



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 11:23 AM EDT

PDB ID : 3I3B
Title : E.coli (lacZ) Beta-Galactosidase (M542A) in Complex with D-Galactopyranosyl-1-on
Authors : Dugdale, M.L.; Dymianiw, D.; Minhas, B.; Huber, R.E.
Deposited on : 2009-06-30
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	:	2.23.2
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)	:	2.23.2

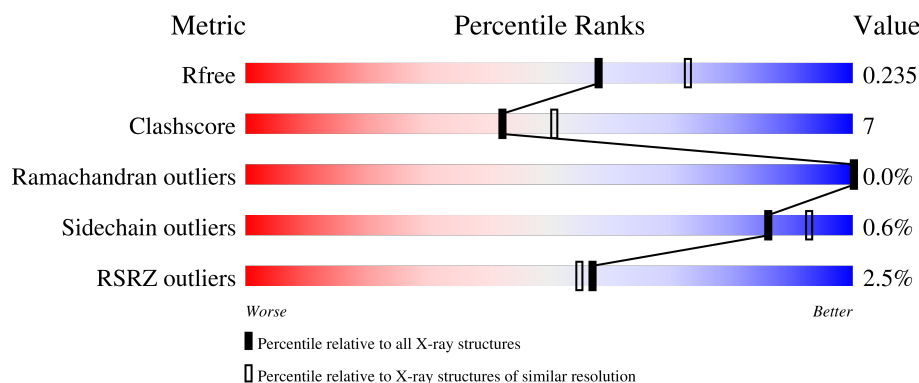
1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	<div> <div>3%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	B	1023	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	C	1023	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	D	1023	<div> <div>2%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36275 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			
1	B	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			
1	C	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			
1	D	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			

There are 36 discrepancies between the modelled and reference sequences:

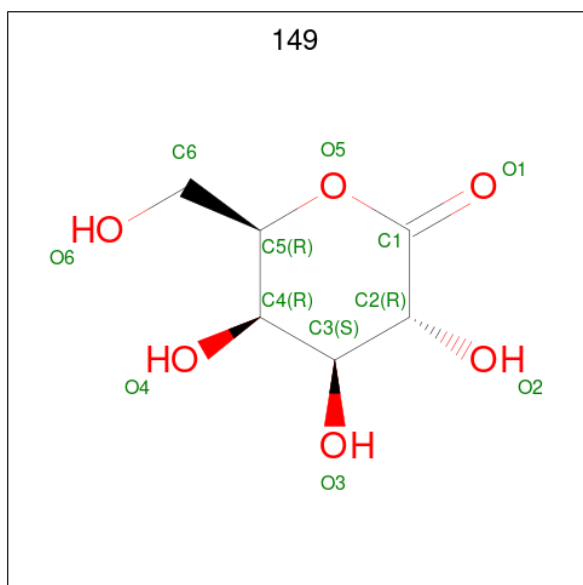
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP B8LFD6
A	2	SER	-	expression tag	UNP B8LFD6
A	3	HIS	-	expression tag	UNP B8LFD6
A	4	MET	-	expression tag	UNP B8LFD6
A	5	LEU	-	expression tag	UNP B8LFD6
A	6	GLU	-	expression tag	UNP B8LFD6
A	7	ASP	-	expression tag	UNP B8LFD6
A	8	PRO	-	expression tag	UNP B8LFD6
A	542	ALA	MET	engineered mutation	UNP B8LFD6
B	1	GLY	-	expression tag	UNP B8LFD6
B	2	SER	-	expression tag	UNP B8LFD6
B	3	HIS	-	expression tag	UNP B8LFD6
B	4	MET	-	expression tag	UNP B8LFD6
B	5	LEU	-	expression tag	UNP B8LFD6
B	6	GLU	-	expression tag	UNP B8LFD6
B	7	ASP	-	expression tag	UNP B8LFD6
B	8	PRO	-	expression tag	UNP B8LFD6
B	542	ALA	MET	engineered mutation	UNP B8LFD6
C	1	GLY	-	expression tag	UNP B8LFD6
C	2	SER	-	expression tag	UNP B8LFD6
C	3	HIS	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	expression tag	UNP B8LFD6
C	5	LEU	-	expression tag	UNP B8LFD6
C	6	GLU	-	expression tag	UNP B8LFD6
C	7	ASP	-	expression tag	UNP B8LFD6
C	8	PRO	-	expression tag	UNP B8LFD6
C	542	ALA	MET	engineered mutation	UNP B8LFD6
D	1	GLY	-	expression tag	UNP B8LFD6
D	2	SER	-	expression tag	UNP B8LFD6
D	3	HIS	-	expression tag	UNP B8LFD6
D	4	MET	-	expression tag	UNP B8LFD6
D	5	LEU	-	expression tag	UNP B8LFD6
D	6	GLU	-	expression tag	UNP B8LFD6
D	7	ASP	-	expression tag	UNP B8LFD6
D	8	PRO	-	expression tag	UNP B8LFD6
D	542	ALA	MET	engineered mutation	UNP B8LFD6

