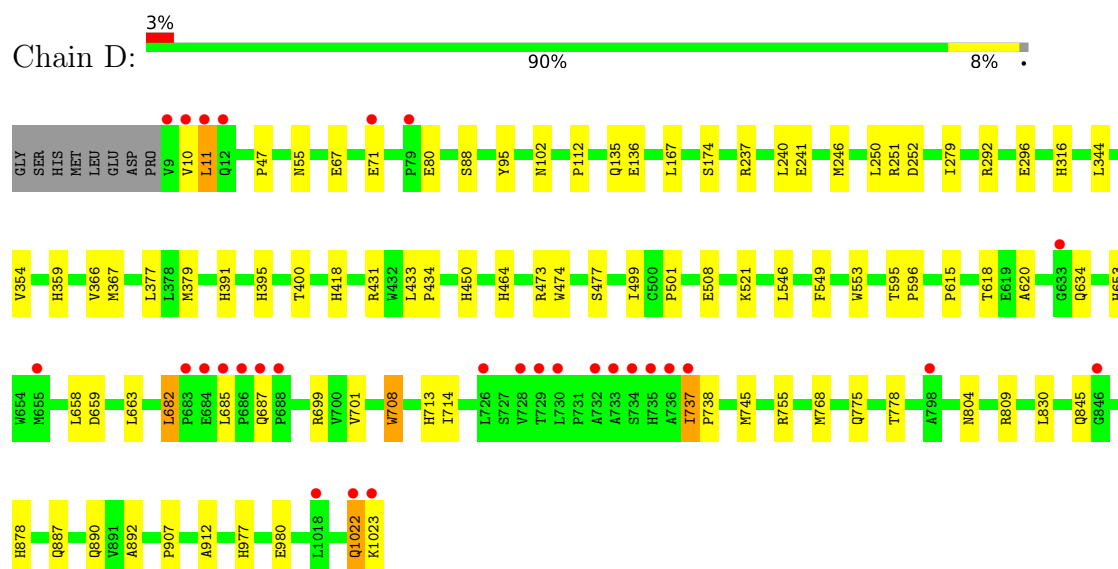
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



• 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	149.29Å 168.10Å 200.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.81 – 1.60 55.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.1 (55.81-1.60) 92.1 (55.81-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.160 , 0.188 (Not available) , 0.193	Depositor DCC
R_{free} test set	8778 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	38364	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6165e-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: CL, CSD, MG, DMS, K

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	1.32	26/8684 (0.3%)	1.17	12/11840 (0.1%)
1	B	1.30	17/8628 (0.2%)	1.15	10/11769 (0.1%)
1	C	1.30	32/8651 (0.4%)	1.13	7/11798 (0.1%)
1	D	1.29	17/8652 (0.2%)	1.14	1/11804 (0.0%)
All	All	1.30	92/34615 (0.3%)	1.15	30/47211 (0.1%)

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

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

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	GLY	N-CA	9.57	1.55	1.45
1	D	279	ILE	CA-CB	-8.28	1.44	1.54
1	A	878	HIS	CE1-NE2	8.23	1.40	1.32
1	B	713	HIS	ND1-CE1	7.90	1.40	1.32
1	A	316	HIS	CG-CD2	7.87	1.44	1.35
1	D	464	HIS	ND1-CE1	7.87	1.40	1.32
1	D	713	HIS	ND1-CE1	7.65	1.40	1.32
1	C	713	HIS	ND1-CE1	7.50	1.40	1.32
1	A	316	HIS	ND1-CE1	7.22	1.39	1.32
1	D	450	HIS	ND1-CE1	7.12	1.39	1.32
1	A	391	HIS	ND1-CE1	7.02	1.39	1.32
1	D	379	MET	SD-CE	-6.94	1.62	1.79
1	B	949	HIS	ND1-CE1	6.91	1.39	1.32
1	A	977	HIS	CG-CD2	6.87	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	450	HIS	ND1-CE1	6.85	1.39	1.32
1	C	977	HIS	CG-CD2	6.63	1.43	1.35
1	D	977	HIS	CG-CD2	6.60	1.43	1.35
1	B	450	HIS	ND1-CE1	6.55	1.39	1.32
1	A	391	HIS	CG-CD2	6.49	1.43	1.35
1	B	372	MET	SD-CE	-6.39	1.63	1.79
1	D	878	HIS	CE1-NE2	6.37	1.39	1.32
1	B	333	ARG	CD-NE	6.37	1.55	1.46
1	D	418	HIS	ND1-CE1	6.33	1.38	1.32
1	C	990	HIS	ND1-CE1	6.31	1.38	1.32
1	A	840	HIS	ND1-CE1	6.26	1.38	1.32
1	D	391	HIS	ND1-CE1	6.19	1.38	1.32
1	C	878	HIS	ND1-CE1	6.14	1.38	1.32
1	D	167	LEU	N-CA	6.03	1.50	1.45
1	C	297	ASN	CA-CB	6.00	1.58	1.52
1	A	947	GLY	N-CA	5.97	1.52	1.44
1	B	878	HIS	ND1-CE1	5.92	1.38	1.32
1	C	464	HIS	ND1-CE1	5.91	1.38	1.32
1	B	990	HIS	ND1-CE1	5.89	1.38	1.32
1	C	465	GLY	N-CA	5.87	1.50	1.44
1	C	468	HIS	CE1-NE2	5.83	1.38	1.32
1	C	990	HIS	CG-CD2	5.80	1.42	1.35
1	C	990	HIS	CE1-NE2	5.79	1.38	1.32
1	B	30	HIS	ND1-CE1	5.78	1.38	1.32
1	A	713	HIS	ND1-CE1	5.77	1.38	1.32
1	D	450	HIS	CG-CD2	5.76	1.42	1.35
1	B	974	HIS	CE1-NE2	5.71	1.38	1.32
1	C	166	ARG	N-CA	5.70	1.52	1.46
1	C	391	HIS	ND1-CE1	5.70	1.38	1.32
1	B	391	HIS	ND1-CE1	5.69	1.38	1.32
1	B	990	HIS	CE1-NE2	5.67	1.38	1.32
1	C	333	ARG	CD-NE	5.65	1.54	1.46
1	C	899	GLY	N-CA	5.60	1.50	1.45
1	D	395	HIS	CE1-NE2	5.58	1.38	1.32
1	C	421	VAL	CA-CB	5.57	1.58	1.54
1	C	395	HIS	ND1-CE1	5.55	1.38	1.32
1	A	713	HIS	CG-CD2	5.54	1.42	1.35
1	C	949	HIS	CG-ND1	-5.54	1.32	1.38
1	A	974	HIS	CE1-NE2	5.50	1.38	1.32
1	A	316	HIS	CE1-NE2	5.47	1.38	1.32
1	A	244	VAL	C-O	5.47	1.29	1.24
1	A	273	PRO	C-O	5.47	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	540	HIS	ND1-CE1	5.44	1.38	1.32
1	A	465	GLY	N-CA	5.43	1.50	1.44
1	C	212	VAL	C-O	5.40	1.29	1.24
1	A	972	HIS	ND1-CE1	5.39	1.38	1.32
1	C	972	HIS	ND1-CE1	5.35	1.37	1.32
1	C	395	HIS	CG-CD2	5.34	1.41	1.35
1	A	360	HIS	CE1-NE2	5.34	1.37	1.32
1	D	316	HIS	CG-CD2	5.34	1.41	1.35
1	A	906	TYR	N-CA	5.31	1.49	1.46
1	B	977	HIS	ND1-CE1	5.30	1.37	1.32
1	C	30	HIS	ND1-CE1	5.29	1.37	1.32
1	A	972	HIS	CG-CD2	5.27	1.41	1.35
1	C	894	ARG	N-CA	5.26	1.52	1.45
1	B	316	HIS	CE1-NE2	5.24	1.37	1.32
1	B	977	HIS	CG-CD2	5.21	1.41	1.35
1	A	360	HIS	CG-CD2	5.21	1.41	1.35
1	A	1016	TYR	N-CA	5.21	1.52	1.45
1	A	1015	HIS	ND1-CE1	5.20	1.37	1.32
1	C	427	THR	N-CA	5.20	1.53	1.46
1	C	30	HIS	CG-CD2	5.19	1.41	1.35
1	C	653	HIS	CG-CD2	5.18	1.41	1.35
1	D	47	PRO	C-O	5.17	1.29	1.23
1	D	359	HIS	ND1-CE1	5.14	1.37	1.32
1	C	359	HIS	CE1-NE2	5.13	1.37	1.32
1	B	464	HIS	ND1-CE1	5.13	1.37	1.32
1	A	464	HIS	CA-C	-5.12	1.46	1.52
1	C	151	HIS	CG-CD2	5.11	1.41	1.35
1	B	439	ARG	CZ-NH1	5.11	1.40	1.32
1	A	330	VAL	C-O	-5.09	1.18	1.24
1	C	920	LEU	C-O	-5.07	1.19	1.24
1	D	354	VAL	N-CA	5.06	1.51	1.46
1	B	810	TRP	CD2-CE2	5.06	1.50	1.41
1	A	977	HIS	ND1-CE1	5.05	1.37	1.32
1	C	357	HIS	CE1-NE2	5.04	1.37	1.32
1	A	395	HIS	CG-CD2	5.04	1.41	1.35
1	D	708	TRP	CA-CB	5.04	1.61	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	GLY	N-CA-C	-9.62	90.39	113.18
1	A	323	ILE	N-CA-C	-7.90	104.11	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	737	ILE	CA-C-N	-6.39	114.05	120.31
1	C	737	ILE	C-N-CA	-6.39	114.05	120.31
1	B	1018	LEU	CA-CB-CG	6.07	137.53	116.30
1	B	690	SER	N-CA-C	6.00	116.34	107.88
1	B	95	TYR	N-CA-C	5.97	118.74	111.82
1	A	553	TRP	CA-CB-CG	-5.90	102.39	113.60
1	A	12	GLN	N-CA-C	5.73	119.37	112.38
1	A	13	ARG	N-CA-C	5.66	119.80	113.01
1	B	512	PHE	CA-C-N	-5.59	114.03	119.78
1	B	512	PHE	C-N-CA	-5.59	114.03	119.78
1	C	279	ILE	N-CA-C	-5.54	107.41	111.90
1	A	917	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	C	553	TRP	CA-CB-CG	-5.30	103.53	113.60
1	A	421	VAL	CA-C-O	-5.29	117.19	119.94
1	B	956	GLN	N-CA-C	-5.22	101.37	109.72
1	C	521	LYS	CD-CE-NZ	-5.19	95.28	111.90
1	B	442	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	D	553	TRP	CA-CB-CG	-5.16	103.80	113.60
1	A	110	ASN	CA-C-N	-5.15	115.90	119.66
1	A	110	ASN	C-N-CA	-5.15	115.90	119.66
1	B	278	ILE	CA-C-N	5.09	127.60	122.66
1	B	278	ILE	C-N-CA	5.09	127.60	122.66
1	A	444	VAL	N-CA-C	-5.06	105.61	110.72
1	B	553	TRP	CA-CB-CG	-5.06	103.99	113.60
1	A	233	ASP	N-CA-C	5.03	117.50	111.71
1	C	110	ASN	CA-C-N	-5.02	116.04	119.66
1	C	110	ASN	C-N-CA	-5.02	116.04	119.66
1	A	871	GLU	CB-CG-CD	-5.01	104.08	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1022	GLN	Peptide

