



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 08:15 am BST

PDB ID : 3MV1
Title : E.Coli (lacZ) beta-galactosidase (R599A) in complex with Guanidinium
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

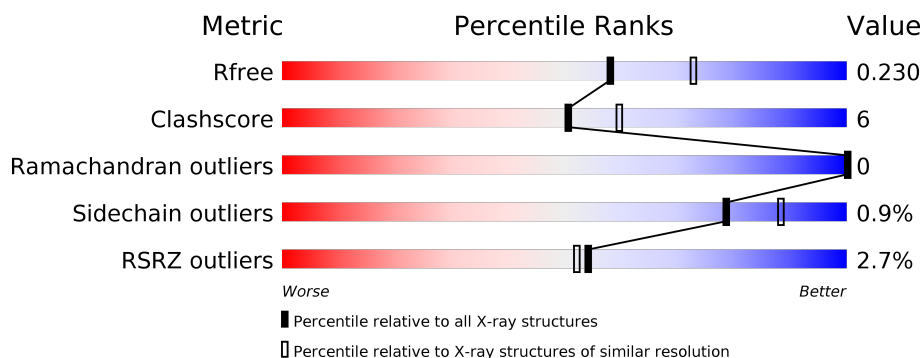
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div></div> </div> <div></div> </div>
1	2	1052	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	3	1052	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	4	1052	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div></div> </div> <div></div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36610 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

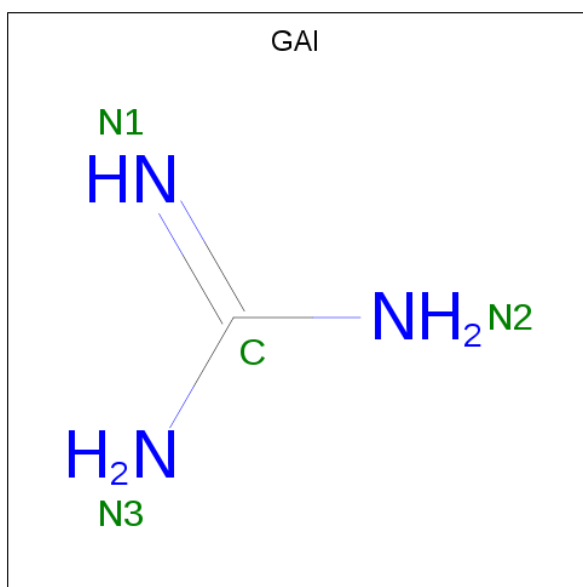
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

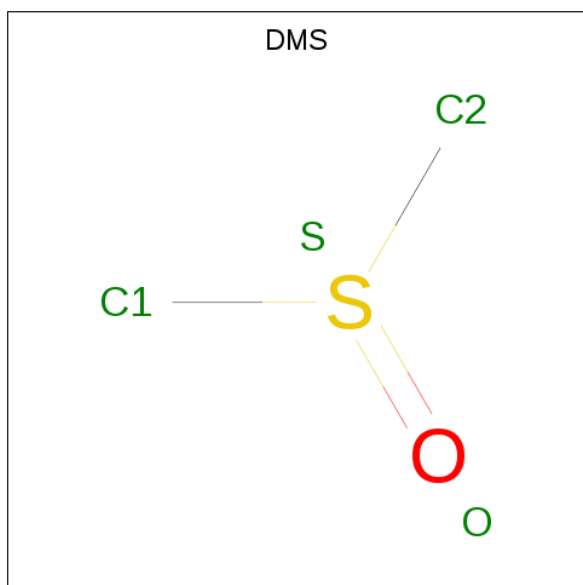
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	2	4	Total Na 4 4	0	0
3	1	4	Total Na 4 4	0	0
3	4	4	Total Na 4 4	0	0
3	3	4	Total Na 4 4	0	0

- Molecule 4 is GUANIDINE (three-letter code: GAI) (formula: CH₅N₃).



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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: 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		
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		
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		
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		
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		
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	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
5	3	1	Total 4	C 2	O 1	S 1	0	0

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

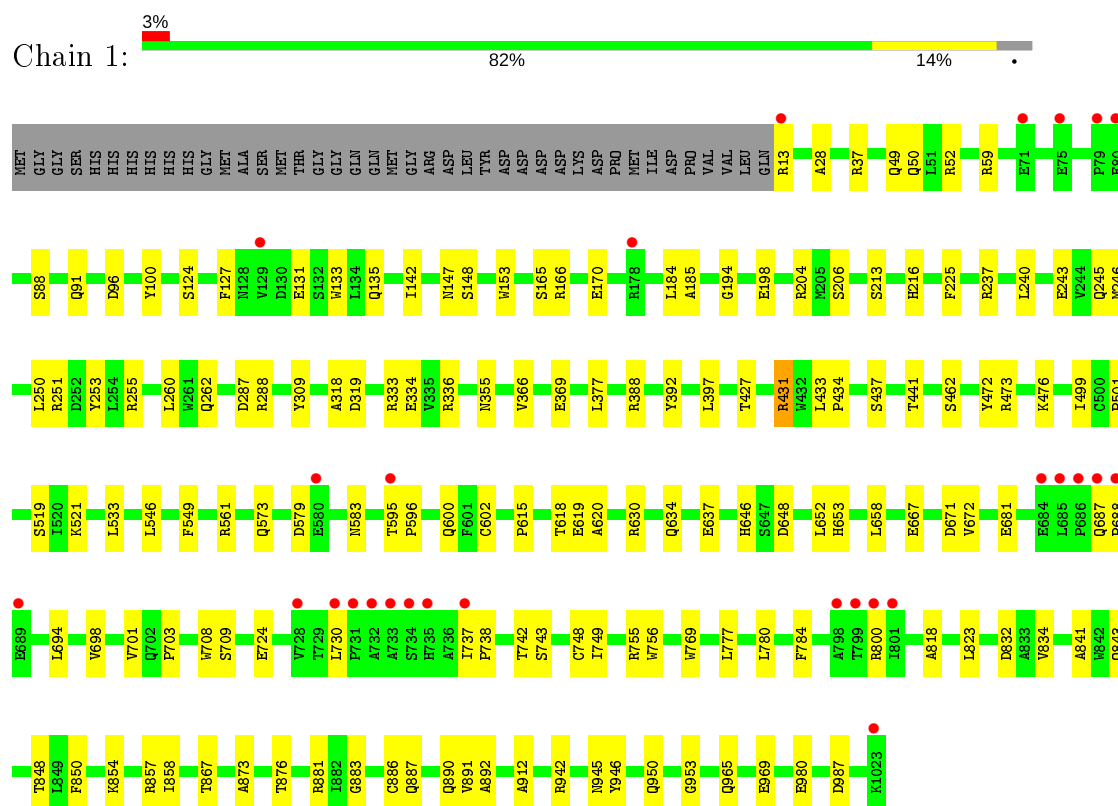
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	860	Total	O	0	0
			860	860		
6	2	977	Total	O	0	0
			977	977		
6	3	982	Total	O	0	0
			982	982		
6	4	835	Total	O	0	0
			835	835		

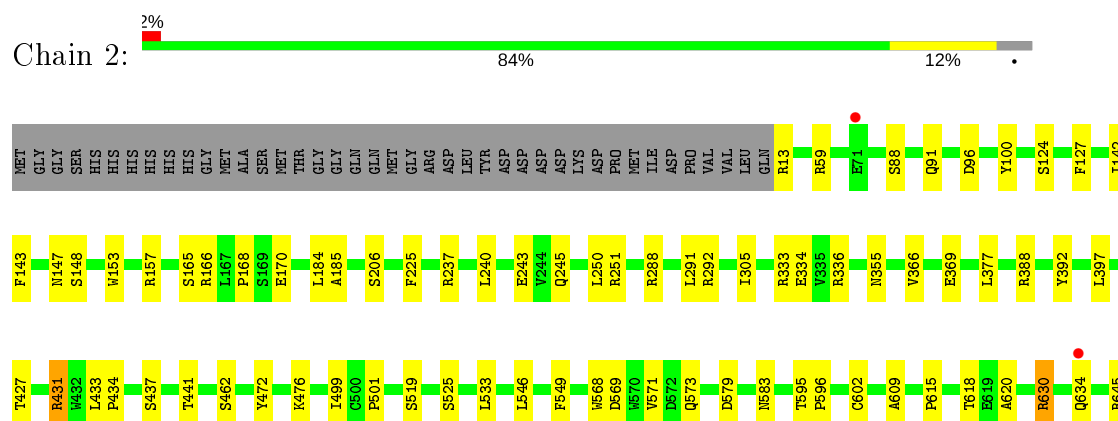
3 Residue-property plots [i](#)