- Molecule 2 is D-galactonolactone (three-letter code: 149) (formula: C₆H₁₀O₆).



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

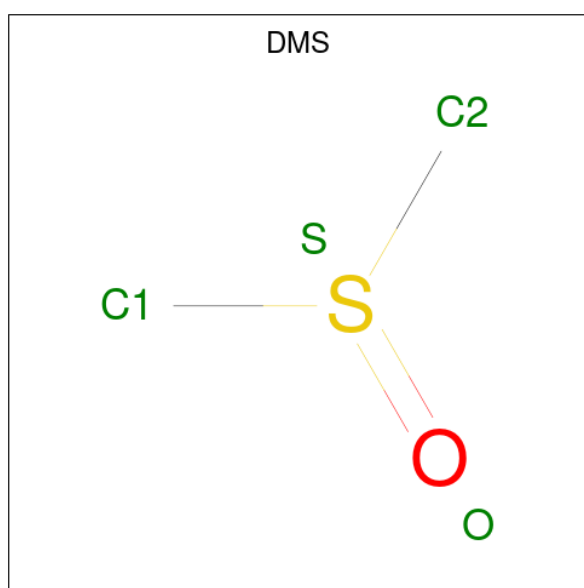
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	798	Total 798	O 798	0	0
6	B	821	Total 821	O 821	0	0
6	C	785	Total 785	O 785	0	0
6	D	804	Total 804	O 804	0	0

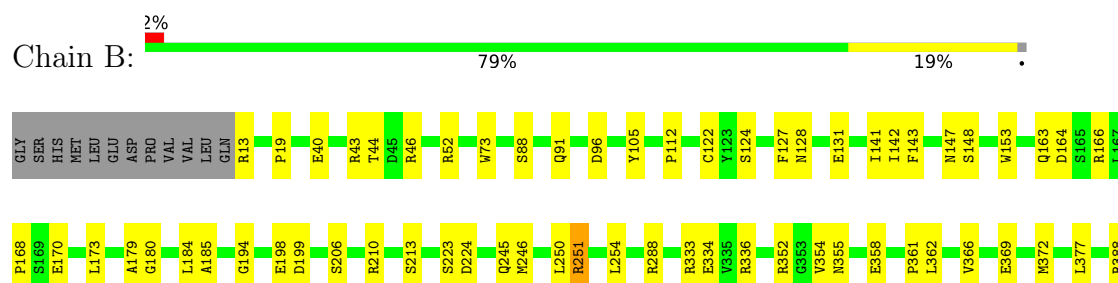
3 Residue-property plots [i](#)

