



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:38 PM UTC

PDB ID : 3MV0 / pdb_00003mv0
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (R599A) IN COMPLEX WITH D
-GALCTOPYRANOSYL-1-ONE
Authors : Dugdale, M.L.; Vance, M.; Driedger, M.L.; Nibber, A.; Tran, A.; Huber, R.E.
Deposited on : 2010-05-03
Resolution : 2.20 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

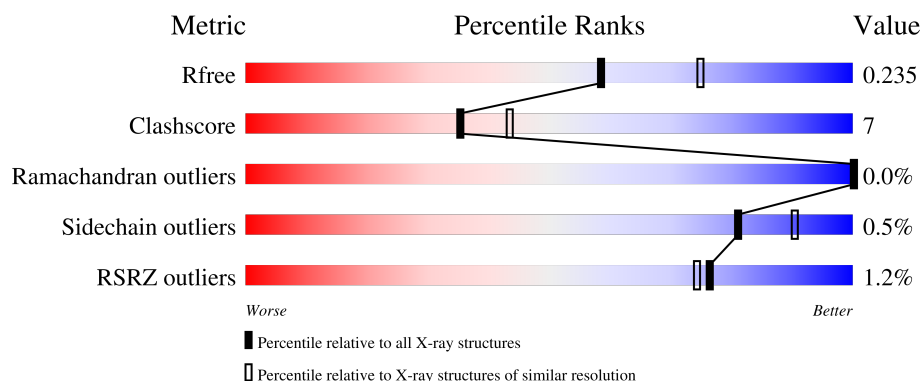
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	1	1052	% 78% 18% ..
1	2	1052	% 78% 17% .
1	3	1052	% 77% 18% .
1	4	1052	% 76% 19% ..

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	1	5029	-	-	X	-
5	DMS	3	5034	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36190 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	1	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	2	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	3	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	4	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-28	MET	-	expression tag	UNP B8LFD6
1	-27	GLY	-	expression tag	UNP B8LFD6
1	-26	GLY	-	expression tag	UNP B8LFD6
1	-25	SER	-	expression tag	UNP B8LFD6
1	-24	HIS	-	expression tag	UNP B8LFD6
1	-23	HIS	-	expression tag	UNP B8LFD6
1	-22	HIS	-	expression tag	UNP B8LFD6
1	-21	HIS	-	expression tag	UNP B8LFD6
1	-20	HIS	-	expression tag	UNP B8LFD6
1	-19	HIS	-	expression tag	UNP B8LFD6
1	-18	GLY	-	expression tag	UNP B8LFD6
1	-17	MET	-	expression tag	UNP B8LFD6
1	-16	ALA	-	expression tag	UNP B8LFD6
1	-15	SER	-	expression tag	UNP B8LFD6
1	-14	MET	-	expression tag	UNP B8LFD6
1	-13	THR	-	expression tag	UNP B8LFD6
1	-12	GLY	-	expression tag	UNP B8LFD6
1	-11	GLY	-	expression tag	UNP B8LFD6
1	-10	GLN	-	expression tag	UNP B8LFD6
1	-9	GLN	-	expression tag	UNP B8LFD6
1	-8	MET	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
1	-7	GLY	-	expression tag	UNP B8LFD6
1	-6	ARG	-	expression tag	UNP B8LFD6
1	-5	ASP	-	expression tag	UNP B8LFD6
1	-4	LEU	-	expression tag	UNP B8LFD6
1	-3	TYR	-	expression tag	UNP B8LFD6
1	-2	ASP	-	expression tag	UNP B8LFD6
1	-1	ASP	-	expression tag	UNP B8LFD6
1	0	ASP	-	expression tag	UNP B8LFD6
1	1	ASP	-	expression tag	UNP B8LFD6
1	2	LYS	-	expression tag	UNP B8LFD6
1	3	ASP	-	expression tag	UNP B8LFD6
1	4	PRO	-	expression tag	UNP B8LFD6
1	5	MET	-	expression tag	UNP B8LFD6
1	6	ILE	-	expression tag	UNP B8LFD6
1	7	ASP	-	expression tag	UNP B8LFD6
1	8	PRO	-	expression tag	UNP B8LFD6
1	599	ALA	ARG	engineered mutation	UNP B8LFD6
2	-28	MET	-	expression tag	UNP B8LFD6
2	-27	GLY	-	expression tag	UNP B8LFD6
2	-26	GLY	-	expression tag	UNP B8LFD6
2	-25	SER	-	expression tag	UNP B8LFD6
2	-24	HIS	-	expression tag	UNP B8LFD6
2	-23	HIS	-	expression tag	UNP B8LFD6
2	-22	HIS	-	expression tag	UNP B8LFD6
2	-21	HIS	-	expression tag	UNP B8LFD6
2	-20	HIS	-	expression tag	UNP B8LFD6
2	-19	HIS	-	expression tag	UNP B8LFD6
2	-18	GLY	-	expression tag	UNP B8LFD6
2	-17	MET	-	expression tag	UNP B8LFD6
2	-16	ALA	-	expression tag	UNP B8LFD6
2	-15	SER	-	expression tag	UNP B8LFD6
2	-14	MET	-	expression tag	UNP B8LFD6
2	-13	THR	-	expression tag	UNP B8LFD6
2	-12	GLY	-	expression tag	UNP B8LFD6
2	-11	GLY	-	expression tag	UNP B8LFD6
2	-10	GLN	-	expression tag	UNP B8LFD6
2	-9	GLN	-	expression tag	UNP B8LFD6
2	-8	MET	-	expression tag	UNP B8LFD6
2	-7	GLY	-	expression tag	UNP B8LFD6
2	-6	ARG	-	expression tag	UNP B8LFD6
2	-5	ASP	-	expression tag	UNP B8LFD6
2	-4	LEU	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
2	-3	TYR	-	expression tag	UNP B8LFD6
2	-2	ASP	-	expression tag	UNP B8LFD6
2	-1	ASP	-	expression tag	UNP B8LFD6
2	0	ASP	-	expression tag	UNP B8LFD6
2	1	ASP	-	expression tag	UNP B8LFD6
2	2	LYS	-	expression tag	UNP B8LFD6
2	3	ASP	-	expression tag	UNP B8LFD6
2	4	PRO	-	expression tag	UNP B8LFD6
2	5	MET	-	expression tag	UNP B8LFD6
2	6	ILE	-	expression tag	UNP B8LFD6
2	7	ASP	-	expression tag	UNP B8LFD6
2	8	PRO	-	expression tag	UNP B8LFD6
2	599	ALA	ARG	engineered mutation	UNP B8LFD6
3	-28	MET	-	expression tag	UNP B8LFD6
3	-27	GLY	-	expression tag	UNP B8LFD6
3	-26	GLY	-	expression tag	UNP B8LFD6
3	-25	SER	-	expression tag	UNP B8LFD6
3	-24	HIS	-	expression tag	UNP B8LFD6
3	-23	HIS	-	expression tag	UNP B8LFD6
3	-22	HIS	-	expression tag	UNP B8LFD6
3	-21	HIS	-	expression tag	UNP B8LFD6
3	-20	HIS	-	expression tag	UNP B8LFD6
3	-19	HIS	-	expression tag	UNP B8LFD6
3	-18	GLY	-	expression tag	UNP B8LFD6
3	-17	MET	-	expression tag	UNP B8LFD6
3	-16	ALA	-	expression tag	UNP B8LFD6
3	-15	SER	-	expression tag	UNP B8LFD6
3	-14	MET	-	expression tag	UNP B8LFD6
3	-13	THR	-	expression tag	UNP B8LFD6
3	-12	GLY	-	expression tag	UNP B8LFD6
3	-11	GLY	-	expression tag	UNP B8LFD6
3	-10	GLN	-	expression tag	UNP B8LFD6
3	-9	GLN	-	expression tag	UNP B8LFD6
3	-8	MET	-	expression tag	UNP B8LFD6
3	-7	GLY	-	expression tag	UNP B8LFD6
3	-6	ARG	-	expression tag	UNP B8LFD6
3	-5	ASP	-	expression tag	UNP B8LFD6
3	-4	LEU	-	expression tag	UNP B8LFD6
3	-3	TYR	-	expression tag	UNP B8LFD6
3	-2	ASP	-	expression tag	UNP B8LFD6
3	-1	ASP	-	expression tag	UNP B8LFD6
3	0	ASP	-	expression tag	UNP B8LFD6

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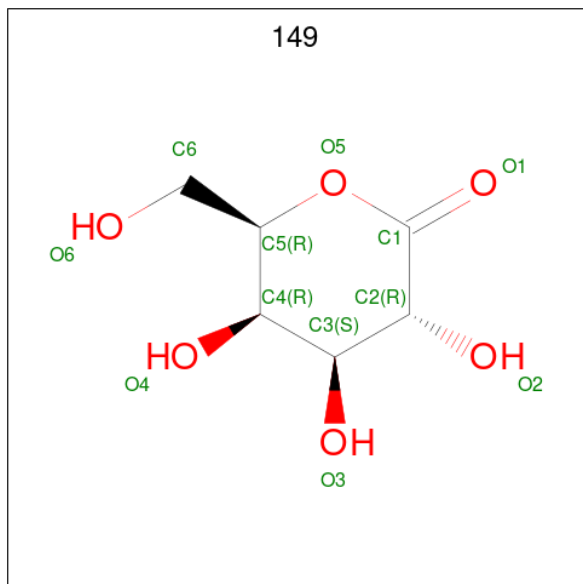
Chain	Residue	Modelled	Actual	Comment	Reference
3	1	ASP	-	expression tag	UNP B8LFD6
3	2	LYS	-	expression tag	UNP B8LFD6
3	3	ASP	-	expression tag	UNP B8LFD6
3	4	PRO	-	expression tag	UNP B8LFD6
3	5	MET	-	expression tag	UNP B8LFD6
3	6	ILE	-	expression tag	UNP B8LFD6
3	7	ASP	-	expression tag	UNP B8LFD6
3	8	PRO	-	expression tag	UNP B8LFD6
3	599	ALA	ARG	engineered mutation	UNP B8LFD6
4	-28	MET	-	expression tag	UNP B8LFD6
4	-27	GLY	-	expression tag	UNP B8LFD6
4	-26	GLY	-	expression tag	UNP B8LFD6
4	-25	SER	-	expression tag	UNP B8LFD6
4	-24	HIS	-	expression tag	UNP B8LFD6
4	-23	HIS	-	expression tag	UNP B8LFD6
4	-22	HIS	-	expression tag	UNP B8LFD6
4	-21	HIS	-	expression tag	UNP B8LFD6
4	-20	HIS	-	expression tag	UNP B8LFD6
4	-19	HIS	-	expression tag	UNP B8LFD6
4	-18	GLY	-	expression tag	UNP B8LFD6
4	-17	MET	-	expression tag	UNP B8LFD6
4	-16	ALA	-	expression tag	UNP B8LFD6
4	-15	SER	-	expression tag	UNP B8LFD6
4	-14	MET	-	expression tag	UNP B8LFD6
4	-13	THR	-	expression tag	UNP B8LFD6
4	-12	GLY	-	expression tag	UNP B8LFD6
4	-11	GLY	-	expression tag	UNP B8LFD6
4	-10	GLN	-	expression tag	UNP B8LFD6
4	-9	GLN	-	expression tag	UNP B8LFD6
4	-8	MET	-	expression tag	UNP B8LFD6
4	-7	GLY	-	expression tag	UNP B8LFD6
4	-6	ARG	-	expression tag	UNP B8LFD6
4	-5	ASP	-	expression tag	UNP B8LFD6
4	-4	LEU	-	expression tag	UNP B8LFD6
4	-3	TYR	-	expression tag	UNP B8LFD6
4	-2	ASP	-	expression tag	UNP B8LFD6
4	-1	ASP	-	expression tag	UNP B8LFD6
4	0	ASP	-	expression tag	UNP B8LFD6
4	1	ASP	-	expression tag	UNP B8LFD6
4	2	LYS	-	expression tag	UNP B8LFD6
4	3	ASP	-	expression tag	UNP B8LFD6
4	4	PRO	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
4	5	MET	-	expression tag	UNP B8LFD6
4	6	ILE	-	expression tag	UNP B8LFD6
4	7	ASP	-	expression tag	UNP B8LFD6
4	8	PRO	-	expression tag	UNP B8LFD6
4	599	ALA	ARG	engineered mutation	UNP B8LFD6