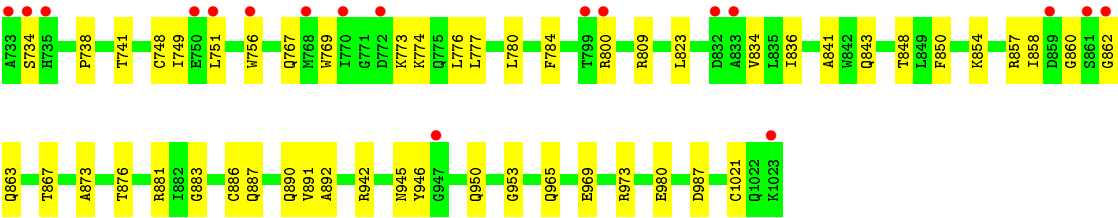
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.73Å 161.52Å 203.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.29 – 2.20 71.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (71.29-2.20) 99.6 (71.29-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.205 , 0.242 0.196 , 0.230	Depositor DCC
R_{free} test set	3595 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36610	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.28 % 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 3.7750e-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, MG, DMS, GAI

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	0.32	0/8361	0.63	6/11408 (0.1%)
1	2	0.33	0/8361	0.63	6/11408 (0.1%)
1	3	0.34	0/8361	0.70	7/11408 (0.1%)
1	4	0.32	0/8361	0.75	11/11408 (0.1%)
All	All	0.33	0/33444	0.68	30/45632 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	630	ARG	NE-CZ-NH1	-21.84	109.38	120.30
1	3	431	ARG	NE-CZ-NH1	-21.74	109.43	120.30
1	3	431	ARG	NE-CZ-NH2	21.59	131.10	120.30
1	4	630	ARG	NE-CZ-NH2	20.86	130.73	120.30
1	4	237	ARG	NE-CZ-NH1	-19.45	110.58	120.30
1	4	237	ARG	NE-CZ-NH2	18.53	129.57	120.30
1	4	147	ASN	C-N-CA	13.52	155.50	121.70
1	3	431	ARG	CD-NE-CZ	11.03	139.04	123.60
1	4	630	ARG	CD-NE-CZ	10.73	138.63	123.60
1	4	147	ASN	CA-C-N	-8.90	97.61	117.20
1	4	237	ARG	CD-NE-CZ	8.80	135.93	123.60
1	4	147	ASN	O-C-N	8.07	135.61	122.70
1	4	431	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	3	630	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	1	431	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	1	630	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	2	630	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	3	630	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	2	431	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	2	630	ARG	NE-CZ-NH1	7.14	123.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	431	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	4	431	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	1	630	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	2	431	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	2	237	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	3	237	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	1	237	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	2	237	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	3	237	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	1	237	ARG	NE-CZ-NH1	5.55	123.08	120.30

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	98	0
1	2	8119	0	7708	84	0
1	3	8119	0	7708	95	0
1	4	8119	0	7707	99	0
2	1	3	0	0	0	0
2	2	3	0	0	0	0
2	3	3	0	0	0	0
2	4	3	0	0	0	0
3	1	4	0	0	0	0
3	2	4	0	0	0	0
3	3	4	0	0	0	0
3	4	4	0	0	0	0
4	1	4	0	4	0	0
4	2	4	0	4	0	0
4	3	4	0	4	0	0
4	4	4	0	4	0	0
5	1	100	0	150	1	0
5	2	120	0	180	3	0
5	3	112	0	168	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	104	0	156	5	0
6	1	860	0	0	9	0
6	2	977	0	0	5	0
6	3	982	0	0	9	0
6	4	835	0	0	5	0
All	All	36610	0	31501	368	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 6.