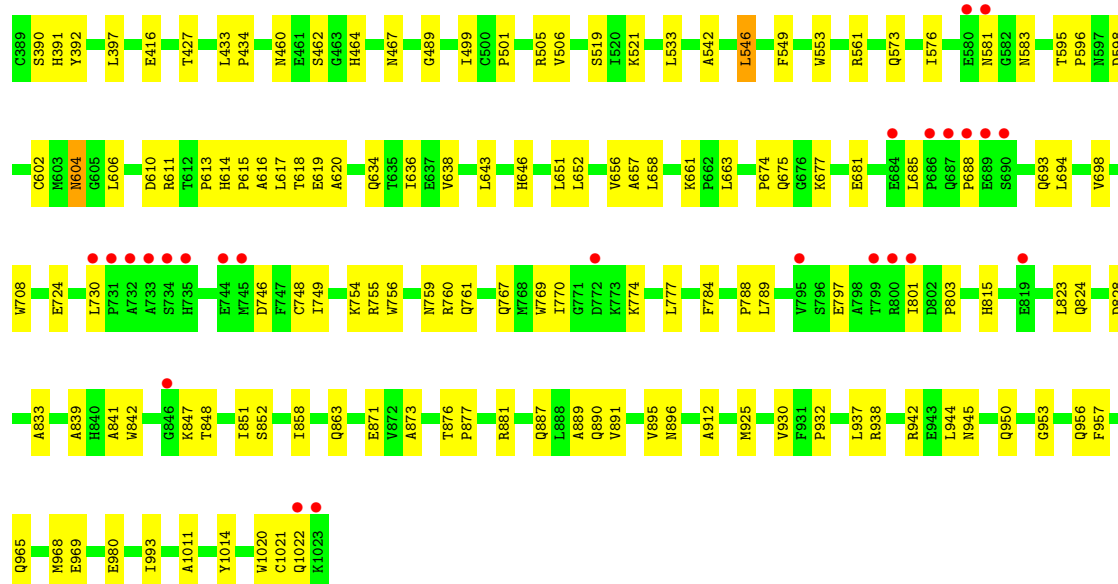
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-galactosidase

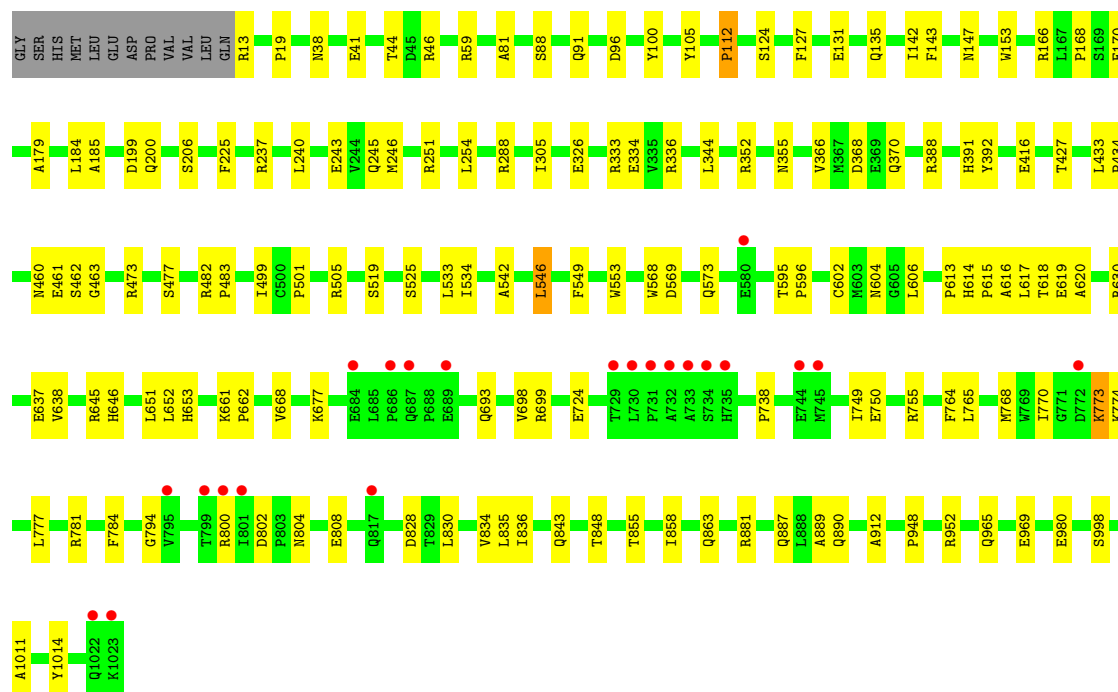
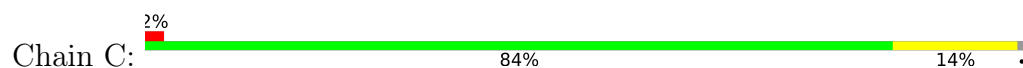