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	8365	0	8028	88	0
1	B	8315	0	7967	78	0
1	C	8342	0	7991	76	0
1	D	8328	0	8000	61	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	1	0	0	0	0
5	A	128	0	192	41	0
5	B	148	0	222	35	0
5	C	148	0	222	29	0
5	D	108	0	162	18	0
6	A	1130	0	0	16	1
6	B	1114	0	0	13	1
6	C	1094	0	0	26	2
6	D	1113	0	0	18	2
All	All	38364	0	32784	327	3

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 5.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:ILE:CD1	5:B:1119:DMS:C2	2.07	1.33
1:B:576:ILE:CD1	5:B:1119:DMS:H23	1.61	1.30
1:B:576:ILE:HD12	5:B:1119:DMS:C2	1.65	1.26
1:A:430:PRO:HD3	5:A:3025:DMS:C1	1.69	1.23
1:A:430:PRO:HD3	5:A:3025:DMS:H11	1.22	1.14
1:C:102:ASN:HD22	5:C:3034:DMS:H13	1.15	1.10
1:A:651[B]:LEU:HD21	1:A:667:GLU:HB3	1.33	1.07
5:B:1130:DMS:O	6:B:1518:HOH:O	1.74	1.03
1:B:576:ILE:HD12	5:B:1119:DMS:H21	1.36	1.03
5:B:1125:DMS:H12	6:B:1904:HOH:O	1.56	1.02
1:B:576:ILE:HD11	5:B:1119:DMS:H23	1.38	1.00
1:C:842[B]:TRP:HZ3	6:C:4139:HOH:O	1.45	1.00
5:A:3031:DMS:O	6:A:3445:HOH:O	1.83	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1126:DMS:O	6:D:1550:HOH:O	1.85	0.94
5:C:3030:DMS:O	6:C:3418:HOH:O	1.84	0.94
1:C:102:ASN:ND2	5:C:3034:DMS:H13	1.82	0.93
1:A:397:LEU:HD11	5:A:3041:DMS:H21	1.51	0.93
5:A:3025:DMS:H22	6:D:2069:HOH:O	1.67	0.93
1:D:102:ASN:HD22	5:D:1101:DMS:H13	1.32	0.92
5:A:3026:DMS:H11	6:A:3812:HOH:O	1.70	0.92
5:A:3028:DMS:H22	6:A:3733:HOH:O	1.70	0.92
1:A:618[A]:THR:HG21	6:A:3526:HOH:O	1.71	0.90
5:C:3029:DMS:H22	6:C:3946:HOH:O	1.71	0.90
1:B:102:ASN:HD22	5:B:1132:DMS:H13	1.38	0.89
1:A:430:PRO:HD3	5:A:3025:DMS:H12	1.55	0.88
1:C:655:MET:CE	1:C:662:PRO:HB3	2.05	0.87
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.10	0.87
5:C:3015:DMS:H11	6:C:3142:HOH:O	1.72	0.86
1:B:730:LEU:HD12	1:B:730:LEU:H	1.40	0.85
1:B:93:HIS:CE1	5:B:1122:DMS:H12	2.13	0.83
1:D:473[A]:ARG:NH1	1:D:477[A]:SER:OG	2.12	0.83
5:C:3039:DMS:H22	6:C:3656:HOH:O	1.79	0.81
1:D:252:ASP:H	5:D:1122:DMS:H13	1.43	0.81
1:B:618[B]:THR:HG21	1:B:903:GLN:NE2	1.95	0.81
1:D:174:SER:HB3	5:D:1129:DMS:C2	2.11	0.80
1:D:618[A]:THR:HG21	6:D:1632:HOH:O	1.80	0.80
1:A:102:ASN:OD1	5:A:3038:DMS:H21	1.82	0.79
1:D:508:GLU:OE2	5:D:1115:DMS:H21	1.84	0.78
1:A:431[A]:ARG:HG3	6:A:3934:HOH:O	1.82	0.78
1:B:241[B]:GLU:HG2	1:B:292:ARG:HG2	1.65	0.77
1:B:93:HIS:ND1	5:B:1122:DMS:H12	1.99	0.77
1:A:93:HIS:CG	5:A:3023:DMS:H12	2.20	0.77
1:C:965[B]:GLN:NE2	1:C:969:GLU:OE2	2.17	0.77
1:C:634:GLN:CD	1:C:634:GLN:H	1.92	0.76
1:D:102:ASN:ND2	5:D:1101:DMS:H13	1.99	0.76
1:A:976:LEU:HB2	5:A:3027:DMS:H13	1.66	0.76
1:B:93:HIS:CD2	5:B:1122:DMS:H23	2.21	0.75
1:C:521:LYS:HE2	6:C:3616:HOH:O	1.87	0.75
1:D:252:ASP:H	5:D:1122:DMS:C1	2.01	0.74
1:D:241[B]:GLU:HG2	1:D:292:ARG:HG2	1.69	0.74
1:C:655:MET:HE2	1:C:662:PRO:HB3	1.69	0.74
1:C:618[B]:THR:HG21	1:C:903:GLN:NE2	2.03	0.74
1:A:246[B]:MET:SD	1:A:250[B]:LEU:CD1	2.77	0.73
1:D:135:GLN:C	1:D:136:GLU:HG2	2.12	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:LYS:HE2	6:D:1744:HOH:O	1.87	0.73
1:A:430:PRO:CD	5:A:3025:DMS:C1	2.61	0.73
1:B:508:GLU:HG3	5:B:1103:DMS:H22	1.70	0.73
1:B:576:ILE:HD13	5:B:1119:DMS:H23	1.67	0.73
5:C:3044:DMS:H21	6:C:4167:HOH:O	1.88	0.72
1:C:655:MET:HE1	1:C:662:PRO:HB3	1.68	0.72
1:C:102:ASN:HD22	5:C:3034:DMS:C1	1.99	0.72
1:A:744:GLU:HG2	5:A:3037:DMS:H21	1.71	0.71
1:B:102:ASN:ND2	5:B:1132:DMS:H13	2.04	0.71
1:A:246[B]:MET:SD	1:A:250[B]:LEU:HD13	2.30	0.71
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.72	0.71
1:B:618[B]:THR:HG21	1:B:903:GLN:HE22	1.56	0.71
1:C:618[B]:THR:HG23	6:C:3527:HOH:O	1.90	0.71
1:D:431[B]:ARG:HD2	6:D:1849:HOH:O	1.90	0.71
1:C:739:HIS:HE1	6:C:3144:HOH:O	1.73	0.70
1:B:84:VAL:HG12	5:B:1122:DMS:H13	1.73	0.70
1:D:174:SER:HB3	5:D:1129:DMS:H22	1.72	0.70
1:B:230:ARG:HH12	1:B:241[B]:GLU:CD	1.98	0.70
1:B:618[B]:THR:HG23	6:B:1627:HOH:O	1.90	0.69
1:A:651[B]:LEU:HD22	1:A:653[B]:HIS:CE1	2.27	0.69
1:B:576:ILE:HD13	5:B:1119:DMS:C2	2.21	0.69
1:B:753[A]:ASN:ND2	6:B:1201:HOH:O	2.15	0.69
1:B:976:LEU:HB2	5:B:1127:DMS:H13	1.74	0.68
1:A:430:PRO:CD	5:A:3025:DMS:H12	2.23	0.68
1:C:372[B]:MET:HE1	1:C:397:LEU:HB3	1.76	0.68
1:A:651[B]:LEU:HD21	1:A:667:GLU:CB	2.18	0.67
1:C:289:VAL:HG23	5:C:3019:DMS:C2	2.24	0.67
1:C:710:GLU:HG2	5:C:3033:DMS:H11	1.75	0.66
1:C:965[B]:GLN:HE21	1:C:969:GLU:CD	2.04	0.66
1:B:47:PRO:O	6:B:2284:HOH:O	2.12	0.65
1:A:237:ARG:HD2	1:A:296:GLU:OE1	1.97	0.64
5:C:3036:DMS:C2	6:C:3832:HOH:O	2.46	0.64
1:C:47:PRO:HA	5:C:3029:DMS:H23	1.79	0.64
1:B:635:THR:OG1	1:B:681:GLU:OE2	2.09	0.63
1:B:508:GLU:OE2	5:B:1116:DMS:H21	1.98	0.63
1:A:431[B]:ARG:HD2	6:A:4049:HOH:O	1.98	0.63
1:A:976:LEU:HB2	5:A:3027:DMS:C1	2.27	0.63
1:A:93:HIS:ND1	5:A:3023:DMS:H12	2.14	0.62
1:A:84:VAL:HG12	5:A:3023:DMS:H13	1.80	0.62
1:D:473[A]:ARG:NE	6:D:2019:HOH:O	2.13	0.62
1:B:93:HIS:CG	5:B:1122:DMS:H12	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:MET:HB3	1:C:372[A]:MET:HE2	1.82	0.61
1:C:289:VAL:CG2	5:C:3019:DMS:H22	2.30	0.61
5:C:3032:DMS:H22	6:C:4030:HOH:O	1.99	0.61
1:D:252:ASP:N	5:D:1122:DMS:H13	2.14	0.61
1:A:728:VAL:HG21	5:B:1101:DMS:H12	1.82	0.61