- Molecule 2 is D-galactonolactone (CCD ID: 149) (formula: C₆H₁₀O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	1	Total C O 12 6 6	0	0
2	2	1	Total C O 12 6 6	0	0
2	3	1	Total C O 12 6 6	0	0
2	4	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	1	2	Total Mg 2 2	0	0
3	2	3	Total Mg 3 3	0	0

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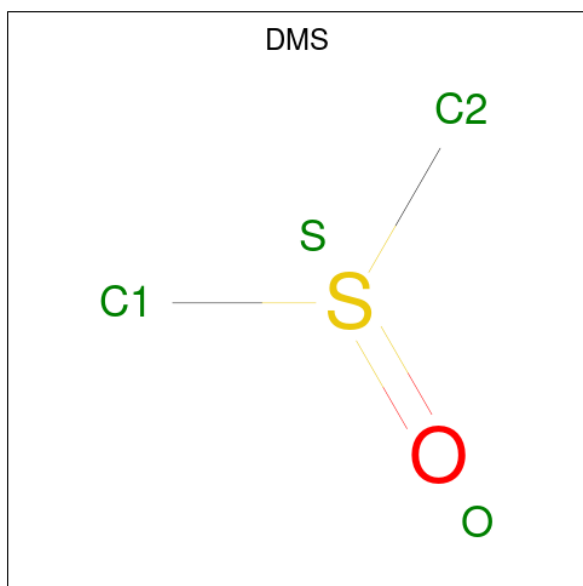
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	3	3	Total	Mg	0	0
			3	3		
3	4	3	Total	Mg	0	0
			3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	4	Total	Na	0	0
			4	4		
4	2	4	Total	Na	0	0
			4	4		
4	3	4	Total	Na	0	0
			4	4		
4	4	4	Total	Na	0	0
			4	4		

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0

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

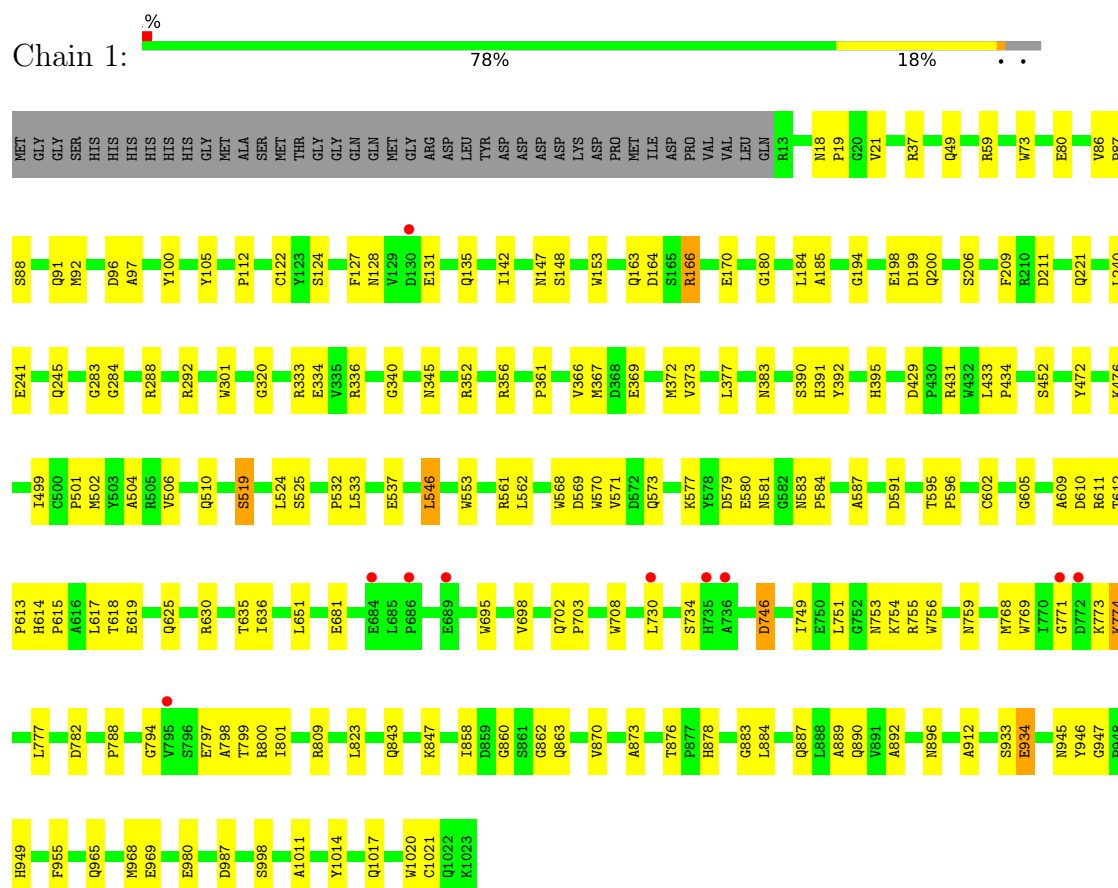
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	773	Total O 773 773	0	0
6	2	858	Total O 858 858	0	0
6	3	760	Total O 760 760	0	0
6	4	760	Total O 760 760	0	0

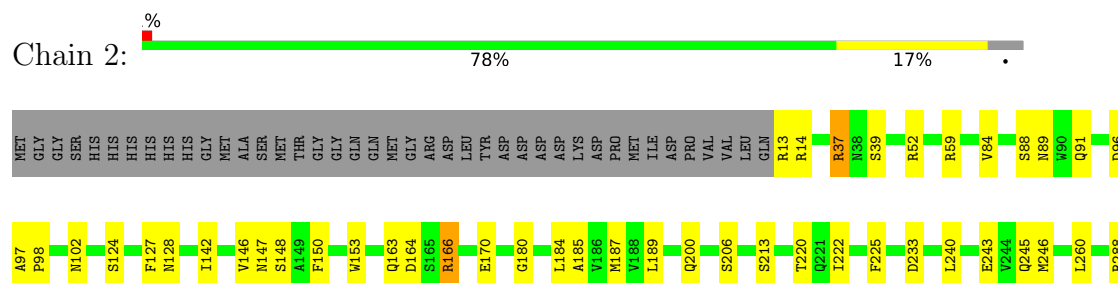
3 Residue-property plots

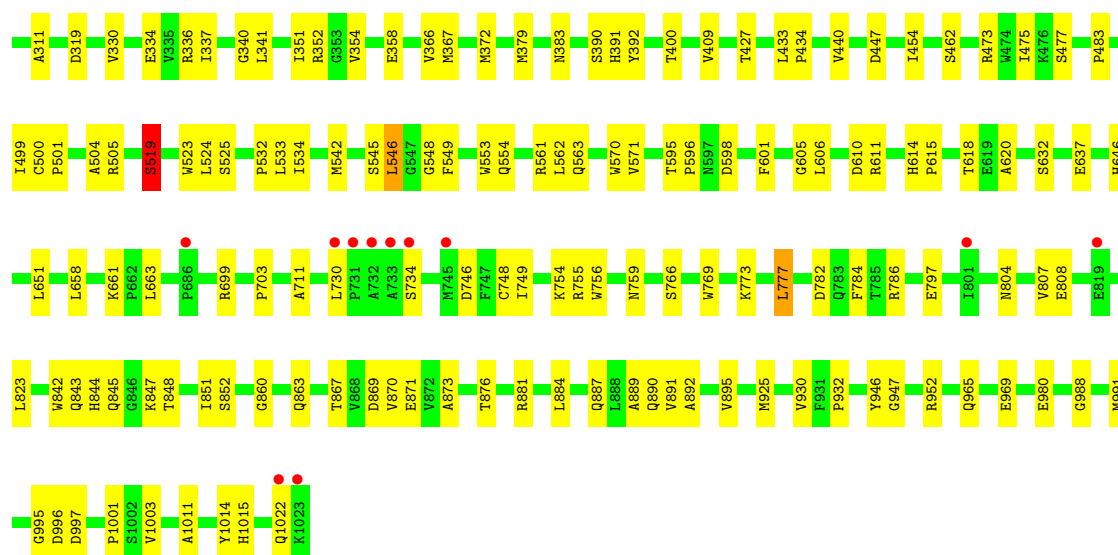
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

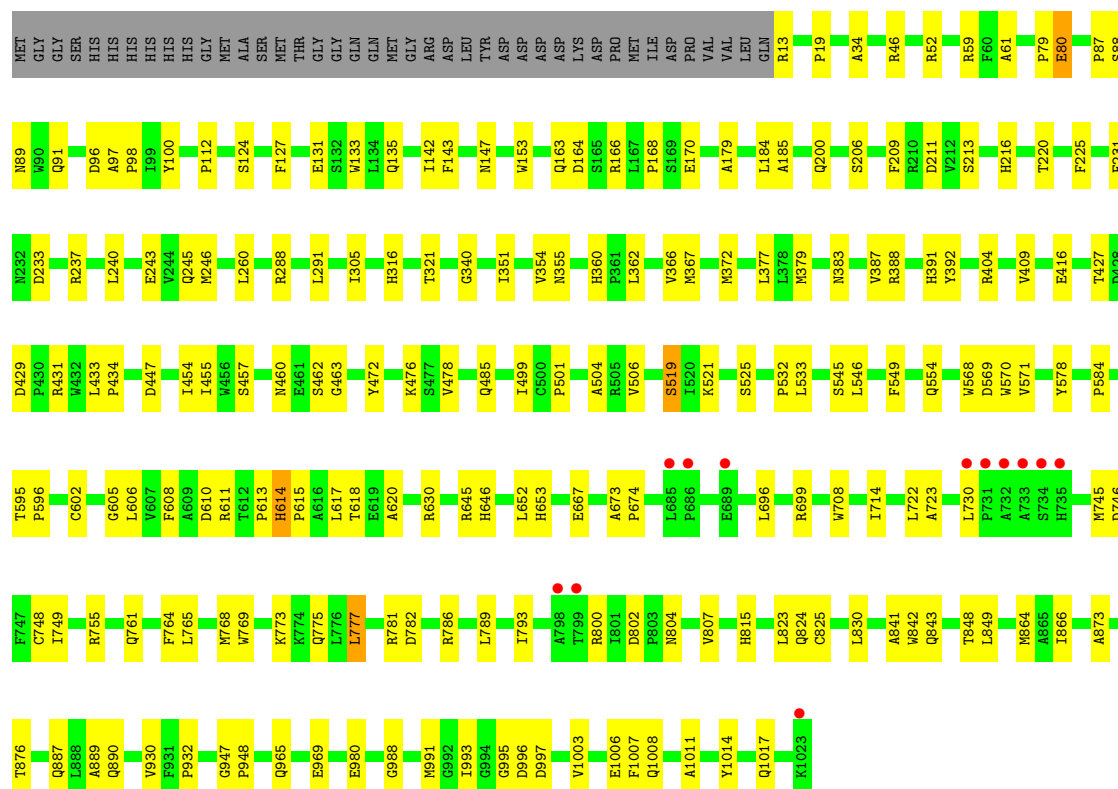
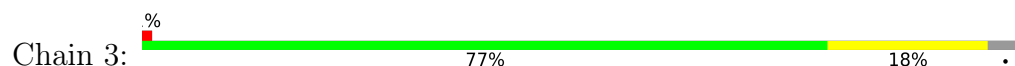


• Molecule 1: Beta-galactosidase

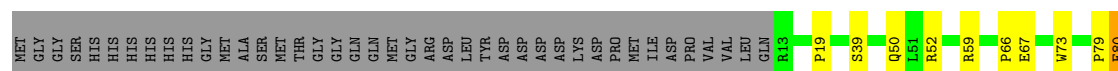
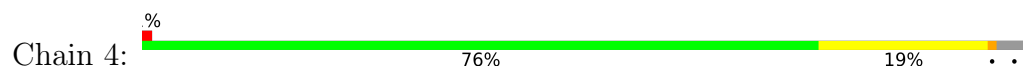