• Molecule 1: Beta-galactosidase

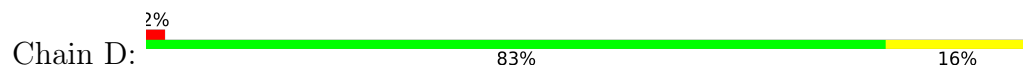


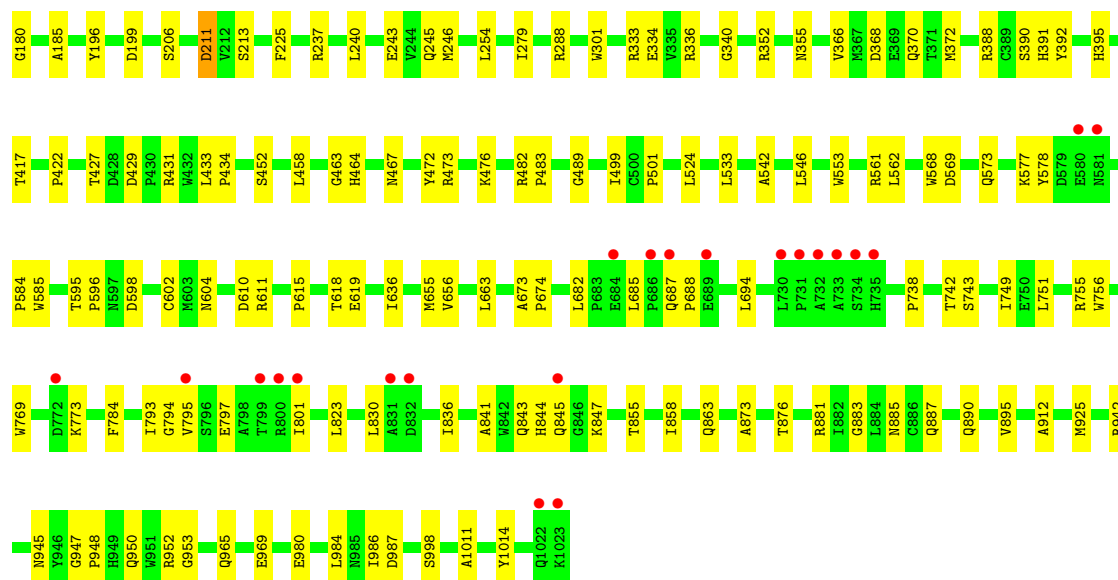


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.60Å 168.42Å 201.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.18 – 2.20 14.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (14.18-2.20) 96.2 (14.18-2.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.193 , 0.244 0.184 , 0.235	Depositor DCC
R_{free} test set	3517 reflections (1.08%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.1	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	0.94	EDS
Total number of atoms	36275	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 36.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1383e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 149, NA, DMS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/8364	0.62	1/11412 (0.0%)
1	B	0.33	0/8364	0.63	0/11412
1	C	0.33	0/8364	0.62	1/11412 (0.0%)
1	D	0.33	0/8364	0.62	0/11412
All	All	0.33	0/33456	0.62	2/45648 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	GLY	N-CA-C	-5.33	99.76	113.10
1	C	770	ILE	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8122	0	7711	130	0
1	B	8122	0	7712	125	0
1	C	8122	0	7712	102	0
1	D	8122	0	7712	104	0
2	A	12	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	9	0	0
2	C	12	0	9	0	0
2	D	12	0	9	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	120	0	180	2	0
5	B	132	0	198	0	0
5	C	132	0	198	1	0
5	D	120	0	180	0	0
6	A	798	0	0	2	0
6	B	821	0	0	4	0
6	C	785	0	0	2	0
6	D	804	0	0	4	0
All	All	36275	0	31639	449	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 (449) 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:A:142:ILE:HG12	1:A:170:GLU:HG2	1.42	1.01
1:A:249:GLU:CD	1:A:251:ARG:HE	1.68	0.96
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.59	0.82
1:A:730:LEU:HD21	1:B:823:LEU:O	1.82	0.80
1:A:147:ASN:HB3	1:A:206:SER:HA	1.63	0.79
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.63	0.79
1:B:767:GLN:NE2	1:B:774:LYS:HB3	2.00	0.77
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.69	0.75
1:C:773:LYS:HE2	1:C:774:LYS:N	2.01	0.75
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.53	0.74
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.69	0.74
1:D:237:ARG:HB3	1:D:237:ARG:NH1	2.03	0.74
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.69	0.74
1:C:44:THR:OG1	1:C:46:ARG:HD3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:SER:HA	1:D:366:VAL:HG21	1.71	0.72
1:D:863:GLN:HE22	1:D:952:ARG:HH21	1.37	0.70
1:A:241:GLU:HG2	1:A:292:ARG:HG2	1.73	0.70
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.74	0.70
1:B:52:ARG:O	1:B:213:SER:HB2	1.94	0.68