All (368) 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)
1:3:581:ASN:HB2	1:3:583:ASN:ND2	1.94	0.82
1:4:147:ASN:HB3	1:4:206:SER:HA	1.62	0.81
1:1:142:ILE:HG12	1:1:170:GLU:HG2	1.62	0.81
1:1:730:LEU:HD21	1:2:823:LEU:O	1.80	0.81
1:4:767:GLN:NE2	1:4:774:LYS:HG3	1.98	0.79
1:4:245:GLN:HG2	1:4:288:ARG:HG2	1.63	0.79
1:3:142:ILE:HG12	1:3:170:GLU:HG2	1.64	0.79
1:1:245:GLN:HG2	1:1:288:ARG:HG2	1.64	0.78
1:4:142:ILE:HG12	1:4:170:GLU:HG2	1.63	0.78
1:3:245:GLN:HG2	1:3:288:ARG:HG2	1.66	0.78
1:2:245:GLN:HG2	1:2:288:ARG:HG2	1.64	0.77
1:2:754:LYS:HE2	1:2:1022:GLN:HE21	1.51	0.76
1:2:142:ILE:HG12	1:2:170:GLU:HG2	1.67	0.75
1:1:615:PRO:O	1:1:618:THR:HG22	1.87	0.74
1:2:754:LYS:HE2	1:2:1022:GLN:NE2	2.02	0.74
1:3:615:PRO:O	1:3:618:THR:HG22	1.88	0.74
1:4:615:PRO:O	1:4:618:THR:HG22	1.87	0.73
1:2:615:PRO:O	1:2:618:THR:HG22	1.89	0.72
1:3:128:ASN:HA	1:3:180:GLY:O	1.92	0.70
1:4:628:GLN:HE22	5:4:7001:DMS:H21	1.57	0.69
1:2:147:ASN:HB3	1:2:206:SER:HA	1.75	0.69
1:3:581:ASN:HB2	1:3:583:ASN:HD21	1.56	0.69
1:3:749:ILE:HD12	1:3:858:ILE:HD12	1.75	0.69
1:1:147:ASN:HB3	1:1:206:SER:HA	1.74	0.68
1:3:749:ILE:CD1	1:3:858:ILE:HD12	2.24	0.68
1:3:147:ASN:HB3	1:3:206:SER:HA	1.75	0.67
1:4:965:GLN:O	1:4:969:GLU:HG3	1.95	0.67
1:2:965:GLN:O	1:2:969:GLU:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:750:GLU:HG3	1:2:755:ARG:HG2	1.76	0.66
1:1:737:ILE:HD13	1:1:832:ASP:HA	1.77	0.66
1:4:581:ASN:HB2	1:4:583:ASN:ND2	2.10	0.66
1:1:737:ILE:HD12	1:1:738:PRO:HD2	1.77	0.65
1:1:965:GLN:O	1:1:969:GLU:HG3	1.96	0.65
1:3:131:GLU:O	1:3:135:GLN:HG3	1.97	0.65
1:4:756:TRP:CD2	1:4:858:ILE:HD13	2.32	0.65
1:1:579:ASP:OD2	1:1:583:ASN:HB2	1.97	0.64
1:3:88:SER:HA	1:3:366:VAL:HG21	1.80	0.64
1:4:88:SER:HA	1:4:366:VAL:HG21	1.80	0.64
1:2:157:ARG:HD3	6:2:4685:HOH:O	1.99	0.63
1:2:88:SER:HA	1:2:366:VAL:HG21	1.79	0.63
1:1:88:SER:HA	1:1:366:VAL:HG21	1.80	0.63
1:3:965:GLN:O	1:3:969:GLU:HG3	1.98	0.62
1:1:377:LEU:HD22	1:1:708:TRP:HA	1.82	0.62
1:3:578:TYR:HA	1:3:583:ASN:O	2.00	0.62
1:4:377:LEU:HD22	1:4:708:TRP:HA	1.81	0.62
1:1:131:GLU:O	1:1:135:GLN:HG3	2.00	0.61
1:1:13:ARG:HG3	1:4:13:ARG:CZ	2.30	0.61
1:1:127:PHE:CE2	1:1:184:LEU:HG	2.36	0.61
1:2:127:PHE:CE2	1:2:184:LEU:HG	2.36	0.61
1:3:377:LEU:HD22	1:3:708:TRP:HA	1.81	0.61
1:4:127:PHE:CE2	1:4:184:LEU:HG	2.36	0.60
1:1:127:PHE:HE2	1:1:184:LEU:HG	1.66	0.60
1:1:13:ARG:CZ	1:4:13:ARG:HG3	2.31	0.60
1:3:833:ALA:HB1	1:3:858:ILE:O	2.02	0.60
1:4:127:PHE:HE2	1:4:184:LEU:HG	1.66	0.60
1:2:127:PHE:HE2	1:2:184:LEU:HG	1.66	0.59
1:2:823:LEU:HD11	1:2:841:ALA:HB2	1.84	0.59
1:3:127:PHE:CE2	1:3:184:LEU:HG	2.37	0.59
1:3:127:PHE:HE2	1:3:184:LEU:HG	1.67	0.59
1:3:52:ARG:O	1:3:213:SER:HB2	2.02	0.59
1:2:377:LEU:HD22	1:2:708:TRP:HA	1.85	0.59
1:4:741:THR:HB	1:4:748:CYS:HB3	1.85	0.59
1:3:577:LYS:O	1:3:584:PRO:HA	2.02	0.59
1:4:823:LEU:HD11	1:4:841:ALA:HB2	1.85	0.58
1:1:823:LEU:HD11	1:1:841:ALA:HB2	1.84	0.58
1:4:734:SER:OG	1:4:860:GLY:HA3	2.04	0.57
1:2:579:ASP:OD2	1:2:583:ASN:HB2	2.05	0.57
1:3:823:LEU:HD11	1:3:841:ALA:HB2	1.85	0.57
1:1:749:ILE:HD12	1:1:749:ILE:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:749:ILE:N	1:4:749:ILE:HD12	2.19	0.57
1:1:873:ALA:O	1:1:876:THR:HG22	2.05	0.56
1:4:237:ARG:HD2	1:4:296:GLU:OE1	2.04	0.56
1:4:767:GLN:NE2	1:4:774:LYS:HE3	2.20	0.56
1:4:863:GLN:HG2	1:4:1021:CYS:HB3	1.85	0.56
1:2:945:ASN:OD1	1:2:950:GLN:HG3	2.05	0.56
1:3:890:GLN:HB2	6:3:4427:HOH:O	2.03	0.56
1:1:262:GLN:HG2	6:1:4836:HOH:O	2.04	0.56
1:1:204:ARG:HB3	6:1:4190:HOH:O	2.05	0.56
1:2:292:ARG:HH12	5:2:7009:DMS:C1	2.19	0.56
1:3:942:ARG:HA	1:3:953:GLY:O	2.06	0.56
1:2:334:GLU:OE1	1:2:336:ARG:NH1	2.38	0.55
1:3:653:HIS:HB3	6:3:4967:HOH:O	2.06	0.55
1:3:334:GLU:OE1	1:3:336:ARG:NH1	2.40	0.55
1:4:334:GLU:OE1	1:4:336:ARG:NH1	2.39	0.55
1:3:873:ALA:O	1:3:876:THR:HG22	2.07	0.55
1:4:945:ASN:OD1	1:4:950:GLN:HG3	2.07	0.55
1:2:675:GLN:HG3	6:2:5019:HOH:O	2.07	0.55
1:2:942:ARG:HA	1:2:953:GLY:O	2.06	0.55
1:3:277:GLU:HG2	6:3:4755:HOH:O	2.07	0.55
1:2:873:ALA:O	1:2:876:THR:HG22	2.07	0.54
1:3:945:ASN:OD1	1:3:950:GLN:HG3	2.07	0.54
1:4:942:ARG:HA	1:4:953:GLY:O	2.08	0.54
1:1:738:PRO:HB2	1:1:834:VAL:HG23	1.90	0.54
1:2:1023:LYS:HA	6:2:4992:HOH:O	2.08	0.54