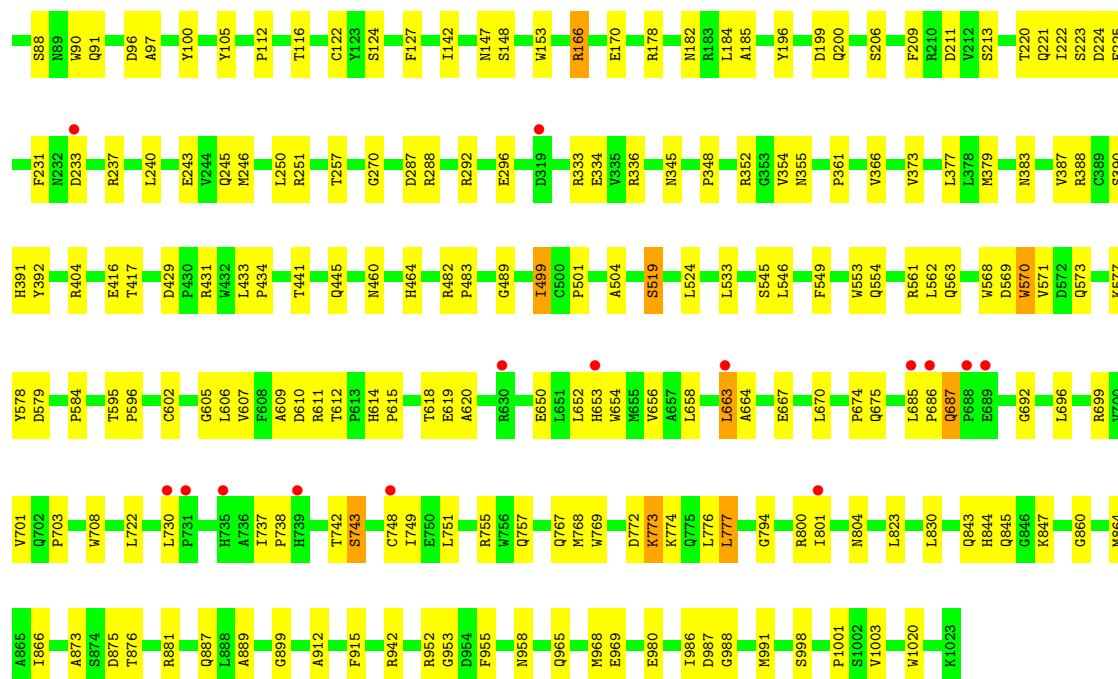


• Molecule 1: Beta-galactosidase



• 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	149.84Å 166.31Å 201.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.23 – 2.20 21.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.1 (21.23-2.20) 91.9 (21.23-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.19Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.195 , 0.237 0.192 , 0.235	Depositor DCC
R_{free} test set	3358 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtrriage
Anisotropy	0.724	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36190	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 37.12 % 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 4.5024e-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: NA, DMS, 149, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.36	0/8361	0.89	25/11408 (0.2%)
1	2	0.37	0/8361	0.89	28/11408 (0.2%)
1	3	0.36	0/8361	0.88	22/11408 (0.2%)
1	4	0.36	0/8361	0.89	28/11408 (0.2%)
All	All	0.36	0/33444	0.89	103/45632 (0.2%)

There are no bond length outliers.