1:A:768[A]:MET:HE1	1:A:1020:TRP:CZ2	2.36	0.61
1:D:687:GLN:HB3	6:D:2308:HOH:O	2.00	0.61
1:A:817:GLN:NE2	6:A:3552:HOH:O	2.33	0.61
1:C:241[B]:GLU:HG2	1:C:292:ARG:HG2	1.81	0.61
5:D:1129:DMS:H22	6:D:2311:HOH:O	2.00	0.61
1:B:230:ARG:NH1	1:B:241[B]:GLU:CD	2.59	0.60
1:B:576:ILE:HD11	5:B:1119:DMS:C2	2.08	0.60
1:D:251:ARG:HA	5:D:1122:DMS:H13	1.83	0.60
1:C:739:HIS:CE1	6:C:3144:HOH:O	2.51	0.60
1:A:521:LYS:HE2	6:A:3635:HOH:O	2.02	0.60
5:C:3036:DMS:H23	6:C:3832:HOH:O	2.02	0.60
1:D:804:ASN:OD1	1:D:809:ARG:NH2	2.22	0.59
5:A:3024:DMS:H12	6:A:3853:HOH:O	2.02	0.59
1:B:976:LEU:HD12	5:B:1127:DMS:H13	1.85	0.59
1:C:289:VAL:HG23	5:C:3019:DMS:H22	1.85	0.59
1:A:251:ARG:HH11	5:A:3024:DMS:C2	2.16	0.59
1:C:699:ARG:NH1	6:C:4158:HOH:O	2.35	0.59
1:C:768[A]:MET:HE1	1:C:1020:TRP:CZ2	2.37	0.59
1:D:755:ARG:HG3	1:D:755:ARG:HH11	1.67	0.58
1:A:246[B]:MET:SD	1:A:250[B]:LEU:HD12	2.43	0.58
1:B:93:HIS:NE2	5:B:1122:DMS:H23	2.19	0.58
1:C:646[B]:HIS:NE2	1:C:671:ASP:OD1	2.29	0.58
1:A:356:ARG:HD2	1:A:379[B]:MET:HE1	1.86	0.58
5:A:3025:DMS:H13	1:D:474:TRP:HZ2	1.68	0.58
1:D:521:LYS:CE	6:D:1744:HOH:O	2.49	0.58
1:C:651:LEU:HD12	1:C:651:LEU:C	2.29	0.58
1:B:356:ARG:HD2	1:B:379[B]:MET:HE1	1.85	0.57
5:A:3025:DMS:H11	6:A:4195:HOH:O	2.05	0.57
1:B:576:ILE:CD1	5:B:1119:DMS:H22	2.26	0.57
1:C:230[B]:ARG:NH1	1:C:241[B]:GLU:CD	2.62	0.57
1:A:653[B]:HIS:CD2	1:A:667:GLU:HG2	2.39	0.57
1:B:730:LEU:HD12	1:B:730:LEU:N	2.17	0.57
1:A:93:HIS:CE1	5:A:3023:DMS:H12	2.40	0.56
1:B:618[B]:THR:HG22	6:B:1618:HOH:O	2.03	0.56
5:A:3028:DMS:H23	6:A:3490:HOH:O	2.06	0.56
1:C:356:ARG:HD2	1:C:379[B]:MET:HE1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:MET:HE2	1:C:372[A]:MET:HG3	1.87	0.56
1:D:112:PRO:HG3	1:D:431[B]:ARG:HH22	1.70	0.56
1:B:820:ALA:HB2	1:B:842[B]:TRP:CH2	2.41	0.56
1:C:778[A]:THR:HG21	6:C:3984:HOH:O	2.05	0.56
1:D:174:SER:HB3	5:D:1129:DMS:H21	1.86	0.56
1:A:93:HIS:CD2	5:A:3023:DMS:H23	2.41	0.56
1:B:731:PRO:O	1:B:732:ALA:HB3	2.06	0.56
1:B:576:ILE:HD12	5:B:1119:DMS:H22	1.76	0.55
1:A:651[B]:LEU:CD2	1:A:667:GLU:HB3	2.23	0.55
1:B:84:VAL:CG1	5:B:1122:DMS:H13	2.36	0.55
1:B:356:ARG:HD2	1:B:379[B]:MET:CE	2.38	0.54
1:C:49:GLN:CG	6:C:3134:HOH:O	2.55	0.54
1:A:372[B]:MET:HE1	1:A:397:LEU:HB3	1.89	0.54
1:A:655:MET:HE2	1:A:665:SER:HB3	1.90	0.54
1:D:634:GLN:HG3	1:D:682:LEU:O	2.07	0.54
5:C:3022:DMS:H21	6:C:4156:HOH:O	2.08	0.54
1:A:252:ASP:OD1	5:A:3024:DMS:H13	2.08	0.54
1:C:49:GLN:HG2	6:C:3134:HOH:O	2.08	0.54
1:C:618[B]:THR:HG22	6:C:3518:HOH:O	2.07	0.54
1:C:379[A]:MET:HE1	1:C:398:TRP:HH2	1.73	0.53
1:A:102:ASN:C	1:A:102:ASN:HD22	2.17	0.53
1:A:885[A]:ASN:OD1	6:A:3612:HOH:O	2.17	0.53
5:A:3024:DMS:C1	6:A:3853:HOH:O	2.56	0.53
1:B:9:VAL:HG22	1:C:9:VAL:HG22	1.89	0.53
1:B:80:GLU:O	5:B:1142:DMS:H21	2.09	0.53
1:D:251:ARG:HE	5:D:1122:DMS:H11	1.73	0.53
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.71	0.53
5:A:3025:DMS:H13	1:D:474:TRP:CZ2	2.43	0.53
1:A:102:ASN:C	1:A:102:ASN:ND2	2.66	0.53
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.43	0.53
1:A:595:THR:HA	1:A:596:PRO:C	2.34	0.53
1:A:367[A]:MET:HB3	1:A:372[A]:MET:HE2	1.90	0.52
1:C:431[A]:ARG:HD2	6:C:3947:HOH:O	2.09	0.52
1:C:521:LYS:CE	6:C:3616:HOH:O	2.52	0.52
1:A:866:ILE:O	1:A:1017:GLN:HG2	2.09	0.52
1:B:250:LEU:HD23	6:B:2140:HOH:O	2.09	0.52
1:B:820:ALA:HB2	1:B:842[B]:TRP:CZ2	2.44	0.52
1:D:95:TYR:HA	5:D:1123:DMS:H12	1.92	0.52
5:D:1123:DMS:H13	6:D:1929:HOH:O	2.09	0.52
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.25	0.52
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768[B]:MET:HE1	1:B:1020:TRP:CZ2	2.44	0.52
1:D:778[B]:THR:HG21	6:D:2095:HOH:O	2.09	0.51
1:B:730:LEU:H	1:B:730:LEU:CD1	2.16	0.51
1:D:701[B]:VAL:HG12	1:D:714:ILE:HG12	1.93	0.51
1:A:695:TRP:HH2	5:A:3028:DMS:H21	1.74	0.51
1:A:820:ALA:HB2	1:A:842[B]:TRP:CH2	2.46	0.51
1:C:618[B]:THR:HG21	1:C:903:GLN:HE22	1.76	0.50
1:D:88:SER:HA	1:D:366:VAL:HG21	1.93	0.50
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.46	0.50
1:A:859:ASP:OD1	1:A:861:SER:OG	2.29	0.50
1:C:125:LEU:HD21	5:C:3015:DMS:H13	1.93	0.50
1:B:778[B]:THR:HG21	6:B:2204:HOH:O	2.10	0.50
1:A:54:LEU:HD11	1:A:214[B]:LEU:HG	1.92	0.49
1:C:230[B]:ARG:HH12	1:C:241[B]:GLU:CD	2.20	0.49
5:C:3023:DMS:H22	6:C:3849:HOH:O	2.10	0.49
1:C:508:GLU:OE2	5:C:3014:DMS:H21	2.13	0.49
1:B:576:ILE:CD1	5:B:1119:DMS:H21	2.06	0.49
1:B:181:GLU:OE2	6:B:2150:HOH:O	2.20	0.49
1:B:976:LEU:HB2	5:B:1127:DMS:C1	2.42	0.49
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.48	0.49
1:C:289:VAL:HG23	5:C:3019:DMS:H23	1.95	0.49
1:A:387:VAL:HG22	6:A:4168:HOH:O	2.13	0.48
1:D:618[A]:THR:HG22	1:D:912:ALA:HB1	1.95	0.48
5:C:3036:DMS:H22	6:C:3832:HOH:O	2.10	0.48
1:C:47:PRO:CA	5:C:3029:DMS:H23	2.43	0.48
1:A:976:LEU:HD12	5:A:3027:DMS:H13	1.95	0.48
1:B:753[A]:ASN:CG	6:B:1201:HOH:O	2.54	0.48
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.90	0.47
5:A:3025:DMS:C1	6:A:4195:HOH:O	2.59	0.47
1:D:11:LEU:HD21	1:D:67:GLU:HA	1.94	0.47
1:A:580:GLU:H	1:A:580:GLU:HG2	1.40	0.47
1:B:348:PRO:HD3	5:B:1141:DMS:H22	1.96	0.47
1:D:251:ARG:CA	5:D:1122:DMS:H13	2.44	0.47
1:D:595[A]:THR:HA	1:D:596:PRO:C	2.39	0.47
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.79	0.47