1:1:573:GLN:HB2	1:1:602:CYS:O	2.08	0.54
1:4:573:GLN:HB2	1:4:602:CYS:O	2.08	0.53
1:4:873:ALA:O	1:4:876:THR:HG22	2.08	0.53
1:4:91:GLN:HG3	1:4:96:ASP:OD1	2.08	0.53
1:3:91:GLN:HG3	1:3:96:ASP:OD1	2.08	0.53
1:1:334:GLU:OE1	1:1:336:ARG:NH1	2.40	0.53
1:1:942:ARG:HA	1:1:953:GLY:O	2.09	0.53
1:2:91:GLN:HG3	1:2:96:ASP:OD1	2.07	0.53
1:2:749:ILE:HD12	1:2:858:ILE:HD12	1.91	0.53
1:4:628:GLN:HE22	5:4:7001:DMS:C2	2.22	0.53
1:1:91:GLN:HG3	1:1:96:ASP:OD1	2.08	0.53
1:2:749:ILE:CD1	1:2:858:ILE:HD12	2.38	0.53
1:3:573:GLN:HB2	1:3:602:CYS:O	2.09	0.53
1:2:730:LEU:N	1:2:730:LEU:HD12	2.24	0.52
1:1:260:LEU:HD11	1:1:309:TYR:HB3	1.91	0.52
1:1:52:ARG:O	1:1:213:SER:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:573:GLN:HB2	1:2:602:CYS:O	2.10	0.52
1:3:369:GLU:HG3	1:3:397:LEU:HD21	1.91	0.52
1:3:730:LEU:HD12	1:3:730:LEU:N	2.24	0.52
1:2:950:GLN:HB2	1:2:1023:LYS:HB2	1.92	0.52
1:4:369:GLU:HG3	1:4:397:LEU:HD21	1.91	0.52
1:1:756:TRP:CD2	1:1:858:ILE:HD13	2.45	0.51
1:4:892:ALA:HB3	1:4:946:TYR:CE1	2.45	0.51
1:2:630:ARG:HE	5:2:7024:DMS:H23	1.75	0.51
1:1:730:LEU:HD12	1:1:730:LEU:N	2.25	0.51
1:3:800:ARG:HG2	1:3:800:ARG:HH11	1.75	0.51
1:1:892:ALA:HB3	1:1:946:TYR:CE1	2.45	0.51
1:1:945:ASN:OD1	1:1:950:GLN:HG3	2.10	0.51
1:3:730:LEU:HD21	1:4:823:LEU:O	2.10	0.51
1:4:277:GLU:HG2	6:4:4549:HOH:O	2.09	0.51
1:4:751:LEU:HD21	1:4:860:GLY:O	2.11	0.50
1:2:730:LEU:H	1:2:730:LEU:HD12	1.77	0.50
1:1:148:SER:HA	1:1:165:SER:OG	2.11	0.50
1:1:653:HIS:HB3	6:1:4865:HOH:O	2.11	0.50
1:2:369:GLU:HG3	1:2:397:LEU:HD21	1.93	0.50
1:3:579:ASP:OD2	1:3:583:ASN:HB2	2.11	0.50
1:4:316:HIS:HB2	1:4:321:THR:O	2.11	0.50
1:1:800:ARG:HH11	1:1:800:ARG:HG2	1.77	0.50
1:4:730:LEU:N	1:4:730:LEU:HD12	2.25	0.50
1:3:749:ILE:HB	1:3:756:TRP:HB2	1.92	0.50
1:3:892:ALA:HB3	1:3:946:TYR:CE1	2.46	0.50
1:2:433:LEU:HB3	1:2:434:PRO:HD3	1.94	0.50
1:3:433:LEU:HB3	1:3:434:PRO:HD3	1.94	0.50
1:1:260:LEU:HD11	1:1:309:TYR:CB	2.41	0.50
1:4:800:ARG:HH11	1:4:800:ARG:HG2	1.76	0.50
1:2:892:ALA:HB3	1:2:946:TYR:CE1	2.47	0.50
1:4:579:ASP:OD2	1:4:583:ASN:HB2	2.12	0.50
1:4:767:GLN:HE22	1:4:774:LYS:HE3	1.77	0.50
1:2:800:ARG:HG2	1:2:800:ARG:HH11	1.76	0.49
1:2:634:GLN:HB2	1:2:681:GLU:OE2	2.12	0.49
1:3:730:LEU:HD12	1:3:730:LEU:H	1.77	0.49
1:1:369:GLU:HG3	1:1:397:LEU:HD21	1.92	0.49
1:1:634:GLN:HB2	1:1:681:GLU:OE2	2.13	0.49
1:4:748:CYS:C	1:4:749:ILE:HD12	2.32	0.49
1:1:646:HIS:CE1	1:1:671:ASP:OD1	2.65	0.49
1:4:738:PRO:HB2	1:4:834:VAL:HG23	1.94	0.49
1:4:634:GLN:HB2	1:4:681:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:730:LEU:HD12	1:4:730:LEU:H	1.77	0.49
1:1:823:LEU:O	1:2:730:LEU:HD21	2.12	0.49
1:3:688:PRO:HD3	1:3:694:LEU:HD11	1.95	0.49
1:4:433:LEU:HB3	1:4:434:PRO:HD3	1.95	0.49
1:4:549:PHE:CE2	1:4:620:ALA:HA	2.48	0.49
1:1:637:GLU:HB2	5:1:7019:DMS:H13	1.95	0.48
1:1:887:GLN:NE2	1:1:980:GLU:O	2.46	0.48
1:3:148:SER:HA	1:3:165:SER:OG	2.13	0.48
1:2:658:LEU:HD22	1:2:688:PRO:HB2	1.95	0.48
1:3:887:GLN:NE2	1:3:980:GLU:O	2.46	0.48
1:1:737:ILE:HD12	1:1:738:PRO:CD	2.43	0.48
1:4:769:TRP:HA	1:4:773:LYS:O	2.14	0.48
1:1:433:LEU:HB3	1:1:434:PRO:HD3	1.95	0.48
1:2:688:PRO:HD3	1:2:694:LEU:HD11	1.96	0.48
1:3:658:LEU:HD22	1:3:688:PRO:HB2	1.95	0.48
1:1:724:GLU:O	1:2:847:LYS:NZ	2.47	0.48
1:4:809:ARG:HD2	6:4:4569:HOH:O	2.14	0.48
1:3:634:GLN:HB2	1:3:681:GLU:OE2	2.13	0.48
1:1:561:ARG:HD3	1:2:525:SER:O	2.14	0.48
1:4:887:GLN:NE2	1:4:980:GLU:O	2.47	0.48
1:3:249:GLU:CD	1:3:251:ARG:HD3	2.34	0.47
1:3:701:VAL:O	1:3:703:PRO:HD3	2.14	0.47
1:1:688:PRO:HD3	1:1:694:LEU:HD11	1.95	0.47
1:2:476:LYS:HD2	6:2:4199:HOH:O	2.14	0.47
1:4:36:TRP:O	1:4:37:ARG:HD3	2.13	0.47
1:4:646:HIS:NE2	1:4:671:ASP:OD1	2.47	0.47
1:4:688:PRO:HD3	1:4:694:LEU:HD11	1.95	0.47
1:2:148:SER:HA	1:2:165:SER:OG	2.13	0.47
1:3:355:ASN:OD1	1:3:388:ARG:HD3	2.14	0.47
1:3:533:LEU:HD23	1:3:533:LEU:C	2.34	0.47
1:4:658:LEU:HD22	1:4:688:PRO:HB2	1.96	0.47
1:4:701:VAL:O	1:4:703:PRO:HD3	2.15	0.47
1:1:658:LEU:HD22	1:1:688:PRO:HB2	1.96	0.47
1:4:751:LEU:HD23	1:4:862:GLY:HA2	1.96	0.47
1:1:730:LEU:H	1:1:730:LEU:HD12	1.78	0.47
1:1:748:CYS:C	1:1:749:ILE:HD12	2.35	0.47
1:1:755:ARG:HB2	1:1:769:TRP:HB2	1.97	0.47
1:4:774:LYS:HE2	1:4:776:LEU:O	2.15	0.47