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	614	HIS	N-CA-C	-9.31	97.88	110.36
1	1	614	HIS	N-CA-C	-8.66	99.06	110.40
1	4	614	HIS	N-CA-C	-8.46	99.32	110.40
1	1	570	TRP	N-CA-C	7.64	119.51	111.03
1	2	988	GLY	N-CA-C	-7.43	102.72	113.86
1	3	570	TRP	N-CA-C	7.41	119.26	111.03
1	4	570	TRP	N-CA-C	7.41	119.25	111.03
1	3	614	HIS	N-CA-C	-7.37	100.48	110.36
1	2	777	LEU	N-CA-C	-7.12	105.12	113.88
1	4	988	GLY	N-CA-C	-7.01	103.34	113.86
1	2	570	TRP	N-CA-C	6.91	118.70	111.03
1	3	97	ALA	N-CA-C	6.83	118.39	109.93
1	3	605	GLY	N-CA-C	6.82	122.23	112.82
1	2	519	SER	N-CA-C	-6.81	100.36	110.23
1	3	777	LEU	N-CA-C	-6.68	105.67	113.88
1	3	988	GLY	N-CA-C	-6.67	103.86	113.86
1	4	97	ALA	N-CA-C	6.62	117.99	109.72
1	4	519	SER	N-CA-C	-6.40	100.96	110.23
1	1	519	SER	N-CA-C	-6.34	101.03	110.23
1	4	383	ASN	N-CA-C	6.31	120.26	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	646	HIS	N-CA-C	-6.24	101.29	110.52
1	4	233	ASP	N-CA-C	6.14	118.76	111.33
1	1	504	ALA	N-CA-C	-6.14	101.20	110.28
1	4	499	ILE	N-CA-C	-6.12	99.92	108.12
1	1	571	VAL	N-CA-C	6.08	117.52	108.46
1	1	383	ASN	N-CA-C	6.05	119.99	112.24
1	4	606	LEU	N-CA-C	-6.01	105.44	112.89
1	4	605	GLY	N-CA-C	5.96	121.05	112.82
1	4	222	ILE	N-CA-C	-5.90	99.80	108.54
1	3	98	PRO	N-CA-C	-5.89	101.85	111.68
1	2	605	GLY	N-CA-C	5.88	120.06	112.54
1	3	233	ASP	N-CA-C	5.87	118.43	111.33
1	1	510	GLN	CA-C-N	5.84	127.14	119.84
1	1	510	GLN	C-N-CA	5.84	127.14	119.84
1	1	97	ALA	N-CA-C	5.79	117.37	110.07
1	2	39	SER	N-CA-C	5.79	117.59	111.28
1	4	777	LEU	N-CA-C	-5.78	106.86	114.31
1	4	504	ALA	N-CA-C	-5.76	101.76	110.28
1	2	571	VAL	N-CA-C	5.75	116.75	108.48
1	2	554	GLN	N-CA-C	-5.72	105.12	111.36
1	2	563	GLN	N-CA-C	5.72	119.03	112.57
1	3	383	ASN	N-CA-C	5.70	119.54	112.24
1	4	773	LYS	N-CA-C	5.70	118.83	109.76
1	4	220	THR	N-CA-C	-5.69	99.25	108.41
1	2	97	ALA	N-CA-C	5.68	116.97	109.93
1	2	233	ASP	N-CA-C	5.66	118.17	111.33
1	2	606	LEU	N-CA-C	-5.65	105.88	112.89
1	2	746	ASP	N-CA-C	5.62	117.73	109.24
1	4	209	PHE	N-CA-C	5.62	120.13	113.16
1	1	746	ASP	N-CA-C	5.62	117.33	108.96
1	2	545	SER	N-CA-C	5.62	115.83	108.07
1	3	89	ASN	N-CA-C	-5.61	100.03	109.07
1	2	98	PRO	N-CA-C	-5.60	100.65	111.69
1	4	166	ARG	N-CA-C	5.58	120.08	112.88
1	2	504	ALA	N-CA-C	-5.57	101.41	110.20
1	3	554	GLN	N-CA-C	-5.56	105.30	111.36
1	2	409	VAL	N-CA-C	5.55	116.57	108.53
1	3	519	SER	N-CA-C	-5.54	102.19	110.23
1	2	383	ASN	N-CA-C	5.54	119.21	111.74
1	3	351	ILE	N-CA-C	5.54	115.54	108.12
1	4	554	GLN	N-CA-C	-5.52	105.34	111.36
1	1	209	PHE	N-CA-C	5.51	119.86	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	612	THR	N-CA-C	-5.48	102.75	109.65
1	1	949	HIS	N-CA-C	5.47	118.58	110.48
1	4	563	GLN	N-CA-C	5.46	118.75	112.57
1	1	221	GLN	N-CA-C	5.46	117.71	109.41
1	2	222	ILE	N-CA-C	-5.45	99.89	108.23
1	4	211	ASP	N-CA-C	5.43	117.31	110.24
1	3	504	ALA	N-CA-C	-5.42	101.64	110.20
1	1	605	GLY	N-CA-C	5.42	121.63	113.02
1	1	878	HIS	CA-C-N	5.41	125.32	119.85
1	1	878	HIS	C-N-CA	5.41	125.32	119.85
1	4	39	SER	N-CA-C	5.38	117.15	111.28
1	2	166	ARG	N-CA-C	5.37	119.81	112.88
1	1	211	ASP	N-CA-C	5.35	117.19	110.24
1	2	447	ASP	N-CA-C	5.34	119.90	113.17
1	4	612	THR	N-CA-C	-5.34	102.92	109.65
1	3	545	SER	N-CA-C	5.34	115.44	108.07
1	3	211	ASP	N-CA-C	5.34	117.61	110.35
1	2	220	THR	N-CA-C	-5.31	99.86	108.41
1	1	870	VAL	N-CA-C	5.29	116.10	108.48
1	1	934	GLU	N-CA-C	-5.28	102.79	110.24
1	1	166	ARG	N-CA-C	5.26	119.67	112.88
1	4	116	THR	N-CA-C	-5.24	105.75	111.82
1	4	571	VAL	N-CA-C	5.23	116.25	108.46
1	3	571	VAL	N-CA-C	5.21	116.22	108.46
1	1	320	GLY	N-CA-C	5.18	123.35	115.63
1	3	220	THR	N-CA-C	-5.18	100.07	108.41
1	4	221	GLN	N-CA-C	5.18	116.86	109.14
1	2	351	ILE	N-CA-C	5.17	115.05	108.12
1	1	506	VAL	N-CA-C	5.16	115.38	110.53
1	3	34	ALA	N-CA-C	-5.12	108.29	114.75
1	3	404	ARG	N-CA-C	5.08	117.94	111.69
1	4	545	SER	N-CA-C	5.08	115.08	108.07
1	3	447	ASP	N-CA-C	5.07	120.09	113.30
1	3	409	VAL	N-CA-C	5.07	115.78	108.48
1	4	404	ARG	N-CA-C	5.07	117.92	111.69
1	1	702	GLN	CA-C-N	5.06	124.50	119.24
1	1	702	GLN	C-N-CA	5.06	124.50	119.24
1	4	743	SER	N-CA-C	-5.06	101.21	108.60
1	2	37	ARG	N-CA-C	-5.02	106.47	112.59
1	2	89	ASN	N-CA-C	-5.01	101.07	109.24
1	2	870	VAL	N-CA-C	5.00	115.69	108.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	8119	0	7708	116	0
1	2	8119	0	7708	120	0
1	3	8119	0	7708	123	0
1	4	8119	0	7708	129	0
2	1	12	0	9	0	0
2	2	12	0	9	0	0
2	3	12	0	9	0	0
2	4	12	0	9	0	0
3	1	2	0	0	0	0
3	2	3	0	0	0	0
3	3	3	0	0	0	0
3	4	3	0	0	0	0
4	1	4	0	0	0	0
4	2	4	0	0	0	0
4	3	4	0	0	0	0
4	4	4	0	0	0	0
5	1	112	0	168	9	0
5	2	124	0	186	6	0
5	3	136	0	204	7	0
5	4	116	0	174	3	0
6	1	773	0	0	4	0
6	2	858	0	0	5	0
6	3	760	0	0	3	0
6	4	760	0	0	2	0
All	All	36190	0	31600	479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (479) 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)
1:3:142:ILE:HG12	1:3:170:GLU:HG2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:142:ILE:HG12	1:1:170:GLU:HG2	1.57	0.84
1:4:687:GLN:H	1:4:687:GLN:NE2	1.76	0.83
1:1:284:GLY:H	5:1:5029:DMS:H13	1.45	0.82
1:1:823:LEU:O	1:2:730:LEU:HD21	1.80	0.81
1:1:292:ARG:HH12	5:1:5012:DMS:H13	1.46	0.80
1:3:765:LEU:HD21	1:3:768:MET:HE2	1.66	0.78
1:3:730:LEU:HD11	1:4:823:LEU:HB3	1.66	0.76
1:2:187:MET:HE3	1:2:189:LEU:HD21	1.67	0.75
1:2:245:GLN:HG2	1:2:288:ARG:HG2	1.69	0.74
1:1:768:MET:HE1	1:1:1020:TRP:CZ2	2.23	0.73
1:4:355:ASN:OD1	1:4:388:ARG:HD3	1.89	0.72
1:4:142:ILE:HG12	1:4:170:GLU:HG2	1.70	0.71
1:3:765:LEU:HD21	1:3:768:MET:CE	2.20	0.71
1:2:873:ALA:O	1:2:876:THR:HG22	1.92	0.70
1:1:890:GLN:HE22	1:1:947:GLY:HA3	1.56	0.69
1:1:356:ARG:HH22	1:1:367:MET:HE2	1.58	0.67
1:2:127:PHE:CE1	1:2:184:LEU:HG	2.30	0.67
1:3:696:LEU:HB2	1:3:722:LEU:HD11	1.75	0.67
1:1:283:GLY:HA3	5:1:5029:DMS:H13	1.77	0.66
1:3:245:GLN:HG2	1:3:288:ARG:HG2	1.76	0.66
1:1:91:GLN:HG3	1:1:96:ASP:OD1	1.96	0.66
1:1:284:GLY:N	5:1:5029:DMS:H13	2.10	0.66
1:4:755:ARG:HB2	1:4:769:TRP:HB2	1.79	0.65
1:1:166:ARG:HG3	1:1:392:TYR:HB2	1.79	0.65
1:1:863:GLN:HG2	1:1:1021:CYS:HB3	1.79	0.64
1:3:549:PHE:CE2	1:3:620:ALA:HA	2.33	0.64
1:3:991:MET:HE3	1:3:1003:VAL:HG21	1.79	0.64
1:1:245:GLN:HG2	1:1:288:ARG:HG2	1.79	0.64
1:1:892:ALA:HB3	1:1:946:TYR:CE1	2.33	0.64
1:2:142:ILE:HG12	1:2:170:GLU:HG2	1.80	0.64
1:3:237:ARG:HB3	1:3:237:ARG:NH1	2.13	0.64
1:4:153:TRP:HB2	1:4:185:ALA:HB3	1.78	0.63
1:4:237:ARG:NH1	1:4:237:ARG:HB3	2.14	0.63
1:4:615:PRO:O	1:4:618:THR:HG22	1.98	0.63
1:2:367:MET:HE2	1:2:372:MET:HG3	1.81	0.63
1:2:91:GLN:HG3	1:2:96:ASP:OD1	1.97	0.63
1:3:630:ARG:HH11	1:3:630:ARG:HB3	1.63	0.63
1:4:88:SER:HA	1:4:366:VAL:HG21	1.80	0.63
1:3:965:GLN:O	1:3:969:GLU:HG3	1.99	0.62
1:3:88:SER:HA	1:3:366:VAL:HG21	1.81	0.62
1:3:237:ARG:CB	1:3:237:ARG:HH11	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:237:ARG:HB3	1:4:237:ARG:HH11	1.65	0.62
1:1:579:ASP:OD2	1:1:583:ASN:HB2	1.99	0.62
1:3:890:GLN:HE22	1:3:948:PRO:HD3	1.65	0.62
1:2:844:HIS:HE1	1:2:845:GLN:HE21	1.48	0.62
1:4:873:ALA:O	1:4:876:THR:HG22	1.99	0.61
1:1:147:ASN:HB3	1:1:206:SER:HA	1.81	0.61
1:1:630:ARG:HB3	1:1:630:ARG:HH21	1.66	0.61
1:2:433:LEU:HB3	1:2:434:PRO:HD3	1.83	0.61
1:1:615:PRO:O	1:1:618:THR:HG22	2.01	0.60
1:2:102:ASN:HD21	5:2:5030:DMS:H22	1.65	0.59
1:4:578:TYR:CE1	1:4:584:PRO:HB3	2.36	0.59
1:1:749:ILE:N	1:1:749:ILE:HD12	2.16	0.59
1:1:777:LEU:HG	1:1:889:ALA:HA	1.84	0.59
1:2:890:GLN:HG2	1:2:891:VAL:N	2.15	0.59
1:3:506:VAL:HG12	1:3:521:LYS:HE3	1.85	0.59
1:4:573:GLN:HB2	1:4:602:CYS:O	2.03	0.59
1:3:1008:GLN:HE22	5:3:5006:DMS:H23	1.68	0.59
1:1:887:GLN:NE2	1:1:980:GLU:O	2.34	0.58
1:3:777:LEU:HD11	1:3:980:GLU:HG2	1.85	0.58
1:4:147:ASN:HB3	1:4:206:SER:HA	1.84	0.58
1:4:292:ARG:HH12	5:4:5012:DMS:H13	1.69	0.58
1:1:788:PRO:HD2	1:1:968:MET:HG3	1.86	0.58
1:2:965:GLN:O	1:2:969:GLU:HG3	2.04	0.58
1:2:844:HIS:CE1	1:2:845:GLN:HE21	2.22	0.58
1:1:730:LEU:HD21	1:2:823:LEU:O	2.05	0.57
1:3:240:LEU:HD23	1:3:240:LEU:C	2.29	0.57
1:4:577:LYS:O	1:4:584:PRO:HA	2.04	0.57
1:4:334:GLU:OE1	1:4:336:ARG:NH1	2.36	0.57
1:1:595:THR:HA	1:1:596:PRO:C	2.30	0.57
1:2:127:PHE:HE1	1:2:184:LEU:HG	1.67	0.57
1:2:595:THR:HA	1:2:596:PRO:C	2.29	0.57
1:3:200:GLN:HG2	1:3:391:HIS:HB2	1.87	0.57
1:3:127:PHE:CE1	1:3:184:LEU:HG	2.40	0.57
1:2:147:ASN:HB3	1:2:206:SER:HA	1.88	0.56
1:2:887:GLN:NE2	1:2:980:GLU:O	2.37	0.56
1:4:245:GLN:HG2	1:4:288:ARG:HG2	1.86	0.56
1:3:91:GLN:HG3	1:3:96:ASP:OD1	2.05	0.56
1:1:801:ILE:N	1:1:801:ILE:HD12	2.21	0.56
1:4:237:ARG:HG2	1:4:296:GLU:OE1	2.06	0.56
1:1:651:LEU:HD23	1:1:703:PRO:HG3	1.87	0.56
1:3:79:PRO:HD2	1:3:80:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:777:LEU:HB2	1:3:887:GLN:HG2	1.88	0.55