1:D:147:ASN:HB3	1:D:206:SER:HA	1.75	0.68
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.77	0.67
1:A:945:ASN:HB3	1:A:1023:LYS:NZ	2.11	0.66
1:B:890:GLN:HG2	1:B:891:VAL:N	2.12	0.65
1:D:965:GLN:O	1:D:969:GLU:HG3	1.95	0.65
1:A:54:LEU:HD11	1:A:214:LEU:HD13	1.78	0.65
1:C:473:ARG:HH12	1:C:477:SER:HB2	1.62	0.65
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.33	0.64
1:A:579:ASP:OD2	1:A:583:ASN:HB2	1.97	0.64
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.12	0.64
1:D:749:ILE:HD12	1:D:749:ILE:N	2.13	0.64
1:A:88:SER:HA	1:A:366:VAL:HG21	1.79	0.64
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.81	0.63
1:C:147:ASN:HB3	1:C:206:SER:HA	1.79	0.63
1:A:749:ILE:HD12	1:A:858:ILE:HD12	1.81	0.63
1:A:249:GLU:HG2	1:A:251:ARG:HG2	1.79	0.62
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.80	0.62
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.79	0.62
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.14	0.62
1:A:823:LEU:O	1:B:730:LEU:HD11	2.00	0.62
1:C:131:GLU:O	1:C:135:GLN:HG3	1.99	0.62
1:D:578:TYR:CE1	1:D:584:PRO:HB3	2.35	0.62
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.00	0.61
1:D:573:GLN:HB2	1:D:602:CYS:O	2.01	0.61
1:B:777:LEU:HG	1:B:889:ALA:HA	1.82	0.61
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.01	0.60
1:D:863:GLN:HE22	1:D:952:ARG:NH2	1.99	0.60
1:A:801:ILE:HD12	1:A:801:ILE:N	2.16	0.60
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.33	0.60
1:A:751:LEU:HD23	1:A:862:GLY:HA2	1.83	0.60
1:B:873:ALA:O	1:B:876:THR:HG22	2.01	0.59
1:C:887:GLN:NE2	1:C:980:GLU:O	2.35	0.59
1:A:965:GLN:O	1:A:969:GLU:HG3	2.02	0.59
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.37	0.59
1:C:473:ARG:NH1	1:C:477:SER:HB2	2.18	0.59
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:LEU:HD23	1:B:675:GLN:NE2	2.18	0.59
1:D:254:LEU:HD12	6:D:4828:HOH:O	2.03	0.59
1:C:131:GLU:OE1	1:C:179:ALA:HB2	2.03	0.59
1:B:774:LYS:HB2	6:B:4851:HOH:O	2.03	0.59
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.85	0.58
1:A:131:GLU:O	1:A:135:GLN:HG2	2.03	0.58
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.84	0.58
1:D:793:ILE:HG22	1:D:795:VAL:HG22	1.84	0.58
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.83	0.58
1:D:656:VAL:HG21	1:D:685:LEU:HD13	1.84	0.58
1:B:754:LYS:HE2	1:B:1022:GLN:OE1	2.04	0.58
1:B:754:LYS:HE3	1:B:770:ILE:HG23	1.85	0.58
1:C:777:LEU:HG	1:C:889:ALA:HA	1.86	0.58
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.34	0.58
1:A:334:GLU:OE1	1:A:336:ARG:NH1	2.37	0.58
1:C:749:ILE:N	1:C:749:ILE:HD12	2.18	0.58
1:A:249:GLU:CG	1:A:251:ARG:HE	2.17	0.57
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.85	0.57