1:3:476:LYS:HD2	6:3:4199:HOH:O	2.15	0.47
1:3:823:LEU:O	1:4:730:LEU:HD21	2.15	0.47
1:4:355:ASN:OD1	1:4:388:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:546:LEU:HA	6:3:4128:HOH:O	2.14	0.47
1:4:749:ILE:HD11	1:4:836:ILE:HD11	1.97	0.47
1:4:306:PRO:HD2	6:4:4751:HOH:O	2.14	0.47
1:3:576:ILE:HG12	5:3:7008:DMS:H22	1.97	0.46
1:3:754:LYS:HA	1:3:769:TRP:O	2.16	0.46
1:4:427:THR:HG21	1:4:462:SER:HB3	1.97	0.46
1:4:499:ILE:HG22	1:4:501:PRO:HD3	1.98	0.46
1:2:595:THR:HA	1:2:596:PRO:C	2.36	0.46
1:3:153:TRP:HB2	1:3:185:ALA:HB3	1.97	0.46
1:1:37:ARG:HG2	1:1:50:GLN:NE2	2.31	0.46
1:2:427:THR:HG21	1:2:462:SER:HB3	1.98	0.46
1:2:549:PHE:CE2	1:2:620:ALA:HA	2.49	0.46
1:1:549:PHE:CE2	1:1:620:ALA:HA	2.50	0.46
1:2:890:GLN:HG3	1:2:891:VAL:N	2.31	0.46
1:2:250:LEU:O	1:2:251:ARG:HD2	2.15	0.46
1:2:533:LEU:HD23	1:2:533:LEU:C	2.36	0.46
1:2:887:GLN:NE2	1:2:980:GLU:O	2.49	0.46
1:1:153:TRP:HB2	1:1:185:ALA:HB3	1.97	0.46
1:4:131:GLU:HG3	6:4:4732:HOH:O	2.15	0.46
1:3:861:SER:OG	1:3:863:GLN:HG3	2.16	0.46
1:4:533:LEU:HD23	1:4:533:LEU:C	2.36	0.46
1:3:245:GLN:HG2	1:3:288:ARG:CG	2.42	0.46
1:3:749:ILE:HD13	1:3:858:ILE:HD12	1.97	0.46
1:1:648:ASP:HB3	6:1:4828:HOH:O	2.14	0.45
1:2:355:ASN:OD1	1:2:388:ARG:HD3	2.16	0.45
1:4:245:GLN:HG2	1:4:288:ARG:CG	2.39	0.45
1:1:49:GLN:HG2	6:1:4609:HOH:O	2.15	0.45
1:1:240:LEU:HD23	1:1:240:LEU:C	2.37	0.45
1:3:427:THR:HG21	1:3:462:SER:HB3	1.99	0.45
1:1:255:ARG:HG3	1:1:318:ALA:HA	1.97	0.45
1:1:701:VAL:O	1:1:703:PRO:HD3	2.17	0.45
1:2:153:TRP:HB2	1:2:185:ALA:HB3	1.98	0.45
1:2:499:ILE:HG22	1:2:501:PRO:HD3	1.99	0.45
1:1:499:ILE:HG22	1:1:501:PRO:HD3	1.98	0.45
1:2:739:HIS:O	1:2:749:ILE:HA	2.16	0.45
1:4:153:TRP:HB2	1:4:185:ALA:HB3	1.98	0.45
1:4:595:THR:HA	1:4:596:PRO:C	2.37	0.45
1:1:742:THR:HG22	1:1:743:SER:N	2.32	0.45
1:3:240:LEU:HD23	1:3:240:LEU:C	2.36	0.45
1:3:549:PHE:CE2	1:3:620:ALA:HA	2.51	0.45
1:4:890:GLN:HG3	1:4:891:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:28:ALA:HB1	6:1:4889:HOH:O	2.16	0.45
1:1:533:LEU:HD23	1:1:533:LEU:C	2.37	0.45
1:3:499:ILE:HG22	1:3:501:PRO:HD3	1.99	0.45
1:1:473:ARG:NH1	6:1:4608:HOH:O	2.50	0.45
1:1:595:THR:HA	1:1:596:PRO:C	2.37	0.45
1:1:355:ASN:OD1	1:1:388:ARG:HD3	2.17	0.44
1:2:754:LYS:HA	1:2:769:TRP:O	2.18	0.44
1:4:52:ARG:O	1:4:213:SER:HB2	2.17	0.44
1:2:701:VAL:O	1:2:703:PRO:HD3	2.18	0.44
1:4:240:LEU:HD23	1:4:240:LEU:C	2.37	0.44
1:4:194:GLY:O	1:4:198:GLU:HG3	2.18	0.44
1:3:595:THR:HA	1:3:596:PRO:C	2.37	0.44
1:3:857:ARG:HG2	1:3:857:ARG:HH11	1.82	0.44
1:4:124:SER:HA	1:4:184:LEU:O	2.17	0.44
1:4:246:MET:C	1:4:246:MET:SD	2.95	0.44
1:1:472:TYR:O	1:1:476:LYS:HG2	2.18	0.44
1:2:240:LEU:C	1:2:240:LEU:HD23	2.38	0.44
1:1:883:GLY:HA3	1:1:987:ASP:HA	2.00	0.44
1:1:890:GLN:HG3	1:1:891:VAL:N	2.32	0.44
1:3:250:LEU:O	1:3:251:ARG:HD2	2.17	0.43
1:3:390:SER:HA	1:3:391:HIS:HA	1.74	0.43
1:4:472:TYR:O	1:4:476:LYS:HG2	2.18	0.43
1:4:749:ILE:HG13	1:4:834:VAL:HG11	2.00	0.43
1:1:251:ARG:HG3	1:1:253:TYR:CZ	2.53	0.43
1:2:784:PHE:HA	1:2:881:ARG:O	2.18	0.43
1:3:755:ARG:HB2	1:3:769:TRP:HB2	2.00	0.43
1:4:59:ARG:HB2	1:4:124:SER:OG	2.19	0.43
1:4:305:ILE:HA	6:4:4751:HOH:O	2.19	0.43
1:1:777:LEU:HB2	1:1:887:GLN:HG2	2.00	0.43
1:3:890:GLN:HG3	1:3:891:VAL:N	2.32	0.43
1:4:883:GLY:HA3	1:4:987:ASP:HA	1.99	0.43
1:1:59:ARG:HB2	1:1:124:SER:OG	2.19	0.43
1:1:124:SER:HA	1:1:184:LEU:O	2.18	0.43
1:1:784:PHE:HA	1:1:881:ARG:O	2.19	0.43
1:3:472:TYR:O	1:3:476:LYS:HG2	2.18	0.43
1:3:784:PHE:HA	1:3:881:ARG:O	2.18	0.43
1:4:863:GLN:HG2	1:4:1021:CYS:CB	2.48	0.43
1:4:100:TYR:CE1	1:4:602:CYS:HB3	2.54	0.43
1:1:133:TRP:CE3	1:1:216:HIS:HB2	2.54	0.43
1:1:854:LYS:HA	1:1:867:THR:O	2.19	0.43
1:4:292:ARG:HH12	5:4:7009:DMS:C1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:857:ARG:HH11	1:4:857:ARG:HG2	1.83	0.43
1:2:883:GLY:HA3	1:2:987:ASP:HA	1.99	0.43
1:2:833:ALA:HB1	1:2:858:ILE:O	2.19	0.43
1:3:817:GLN:HG2	6:3:4333:HOH:O	2.19	0.43
1:1:246:MET:C	1:1:246:MET:SD	2.97	0.42
1:2:292:ARG:HH12	5:2:7009:DMS:H13	1.84	0.42
1:4:854:LYS:HA	1:4:867:THR:O	2.19	0.42
1:1:245:GLN:HG2	1:1:288:ARG:CG	2.41	0.42
1:1:857:ARG:HH11	1:1:857:ARG:HG2	1.83	0.42
1:3:59:ARG:HB2	1:3:124:SER:OG	2.19	0.42