1:3:873:ALA:O	1:3:876:THR:HG22	2.05	0.55
1:2:777:LEU:HD11	1:2:980:GLU:HG2	1.89	0.55
1:4:200:GLN:HG2	1:4:391:HIS:HB2	1.89	0.55
1:2:473:ARG:HH12	1:2:477:SER:HB2	1.71	0.55
1:2:632:SER:HB2	5:2:5033:DMS:H21	1.89	0.55
5:3:5034:DMS:H22	1:4:875:ASP:HB2	1.88	0.55
1:4:656:VAL:HG21	1:4:685:LEU:CD1	2.37	0.55
1:4:757:GLN:HE21	1:4:767:GLN:HB3	1.72	0.55
1:4:768:MET:HE1	1:4:1020:TRP:CZ2	2.42	0.55
1:3:610:ASP:O	1:3:611:ARG:HB2	2.07	0.55
1:2:651:LEU:HD12	1:2:651:LEU:C	2.32	0.54
1:2:524:LEU:HD11	1:2:562:LEU:HG	1.89	0.54
1:2:892:ALA:HB3	1:2:946:TYR:CE1	2.43	0.54
1:4:429:ASP:OD1	1:4:431:ARG:HG3	2.07	0.54
1:3:305:ILE:HD11	1:3:645:ARG:HB3	1.88	0.54
1:3:355:ASN:OD1	1:3:388:ARG:HD3	2.07	0.54
1:3:1017:GLN:HB2	6:3:4736:HOH:O	2.07	0.54
1:3:237:ARG:HB3	1:3:237:ARG:HH11	1.73	0.54
1:3:61:ALA:HA	5:3:5030:DMS:H12	1.90	0.53
1:2:153:TRP:HB2	1:2:185:ALA:HB3	1.90	0.53
1:4:794:GLY:HA2	1:4:998:SER:O	2.07	0.53
1:1:367:MET:HB3	1:1:372:MET:HE2	1.91	0.53
1:4:804:ASN:ND2	1:4:1001:PRO:HG2	2.24	0.53
1:3:533:LEU:C	1:3:533:LEU:HD23	2.34	0.53
1:2:615:PRO:O	1:2:618:THR:HG22	2.09	0.53
1:3:823:LEU:HD11	1:3:841:ALA:HB2	1.90	0.52
1:1:896:ASN:HB3	1:1:945:ASN:HB2	1.90	0.52
1:2:166:ARG:HG3	1:2:392:TYR:HB2	1.91	0.52
1:3:245:GLN:HG2	1:3:288:ARG:CD	2.39	0.52
1:4:250:LEU:O	1:4:251:ARG:HD3	2.09	0.52
1:1:166:ARG:HG3	1:1:392:TYR:CB	2.40	0.52
1:2:59:ARG:HB2	1:2:124:SER:OG	2.09	0.52
1:2:843:GLN:HA	1:2:847:LYS:O	2.08	0.52
1:2:777:LEU:CD1	1:2:980:GLU:HG2	2.40	0.52
1:3:379:MET:HE1	1:3:387:VAL:HB	1.91	0.52
1:4:654:TRP:CH2	1:4:685:LEU:HD21	2.45	0.52
1:1:352:ARG:HG2	1:1:553:TRP:CH2	2.44	0.52
1:3:864:MET:HE3	1:3:866:ILE:HD11	1.92	0.52
1:4:361:PRO:HB3	1:4:609:ALA:HB1	1.91	0.52
1:2:367:MET:HE2	1:2:372:MET:CG	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:240:LEU:C	1:4:240:LEU:HD23	2.34	0.52
1:4:777:LEU:HB2	1:4:887:GLN:HG2	1.91	0.52
1:1:127:PHE:CE1	1:1:184:LEU:HG	2.44	0.52
1:1:630:ARG:HB3	1:1:630:ARG:NH2	2.25	0.52
1:1:751:LEU:HD23	1:1:862:GLY:HA2	1.91	0.52
1:4:887:GLN:NE2	1:4:980:GLU:O	2.40	0.52
1:4:800:ARG:C	1:4:801:ILE:HD12	2.34	0.52
1:2:895:VAL:HG11	1:2:925:MET:HE2	1.91	0.52
1:4:100:TYR:CE1	1:4:602:CYS:HB3	2.45	0.52
1:1:573:GLN:HB2	1:1:602:CYS:O	2.11	0.51
1:3:131:GLU:O	1:3:135:GLN:HG3	2.10	0.51
1:1:292:ARG:HH12	5:1:5012:DMS:C1	2.19	0.51
1:4:166:ARG:HG3	1:4:392:TYR:HB2	1.92	0.51
1:4:91:GLN:HG3	1:4:96:ASP:OD1	2.10	0.51
1:4:730:LEU:N	1:4:730:LEU:HD12	2.25	0.51
1:4:881:ARG:HE	1:4:987:ASP:CG	2.18	0.51
1:3:499:ILE:HG22	1:3:501:PRO:HD3	1.93	0.51
1:3:653:HIS:CD2	1:3:667:GLU:HB3	2.46	0.51
1:3:800:ARG:HH11	1:3:800:ARG:HG2	1.75	0.51
1:1:105:TYR:CE1	1:1:199:ASP:HB2	2.46	0.51
1:1:890:GLN:HG2	6:1:4394:HOH:O	2.11	0.51
1:3:1011:ALA:HB3	1:3:1014:TYR:CZ	2.45	0.51
1:1:194:GLY:O	1:1:198:GLU:HG3	2.11	0.51
1:2:759:ASN:HB2	1:2:766:SER:OG	2.11	0.50
1:3:245:GLN:HG2	1:3:288:ARG:CG	2.41	0.50
1:4:570:TRP:O	1:4:607:VAL:HG22	2.11	0.50
1:4:610:ASP:O	1:4:611:ARG:HB2	2.11	0.50
1:3:608:PHE:CE2	1:3:614:HIS:HD2	2.30	0.50
1:1:18:ASN:ND2	1:1:21:VAL:HG23	2.26	0.50
1:2:991:MET:HE3	1:2:1003:VAL:HG21	1.93	0.50
1:2:533:LEU:C	1:2:533:LEU:HD23	2.36	0.50
1:3:133:TRP:CE3	1:3:216:HIS:HB2	2.46	0.50
1:4:749:ILE:N	1:4:749:ILE:HD12	2.26	0.50
1:1:369:GLU:O	1:1:373:VAL:HG23	2.12	0.50
1:3:131:GLU:OE1	1:3:179:ALA:HB2	2.12	0.50
1:4:773:LYS:NZ	1:4:774:LYS:HG2	2.27	0.50
1:2:102:ASN:ND2	5:2:5030:DMS:H22	2.27	0.50
1:2:128:ASN:HA	1:2:180:GLY:O	2.12	0.49
1:1:625:GLN:NE2	6:1:4833:HOH:O	2.46	0.49
1:2:52:ARG:O	1:2:213:SER:HB2	2.11	0.49
1:3:578:TYR:CE1	1:3:584:PRO:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:749:ILE:HD12	1:3:749:ILE:N	2.27	0.49
1:3:887:GLN:NE2	1:3:980:GLU:O	2.45	0.49
1:4:246:MET:SD	1:4:246:MET:C	2.95	0.49
1:2:246:MET:SD	1:2:246:MET:C	2.95	0.49
1:3:748:CYS:C	1:3:749:ILE:HD12	2.37	0.49
1:1:651:LEU:C	1:1:651:LEU:HD12	2.37	0.49
1:1:88:SER:HA	1:1:366:VAL:HG21	1.94	0.49
1:1:533:LEU:HD23	1:1:533:LEU:C	2.37	0.49
1:2:542:MET:HE3	1:2:601:PHE:HA	1.95	0.49
1:2:549:PHE:CE2	1:2:620:ALA:HA	2.48	0.49
1:3:506:VAL:CG1	1:3:521:LYS:HE3	2.42	0.49
1:3:699:ARG:HD2	1:3:714:ILE:HD13	1.94	0.49
1:4:433:LEU:HB3	1:4:434:PRO:HD3	1.95	0.49
1:4:777:LEU:HG	1:4:889:ALA:HA	1.94	0.49
1:4:843:GLN:HA	1:4:847:LYS:O	2.12	0.49
1:2:1011:ALA:HB3	1:2:1014:TYR:CZ	2.48	0.49
1:4:751:LEU:HD21	1:4:860:GLY:O	2.13	0.49
1:2:730:LEU:HD12	1:2:730:LEU:N	2.27	0.49
1:1:153:TRP:HB2	1:1:185:ALA:HB3	1.95	0.49
1:3:225:PHE:HA	1:3:243:GLU:O	2.13	0.49
1:4:66:PRO:HG2	1:4:67:GLU:OE1	2.13	0.49
1:4:687:GLN:NE2	1:4:687:GLN:N	2.55	0.49
1:2:334:GLU:OE1	1:2:336:ARG:NH1	2.45	0.49
1:4:377:LEU:HD22	1:4:708:TRP:HA	1.94	0.48
1:4:730:LEU:HD12	1:4:730:LEU:H	1.77	0.48
1:2:754:LYS:HZ1	1:2:1022:GLN:NE2	2.11	0.48
1:2:473:ARG:NH1	1:2:477:SER:HB2	2.27	0.48
1:3:777:LEU:CD1	1:3:980:GLU:HG2	2.43	0.48
1:4:942:ARG:HA	1:4:953:GLY:O	2.14	0.48
1:2:367:MET:HB3	1:2:372:MET:HE2	1.96	0.48
1:2:499:ILE:HG22	1:2:501:PRO:HD3	1.95	0.48
1:1:636:ILE:HD13	1:1:698:VAL:HG11	1.95	0.48
1:2:863:GLN:OE1	1:2:952:ARG:NH2	2.47	0.48
1:4:100:TYR:CZ	1:4:602:CYS:HB3	2.48	0.48
1:4:801:ILE:HD12	1:4:801:ILE:N	2.28	0.48
1:1:241:GLU:HG2	1:1:292:ARG:HG2	1.95	0.48
1:1:797:GLU:C	1:1:799:THR:H	2.22	0.48
1:2:354:VAL:CG1	1:2:379:MET:HE3	2.44	0.48
1:4:656:VAL:HG21	1:4:685:LEU:HD13	1.94	0.48
1:4:768:MET:HE1	1:4:1020:TRP:CH2	2.47	0.48
1:4:199:ASP:C	1:4:416:GLU:HG2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:630:ARG:HB3	1:3:630:ARG:NH1	2.28	0.48
1:3:930:VAL:O	1:3:932:PRO:HD3	2.12	0.48
1:4:225:PHE:HA	1:4:243:GLU:O	2.14	0.48
1:4:595:THR:HA	1:4:596:PRO:C	2.39	0.48
1:1:361:PRO:HB3	1:1:609:ALA:HB1	1.96	0.48
1:2:651:LEU:HD12	1:2:651:LEU:O	2.14	0.48
1:2:890:GLN:OE1	1:2:947:GLY:HA3	2.13	0.48
1:4:105:TYR:CE1	1:4:199:ASP:HB2	2.49	0.47
1:4:968:MET:HG2	5:4:5029:DMS:H12	1.96	0.47
1:2:734:SER:HB2	1:2:860:GLY:HA3	1.95	0.47
1:3:52:ARG:O	1:3:213:SER:HB2	2.14	0.47
1:4:952:ARG:NH1	1:4:952:ARG:HB2	2.29	0.47
1:2:84:VAL:HG12	5:2:5014:DMS:H22	1.96	0.47
1:2:610:ASP:O	1:2:611:ARG:HB2	2.14	0.47
1:4:50:GLN:HG2	6:4:4738:HOH:O	2.13	0.47
1:4:533:LEU:C	1:4:533:LEU:HD23	2.38	0.47
1:2:754:LYS:NZ	1:2:1022:GLN:NE2	2.62	0.47
1:1:734:SER:HB2	1:1:860:GLY:HA3	1.97	0.47
1:1:773:LYS:HG2	1:1:774:LYS:N	2.29	0.47
1:4:52:ARG:O	1:4:213:SER:HB2	2.15	0.47
1:2:240:LEU:C	1:2:240:LEU:HD23	2.40	0.47
1:2:311:ALA:HB2	1:2:330:VAL:HG21	1.95	0.47
1:2:661:LYS:O	1:2:663:LEU:HD22	2.15	0.47
1:2:748:CYS:C	1:2:749:ILE:HD12	2.39	0.47
1:3:606:LEU:O	1:3:614:HIS:HB2	2.14	0.47
1:3:646:HIS:CE1	1:3:673:ALA:HB2	2.50	0.47
1:3:730:LEU:N	1:3:730:LEU:HD12	2.30	0.47
1:3:730:LEU:HD21	1:4:823:LEU:O	2.15	0.47
1:3:755:ARG:HB3	1:3:769:TRP:HB2	1.97	0.47
1:3:890:GLN:OE1	1:3:947:GLY:HA3	2.15	0.47
1:2:851:ILE:HB	1:2:871:GLU:HB2	1.97	0.47
5:3:5034:DMS:H22	1:4:875:ASP:CB	2.44	0.47
1:4:147:ASN:HA	1:4:148:SER:HA	1.62	0.47
1:2:358:GLU:HB3	1:2:367:MET:HG2	1.97	0.47
1:2:786:ARG:NH2	1:2:991:MET:HE2	2.30	0.47
1:3:595:THR:HA	1:3:596:PRO:C	2.40	0.47
1:3:789:LEU:HD11	1:3:993:ILE:HG22	1.97	0.47
1:4:742:THR:HG22	1:4:743:SER:N	2.30	0.47
1:1:499:ILE:HG22	1:1:501:PRO:HD3	1.97	0.47
1:4:952:ARG:CB	1:4:952:ARG:HH11	2.28	0.47
1:1:433:LEU:HB3	1:1:434:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:782:ASP:HA	1:2:884:LEU:HD23	1.97	0.46
1:3:80:GLU:CD	1:3:80:GLU:H	2.21	0.46
1:3:427:THR:HG21	1:3:462:SER:HB3	1.98	0.46
1:1:340:GLY:O	1:1:532:PRO:HB3	2.16	0.46
1:2:225:PHE:HA	1:2:243:GLU:O	2.15	0.46
1:2:352:ARG:HG2	1:2:553:TRP:CH2	2.50	0.46
1:2:995:GLY:C	1:2:997:ASP:N	2.72	0.46
1:3:433:LEU:HB3	1:3:434:PRO:HD3	1.96	0.46
1:4:257:THR:HA	1:4:270:GLY:O	2.16	0.46
1:1:59:ARG:HB2	1:1:124:SER:OG	2.15	0.46
1:3:237:ARG:NH1	1:3:237:ARG:CB	2.75	0.46
1:2:804:ASN:ND2	1:2:1001:PRO:HG2	2.30	0.46
1:3:100:TYR:CZ	1:3:602:CYS:HB3	2.51	0.46
1:3:478:VAL:HB	5:3:5018:DMS:H22	1.98	0.46
1:1:147:ASN:HA	1:1:148:SER:HA	1.63	0.46
1:3:100:TYR:CE1	1:3:602:CYS:HB3	2.50	0.46
1:3:153:TRP:HB2	1:3:185:ALA:HB3	1.97	0.46
1:3:340:GLY:O	1:3:532:PRO:HB3	2.15	0.46
1:4:373:VAL:O	1:4:377:LEU:HG	2.16	0.46
1:4:674:PRO:O	1:4:675:GLN:HB2	2.16	0.46
1:4:844:HIS:ND1	1:4:845:GLN:HG2	2.31	0.46
1:1:472:TYR:O	1:1:476:LYS:HG2	2.16	0.46
1:2:245:GLN:HG2	1:2:288:ARG:CG	2.42	0.46
1:1:800:ARG:C	1:1:801:ILE:HD12	2.41	0.46
1:3:653:HIS:HB3	6:3:4793:HOH:O	2.15	0.46
1:4:748:CYS:C	1:4:749:ILE:HD12	2.40	0.46
1:3:995:GLY:C	1:3:997:ASP:N	2.73	0.46
1:4:464:HIS:HB2	1:4:489:GLY:HA3	1.98	0.46
1:1:756:TRP:CD2	1:1:858:ILE:HD13	2.51	0.46
1:2:319:ASP:OD2	1:2:319:ASP:C	2.58	0.46
1:3:147:ASN:HB3	1:3:206:SER:HA	1.97	0.46
1:3:722:LEU:HA	5:3:5034:DMS:H12	1.98	0.46
1:4:390:SER:HA	1:4:391:HIS:HA	1.70	0.46
1:1:240:LEU:C	1:1:240:LEU:HD23	2.40	0.45