1:B:646[B]:HIS:NE2	1:B:671:ASP:OD1	2.40	0.47
1:D:241[A]:GLU:OE1	1:D:292:ARG:NE	2.43	0.47
1:D:887:GLN:NE2	1:D:980:GLU:O	2.45	0.47
1:A:356:ARG:HD2	1:A:379[B]:MET:CE	2.45	0.46
1:A:430:PRO:CG	5:A:3025:DMS:H12	2.44	0.46
1:D:737:ILE:HD12	1:D:738:PRO:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:MET:HE1	1:C:662:PRO:CB	2.40	0.46
1:C:768[A]:MET:HE1	1:C:1020:TRP:CH2	2.50	0.46
1:B:634:GLN:HG3	1:B:682:LEU:O	2.15	0.46
1:C:634:GLN:NE2	1:C:681:GLU:OE2	2.49	0.46
1:A:240:LEU:C	1:A:240:LEU:HD23	2.40	0.46
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.50	0.46
1:A:618[A]:THR:HG22	1:A:912:ALA:HB1	1.97	0.46
1:B:651:LEU:HD11	1:B:667:GLU:OE1	2.16	0.46
5:D:1101:DMS:H21	6:D:2237:HOH:O	2.15	0.46
5:A:3023:DMS:H21	6:A:4062:HOH:O	2.14	0.45
1:B:472:TYR:OH	5:B:1140:DMS:H12	2.15	0.45
1:C:473[B]:ARG:NH2	6:C:3174:HOH:O	2.48	0.45
1:B:962:TYR:OH	5:B:1127:DMS:C1	2.65	0.45
1:B:651:LEU:C	1:B:651:LEU:HD23	2.41	0.45
1:B:731:PRO:O	1:B:732:ALA:CB	2.65	0.45
1:C:102:ASN:CB	5:C:3034:DMS:H13	2.45	0.45
1:A:984:LEU:HD21	1:A:986[B]:ILE:HD13	1.97	0.45
1:C:655:MET:CE	1:C:662:PRO:CB	2.86	0.45
1:B:437[B]:SER:OG	1:C:433:LEU:HD23	2.16	0.45
1:B:157:ARG:HD3	6:B:2109:HOH:O	2.16	0.45
1:A:820:ALA:HB2	1:A:842[B]:TRP:CZ2	2.52	0.45
1:D:434:PRO:HB2	6:D:2150:HOH:O	2.17	0.45
1:A:437[B]:SER:OG	1:D:433:LEU:HD23	2.17	0.45
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.99	0.45
1:C:26:ARG:NH2	1:C:438[A]:GLU:OE1	2.49	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.66	0.44
1:B:755:ARG:NH1	6:B:1203:HOH:O	2.49	0.44
1:C:830:LEU:CD2	1:D:830:LEU:HD21	2.47	0.44
1:A:653[B]:HIS:NE2	1:A:667:GLU:HG2	2.31	0.44
1:D:431[A]:ARG:HG3	6:D:2061:HOH:O	2.18	0.44
1:A:695:TRP:CH2	5:A:3028:DMS:H21	2.52	0.44
1:B:595:THR:HA	1:B:596:PRO:C	2.43	0.44
1:C:634:GLN:HE21	1:C:681:GLU:CD	2.26	0.44
1:D:890:GLN:HE21	1:D:892:ALA:HB2	1.83	0.44
1:A:434:PRO:HB3	1:D:434:PRO:HB3	2.00	0.44
1:B:377:LEU:HD22	1:B:708:TRP:HA	2.00	0.44
1:C:88:SER:HA	1:C:366:VAL:HG21	1.99	0.44
1:D:400:THR:OG1	6:D:2313:HOH:O	1.64	0.43
1:B:93:HIS:O	5:B:1126:DMS:H12	2.17	0.43
1:B:545:SER:O	1:B:909:ARG:HD3	2.19	0.43
1:C:54:LEU:HD11	1:C:214[B]:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:SER:HA	1:A:366:VAL:HG21	2.00	0.43
1:D:745[B]:MET:HG2	6:D:1205:HOH:O	2.17	0.43
1:C:890:GLN:HG2	1:C:891:VAL:N	2.33	0.43
1:D:237:ARG:HG2	1:D:296:GLU:OE1	2.19	0.43
1:A:372[B]:MET:CE	1:A:397:LEU:HD23	2.48	0.43
1:A:630:ARG:HH11	1:A:630:ARG:CB	2.31	0.43
1:C:80:GLU:O	5:C:3041:DMS:H21	2.19	0.43
1:A:763:GLY:HA3	1:A:822:LEU:HD13	2.00	0.43
1:C:47:PRO:HA	5:C:3029:DMS:C2	2.45	0.43
1:D:653:HIS:HB2	1:D:699:ARG:HG2	1.99	0.43
1:A:132:SER:HB2	5:A:3032:DMS:H11	2.01	0.43
1:A:241[A]:GLU:OE2	1:A:292:ARG:NE	2.48	0.43
1:A:401:LEU:CD2	5:A:3041:DMS:H22	2.49	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.71	0.43
1:C:102:ASN:HB3	5:C:3034:DMS:H13	2.00	0.43
1:C:745:MET:HE3	1:C:745:MET:HB3	1.85	0.43
1:D:55:ASN:O	5:D:1116:DMS:H11	2.19	0.43
1:A:241[B]:GLU:HG3	1:A:290:THR:CG2	2.48	0.43
1:D:240:LEU:HD23	1:D:240:LEU:C	2.44	0.43
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.01	0.43
1:D:699:ARG:NH2	6:D:2126:HOH:O	2.51	0.43
1:C:855:THR:HG23	6:C:3923:HOH:O	2.19	0.42
1:B:756:TRP:CD1	1:B:768[B]:MET:SD	3.12	0.42
1:C:770:ILE:O	1:C:773:LYS:HE3	2.20	0.42
1:A:377:LEU:HD22	1:A:708:TRP:HA	2.01	0.42
5:B:1132:DMS:H21	6:B:2122:HOH:O	2.19	0.42
1:D:768[B]:MET:SD	1:D:775:GLN:HG3	2.59	0.42
1:A:457:SER:HA	1:A:485:GLN:O	2.19	0.42
1:A:630:ARG:HH11	1:A:630:ARG:HB3	1.83	0.42
1:A:508:GLU:OE2	5:A:3016:DMS:H21	2.19	0.42
1:B:806:TRP:HA	1:B:809[A]:ARG:HD2	2.01	0.42
1:D:473[A]:ARG:NH1	1:D:477[A]:SER:HG	2.16	0.42
1:A:13:ARG:O	1:A:14:ARG:C	2.63	0.42
1:D:1022:GLN:O	1:D:1023:LYS:HD2	2.20	0.42
1:A:93:HIS:CD2	5:A:3023:DMS:H12	2.55	0.41
1:A:251:ARG:HH11	5:A:3024:DMS:H22	1.84	0.41
1:C:687:GLN:HG3	1:C:688:PRO:HD2	2.02	0.41
1:C:730:LEU:H	1:C:730:LEU:HG	1.20	0.41
1:C:232:ASN:O	5:C:3024:DMS:H21	2.20	0.41
1:A:663:LEU:HB3	1:A:686:PRO:HG3	2.02	0.41
1:A:778:THR:HG23	1:A:887:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:THR:HB	1:B:748[B]:CYS:HB3	2.03	0.41
1:A:658:LEU:O	1:A:659:ASP:C	2.63	0.41
1:B:16:TRP:CG	1:B:189:LEU:HD13	2.55	0.41
1:B:962:TYR:OH	5:B:1127:DMS:H12	2.21	0.41
1:C:655:MET:SD	1:C:665:SER:HB3	2.61	0.41
1:D:615:PRO:O	1:D:618[B]:THR:HG22	2.21	0.41
1:A:708:TRP:CZ2	5:A:3012:DMS:H23	2.56	0.41
1:D:658:LEU:O	1:D:659:ASP:C	2.64	0.41
1:A:277:GLU:CD	1:A:277:GLU:H	2.28	0.41
5:C:3029:DMS:C2	6:C:3946:HOH:O	2.45	0.41
1:B:13:ARG:O	1:B:14:ARG:C	2.64	0.41
1:C:240:LEU:HD23	1:C:240:LEU:C	2.47	0.40
1:C:246[B]:MET:SD	1:C:250:LEU:HD23	2.61	0.40
1:D:699:ARG:NH1	6:D:2295:HOH:O	2.52	0.40
1:C:147:ASN:HA	1:C:148:SER:HA	1.77	0.40
1:A:80:GLU:O	5:A:3040:DMS:H21	2.22	0.40
1:A:430:PRO:HG3	5:A:3025:DMS:H12	2.02	0.40
1:B:359:HIS:CD2	1:B:573:GLN:HA	2.57	0.40
1:C:427:THR:HG21	1:C:462:SER:HB3	2.03	0.40
1:D:367[B]:MET:HE2	1:D:367[B]:MET:HA	2.03	0.40
1:A:577:LYS:HB3	1:A:577:LYS:HE3	1.96	0.40
1:A:696:LEU:HB2	1:A:722:LEU:HD11	2.02	0.40
1:B:457:SER:HA	1:B:485:GLN:O	2.22	0.40
1:D:246[B]:MET:SD	1:D:250:LEU:HD23	2.62	0.40
1:B:885[A]:ASN:ND2	1:B:983:TRP:HZ3	2.18	0.40