1:1:427:THR:HG21	1:1:462:SER:HB3	2.00	0.42
1:3:124:SER:HA	1:3:184:LEU:O	2.19	0.42
1:1:131:GLU:HG3	1:1:135:GLN:CG	2.50	0.42
1:1:521:LYS:HE2	6:1:4411:HOH:O	2.19	0.42
1:2:245:GLN:HG2	1:2:288:ARG:CG	2.41	0.42
1:2:472:TYR:O	1:2:476:LYS:HG2	2.20	0.42
1:2:843:GLN:HG2	1:2:848:THR:HA	2.02	0.42
1:2:857:ARG:HG2	1:2:857:ARG:HH11	1.84	0.42
1:3:652:LEU:HD11	1:3:698:VAL:HB	2.01	0.42
1:2:124:SER:HA	1:2:184:LEU:O	2.19	0.42
1:3:576:ILE:HD11	6:3:4216:HOH:O	2.18	0.42
1:3:843:GLN:HG2	1:3:848:THR:HA	2.02	0.42
1:4:751:LEU:HD23	1:4:862:GLY:CA	2.50	0.42
1:4:843:GLN:HG2	1:4:848:THR:HA	2.02	0.42
1:1:100:TYR:CE1	1:1:602:CYS:HB3	2.54	0.42
1:1:652:LEU:HD11	1:1:698:VAL:HB	2.01	0.42
1:4:777:LEU:HB2	1:4:887:GLN:HG2	2.01	0.42
1:2:708:TRP:CE3	1:2:709:SER:HB3	2.55	0.42
1:2:777:LEU:HB2	1:2:887:GLN:HG2	2.02	0.42
1:4:225:PHE:HA	1:4:243:GLU:O	2.20	0.42
1:1:131:GLU:HG3	1:1:135:GLN:HG3	2.01	0.42
1:1:737:ILE:HG23	1:1:737:ILE:O	2.20	0.42
1:3:883:GLY:HA3	1:3:987:ASP:HA	2.01	0.42
1:4:257:THR:HA	1:4:270:GLY:O	2.19	0.42
1:3:100:TYR:CE1	1:3:602:CYS:HB3	2.55	0.41
1:3:305:ILE:HD11	1:3:645:ARG:HB3	2.01	0.41
1:3:777:LEU:HB2	1:3:887:GLN:HG2	2.01	0.41
1:3:200:GLN:HG2	1:3:391:HIS:HB2	2.02	0.41
1:4:377:LEU:CD2	1:4:708:TRP:HA	2.49	0.41
1:1:619:GLU:HA	1:1:912:ALA:HB2	2.03	0.41
1:2:225:PHE:HA	1:2:243:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:437:SER:O	1:1:441:THR:HG23	2.21	0.41
1:3:578:TYR:CE2	1:3:584:PRO:HB3	2.55	0.41
1:4:652:LEU:HD11	1:4:698:VAL:HB	2.02	0.41
1:3:52:ARG:HD2	6:3:4818:HOH:O	2.20	0.41
1:4:973:ARG:O	5:4:7014:DMS:H22	2.20	0.41
1:4:708:TRP:CE3	1:4:709:SER:HB3	2.55	0.41
1:1:250:LEU:HD11	1:1:287:ASP:HA	2.01	0.41
1:3:596:PRO:HG2	6:3:4456:HOH:O	2.21	0.41
1:4:166:ARG:HG3	1:4:392:TYR:HB2	2.02	0.41
1:4:652:LEU:O	1:4:667:GLU:HA	2.21	0.41
1:1:780:LEU:HA	1:1:886:CYS:HB3	2.02	0.41
1:1:818:ALA:HB3	6:1:4943:HOH:O	2.19	0.41
1:2:652:LEU:HD11	1:2:698:VAL:HB	2.02	0.41
1:2:59:ARG:HB2	1:2:124:SER:OG	2.21	0.41
1:2:571:VAL:CG2	1:2:609:ALA:HA	2.51	0.41
1:2:674:PRO:O	1:2:675:GLN:HB2	2.20	0.41
1:3:613:PRO:HB3	1:3:617:LEU:HD23	2.03	0.41
1:3:292:ARG:HH12	5:3:7009:DMS:C1	2.33	0.41
1:1:652:LEU:O	1:1:667:GLU:HA	2.21	0.41
1:2:568:TRP:HA	1:2:569:ASP:HA	1.84	0.41
1:2:757:GLN:O	1:2:765:LEU:HD12	2.21	0.41
1:3:111:PRO:HA	1:3:112:PRO:HA	1.88	0.41
1:3:225:PHE:HA	1:3:243:GLU:O	2.21	0.41
1:4:637:GLU:HB2	5:4:7021:DMS:S	2.60	0.41
1:1:166:ARG:HG3	1:1:392:TYR:HB2	2.03	0.41
1:2:143:PHE:O	1:2:168:PRO:HA	2.21	0.41
1:2:652:LEU:O	1:2:667:GLU:HA	2.21	0.41
1:3:619:GLU:HA	1:3:912:ALA:HB2	2.03	0.41
1:3:652:LEU:O	1:3:667:GLU:HA	2.21	0.41
1:2:305:ILE:HD11	1:2:645:ARG:HB3	2.02	0.41
1:4:780:LEU:HA	1:4:886:CYS:HB3	2.02	0.41
1:2:854:LYS:HA	1:2:867:THR:O	2.21	0.40
1:4:571:VAL:CG2	1:4:609:ALA:HA	2.51	0.40
1:2:166:ARG:HG3	1:2:392:TYR:HB2	2.03	0.40
1:2:437:SER:O	1:2:441:THR:HG23	2.20	0.40
1:3:433:LEU:N	1:3:434:PRO:CD	2.84	0.40
1:3:600:GLN:CD	1:3:600:GLN:H	2.25	0.40
1:3:747:PHE:HB2	1:3:758:PHE:HB2	2.04	0.40
1:4:767:GLN:HE22	1:4:774:LYS:HG3	1.80	0.40
1:1:225:PHE:HA	1:1:243:GLU:O	2.22	0.40
1:1:600:GLN:H	1:1:600:GLN:CD	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:708:TRP:CE3	1:1:709:SER:HB3	2.56	0.40
1:1:843:GLN:HG2	1:1:848:THR:HA	2.02	0.40
1:2:291:LEU:HD22	1:2:291:LEU:N	2.36	0.40
1:3:377:LEU:CD2	1:3:708:TRP:HA	2.50	0.40
1:4:784:PHE:HA	1:4:881:ARG:O	2.21	0.40
1:1:194:GLY:O	1:1:198:GLU:HG3	2.21	0.40
1:3:287:ASP:N	1:3:287:ASP:OD1	2.51	0.40
1:3:610:ASP:O	1:3:611:ARG:HB2	2.21	0.40
1:3:739:HIS:O	1:3:749:ILE:HA	2.21	0.40
1:2:13:ARG:N	6:2:5013:HOH:O	2.54	0.40
1:2:100:TYR:CE1	1:2:602:CYS:HB3	2.57	0.40
1:4:800:ARG:NH1	1:4:800:ARG:HG2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	1009/1052 (96%)	964 (96%)	45 (4%)	0	100	100
1	2	1009/1052 (96%)	961 (95%)	48 (5%)	0	100	100
1	3	1009/1052 (96%)	960 (95%)	49 (5%)	0	100	100
1	4	1009/1052 (96%)	963 (95%)	46 (5%)	0	100	100
All	All	4036/4208 (96%)	3848 (95%)	188 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	855 (99%)	8 (1%)	78	88
1	2	863/897 (96%)	855 (99%)	8 (1%)	78	88
1	3	863/897 (96%)	857 (99%)	6 (1%)	84	91
1	4	863/897 (96%)	855 (99%)	8 (1%)	78	88
All	All	3452/3588 (96%)	3422 (99%)	30 (1%)	78	88