1:3:416:GLU:HA	1:3:460:ASN:O	2.16	0.45
1:4:90:TRP:NE1	1:4:96:ASP:OD2	2.36	0.45
1:1:334:GLU:OE1	1:1:336:ARG:NH1	2.43	0.45
1:3:890:GLN:NE2	1:3:948:PRO:HD3	2.30	0.45
1:4:19:PRO:HD3	1:4:112:PRO:CB	2.46	0.45
1:4:952:ARG:HB2	1:4:952:ARG:HH11	1.81	0.45
1:2:637:GLU:HB2	5:2:5033:DMS:H12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:147:ASN:HA	1:2:148:SER:HA	1.60	0.45
1:3:525:SER:O	1:4:561:ARG:HD3	2.16	0.45
1:2:37:ARG:NH1	5:2:5024:DMS:H11	2.31	0.45
1:2:367:MET:CE	1:2:372:MET:HG3	2.47	0.45
1:3:463:GLY:HA2	6:3:4559:HOH:O	2.16	0.45
1:4:687:GLN:H	1:4:687:GLN:HE21	1.59	0.45
1:1:635:THR:OG1	1:1:681:GLU:HG3	2.17	0.45
1:3:19:PRO:HD3	1:3:112:PRO:CB	2.46	0.45
1:3:143:PHE:O	1:3:168:PRO:HA	2.16	0.45
1:3:377:LEU:HD22	1:3:708:TRP:HA	1.99	0.45
1:4:178:ARG:HG2	1:4:182:ASN:OD1	2.17	0.45
1:4:524:LEU:HD11	1:4:562:LEU:HG	1.99	0.45
1:4:658:LEU:HD11	1:4:692:GLY:HA3	1.99	0.45
1:2:773:LYS:HD3	6:2:4925:HOH:O	2.16	0.45
1:3:786:ARG:NH2	1:3:991:MET:HE2	2.32	0.45
1:4:231:PHE:CD1	1:4:231:PHE:N	2.85	0.45
1:1:610:ASP:O	1:1:611:ARG:HB2	2.17	0.45
1:2:88:SER:HA	1:2:366:VAL:HG21	1.98	0.45
1:3:764:PHE:CE2	1:3:781:ARG:NH1	2.85	0.45
1:3:768:MET:O	1:3:775:GLN:HG2	2.16	0.45
1:4:568:TRP:CD2	1:4:569:ASP:HB3	2.52	0.45
1:1:577:LYS:O	1:1:584:PRO:HA	2.18	0.44
1:2:843:GLN:HG2	1:2:848:THR:HA	1.98	0.44
1:3:246:MET:SD	1:3:246:MET:C	3.00	0.44
1:3:568:TRP:CD2	1:3:569:ASP:HB3	2.51	0.44
1:3:777:LEU:HG	1:3:889:ALA:HA	1.99	0.44
1:4:354:VAL:CG1	1:4:379:MET:HE3	2.47	0.44
1:4:864:MET:HE3	1:4:866:ILE:HD11	1.99	0.44
1:1:782:ASP:HA	1:1:884:LEU:HD23	1.98	0.44
1:2:390:SER:HA	1:2:391:HIS:HA	1.81	0.44
1:3:673:ALA:HB1	1:3:674:PRO:HD2	1.99	0.44
1:4:80:GLU:CD	1:4:80:GLU:H	2.25	0.44
1:4:965:GLN:O	1:4:969:GLU:HG3	2.17	0.44
1:1:377:LEU:HD22	1:1:708:TRP:HA	1.99	0.44
1:4:223:SER:O	1:4:224:ASP:HB2	2.17	0.44
1:4:390:SER:HB2	1:4:391:HIS:CE1	2.53	0.44
1:1:100:TYR:CE1	1:1:602:CYS:HB3	2.53	0.44
1:3:995:GLY:O	1:3:996:ASP:C	2.60	0.44
1:4:653:HIS:HB3	1:4:699:ARG:NH1	2.32	0.44
1:2:548:GLY:HA2	6:2:4069:HOH:O	2.18	0.44
1:2:930:VAL:O	1:2:932:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:619:GLU:HA	1:4:912:ALA:HB2	2.00	0.44
1:3:472:TYR:O	1:3:476:LYS:HG2	2.17	0.44
1:4:663:LEU:CD1	1:4:686:PRO:HG2	2.48	0.44
1:1:965:GLN:O	1:1:969:GLU:HG3	2.17	0.44
1:2:427:THR:HG21	1:2:462:SER:HB3	2.00	0.44
1:3:131:GLU:HG3	1:3:135:GLN:HG3	1.98	0.44
1:2:749:ILE:HD12	1:2:749:ILE:N	2.33	0.44
1:4:166:ARG:HG3	1:4:392:TYR:CB	2.47	0.44
1:1:49:GLN:OE1	1:1:49:GLN:HA	2.17	0.43
1:1:561:ARG:HD3	1:2:525:SER:O	2.18	0.43
1:3:615:PRO:O	1:3:618:THR:HG22	2.18	0.43
1:1:73:TRP:CE2	1:1:122:CYS:HB3	2.53	0.43
1:1:80:GLU:CD	1:1:80:GLU:H	2.25	0.43
1:1:100:TYR:CZ	1:1:602:CYS:HB3	2.53	0.43
1:1:613:PRO:HB3	1:1:617:LEU:HD23	2.00	0.43
1:2:651:LEU:HD23	1:2:703:PRO:HG3	1.99	0.43
1:2:995:GLY:O	1:2:996:ASP:C	2.62	0.43
1:1:525:SER:O	1:2:561:ARG:HD3	2.19	0.43
1:2:240:LEU:CD1	1:2:260:LEU:HD13	2.48	0.43
1:2:400:THR:HA	6:2:4148:HOH:O	2.18	0.43
1:2:755:ARG:HD3	1:2:769:TRP:CE3	2.53	0.43
1:3:843:GLN:HG2	1:3:848:THR:HA	1.99	0.43
1:4:196:TYR:O	1:4:417:THR:HG22	2.19	0.43
1:1:695:TRP:HZ3	5:1:5019:DMS:H13	1.84	0.43
1:1:873:ALA:O	1:1:876:THR:HG22	2.18	0.43
1:1:809:ARG:HD2	6:1:4886:HOH:O	2.19	0.43
1:4:379:MET:HE1	1:4:387:VAL:HB	2.00	0.43
1:1:37:ARG:NH1	5:1:5023:DMS:H22	2.34	0.43
1:1:546:LEU:HA	6:1:4128:HOH:O	2.18	0.43
1:2:546:LEU:HA	6:2:4129:HOH:O	2.18	0.43
1:3:87:PRO:HB2	1:3:209:PHE:C	2.43	0.43
1:3:166:ARG:HG3	1:3:392:TYR:HB2	2.00	0.43
1:4:579:ASP:OD1	1:4:579:ASP:C	2.62	0.43
1:3:457:SER:HA	1:3:485:GLN:O	2.19	0.43
1:4:348:PRO:HG2	6:4:4309:HOH:O	2.19	0.43
1:1:131:GLU:O	1:1:135:GLN:HG3	2.19	0.43
1:1:429:ASP:OD1	1:1:431:ARG:HG3	2.19	0.43
1:4:237:ARG:HH11	1:4:237:ARG:CB	2.30	0.43
1:1:301:TRP:CH2	1:1:452:SER:HA	2.54	0.43
1:2:163:GLN:O	1:2:164:ASP:HB3	2.19	0.43
1:2:784:PHE:HA	1:2:881:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:291:LEU:HD22	1:3:291:LEU:N	2.34	0.43
1:3:802:ASP:OD2	1:3:804:ASN:HB3	2.18	0.43
1:1:581:ASN:HB2	1:1:583:ASN:ND2	2.34	0.42
1:3:824:GLN:HG2	1:3:825:CYS:N	2.33	0.42
1:1:730:LEU:HD12	1:1:730:LEU:H	1.84	0.42
1:1:755:ARG:HB2	1:1:769:TRP:HB2	2.01	0.42
1:1:843:GLN:HA	1:1:847:LYS:O	2.19	0.42
1:2:749:ILE:HB	1:2:756:TRP:HB2	2.00	0.42
1:3:815:HIS:HD2	1:3:849:LEU:HD13	1.85	0.42
1:3:830:LEU:CD2	1:4:830:LEU:HD21	2.49	0.42
1:1:524:LEU:HD11	1:1:562:LEU:HG	2.01	0.42
1:2:13:ARG:O	1:2:14:ARG:C	2.62	0.42
1:2:337:ILE:HA	1:2:341:LEU:O	2.18	0.42
1:2:542:MET:CE	1:2:601:PHE:HA	2.49	0.42
1:2:777:LEU:HG	1:2:889:ALA:HA	2.02	0.42
1:3:231:PHE:CD1	1:3:231:PHE:N	2.86	0.42
1:3:613:PRO:HB3	1:3:617:LEU:HD23	2.01	0.42
1:4:333:ARG:HA	1:4:345:ASN:OD1	2.19	0.42
1:1:128:ASN:HA	1:1:180:GLY:O	2.20	0.42
1:2:440:VAL:HG13	1:2:475:ILE:HD11	2.01	0.42
1:1:390:SER:HA	1:1:391:HIS:HA	1.80	0.42
1:1:730:LEU:HD12	1:1:730:LEU:N	2.34	0.42
1:4:899:GLY:HA2	1:4:915:PHE:CD1	2.54	0.42
1:4:955:PHE:CD1	1:4:986:ILE:HG23	2.54	0.42
1:1:19:PRO:HD3	1:1:112:PRO:CB	2.50	0.42
1:1:163:GLN:O	1:1:164:ASP:HB3	2.20	0.42
1:4:958:ASN:C	1:4:958:ASN:OD1	2.62	0.42
1:1:92:MET:HE2	1:1:92:MET:HA	2.00	0.42
1:1:933:SER:O	1:1:934:GLU:C	2.62	0.42
1:1:1020:TRP:HD1	1:1:1021:CYS:N	2.18	0.42
1:2:166:ARG:HG3	1:2:392:TYR:CB	2.50	0.42
1:3:652:LEU:O	1:3:667:GLU:HA	2.20	0.42
1:1:568:TRP:CD2	1:1:569:ASP:HB3	2.55	0.42
1:1:580:GLU:OE1	1:1:580:GLU:HA	2.19	0.42
1:2:200:GLN:HG2	1:2:391:HIS:HB2	2.02	0.42
1:3:59:ARG:HB2	1:3:124:SER:OG	2.20	0.42
1:2:867:THR:HG23	1:2:1015:HIS:HE1	1.85	0.42
1:4:352:ARG:HG2	1:4:553:TRP:CH2	2.55	0.42
1:1:200:GLN:HG2	1:1:391:HIS:HB2	2.02	0.42
1:1:283:GLY:HA3	5:1:5029:DMS:C1	2.48	0.42
1:2:340:GLY:O	1:2:532:PRO:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:782:ASP:HB2	1:2:842:TRP:CZ2	2.55	0.42
1:2:842:TRP:HZ3	1:2:852:SER:HB3	1.84	0.42
1:3:723:ALA:N	5:3:5034:DMS:H23	2.34	0.42
1:4:737:ILE:HA	1:4:738:PRO:HD3	1.91	0.42
1:1:619:GLU:HA	1:1:912:ALA:HB2	2.02	0.41
1:3:316:HIS:HB2	1:3:321:THR:O	2.20	0.41
1:1:502:MET:HA	1:1:537:GLU:O	2.20	0.41
1:3:127:PHE:CD1	1:3:127:PHE:N	2.88	0.41
1:3:367:MET:HB3	1:3:372:MET:HE2	2.01	0.41
1:3:793:ILE:HA	1:3:807:VAL:HG11	2.02	0.41
1:1:955:PHE:HB2	1:1:987:ASP:O	2.21	0.41
1:3:745:MET:O	1:3:746:ASP:CG	2.64	0.41
1:4:59:ARG:HB2	1:4:124:SER:OG	2.20	0.41
1:4:767:GLN:HA	1:4:776:LEU:HD12	2.01	0.41
1:1:587:ALA:HB1	1:1:591:ASP:CB	2.50	0.41
1:4:79:PRO:HD2	1:4:80:GLU:OE2	2.21	0.41
1:2:500:CYS:HA	1:2:534:ILE:O	2.21	0.41
1:2:505:ARG:O	1:2:519:SER:HA	2.20	0.41
1:2:658:LEU:N	1:2:663:LEU:CD2	2.83	0.41
1:2:699:ARG:HE	1:2:699:ARG:HB3	1.67	0.41
1:3:454:ILE:HG13	1:3:455:ILE:HG13	2.02	0.41
1:3:1006:GLU:HG2	1:3:1007:PHE:CD2	2.56	0.41
1:1:695:TRP:CZ3	5:1:5019:DMS:H13	2.55	0.41
1:2:146:VAL:HG11	1:2:150:PHE:CD1	2.55	0.41
1:3:782:ASP:OD1	1:3:842:TRP:HH2	2.04	0.41
1:4:696:LEU:HB2	1:4:722:LEU:HD11	2.02	0.41
1:3:163:GLN:O	1:3:164:ASP:HB3	2.21	0.41
1:3:354:VAL:CG1	1:3:379:MET:HE3	2.51	0.41
1:3:429:ASP:OD1	1:3:431:ARG:HG3	2.21	0.41
1:3:793:ILE:HA	1:3:807:VAL:CG1	2.50	0.41
1:4:127:PHE:CE1	1:4:184:LEU:HG	2.56	0.41
1:1:86:VAL:HG13	1:1:87:PRO:HA	2.02	0.41
1:1:333:ARG:HA	1:1:345:ASN:OD1	2.21	0.41
1:1:746:ASP:OD1	1:1:759:ASN:HA	2.21	0.41
1:2:501:PRO:HB3	1:2:523:TRP:CZ3	2.56	0.41
1:2:703:PRO:O	1:2:711:ALA:HB1	2.20	0.41
1:4:73:TRP:CE2	1:4:122:CYS:HB3	2.55	0.41
1:4:441:THR:O	1:4:445:GLN:HG3	2.21	0.41
1:4:650:GLU:HB3	1:4:670:LEU:HD12	2.03	0.41
1:1:755:ARG:O	1:1:768:MET:HA	2.21	0.41
1:2:454:ILE:O	1:2:483:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:754:LYS:HA	1:1:769:TRP:O	2.22	0.40
1:1:794:GLY:HA2	1:1:998:SER:O	2.22	0.40
1:1:1011:ALA:HB3	1:1:1014:TYR:CZ	2.56	0.40
1:2:658:LEU:H	1:2:663:LEU:CD2	2.34	0.40
1:2:869:ASP:OD1	1:2:1015:HIS:ND1	2.50	0.40
1:3:360:HIS:CE1	1:3:362:LEU:HB2	2.56	0.40
1:4:287:ASP:OD1	1:4:287:ASP:N	2.51	0.40
1:4:652:LEU:O	1:4:667:GLU:HA	2.21	0.40
1:4:701:VAL:O	1:4:703:PRO:HD3	2.21	0.40
1:2:127:PHE:CD1	1:2:127:PHE:N	2.89	0.40
1:2:598:ASP:OD1	1:2:797:GLU:HA	2.21	0.40
1:2:699:ARG:HD2	6:2:4846:HOH:O	2.19	0.40
1:4:991:MET:CE	1:4:1003:VAL:HG21	2.50	0.40
1:1:292:ARG:HG3	1:1:292:ARG:HH11	1.86	0.40
1:1:372:MET:HE1	1:1:395:HIS:CG	2.55	0.40
1:4:499:ILE:HG22	1:4:501:PRO:HD3	2.03	0.40
1:2:807:VAL:HG13	1:2:808:GLU:N	2.36	0.40
1:4:482:ARG:HA	1:4:483:PRO:HD3	1.95	0.40
1:4:549:PHE:CE2	1:4:620:ALA:HA	2.56	0.40
1:4:568:TRP:HA	1:4:569:ASP:HA	1.80	0.40
1:4:664:ALA:CB	1:4:685:LEU:HD22	2.51	0.40
1:4:968:MET:CG	5:4:5029:DMS:H12	2.51	0.40
1:1:753:ASN:HB2	1:1:771:GLY:HA2	2.02	0.40
1:1:883:GLY:HA3	1:1:987:ASP:HA	2.04	0.40
1:2:13:ARG:NH1	1:3:13:ARG:HD2	2.37	0.40
1:3:240:LEU:HD13	1:3:260:LEU:HD13	2.02	0.40
1:4:416:GLU:HA	1:4:460:ASN:O	2.22	0.40