All (3) 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:B:1256:HOH:O	6:C:3103:HOH:O[4_455]	1.79	0.41
6:A:3193:HOH:O	6:D:1263:HOH:O[4_545]	2.03	0.17
6:C:3129:HOH:O	6:D:1243:HOH:O[2_554]	2.11	0.09

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	1047/1023 (102%)	1019 (97%)	28 (3%)	0	100	100
1	B	1041/1023 (102%)	1011 (97%)	29 (3%)	1 (0%)	48	27
1	C	1043/1023 (102%)	1014 (97%)	29 (3%)	0	100	100
1	D	1045/1023 (102%)	1022 (98%)	23 (2%)	0	100	100
All	All	4176/4092 (102%)	4066 (97%)	109 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	ALA

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	902/874 (103%)	885 (98%)	17 (2%)	50	27
1	B	896/874 (102%)	882 (98%)	14 (2%)	55	33
1	C	898/874 (103%)	880 (98%)	18 (2%)	48	24
1	D	900/874 (103%)	887 (99%)	13 (1%)	59	38
All	All	3596/3496 (103%)	3534 (98%)	62 (2%)	53	30

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	230	ARG
1	A	250[A]	LEU
1	A	250[B]	LEU
1	A	344	LEU

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Mol	Chain	Res	Type
1	A	438[A]	GLU
1	A	438[B]	GLU
1	A	546	LEU
1	A	560	PRO
1	A	580	GLU
1	A	630	ARG
1	A	671	ASP
1	A	737	ILE
1	A	773	LYS
1	A	797	GLU
1	A	817	GLN
1	A	819	GLU
1	B	10	VAL
1	B	11	LEU
1	B	71	GLU
1	B	344	LEU
1	B	546	LEU
1	B	663	LEU
1	B	689	GLU
1	B	699	ARG
1	B	730	LEU
1	B	737	ILE
1	B	797	GLU
1	B	799	THR
1	B	1018	LEU
1	B	1022	GLN
1	C	10	VAL
1	C	71	GLU
1	C	80	GLU
1	C	135	GLN
1	C	344	LEU
1	C	438[A]	GLU
1	C	438[B]	GLU
1	C	527	PRO
1	C	546	LEU
1	C	630	ARG
1	C	634	GLN
1	C	681	GLU
1	C	685	LEU
1	C	687	GLN
1	C	730	LEU
1	C	737	ILE

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Mol	Chain	Res	Type
1	C	745	MET
1	C	1023	LYS
1	D	10	VAL
1	D	11	LEU
1	D	71	GLU
1	D	80	GLU
1	D	344	LEU
1	D	546	LEU
1	D	663	LEU
1	D	682	LEU
1	D	685	LEU
1	D	737	ILE
1	D	845	GLN
1	D	907	PRO
1	D	1022	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	266	GLN
1	A	445	GLN
1	A	485	GLN
1	A	817	GLN
1	A	945	ASN
1	A	950	GLN
1	A	977	HIS
1	B	163	GLN
1	B	485	GLN
1	B	628	GLN
1	B	702	GLN
1	B	757	GLN
1	B	903	GLN
1	B	950	GLN
1	C	163	GLN
1	C	307	ASN
1	C	445	GLN
1	C	485	GLN
1	C	634	GLN
1	C	702	GLN
1	C	739	HIS
1	C	817	GLN

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Mol	Chain	Res	Type
1	C	843	GLN
1	C	844	HIS
1	C	903	GLN
1	C	945	ASN
1	C	950	GLN
1	C	977	HIS
1	D	266	GLN
1	D	485	GLN
1	D	761	GLN
1	D	843	GLN
1	D	890	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	CSD	A	247	1	4,7,8	2.10	1 (25%)	1,8,10	3.01	1 (100%)
1	CSD	D	247	1	4,7,8	0.97	0	1,8,10	1.99	0
1	CSD	C	247	1	4,7,8	1.12	0	1,8,10	0.96	0
1	CSD	B	247	1	4,7,8	0.95	0	1,8,10	0.68	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	CSD	A	247	1	-	2/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	D	247	1	-	1/2/6/8	-
1	CSD	C	247	1	-	1/2/6/8	-
1	CSD	B	247	1	-	1/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	CSD	OD1-SG	3.89	1.51	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	CSD	OD1-SG-CB	-3.01	100.06	105.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	247	CSD	CA-CB-SG-OD1
1	B	247	CSD	CA-CB-SG-OD1
1	C	247	CSD	CA-CB-SG-OD1
1	D	247	CSD	CA-CB-SG-OD1
1	A	247	CSD	N-CA-CB-SG