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	319	ASP
1	1	333	ARG
1	1	431	ARG
1	1	519	SER
1	1	546	LEU
1	1	672	VAL
1	1	687	GLN
1	1	850	PHE
1	2	333	ARG
1	2	431	ARG
1	2	519	SER
1	2	546	LEU
1	2	646	HIS
1	2	687	GLN
1	2	772	ASP
1	2	850	PHE
1	3	333	ARG
1	3	519	SER
1	3	546	LEU
1	3	672	VAL
1	3	687	GLN
1	3	850	PHE
1	4	148	SER
1	4	333	ARG
1	4	431	ARG
1	4	519	SER
1	4	546	LEU
1	4	648	ASP

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Mol	Chain	Res	Type
1	4	687	GLN
1	4	850	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	363	HIS
1	1	510	GLN
1	1	583	ASN
1	1	634	GLN
1	1	653	HIS
1	1	704	ASN
1	1	804	ASN
1	2	510	GLN
1	2	739	HIS
1	2	804	ASN
1	2	1022	GLN
1	3	262	GLN
1	3	510	GLN
1	3	583	ASN
1	3	653	HIS
1	3	739	HIS
1	3	757	GLN
1	3	804	ASN
1	4	50	GLN
1	4	510	GLN
1	4	554	GLN
1	4	583	ASN
1	4	628	GLN
1	4	634	GLN
1	4	804	ASN
1	4	863	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 141 ligands modelled in this entry, 28 are monoatomic - leaving 113 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	2	7004	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	3	7000	-	3,3,3	0.19	0	3,3,3	0.61	0
5	DMS	2	7017	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	7010	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	3	7003	-	3,3,3	0.19	0	3,3,3	0.67	0
5	DMS	4	7012	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	4	7006	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	3	7006	-	3,3,3	0.20	0	3,3,3	0.60	0
5	DMS	2	7019	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	7007	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	7018	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	4	7008	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	1	7017	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	1	7023	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	7023	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	2	7013	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	7017	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	3	7014	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	7014	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	4	7001	-	3,3,3	0.17	0	3,3,3	0.63	0
5	DMS	2	7015	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	2	7024	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	7020	-	3,3,3	0.19	0	3,3,3	0.61	0
5	DMS	3	7016	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	1	7022	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	4	7013	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	1	7021	-	3,3,3	0.25	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	1	7000	-	3,3,3	0.21	0	3,3,3	0.66	0
5	DMS	2	7008	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	2	7006	-	3,3,3	0.18	0	3,3,3	0.61	0
5	DMS	3	7020	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	7002	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	3	7004	-	3,3,3	0.24	0	3,3,3	0.62	0
4	GAI	3	2001	-	3,3,3	0.82	0	3,3,3	1.12	0
5	DMS	2	7001	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	1	7003	-	3,3,3	0.19	0	3,3,3	0.66	0
5	DMS	2	7028	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	7012	-	3,3,3	0.22	0	3,3,3	0.61	0
4	GAI	4	2001	-	3,3,3	0.80	0	3,3,3	1.09	0
5	DMS	3	7019	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	2	7011	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	7006	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	1	7009	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	1	7016	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	7008	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	3	7007	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	4	7005	-	3,3,3	0.20	0	3,3,3	0.60	0
5	DMS	4	7021	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	7008	-	3,3,3	0.24	0	3,3,3	0.57	0
5	DMS	2	7025	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	2	7005	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	2	7026	-	3,3,3	0.28	0	3,3,3	0.58	0
5	DMS	3	7024	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	4	7023	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	7002	-	3,3,3	0.20	0	3,3,3	0.57	0
5	DMS	1	7001	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	4	7024	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	2	7014	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	1	7004	-	3,3,3	0.19	0	3,3,3	0.62	0
5	DMS	1	7024	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	2	7027	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	4	7002	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	2	7002	-	3,3,3	0.22	0	3,3,3	0.56	0
5	DMS	3	7001	-	3,3,3	0.16	0	3,3,3	0.61	0
5	DMS	4	7004	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	2	7012	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	1	7020	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	7015	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	7014	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	3	7015	-	3,3,3	0.20	0	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	3	7022	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	2	7010	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	2	7029	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	7019	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	1	7010	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	4	7015	-	3,3,3	0.20	0	3,3,3	0.64	0
5	DMS	2	7023	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	4	7011	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	7011	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	3	7005	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	4	7010	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	3	7018	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	1	7018	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	4	7025	-	3,3,3	0.26	0	3,3,3	0.60	0
5	DMS	1	7011	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	4	7009	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	4	7000	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	1	7007	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	4	7016	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	7026	-	3,3,3	0.24	0	3,3,3	0.63	0
4	GAI	1	2001	-	3,3,3	0.86	0	3,3,3	1.12	0
5	DMS	2	7018	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	4	7022	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	7009	-	3,3,3	0.27	0	3,3,3	0.61	0
5	DMS	3	7025	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	1	7012	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	4	7020	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	4	7019	-	3,3,3	0.28	0	3,3,3	0.63	0
5	DMS	4	7017	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	3	7013	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	2	7003	-	3,3,3	0.23	0	3,3,3	0.68	0
5	DMS	3	7021	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	2	7000	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	1	7013	-	3,3,3	0.19	0	3,3,3	0.62	0
5	DMS	2	7021	-	3,3,3	0.19	0	3,3,3	0.61	0
5	DMS	2	7016	3	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	2	7009	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	3	1024	-	3,3,3	0.27	0	3,3,3	0.61	0
5	DMS	2	7022	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	1	7005	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	4	7003	-	3,3,3	0.28	0	3,3,3	0.66	0
5	DMS	2	7007	-	3,3,3	0.23	0	3,3,3	0.60	0
4	GAI	2	2001	-	3,3,3	0.79	0	3,3,3	1.13	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.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	4	7001	DMS	2	0
5	2	7024	DMS	1	0
5	3	7008	DMS	1	0
5	4	7021	DMS	1	0
5	4	7014	DMS	1	0
5	1	7019	DMS	1	0
5	4	7009	DMS	1	0
5	3	7009	DMS	1	0
5	2	7009	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%)	-0.18	28 (2%)	53	51	9, 25, 47, 75	0
1	2	1011/1052 (96%)	-0.19	22 (2%)	62	59	8, 20, 47, 78	0
1	3	1011/1052 (96%)	-0.23	19 (1%)	66	65	7, 20, 44, 78	0
1	4	1011/1052 (96%)	-0.03	40 (3%)	38	36	10, 27, 50, 77	0
All	All	4044/4208 (96%)	-0.16	109 (2%)	54	52	7, 23, 47, 78	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	689	GLU	8.3