There are no symmetry-related clashes.

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	1	1009/1052 (96%)	968 (96%)	40 (4%)	1 (0%)	48	57
1	2	1009/1052 (96%)	958 (95%)	51 (5%)	0	100	100
1	3	1009/1052 (96%)	966 (96%)	43 (4%)	0	100	100
1	4	1009/1052 (96%)	958 (95%)	51 (5%)	0	100	100
All	All	4036/4208 (96%)	3850 (95%)	185 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	798	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	1	863/897 (96%)	859 (100%)	4 (0%)	81	90
1	2	863/897 (96%)	861 (100%)	2 (0%)	87	94
1	3	863/897 (96%)	857 (99%)	6 (1%)	76	87
1	4	863/897 (96%)	857 (99%)	6 (1%)	76	87
All	All	3452/3588 (96%)	3434 (100%)	18 (0%)	81	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	519	SER
1	1	546	LEU
1	1	774	LYS
1	1	1017	GLN
1	2	519	SER
1	2	546	LEU
1	3	46	ARG
1	3	80	GLU
1	3	519	SER
1	3	546	LEU

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Mol	Chain	Res	Type
1	3	761	GLN
1	3	773	LYS
1	4	80	GLU
1	4	519	SER
1	4	546	LEU
1	4	663	LEU
1	4	687	GLN
1	4	772	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	50	GLN
1	1	128	ASN
1	1	262	GLN
1	1	266	GLN
1	1	294	ASN
1	1	365	GLN
1	1	485	GLN
1	1	558	GLN
1	1	583	ASN
1	1	653	HIS
1	1	817	GLN
1	1	843	GLN
1	1	890	GLN
1	1	977	HIS
1	1	1017	GLN
1	1	1022	GLN
1	2	50	GLN
1	2	163	GLN
1	2	226	HIS
1	2	262	GLN
1	2	365	GLN
1	2	485	GLN
1	2	646	HIS
1	2	739	HIS
1	2	804	ASN
1	2	844	HIS
1	2	845	GLN
1	2	950	GLN
1	2	965	GLN
1	2	1022	GLN