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 [i](#)

Of 164 ligands modelled in this entry, 31 are monoatomic - leaving 133 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	3033	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	A	3040	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	C	3017	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	C	3025	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	B	1112	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	D	1114	-	3,3,3	0.57	0	3,3,3	0.48	0
5	DMS	C	3028	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	A	3021	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	A	3039	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	A	3016	-	3,3,3	0.58	0	3,3,3	0.50	0
5	DMS	D	1113	-	3,3,3	0.58	0	3,3,3	0.49	0
5	DMS	D	1123	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	A	3022	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	D	1110	-	3,3,3	0.57	0	3,3,3	0.48	0
5	DMS	B	1121	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	D	1117	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1102	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	A	3013	-	3,3,3	0.57	0	3,3,3	0.50	0
5	DMS	C	3021	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	D	1133	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	B	1124	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	B	1125	-	3,3,3	0.57	0	3,3,3	0.53	0
5	DMS	A	3035	-	3,3,3	0.57	0	3,3,3	0.53	0
5	DMS	C	3016	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	A	3020	-	3,3,3	0.58	0	3,3,3	0.50	0
5	DMS	B	1144	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	D	1101	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	D	1128	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	B	1113	-	3,3,3	0.57	0	3,3,3	0.48	0
5	DMS	A	3017	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	B	1123	-	3,3,3	0.57	0	3,3,3	0.53	0
5	DMS	B	1143	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	C	3043	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	A	3025	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	C	3011	-	3,3,3	0.57	0	3,3,3	0.50	0
5	DMS	C	3035	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	C	3032	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	C	3045	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	D	1115	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	B	1142	-	3,3,3	0.57	0	3,3,3	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	1118	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	A	3015	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	A	3023	-	3,3,3	0.58	0	3,3,3	0.55	0
5	DMS	C	3012	-	3,3,3	0.57	0	3,3,3	0.50	0
5	DMS	C	3013	-	3,3,3	0.58	0	3,3,3	0.49	0
5	DMS	B	1136	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	A	3034	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	B	1120	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	B	1130	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	B	1135	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	C	3014	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1111	-	3,3,3	0.56	0	3,3,3	0.51	0
5	DMS	A	3026	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	C	3036	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	B	1131	-	3,3,3	0.57	0	3,3,3	0.50	0
5	DMS	B	1103	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	C	3044	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	D	1130	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1134	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	D	1119	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	B	1122	-	3,3,3	0.58	0	3,3,3	0.55	0
5	DMS	A	3030	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	D	1125	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	C	3010	-	3,3,3	0.57	0	3,3,3	0.49	0
5	DMS	A	3011	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	C	3027	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	B	1138	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1128	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	D	1112[B]	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	C	3042	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	A	3037	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	D	1129	-	3,3,3	0.57	0	3,3,3	0.49	0
5	DMS	B	1129	-	3,3,3	0.57	0	3,3,3	0.53	0
5	DMS	C	3031	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	A	3028	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	C	3037	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	D	1132	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	B	1141	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	C	3022	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	C	3041	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	D	1118	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	C	3026	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1114	-	3,3,3	0.57	0	3,3,3	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	3039	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	D	1121	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	A	3010	-	3,3,3	0.57	0	3,3,3	0.43	0
5	DMS	C	3019	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	D	1112[A]	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	A	3014	-	3,3,3	0.57	0	3,3,3	0.49	0
5	DMS	C	3030	-	3,3,3	0.57	0	3,3,3	0.50	0
5	DMS	A	3029	-	3,3,3	0.57	0	3,3,3	0.49	0
5	DMS	C	3038	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1132	-	3,3,3	0.58	0	3,3,3	0.50	0
5	DMS	B	1117	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	B	1140	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	D	1109	-	3,3,3	0.57	0	3,3,3	0.47	0
5	DMS	D	1131	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	A	3024	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	C	3009	-	3,3,3	0.57	0	3,3,3	0.48	0
5	DMS	C	3033	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	D	1116	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	B	1101	-	3,3,3	0.57	0	3,3,3	0.53	0
5	DMS	A	3036	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	A	3031	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	A	3032	-	3,3,3	0.58	0	3,3,3	0.50	0
5	DMS	A	3041	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1115	-	3,3,3	0.58	0	3,3,3	0.50	0
5	DMS	A	3038	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	D	1126	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	A	3018	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1126	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1119	-	3,3,3	0.57	0	3,3,3	0.50	0
5	DMS	A	3012	-	3,3,3	0.57	0	3,3,3	0.50	0
5	DMS	C	3023	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	B	1116	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	C	3029	-	3,3,3	0.58	0	3,3,3	0.48	0
5	DMS	D	1124	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	D	1120	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	C	3024	-	3,3,3	0.57	0	3,3,3	0.53	0
5	DMS	C	3034	-	3,3,3	0.58	0	3,3,3	0.50	0
5	DMS	D	1111	-	3,3,3	0.58	0	3,3,3	0.50	0
5	DMS	D	1127	-	3,3,3	0.57	0	3,3,3	0.43	0
5	DMS	B	1127	-	3,3,3	0.58	0	3,3,3	0.53	0
5	DMS	A	3019	-	3,3,3	0.57	0	3,3,3	0.52	0
5	DMS	B	1139	-	3,3,3	0.57	0	3,3,3	0.51	0
5	DMS	C	3040	-	3,3,3	0.58	0	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	1122	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	A	3027	-	3,3,3	0.57	0	3,3,3	0.53	0
5	DMS	B	1133	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	C	3015	-	3,3,3	0.58	0	3,3,3	0.52	0
5	DMS	C	3018	-	3,3,3	0.57	0	3,3,3	0.50	0
5	DMS	B	1137	-	3,3,3	0.58	0	3,3,3	0.51	0
5	DMS	C	3020	-	3,3,3	0.57	0	3,3,3	0.52	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