1	1	686	PRO	6.6
1	2	685	LEU	6.0
1	2	731	PRO	5.8
1	1	735	HIS	5.8
1	1	800	ARG	5.7
1	4	800	ARG	5.6
1	2	1023	LYS	5.5
1	4	689	GLU	5.3
1	1	689	GLU	5.3
1	4	730	LEU	5.0
1	1	732	ALA	4.8
1	1	730	LEU	4.8
1	4	735	HIS	4.6
1	3	772	ASP	4.5
1	2	686	PRO	4.5
1	2	1022	GLN	4.5
1	4	687	GLN	4.4
1	1	685	LEU	4.3
1	4	688	PRO	4.2
1	3	689	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	2	732	ALA	4.1
1	2	681	GLU	4.1
1	4	686	PRO	4.0
1	4	731	PRO	3.8
1	4	770	ILE	3.8
1	2	770	ILE	3.7
1	1	687	GLN	3.6
1	4	732	ALA	3.6
1	3	688	PRO	3.6
1	1	801	ILE	3.6
1	3	731	PRO	3.4
1	2	683	PRO	3.4
1	1	731	PRO	3.4
1	1	728	VAL	3.3
1	1	79	PRO	3.3
1	4	734	SER	3.3
1	3	800	ARG	3.3
1	4	733	ALA	3.2
1	3	686	PRO	3.1
1	3	582	GLY	3.1
1	4	130	ASP	3.1
1	3	583	ASN	3.0
1	3	687	GLN	3.0
1	4	799	THR	3.0
1	4	833	ALA	3.0
1	3	685	LEU	2.9
1	4	72	SER	2.9
1	2	688	PRO	2.9
1	4	751	LEU	2.9
1	1	71	GLU	2.9
1	3	846	GLY	2.9
1	4	1023	LYS	2.9
1	2	729	THR	2.8
1	4	79	PRO	2.8
1	4	75	GLU	2.8
1	2	634	GLN	2.8
1	1	688	PRO	2.8
1	3	730	LEU	2.7
1	2	71	GLU	2.7
1	4	684	GLU	2.7
1	4	177	LEU	2.7
1	1	733	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	4	750	GLU	2.7
1	1	799	THR	2.7
1	4	581	ASN	2.6
1	4	685	LEU	2.6
1	4	729	THR	2.6
1	2	684	GLU	2.6
1	3	770	ILE	2.5
1	1	580	GLU	2.5
1	1	684	GLU	2.5
1	4	861	SER	2.5
1	1	1023	LYS	2.5
1	4	862	GLY	2.5
1	2	687	GLN	2.5
1	4	582	GLY	2.4
1	1	595	THR	2.4
1	1	75	GLU	2.4
1	4	583	ASN	2.4
1	4	768	MET	2.4
1	1	737	ILE	2.4
1	4	859	ASP	2.4
1	2	800	ARG	2.3
1	3	651	LEU	2.3
1	2	690	SER	2.3
1	3	581	ASN	2.3
1	1	80	GLU	2.2
1	4	947	GLY	2.2
1	1	798	ALA	2.2
1	2	653	HIS	2.2
1	2	733	ALA	2.2
1	4	76	CYS	2.2
1	2	730	LEU	2.2
1	4	756	TRP	2.1
1	1	13	ARG	2.1
1	1	178	ARG	2.1
1	3	755	ARG	2.1
1	4	772	ASP	2.1
1	2	755	ARG	2.1
1	4	634	GLN	2.1
1	3	665	SER	2.1
1	3	668	VAL	2.1
1	4	71	GLU	2.0
1	4	832	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	1	734	SER	2.0
1	1	129	VAL	2.0
1	4	69	VAL	2.0
1	3	733	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
5	DMS	4	7007	4/4	0.43	0.32	89,89,90,90	0
5	DMS	2	7027	4/4	0.55	0.29	96,96,96,97	0
2	MG	3	3004	1/1	0.56	0.07	53,53,53,53	0
5	DMS	3	7013	4/4	0.57	0.39	70,70,72,72	0
5	DMS	2	7013	4/4	0.61	0.38	76,76,77,78	0
5	DMS	4	7021	4/4	0.74	0.23	99,99,99,100	0
4	GAI	1	2001	4/4	0.75	0.22	63,63,63,64	0
5	DMS	4	7023	4/4	0.75	0.23	89,89,90,90	0
5	DMS	1	7022	4/4	0.76	0.23	107,107,107,108	0
2	MG	2	3004	1/1	0.77	0.09	61,61,61,61	0
5	DMS	1	7014	4/4	0.79	0.24	86,86,86,87	0
5	DMS	1	7020	4/4	0.79	0.20	91,91,91,91	0
5	DMS	2	7019	4/4	0.79	0.32	104,104,104,104	0
4	GAI	3	2001	4/4	0.79	0.17	60,61,61,61	0
3	NA	1	3103	1/1	0.80	0.10	40,40,40,40	0
5	DMS	3	7005	4/4	0.80	0.21	72,73,73,74	0
5	DMS	3	7026	4/4	0.82	0.28	98,98,99,99	0
5	DMS	1	7019	4/4	0.82	0.16	69,69,69,70	0
5	DMS	4	7010	4/4	0.82	0.27	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	4	3004	1/1	0.82	0.08	51,51,51,51	0
5	DMS	3	7007	4/4	0.83	0.26	86,86,86,87	0
5	DMS	4	7019	4/4	0.83	0.20	69,70,70,70	0
5	DMS	4	7024	4/4	0.83	0.18	66,67,67,67	0
5	DMS	2	7005	4/4	0.83	0.23	63,64,65,65	0
5	DMS	2	7007	4/4	0.83	0.29	96,97,97,97	0
5	DMS	1	7015	4/4	0.84	0.23	93,93,94,94	0
5	DMS	4	7016	4/4	0.84	0.23	95,95,95,96	0
5	DMS	2	7011	4/4	0.84	0.23	82,82,82,83	0
5	DMS	4	7013	4/4	0.84	0.29	82,82,82,82	0
5	DMS	4	7017	4/4	0.85	0.17	66,67,67,67	0
4	GAI	4	2001	4/4	0.85	0.22	55,56,56,57	0
5	DMS	3	7020	4/4	0.86	0.20	79,80,80,80	0
5	DMS	3	7011	4/4	0.86	0.23	76,76,77,77	0
3	NA	4	3103	1/1	0.87	0.09	37,37,37,37	0
5	DMS	2	7018	4/4	0.87	0.31	96,96,96,96	0
5	DMS	2	7025	4/4	0.88	0.21	70,70,71,71	0
5	DMS	2	7024	4/4	0.88	0.15	79,80,80,80	0
3	NA	3	3104	1/1	0.88	0.11	32,32,32,32	0
3	NA	1	3104	1/1	0.88	0.09	40,40,40,40	0
4	GAI	2	2001	4/4	0.88	0.19	54,55,55,56	0
5	DMS	1	7010	4/4	0.89	0.19	60,61,61,62	0
5	DMS	4	7012	4/4	0.89	0.19	86,86,87,87	0
5	DMS	3	7019	4/4	0.89	0.28	91,91,91,91	0
2	MG	1	3001	1/1	0.90	0.05	25,25,25,25	0
3	NA	3	3103	1/1	0.90	0.16	42,42,42,42	0
5	DMS	2	7012	4/4	0.90	0.16	73,73,73,73	0
5	DMS	3	1024	4/4	0.90	0.22	45,47,48,48	0
5	DMS	1	7017	4/4	0.90	0.23	74,74,74,75	0
5	DMS	3	7012	4/4	0.90	0.15	69,69,69,69	0
5	DMS	3	7022	4/4	0.90	0.17	72,72,72,72	0
5	DMS	4	7025	4/4	0.91	0.20	67,67,67,67	0
5	DMS	4	7014	4/4	0.91	0.22	82,83,83,83	0
5	DMS	1	7006	4/4	0.91	0.18	78,78,78,78	0
5	DMS	3	7025	4/4	0.91	0.14	53,53,53,54	0
5	DMS	4	7020	4/4	0.91	0.14	68,69,69,70	0
5	DMS	4	7015	4/4	0.91	0.16	52,53,54,54	0
5	DMS	2	7017	4/4	0.92	0.12	75,76,76,76	0
2	MG	1	3004	1/1	0.92	0.04	49,49,49,49	0
3	NA	2	3104	1/1	0.92	0.08	30,30,30,30	0
5	DMS	3	7003	4/4	0.92	0.20	38,39,41,44	0
5	DMS	3	7008	4/4	0.92	0.21	52,52,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	1	7011	4/4	0.92	0.18	86,86,86,86	0
3	NA	1	3101	1/1	0.92	0.10	30,30,30,30	0
5	DMS	1	7016	4/4	0.93	0.13	67,67,67,67	0
5	DMS	2	7003	4/4	0.93	0.15	32,33,35,38	0
5	DMS	2	7021	4/4	0.93	0.15	59,59,60,60	0
5	DMS	2	7020	4/4	0.93	0.15	61,61,62,63	0
5	DMS	2	7022	4/4	0.93	0.17	60,60,60,61	0
5	DMS	3	7023	4/4	0.93	0.23	67,67,68,68	0
5	DMS	1	7007	4/4	0.93	0.16	63,64,64,64	0
5	DMS	4	7022	4/4	0.93	0.18	65,65,65,66	0
2	MG	1	3002	1/1	0.94	0.06	24,24,24,24	0
5	DMS	1	7003	4/4	0.94	0.14	31,32,36,38	0
3	NA	4	3101	1/1	0.94	0.06	22,22,22,22	0
5	DMS	3	7021	4/4	0.94	0.14	63,63,63,64	0
5	DMS	1	7013	4/4	0.94	0.11	48,49,50,50	0
5	DMS	2	7010	4/4	0.94	0.14	46,46,47,47	0
5	DMS	2	7016	4/4	0.94	0.24	69,70,70,70	0
5	DMS	1	7024	4/4	0.94	0.18	47,47,48,49	0
3	NA	4	3104	1/1	0.94	0.12	45,45,45,45	0
5	DMS	2	7015	4/4	0.94	0.14	69,69,69,69	0
5	DMS	4	7006	4/4	0.94	0.20	65,65,66,66	0
3	NA	2	3103	1/1	0.94	0.15	39,39,39,39	0
5	DMS	1	7021	4/4	0.95	0.15	72,72,72,73	0
5	DMS	3	7014	4/4	0.95	0.14	70,70,70,70	0
5	DMS	4	7003	4/4	0.95	0.22	36,38,39,40	0
5	DMS	3	7017	4/4	0.95	0.14	50,50,51,51	0
5	DMS	4	7001	4/4	0.95	0.17	32,33,33,35	0
5	DMS	1	7009	4/4	0.95	0.13	43,44,45,45	0
5	DMS	1	7012	4/4	0.96	0.13	68,69,69,69	0
5	DMS	1	7018	4/4	0.96	0.21	52,53,54,54	0
5	DMS	2	7008	4/4	0.96	0.17	59,60,60,60	0
5	DMS	2	7028	4/4	0.96	0.11	58,58,58,59	0
5	DMS	4	7009	4/4	0.96	0.16	52,53,53,54	0
5	DMS	2	7026	4/4	0.96	0.18	47,47,48,48	0
3	NA	4	3102	1/1	0.96	0.08	15,15,15,15	0
5	DMS	2	7006	4/4	0.96	0.13	40,41,41,43	0
5	DMS	4	7008	4/4	0.96	0.12	50,51,52,52	0
5	DMS	4	7018	4/4	0.96	0.13	54,55,55,55	0
5	DMS	1	7023	4/4	0.96	0.17	53,54,54,54	0
5	DMS	4	7002	4/4	0.96	0.15	34,35,35,37	0
5	DMS	2	7023	4/4	0.96	0.17	54,54,54,54	0
5	DMS	4	7005	4/4	0.96	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	2	7004	4/4	0.96	0.09	29,31,31,33	0
5	DMS	1	7008	4/4	0.96	0.13	44,44,44,45	0
5	DMS	1	7001	4/4	0.97	0.15	26,26,27,29	0
5	DMS	3	7006	4/4	0.97	0.14	45,45,46,46	0
5	DMS	2	7001	4/4	0.97	0.11	25,25,25,29	0
3	NA	3	3101	1/1	0.97	0.09	22,22,22,22	0
5	DMS	4	7011	4/4	0.97	0.17	71,71,72,72	0
5	DMS	3	7004	4/4	0.97	0.10	30,31,32,32	0
5	DMS	3	7010	4/4	0.97	0.17	41,42,43,43	0
5	DMS	3	7001	4/4	0.97	0.12	23,23,24,28	0
5	DMS	3	7018	4/4	0.97	0.23	53,53,54,54	0
5	DMS	3	7016	4/4	0.97	0.32	52,54,54,55	0
3	NA	3	3102	1/1	0.98	0.09	18,18,18,18	0
5	DMS	2	7029	4/4	0.98	0.13	43,43,44,44	0
2	MG	4	3002	1/1	0.98	0.07	25,25,25,25	0
3	NA	2	3101	1/1	0.98	0.09	16,16,16,16	0
5	DMS	3	7002	4/4	0.98	0.11	31,31,32,33	0
5	DMS	1	7000	4/4	0.98	0.13	19,21,21,25	0
3	NA	2	3102	1/1	0.98	0.11	18,18,18,18	0
5	DMS	2	7014	4/4	0.98	0.09	56,56,56,56	0
5	DMS	1	7004	4/4	0.98	0.12	36,36,38,39	0
5	DMS	2	7009	4/4	0.98	0.12	42,42,43,44	0
5	DMS	1	7002	4/4	0.98	0.12	32,32,35,35	0
5	DMS	3	7015	4/4	0.98	0.12	54,54,54,54	0
5	DMS	1	7005	4/4	0.98	0.12	60,60,60,60	0
5	DMS	4	7004	4/4	0.98	0.17	32,33,34,35	0
5	DMS	3	7009	4/4	0.98	0.12	40,41,42,42	0
3	NA	1	3102	1/1	0.98	0.11	15,15,15,15	0
5	DMS	3	7024	4/4	0.98	0.13	57,57,57,57	0
2	MG	3	3002	1/1	0.99	0.05	12,12,12,12	0
2	MG	4	3001	1/1	0.99	0.06	23,23,23,23	0
2	MG	3	3001	1/1	0.99	0.06	16,16,16,16	0
2	MG	2	3002	1/1	0.99	0.07	15,15,15,15	0
2	MG	2	3001	1/1	0.99	0.10	20,20,20,20	0
5	DMS	2	7000	4/4	0.99	0.13	22,23,24,24	0
5	DMS	4	7000	4/4	0.99	0.11	24,26,27,27	0
5	DMS	3	7000	4/4	0.99	0.12	17,18,18,21	0
5	DMS	2	7002	4/4	0.99	0.10	30,30,30,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.