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Mol	Chain	Res	Type
1	3	128	ASN
1	3	226	HIS
1	3	294	ASN
1	3	383	ASN
1	3	464	HIS
1	3	485	GLN
1	3	624	GLN
1	3	646	HIS
1	3	844	HIS
1	3	878	HIS
1	3	903	GLN
1	3	965	GLN
1	3	1008	GLN
1	3	1022	GLN
1	4	163	GLN
1	4	294	ASN
1	4	363	HIS
1	4	464	HIS
1	4	485	GLN
1	4	558	GLN
1	4	687	GLN
1	4	757	GLN
1	4	804	ASN
1	4	863	GLN
1	4	885	ASN
1	4	1022	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 153 ligands modelled in this entry, 27 are monoatomic - leaving 126 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	$\# Z > 2$
2	149	1	2001	4	12,12,12	1.08	1 (8%)	15,17,17	0.85	0
5	DMS	2	5028	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	3	5013	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	4	5026	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	2	5019	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	5018	-	3,3,3	0.25	0	3,3,3	0.65	0
5	DMS	4	5023	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	5006	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	2	5009	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	1	5006	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	2	5033	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	1	5019	-	3,3,3	0.23	0	3,3,3	0.65	0
5	DMS	3	5002	-	3,3,3	0.20	0	3,3,3	0.62	0
5	DMS	2	5002	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	1024	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	5005	-	3,3,3	0.27	0	3,3,3	0.60	0
5	DMS	1	5013	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	1	5026	-	3,3,3	0.17	0	3,3,3	0.55	0
5	DMS	2	5014	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	4	5012	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	3	5018	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	1	5029	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	2	5016	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	5015	-	3,3,3	0.21	0	3,3,3	0.64	0
5	DMS	1	5016	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	3	5004	-	3,3,3	0.22	0	3,3,3	0.65	0
5	DMS	4	5013	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	2	5003	-	3,3,3	0.27	0	3,3,3	0.65	0
5	DMS	4	5001	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	2	5012	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	1	5017	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	5027	-	3,3,3	0.25	0	3,3,3	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	1	5011	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	4	5005	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	4	5002	-	3,3,3	0.17	0	3,3,3	0.57	0
5	DMS	2	5008	-	3,3,3	0.22	0	3,3,3	0.66	0
5	DMS	2	5022	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	4	5009	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	5015	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	1	5003	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	3	5019	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	2	5027	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	4	5017	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	5029	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	2	5029	-	3,3,3	0.28	0	3,3,3	0.61	0
5	DMS	1	5022	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	4	5004	-	3,3,3	0.23	0	3,3,3	0.65	0
5	DMS	3	5023	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	2	5004	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	3	5016	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	1	5007	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	2	5024	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	3	5025	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	5017	-	3,3,3	0.23	0	3,3,3	0.66	0
5	DMS	3	5033	-	3,3,3	0.31	0	3,3,3	0.62	0
5	DMS	1	5009	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	4	5022	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	4	5030	-	3,3,3	0.28	0	3,3,3	0.55	0
5	DMS	2	1024	-	3,3,3	0.27	0	3,3,3	0.65	0
5	DMS	3	5012	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	5012	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	2	5010	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	3	5034	-	3,3,3	0.25	0	3,3,3	0.65	0
5	DMS	3	5022	-	3,3,3	0.21	0	3,3,3	0.63	0
5	DMS	3	5030	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	4	5028	-	3,3,3	0.33	0	3,3,3	0.59	0
5	DMS	2	5005	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	2	5011	-	3,3,3	0.25	0	3,3,3	0.59	0
5	DMS	1	5010	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	3	5003	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	1	5025	-	3,3,3	0.15	0	3,3,3	0.54	0
5	DMS	3	5028	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	1	5014	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	1	5028	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	2	5032	-	3,3,3	0.26	0	3,3,3	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	2	5001	-	3,3,3	0.27	0	3,3,3	0.66	0
5	DMS	2	5030	-	3,3,3	0.12	0	3,3,3	0.57	0
5	DMS	2	5020	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	1	5001	-	3,3,3	0.22	0	3,3,3	0.66	0
5	DMS	1	5021	-	3,3,3	0.28	0	3,3,3	0.61	0
5	DMS	3	5005	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	4	5010	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	4	5019	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	4	5024	-	3,3,3	0.22	0	3,3,3	0.65	0
5	DMS	1	5020	-	3,3,3	0.21	0	3,3,3	0.63	0
5	DMS	1	5002	-	3,3,3	0.19	0	3,3,3	0.63	0
5	DMS	1	5008	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	5007	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	5025	-	3,3,3	0.27	0	3,3,3	0.60	0
5	DMS	2	5006	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	1	5024	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	5009	-	3,3,3	0.25	0	3,3,3	0.63	0
2	149	4	2001	4	12,12,12	0.91	1 (8%)	15,17,17	0.81	0
5	DMS	4	5008	-	3,3,3	0.27	0	3,3,3	0.63	0
5	DMS	3	5024	-	3,3,3	0.25	0	3,3,3	0.65	0
5	DMS	4	5006	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	4	5021	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	3	5017	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	5026	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	4	5014	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	4	5003	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	4	5020	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	3	5020	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	3	5008	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	5010	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	1	5015	-	3,3,3	0.26	0	3,3,3	0.66	0
5	DMS	4	5016	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	3	5014	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	4	5027	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	3	5011	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	5031	-	3,3,3	0.25	0	3,3,3	0.66	0
5	DMS	2	5031	-	3,3,3	0.28	0	3,3,3	0.64	0
5	DMS	2	5023	-	3,3,3	0.24	0	3,3,3	0.66	0
5	DMS	3	5032	-	3,3,3	0.14	0	3,3,3	0.65	0
5	DMS	1	5018	4	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	1	5023	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	3	5001	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	3	5021	4	3,3,3	0.23	0	3,3,3	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	2	5021	4	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	4	5011	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	4	5007	-	3,3,3	0.24	0	3,3,3	0.62	0
2	149	3	2001	4	12,12,12	1.10	1 (8%)	15,17,17	0.75	0
5	DMS	2	5025	-	3,3,3	0.24	0	3,3,3	0.64	0
2	149	2	2001	4	12,12,12	1.20	2 (16%)	15,17,17	0.81	0
5	DMS	1	5004	-	3,3,3	0.23	0	3,3,3	0.65	0
5	DMS	4	5029	-	3,3,3	0.24	0	3,3,3	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	149	3	2001	4	-	1/2/22/22	0/1/1/1
2	149	2	2001	4	-	1/2/22/22	0/1/1/1
2	149	4	2001	4	-	1/2/22/22	0/1/1/1
2	149	1	2001	4	-	1/2/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2001	149	O5-C1	2.84	1.38	1.34
2	1	2001	149	O5-C1	2.58	1.38	1.34
2	3	2001	149	O5-C1	2.46	1.38	1.34
2	2	2001	149	O5-C5	2.27	1.49	1.46
2	4	2001	149	O5-C1	2.25	1.38	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3	2001	149	O5-C5-C6-O6
2	2	2001	149	O5-C5-C6-O6
2	1	2001	149	O5-C5-C6-O6
2	4	2001	149	O5-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	3	5006	DMS	1	0
5	2	5033	DMS	2	0
5	1	5019	DMS	2	0
5	2	5014	DMS	1	0
5	4	5012	DMS	1	0
5	3	5018	DMS	1	0
5	1	5029	DMS	4	0
5	2	5024	DMS	1	0
5	1	5012	DMS	2	0
5	3	5034	DMS	4	0
5	3	5030	DMS	1	0
5	2	5030	DMS	2	0
5	1	5023	DMS	1	0
5	4	5029	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	1	1011/1052 (96%)	-0.31	10 (0%) 79 77	13, 25, 46, 74	0
1	2	1011/1052 (96%)	-0.39	11 (1%) 78 76	13, 24, 45, 75	0
1	3	1011/1052 (96%)	-0.40	12 (1%) 76 74	14, 24, 45, 75	0
1	4	1011/1052 (96%)	-0.36	15 (1%) 72 69	13, 25, 46, 74	0
All	All	4044/4208 (96%)	-0.37	48 (1%) 76 74	13, 25, 46, 75	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	772	ASP	4.9
1	3	732	ALA	4.8
1	2	731	PRO	3.6
1	2	686	PRO	3.4
1	2	733	ALA	3.2
1	3	689	GLU	3.0
1	2	819	GLU	2.9
1	2	734	SER	2.8
1	4	689	GLU	2.8
1	4	686	PRO	2.8
1	1	686	PRO	2.7
1	2	1023	LYS	2.6
1	1	735	HIS	2.6
1	2	730	LEU	2.6
1	2	745	MET	2.6
1	4	801	ILE	2.6
1	4	735	HIS	2.5
1	2	1022	GLN	2.5
1	4	319	ASP	2.4
1	3	730	LEU	2.4
1	4	630	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	3	733	ALA	2.4
1	3	735	HIS	2.3
1	1	730	LEU	2.3
1	3	734	SER	2.3
1	1	684	GLU	2.3
1	1	795	VAL	2.3
1	1	130	ASP	2.2
1	4	748	CYS	2.2
1	3	686	PRO	2.2
1	3	1023	LYS	2.2
1	4	663	LEU	2.2
1	4	685	LEU	2.2
1	3	731	PRO	2.2
1	2	801	ILE	2.2
1	4	730	LEU	2.1
1	3	685	LEU	2.1
1	2	732	ALA	2.1
1	1	689	GLU	2.1
1	3	799	THR	2.1
1	3	798	ALA	2.1
1	4	653	HIS	2.1
1	1	736	ALA	2.0
1	4	739	HIS	2.0
1	4	233	ASP	2.0
1	4	731	PRO	2.0
1	1	771	GLY	2.0
1	4	688	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	2	5017	4/4	0.59	0.30	92,92,93,94	0
5	DMS	4	5007	4/4	0.60	0.38	113,113,113,114	0
3	MG	3	3003	1/1	0.66	0.14	78,78,78,78	0
5	DMS	1	5007	4/4	0.68	0.27	90,90,90,91	0
5	DMS	4	5026	4/4	0.72	0.29	102,102,102,102	0
5	DMS	2	5031	4/4	0.74	0.21	61,62,62,63	0
5	DMS	3	5012	4/4	0.74	0.26	108,108,109,109	0
5	DMS	1	5013	4/4	0.75	0.21	96,96,97,97	0
5	DMS	3	5027	4/4	0.76	0.21	79,80,80,80	0
5	DMS	1	5019	4/4	0.77	0.23	82,83,83,83	0
5	DMS	3	5006	4/4	0.77	0.23	85,85,85,86	0
5	DMS	2	5020	4/4	0.78	0.23	69,70,70,70	0
5	DMS	3	5028	4/4	0.78	0.21	83,83,84,84	0
5	DMS	3	5029	4/4	0.79	0.26	81,82,82,82	0
5	DMS	3	5034	4/4	0.79	0.18	66,66,66,67	0
3	MG	4	3003	1/1	0.79	0.13	68,68,68,68	0
5	DMS	3	5016	4/4	0.79	0.22	71,72,72,73	0
5	DMS	1	5021	4/4	0.80	0.26	70,71,72,72	0
5	DMS	4	5023	4/4	0.81	0.22	90,90,90,91	0
5	DMS	1	5024	4/4	0.81	0.18	86,86,86,86	0
5	DMS	2	5021	4/4	0.82	0.22	89,89,89,90	0
5	DMS	3	5018	4/4	0.82	0.21	73,74,75,75	0
5	DMS	3	5024	4/4	0.83	0.22	76,77,77,77	0
5	DMS	1	5028	4/4	0.84	0.18	65,66,66,66	0
5	DMS	3	5033	4/4	0.84	0.18	59,60,61,61	0
5	DMS	4	5024	4/4	0.84	0.22	80,81,81,81	0
5	DMS	2	5025	4/4	0.84	0.22	93,93,93,94	0
5	DMS	2	5028	4/4	0.85	0.15	59,61,61,61	0
5	DMS	3	5014	4/4	0.85	0.20	68,69,70,70	0
5	DMS	4	5013	4/4	0.85	0.18	86,86,86,86	0
5	DMS	4	5016	4/4	0.85	0.18	59,59,61,62	0
5	DMS	3	5015	4/4	0.85	0.15	67,67,67,68	0
5	DMS	1	5022	4/4	0.85	0.19	82,82,82,83	0
5	DMS	3	5017	4/4	0.85	0.17	83,83,84,84	0
5	DMS	2	5006	4/4	0.86	0.19	92,92,92,93	0
5	DMS	1	5009	4/4	0.86	0.17	55,55,55,56	0
5	DMS	3	1024	4/4	0.86	0.19	74,74,75,75	0
5	DMS	4	5010	4/4	0.87	0.20	78,78,78,79	0
5	DMS	3	5009	4/4	0.87	0.20	88,88,89,89	0
5	DMS	2	5010	4/4	0.88	0.17	87,87,87,87	0
5	DMS	2	5015	4/4	0.88	0.17	56,56,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	3	5031	4/4	0.88	0.16	58,59,60,60	0
5	DMS	4	5019	4/4	0.88	0.12	64,64,64,64	0
5	DMS	2	1024	4/4	0.88	0.14	59,60,61,61	0
5	DMS	2	5032	4/4	0.88	0.16	54,54,54,54	0
5	DMS	1	5014	4/4	0.88	0.16	65,65,66,66	0
5	DMS	4	5027	4/4	0.88	0.16	81,82,82,82	0
5	DMS	2	5024	4/4	0.89	0.17	78,78,78,79	0
5	DMS	4	5021	4/4	0.89	0.16	68,68,68,68	0
5	DMS	1	5018	4/4	0.89	0.16	68,68,69,69	0
5	DMS	2	5027	4/4	0.89	0.14	71,71,71,72	0
5	DMS	3	5013	4/4	0.89	0.15	55,56,56,56	0
5	DMS	1	5016	4/4	0.89	0.15	65,65,65,65	0
5	DMS	3	5021	4/4	0.90	0.15	64,64,65,66	0
4	NA	1	3104	1/1	0.90	0.08	55,55,55,55	0
5	DMS	4	5014	4/4	0.90	0.18	66,67,67,67	0
5	DMS	2	5033	4/4	0.90	0.13	72,72,73,73	0
5	DMS	1	5006	4/4	0.90	0.18	74,75,75,75	0
5	DMS	4	5020	4/4	0.90	0.15	72,72,72,72	0
5	DMS	1	5015	4/4	0.90	0.14	65,65,66,66	0
5	DMS	2	5023	4/4	0.90	0.19	57,58,58,59	0
5	DMS	1	5025	4/4	0.90	0.16	45,46,47,49	0
5	DMS	3	5019	4/4	0.90	0.15	63,63,64,64	0
5	DMS	3	5020	4/4	0.90	0.17	64,64,64,65	0
5	DMS	3	5004	4/4	0.91	0.14	49,50,52,52	0
5	DMS	1	5012	4/4	0.91	0.12	61,61,62,62	0
5	DMS	3	5007	4/4	0.91	0.14	61,62,62,63	0
5	DMS	4	5017	4/4	0.91	0.16	72,73,73,74	0
5	DMS	3	5008	4/4	0.91	0.15	62,62,63,63	0
5	DMS	1	5017	4/4	0.91	0.13	61,61,61,62	0
4	NA	4	3104	1/1	0.91	0.11	41,41,41,41	0
5	DMS	4	5006	4/4	0.91	0.13	46,47,48,49	0
4	NA	1	3103	1/1	0.91	0.09	47,47,47,47	0
5	DMS	4	5009	4/4	0.91	0.14	60,60,60,61	0
5	DMS	1	5010	4/4	0.91	0.16	71,72,72,72	0
5	DMS	4	5018	4/4	0.92	0.13	72,72,73,73	0
5	DMS	1	5002	4/4	0.92	0.14	45,46,46,47	0
3	MG	2	3003	1/1	0.92	0.06	45,45,45,45	0
5	DMS	3	5030	4/4	0.92	0.16	79,79,80,80	0
5	DMS	2	5029	4/4	0.92	0.12	56,56,57,57	0
5	DMS	3	5022	4/4	0.92	0.12	66,66,66,66	0
5	DMS	1	5029	4/4	0.92	0.14	51,52,53,54	0
5	DMS	2	5026	4/4	0.92	0.14	63,63,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	2	5009	4/4	0.93	0.13	56,56,56,56	0
5	DMS	4	5004	4/4	0.93	0.13	53,53,55,55	0
5	DMS	3	5025	4/4	0.93	0.13	76,76,76,76	0
5	DMS	1	5004	4/4	0.93	0.11	49,50,51,51	0
4	NA	4	3103	1/1	0.93	0.12	34,34,34,34	0
4	NA	2	3104	1/1	0.93	0.06	34,34,34,34	0
4	NA	3	3103	1/1	0.93	0.10	42,42,42,42	0
5	DMS	2	5008	4/4	0.93	0.11	53,54,55,55	0
5	DMS	2	5022	4/4	0.93	0.12	61,61,61,62	0
5	DMS	4	5030	4/4	0.93	0.14	58,59,59,60	0
5	DMS	3	5002	4/4	0.94	0.11	26,29,30,33	0
4	NA	1	3102	1/1	0.94	0.05	29,29,29,29	0
4	NA	3	3104	1/1	0.94	0.05	42,42,42,42	0
5	DMS	4	5022	4/4	0.94	0.11	61,62,62,62	0
5	DMS	3	5032	4/4	0.94	0.13	42,43,44,46	0
5	DMS	2	5019	4/4	0.94	0.12	69,70,70,70	0
5	DMS	1	5020	4/4	0.94	0.11	54,55,55,56	0
5	DMS	2	5004	4/4	0.94	0.12	49,50,51,52	0
5	DMS	4	5028	4/4	0.94	0.13	41,42,42,43	0
5	DMS	4	5029	4/4	0.94	0.11	60,61,61,61	0
5	DMS	2	5014	4/4	0.94	0.11	48,49,49,49	0
5	DMS	2	5002	4/4	0.95	0.10	32,33,34,37	0
5	DMS	4	5025	4/4	0.95	0.11	57,57,58,58	0
5	DMS	4	5012	4/4	0.95	0.10	54,54,54,54	0
5	DMS	1	5026	4/4	0.95	0.10	60,61,61,61	0
3	MG	3	3001	1/1	0.95	0.04	19,19,19,19	0
5	DMS	4	5008	4/4	0.95	0.10	49,50,50,51	0
2	149	1	2001	12/12	0.95	0.07	17,19,21,25	0
2	149	3	2001	12/12	0.96	0.06	16,19,22,25	0
5	DMS	4	5002	4/4	0.96	0.10	39,39,39,39	0
5	DMS	2	5016	4/4	0.96	0.11	54,54,54,55	0
2	149	4	2001	12/12	0.96	0.06	13,17,19,24	0
5	DMS	3	5011	4/4	0.96	0.10	47,49,49,50	0
5	DMS	1	5008	4/4	0.96	0.08	46,47,47,48	0
5	DMS	2	5005	4/4	0.96	0.09	38,38,39,40	0
5	DMS	1	5023	4/4	0.96	0.11	63,63,64,64	0
4	NA	2	3103	1/1	0.96	0.13	29,29,29,29	0
3	MG	1	3002	1/1	0.96	0.07	24,24,24,24	0
5	DMS	1	5011	4/4	0.96	0.09	47,48,49,50	0
5	DMS	2	5012	4/4	0.96	0.08	42,44,44,46	0
2	149	2	2001	12/12	0.96	0.05	13,15,18,24	0
5	DMS	2	5011	4/4	0.97	0.09	38,39,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	2	5030	4/4	0.97	0.08	38,39,39,39	0
3	MG	2	3002	1/1	0.97	0.07	30,30,30,30	0
5	DMS	4	5003	4/4	0.97	0.07	42,42,43,44	0
5	DMS	3	5010	4/4	0.97	0.08	40,41,42,42	0
5	DMS	2	5001	4/4	0.97	0.07	29,29,30,33	0
5	DMS	1	5005	4/4	0.97	0.07	39,39,40,40	0
5	DMS	4	5001	4/4	0.98	0.06	28,30,30,33	0
4	NA	2	3101	1/1	0.98	0.04	18,18,18,18	0
5	DMS	3	5023	4/4	0.98	0.09	46,46,47,47	0
4	NA	1	3101	1/1	0.98	0.04	21,21,21,21	0
5	DMS	3	5001	4/4	0.98	0.06	31,31,31,35	0
5	DMS	1	5001	4/4	0.98	0.05	26,27,28,29	0
3	MG	1	3001	1/1	0.98	0.02	20,20,20,20	0
5	DMS	3	5005	4/4	0.98	0.06	43,43,44,45	0
5	DMS	1	5003	4/4	0.98	0.07	38,39,39,39	0
5	DMS	4	5011	4/4	0.98	0.06	41,41,42,43	0
3	MG	4	3002	1/1	0.98	0.07	25,25,25,25	0
3	MG	3	3002	1/1	0.98	0.08	20,20,20,20	0
4	NA	4	3101	1/1	0.98	0.03	16,16,16,16	0
5	DMS	2	5003	4/4	0.98	0.07	38,38,39,40	0
5	DMS	3	5003	4/4	0.99	0.05	35,36,36,37	0
3	MG	2	3001	1/1	0.99	0.02	22,22,22,22	0
4	NA	4	3102	1/1	0.99	0.02	20,20,20,20	0
4	NA	3	3101	1/1	0.99	0.02	20,20,20,20	0
4	NA	3	3102	1/1	0.99	0.08	24,24,24,24	0
4	NA	2	3102	1/1	0.99	0.04	18,18,18,18	0
3	MG	4	3001	1/1	0.99	0.05	23,23,23,23	0
5	DMS	4	5005	4/4	0.99	0.05	36,36,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.