49 monomers are involved in 123 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3040	DMS	1	0
5	A	3016	DMS	1	0
5	D	1123	DMS	2	0
5	B	1125	DMS	1	0
5	D	1101	DMS	3	0
5	A	3025	DMS	12	0
5	C	3032	DMS	1	0
5	D	1115	DMS	1	0
5	B	1142	DMS	1	0
5	A	3023	DMS	7	0
5	B	1130	DMS	1	0
5	C	3014	DMS	1	0
5	A	3026	DMS	1	0
5	C	3036	DMS	3	0
5	B	1103	DMS	1	0
5	C	3044	DMS	1	0
5	B	1122	DMS	7	0
5	A	3037	DMS	1	0
5	D	1129	DMS	4	0
5	A	3028	DMS	4	0
5	B	1141	DMS	1	0
5	C	3022	DMS	1	0
5	C	3041	DMS	1	0
5	C	3039	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3019	DMS	4	0
5	C	3030	DMS	1	0
5	B	1132	DMS	3	0
5	B	1140	DMS	1	0
5	A	3024	DMS	5	0
5	C	3033	DMS	1	0
5	D	1116	DMS	1	0
5	B	1101	DMS	1	0
5	A	3031	DMS	1	0
5	A	3032	DMS	1	0
5	A	3041	DMS	2	0
5	A	3038	DMS	1	0
5	D	1126	DMS	1	0
5	B	1126	DMS	1	0
5	B	1119	DMS	11	0
5	A	3012	DMS	1	0
5	C	3023	DMS	1	0
5	B	1116	DMS	1	0
5	C	3029	DMS	5	0
5	C	3024	DMS	1	0
5	C	3034	DMS	5	0
5	B	1127	DMS	5	0
5	D	1122	DMS	6	0
5	A	3027	DMS	3	0
5	C	3015	DMS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1014/1023 (99%)	-0.38	31 (3%)	51	54	6, 12, 30, 90	35 (3%)
1	B	1014/1023 (99%)	-0.40	29 (2%)	53	56	5, 12, 28, 74	29 (2%)
1	C	1014/1023 (99%)	-0.36	27 (2%)	56	59	5, 12, 32, 79	31 (3%)
1	D	1014/1023 (99%)	-0.34	29 (2%)	53	56	6, 13, 31, 79	33 (3%)
All	All	4056/4092 (99%)	-0.37	116 (2%)	53	56	5, 12, 30, 90	128 (3%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	6.9
1	B	10	VAL	6.7
1	A	11	LEU	6.6
1	C	735	HIS	6.0
1	C	10	VAL	6.0
1	D	686	PRO	5.6
1	C	11	LEU	5.6
1	A	10	VAL	5.4
1	A	771	GLY	5.2
1	D	732	ALA	5.2
1	D	9	VAL	5.1
1	A	685	LEU	5.1
1	B	735	HIS	5.0
1	B	686	PRO	4.8
1	A	9	VAL	4.7
1	A	732	ALA	4.6
1	D	688	PRO	4.6
1	C	730	LEU	4.5
1	B	11	LEU	4.5
1	C	685	LEU	4.5
1	A	735	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	9	VAL	4.4
1	B	731	PRO	4.3
1	A	12	GLN	4.2
1	D	11	LEU	4.2
1	D	685	LEU	4.2
1	D	735	HIS	4.1
1	D	10	VAL	4.0
1	A	730	LEU	4.0
1	B	9	VAL	4.0
1	A	737	ILE	3.9
1	C	732	ALA	3.8
1	C	737	ILE	3.8
1	A	663	LEU	3.7
1	C	731	PRO	3.7
1	B	730	LEU	3.7
1	D	730	LEU	3.7
1	A	688	PRO	3.6
1	B	732	ALA	3.6
1	B	685	LEU	3.5
1	D	736	ALA	3.5
1	A	733	ALA	3.3
1	D	726	LEU	3.2
1	C	772	ASP	3.2
1	A	689	GLU	3.1
1	B	688	PRO	3.0
1	A	846	GLY	3.0
1	D	12	GLN	3.0
1	C	663	LEU	3.0
1	C	829	THR	3.0
1	B	633	GLY	3.0
1	A	684	GLU	2.9
1	B	819	GLU	2.9
1	B	799	THR	2.9
1	D	733	ALA	2.9
1	C	634	GLN	2.9
1	C	686	PRO	2.9
1	C	745	MET	2.8
1	D	633	GLY	2.8
1	A	687	GLN	2.8
1	A	817	GLN	2.8
1	C	739	HIS	2.7
1	B	687	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	664	ALA	2.7
1	A	798	ALA	2.7
1	D	687	GLN	2.6
1	C	12	GLN	2.6
1	C	1023	LYS	2.6
1	B	729	THR	2.6
1	D	734	SER	2.6
1	B	1023	LYS	2.6
1	D	798	ALA	2.6
1	D	71	GLU	2.6
1	C	655	MET	2.5
1	C	1022	GLN	2.5
1	A	633	GLY	2.5
1	D	1023	LYS	2.5
1	D	737	ILE	2.5
1	D	683	PRO	2.5
1	B	689	GLU	2.5
1	A	580	GLU	2.4
1	A	683	PRO	2.4
1	B	736	ALA	2.3
1	C	729	THR	2.3
1	B	737	ILE	2.3
1	B	846	GLY	2.3
1	A	655	MET	2.3
1	D	1022	GLN	2.3
1	B	663	LEU	2.3
1	A	772	ASP	2.3
1	B	370	GLN	2.2
1	A	729	THR	2.2
1	D	1018	LEU	2.2
1	B	655	MET	2.2
1	A	581	ASN	2.2
1	C	689	GLU	2.2
1	C	736	ALA	2.2
1	C	846	GLY	2.1
1	D	728	VAL	2.1
1	D	846	GLY	2.1
1	A	71	GLU	2.1
1	A	734	SER	2.1
1	C	761	GLN	2.1
1	D	79	PRO	2.1
1	B	733	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	773	LYS	2.1
1	B	651	LEU	2.1
1	C	633	GLY	2.0
1	B	684	GLU	2.0
1	D	655	MET	2.0
1	D	729	THR	2.0
1	A	681	GLU	2.0
1	B	71	GLU	2.0
1	D	684	GLU	2.0
1	B	1022	GLN	2.0
1	B	977	HIS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CSD	A	247	8/9	0.93	0.11	9,11,21,22	0
1	CSD	B	247	8/9	0.96	0.09	11,13,25,27	0
1	CSD	C	247	8/9	0.96	0.08	11,14,24,25	0
1	CSD	D	247	8/9	0.97	0.07	10,12,21,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	C	3036	4/4	0.65	0.27	24,27,29,34	4
5	DMS	B	1140	4/4	0.69	0.22	19,20,24,27	4
5	DMS	C	3043	4/4	0.75	0.24	43,46,49,50	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	3003	1/1	0.77	0.15	28,28,28,28	1
5	DMS	A	3015	4/4	0.77	0.23	23,29,36,47	4
5	DMS	B	1138	4/4	0.77	0.21	32,34,38,39	4
5	DMS	A	3035	4/4	0.78	0.21	46,48,49,53	4
5	DMS	B	1103	4/4	0.78	0.23	42,45,48,53	4
5	DMS	B	1137	4/4	0.80	0.23	32,34,35,44	4
5	DMS	C	3035	4/4	0.81	0.20	45,48,51,59	0
5	DMS	C	3032	4/4	0.83	0.19	25,27,29,34	4
5	DMS	B	1136	4/4	0.83	0.17	35,48,50,51	0
5	DMS	A	3030	4/4	0.83	0.21	19,21,30,30	4
5	DMS	C	3031	4/4	0.83	0.17	36,36,40,47	0
5	DMS	C	3030	4/4	0.84	0.19	27,29,33,36	4
5	DMS	A	3037	4/4	0.85	0.23	31,41,41,50	4
5	DMS	C	3024	4/4	0.85	0.16	25,27,37,38	4
5	DMS	B	1125	4/4	0.85	0.21	29,29,36,36	4
5	DMS	C	3038	4/4	0.85	0.16	26,31,32,35	4
5	DMS	B	1130	4/4	0.85	0.20	22,25,26,29	4
5	DMS	B	1121	4/4	0.86	0.18	23,24,26,26	4
5	DMS	B	1142	4/4	0.86	0.16	22,24,31,33	4
5	DMS	C	3028	4/4	0.87	0.18	41,42,44,49	4
5	DMS	C	3029	4/4	0.87	0.17	19,21,26,32	4
5	DMS	B	1143	4/4	0.87	0.17	40,41,51,52	4
5	DMS	D	1129	4/4	0.87	0.20	23,26,27,33	4
5	DMS	B	1102	4/4	0.88	0.16	41,43,44,46	4
5	DMS	A	3024	4/4	0.88	0.13	16,26,26,35	4
5	DMS	B	1128	4/4	0.88	0.15	29,33,34,36	4
5	DMS	C	3039	4/4	0.88	0.17	35,35,40,46	4
5	DMS	C	3040	4/4	0.88	0.19	43,46,48,48	4
5	DMS	B	1129	4/4	0.88	0.17	18,20,23,25	4
5	DMS	C	3025	4/4	0.88	0.16	20,21,22,23	4
5	DMS	D	1130	4/4	0.88	0.18	45,47,54,59	0
5	DMS	B	1134	4/4	0.89	0.17	23,23,25,25	4
5	DMS	B	1144	4/4	0.89	0.18	37,39,41,46	4
5	DMS	C	3023	4/4	0.89	0.15	37,37,41,45	4
5	DMS	C	3037	4/4	0.89	0.16	27,30,31,36	4
5	DMS	B	1126	4/4	0.89	0.15	29,39,44,54	0
5	DMS	B	1127	4/4	0.89	0.18	19,24,29,30	4
2	MG	B	1106	1/1	0.89	0.12	25,25,25,25	1
5	DMS	C	3042	4/4	0.89	0.17	35,36,37,40	4
5	DMS	B	1139	4/4	0.89	0.14	35,37,43,43	4
5	DMS	D	1112[A]	4/4	0.89	0.12	16,16,19,21	4
5	DMS	D	1112[B]	4/4	0.89	0.12	14,15,15,17	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	D	1128	4/4	0.89	0.16	18,19,19,20	4
5	DMS	B	1101	4/4	0.89	0.15	45,46,47,54	0
5	DMS	A	3028	4/4	0.89	0.15	40,44,47,49	4
5	DMS	A	3036	4/4	0.90	0.14	34,35,42,44	4
5	DMS	B	1141	4/4	0.90	0.18	34,34,38,42	4
5	DMS	A	3025	4/4	0.90	0.22	22,24,29,31	4
5	DMS	B	1135	4/4	0.90	0.14	34,39,42,47	0
5	DMS	C	3045	4/4	0.90	0.14	33,34,36,38	4
5	DMS	D	1101	4/4	0.90	0.17	25,26,26,29	4
5	DMS	A	3040	4/4	0.90	0.15	21,22,30,31	4
5	DMS	C	3015	4/4	0.90	0.15	18,22,23,24	4
5	DMS	D	1124	4/4	0.90	0.15	40,46,48,55	4
5	DMS	D	1126	4/4	0.90	0.17	22,26,26,30	4
5	DMS	A	3026	4/4	0.90	0.14	33,33,36,38	4
5	DMS	A	3033	4/4	0.90	0.13	33,46,49,51	0
5	DMS	A	3027	4/4	0.90	0.17	22,28,30,32	4
5	DMS	A	3041	4/4	0.91	0.16	34,34,36,40	4
5	DMS	C	3020	4/4	0.91	0.15	23,24,27,27	4
5	DMS	D	1123	4/4	0.91	0.17	37,39,44,50	4
5	DMS	A	3018	4/4	0.91	0.13	23,23,25,28	4
5	DMS	A	3034	4/4	0.91	0.13	43,43,43,44	4
5	DMS	B	1131	4/4	0.91	0.13	21,26,30,30	0
5	DMS	C	3026	4/4	0.91	0.14	27,27,29,31	4
5	DMS	A	3023	4/4	0.91	0.16	23,31,32,40	0
5	DMS	D	1131	4/4	0.91	0.14	45,48,50,59	0
5	DMS	C	3041	4/4	0.92	0.14	18,21,28,31	4
5	DMS	D	1125	4/4	0.92	0.13	17,20,23,23	4
5	DMS	C	3027	4/4	0.92	0.16	22,28,30,31	4
5	DMS	B	1133	4/4	0.92	0.13	20,21,25,25	4
5	DMS	D	1121	4/4	0.92	0.14	20,23,24,25	4
5	DMS	D	1122	4/4	0.92	0.12	21,30,33,35	4
5	DMS	C	3022	4/4	0.92	0.14	18,20,23,24	4
5	DMS	B	1116	4/4	0.93	0.15	15,18,18,18	4
5	DMS	C	3044	4/4	0.93	0.14	20,20,22,23	4
5	DMS	A	3039	4/4	0.93	0.14	23,33,33,34	4
5	DMS	A	3038	4/4	0.93	0.14	20,20,22,28	4
5	DMS	D	1133	4/4	0.93	0.17	23,26,28,28	4
5	DMS	D	1115	4/4	0.94	0.13	15,15,16,20	4
5	DMS	A	3032	4/4	0.94	0.14	19,24,25,30	4
5	DMS	A	3022	4/4	0.94	0.12	22,22,23,24	4
5	DMS	A	3029	4/4	0.94	0.12	14,16,18,18	4
5	DMS	C	3014	4/4	0.94	0.12	16,19,21,21	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	B	1114	4/4	0.94	0.10	13,14,17,18	4
5	DMS	C	3016	4/4	0.94	0.12	23,23,24,24	4
5	DMS	C	3017	4/4	0.94	0.12	19,22,23,24	4
5	DMS	A	3016	4/4	0.94	0.13	14,14,16,18	4
5	DMS	A	3031	4/4	0.94	0.13	22,23,25,26	4
5	DMS	B	1123	4/4	0.94	0.12	16,19,22,23	4
5	DMS	D	1132	4/4	0.94	0.12	20,30,31,35	4
5	DMS	B	1124	4/4	0.94	0.13	23,27,28,28	4
5	DMS	B	1118	4/4	0.95	0.12	20,21,22,24	0
5	DMS	B	1119	4/4	0.95	0.11	13,16,19,22	4
5	DMS	C	3033	4/4	0.95	0.11	32,38,39,40	0
5	DMS	C	3034	4/4	0.95	0.12	22,22,23,23	4
5	DMS	A	3021	4/4	0.95	0.11	23,26,27,27	4
5	DMS	B	1122	4/4	0.95	0.12	20,29,31,32	4
5	DMS	C	3019	4/4	0.95	0.13	21,26,29,34	0
5	DMS	A	3019	4/4	0.95	0.11	19,21,21,22	4
5	DMS	C	3021	4/4	0.95	0.12	19,33,33,36	0
5	DMS	D	1117	4/4	0.95	0.12	21,21,22,22	4
5	DMS	C	3012	4/4	0.95	0.09	14,15,16,17	0
5	DMS	C	3013	4/4	0.96	0.09	20,21,21,23	0
5	DMS	B	1117	4/4	0.96	0.10	21,24,25,28	4
5	DMS	A	3013	4/4	0.96	0.09	12,13,14,15	4
5	DMS	D	1127	4/4	0.96	0.11	9,10,11,16	4
3	K	D	1108	1/1	0.96	0.05	16,16,16,16	1
5	DMS	D	1116	4/4	0.96	0.09	22,24,25,33	0
5	DMS	A	3012	4/4	0.96	0.10	16,16,17,18	4
5	DMS	B	1132	4/4	0.96	0.12	19,19,21,22	4
5	DMS	C	3010	4/4	0.96	0.09	16,16,16,16	0
5	DMS	A	3017	4/4	0.96	0.11	22,25,29,30	0
5	DMS	D	1114	4/4	0.97	0.10	14,15,16,17	0
5	DMS	A	3014	4/4	0.97	0.08	19,19,21,21	0
2	MG	A	3004	1/1	0.97	0.04	14,14,14,14	1
5	DMS	B	1120	4/4	0.97	0.09	19,23,23,23	4
5	DMS	D	1118	4/4	0.97	0.09	19,20,22,23	4
5	DMS	A	3020	4/4	0.97	0.09	16,18,20,24	4
5	DMS	B	1115	4/4	0.98	0.08	18,18,21,22	4
5	DMS	D	1109	4/4	0.98	0.07	9,10,11,12	0
5	DMS	D	1111	4/4	0.98	0.07	15,15,17,17	4
5	DMS	A	3010	4/4	0.98	0.06	10,11,11,12	0
5	DMS	A	3011	4/4	0.98	0.07	12,12,12,12	4
5	DMS	D	1113	4/4	0.98	0.08	17,18,20,21	0
2	MG	D	1104	1/1	0.98	0.04	14,14,14,14	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	C	3008	1/1	0.98	0.04	16,16,16,16	1
2	MG	C	3003	1/1	0.98	0.10	17,17,17,17	1
5	DMS	B	1112	4/4	0.98	0.08	14,14,14,15	0
4	CL	A	3009	1/1	0.98	0.06	19,19,19,19	0
5	DMS	D	1119	4/4	0.98	0.09	17,21,21,23	4
5	DMS	D	1120	4/4	0.98	0.06	18,20,21,23	4
3	K	B	1110	1/1	0.99	0.04	15,15,15,15	1
2	MG	C	3001	1/1	0.99	0.03	8,8,8,8	1
5	DMS	C	3009	4/4	0.99	0.06	11,12,13,13	0
3	K	D	1107	1/1	0.99	0.03	12,12,12,12	0
5	DMS	C	3011	4/4	0.99	0.06	17,17,17,19	0
2	MG	B	1105	1/1	0.99	0.02	12,12,12,12	0
2	MG	C	3004	1/1	0.99	0.04	9,9,9,9	1
2	MG	D	1102	1/1	0.99	0.04	8,8,8,8	1
2	MG	D	1103	1/1	0.99	0.05	13,13,13,13	0
5	DMS	D	1110	4/4	0.99	0.06	12,12,12,14	0
5	DMS	B	1111	4/4	0.99	0.06	10,12,13,13	0
2	MG	A	3002	1/1	0.99	0.03	10,10,10,10	1
5	DMS	C	3018	4/4	0.99	0.07	16,19,20,23	4
5	DMS	B	1113	4/4	0.99	0.06	16,17,17,18	0
3	K	A	3007	1/1	0.99	0.03	12,12,12,12	0
3	K	A	3008	1/1	0.99	0.04	14,14,14,14	1
3	K	B	1109	1/1	0.99	0.02	11,11,11,11	0
2	MG	A	3001	1/1	1.00	0.03	8,8,8,8	1
3	K	A	3005	1/1	1.00	0.05	18,18,18,18	0
3	K	C	3005	1/1	1.00	0.05	16,16,16,16	0
3	K	C	3006	1/1	1.00	0.02	8,8,8,8	0
3	K	C	3007	1/1	1.00	0.02	11,11,11,11	0
3	K	A	3006	1/1	1.00	0.03	5,5,5,5	1
3	K	D	1105	1/1	1.00	0.07	18,18,18,18	0
3	K	D	1106	1/1	1.00	0.02	7,7,7,7	0
2	MG	C	3002	1/1	1.00	0.02	10,10,10,10	0
2	MG	B	1104	1/1	1.00	0.02	7,7,7,7	1
3	K	B	1107	1/1	1.00	0.05	15,15,15,15	0
3	K	B	1108	1/1	1.00	0.02	7,7,7,7	0

6.5 Other polymers

There are no such residues in this entry.