1:A:613:PRO:HB3	1:A:617:LEU:HD23	1.86	0.57
1:B:651:LEU:C	1:B:651:LEU:HD12	2.25	0.57
1:B:890:GLN:HG2	1:B:891:VAL:H	1.69	0.57
1:C:533:LEU:C	1:C:533:LEU:HD23	2.25	0.56
1:A:279:ILE:HD11	1:D:422:PRO:HG3	1.86	0.56
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.87	0.56
1:B:823:LEU:HD11	1:B:841:ALA:HB2	1.88	0.56
1:A:194:GLY:O	1:A:198:GLU:HG3	2.06	0.56
1:B:759:ASN:OD1	1:B:761:GLN:HB3	2.06	0.56
1:D:615:PRO:O	1:D:618:THR:HG22	2.06	0.56
1:A:823:LEU:HD11	1:A:841:ALA:HB2	1.86	0.56
1:B:131:GLU:OE1	1:B:179:ALA:HB2	2.05	0.56
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.88	0.55
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.88	0.55
1:B:769:TRP:NE1	1:B:774:LYS:HG2	2.22	0.55
1:A:96:ASP:OD2	1:A:190:ARG:NH1	2.40	0.55
1:C:81:ALA:HA	5:C:5030:DMS:H11	1.89	0.55
1:D:863:GLN:NE2	1:D:952:ARG:HH21	2.04	0.55
1:B:749:ILE:N	1:B:749:ILE:HD12	2.21	0.55
1:B:965:GLN:O	1:B:969:GLU:HG3	2.06	0.55
1:A:634:GLN:NE2	1:A:684:GLU:HA	2.21	0.55
1:B:573:GLN:HB2	1:B:602:CYS:O	2.06	0.55
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:PRO:HD3	1:B:694:LEU:HD11	1.89	0.55
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.17	0.55
1:A:472:TYR:O	1:A:476:LYS:HG2	2.07	0.54
1:C:88:SER:HA	1:C:366:VAL:HG21	1.90	0.54
1:C:863:GLN:NE2	1:C:952:ARG:NH2	2.55	0.54
1:B:88:SER:HA	1:B:366:VAL:HG21	1.87	0.54
1:B:784:PHE:HA	1:B:881:ARG:O	2.08	0.54
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.39	0.54
1:B:851:ILE:HB	1:B:871:GLU:HB2	1.90	0.53
1:D:890:GLN:HE22	1:D:948:PRO:HD3	1.73	0.53
1:D:945:ASN:OD1	1:D:950:GLN:HG3	2.09	0.53
1:A:105:TYR:CE1	1:A:199:ASP:HB2	2.44	0.53
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.43	0.53
1:C:750:GLU:OE2	1:C:755:ARG:HD2	2.09	0.53
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.74	0.53
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.91	0.53
1:C:773:LYS:HE2	1:C:774:LYS:H	1.72	0.53
1:D:823:LEU:HD11	1:D:841:ALA:HB2	1.91	0.53
1:A:663:LEU:HD11	1:A:688:PRO:HB3	1.91	0.53
1:A:984:LEU:HD21	1:A:986:ILE:HD11	1.91	0.53
1:C:352:ARG:HG2	1:C:553:TRP:CH2	2.43	0.53
1:A:196:TYR:O	1:A:417:THR:HG22	2.09	0.53
1:B:887:GLN:NE2	1:B:980:GLU:O	2.40	0.53
1:C:863:GLN:HE22	1:C:952:ARG:NH2	2.07	0.53
1:D:73:TRP:HB2	1:D:78:LEU:HD11	1.91	0.53
1:B:369:GLU:HA	1:B:372:MET:HE3	1.91	0.52
1:B:606:LEU:O	1:B:614:HIS:HB2	2.09	0.52
1:C:646:HIS:HB3	6:C:4937:HOH:O	2.09	0.52
1:D:887:GLN:NE2	1:D:980:GLU:O	2.42	0.52
1:B:755:ARG:HD3	1:B:769:TRP:CE3	2.45	0.52
1:C:843:GLN:HG2	1:C:848:THR:HA	1.91	0.52
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.45	0.52
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.92	0.52
1:D:473:ARG:O	1:D:473:ARG:NH1	2.42	0.52
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.45	0.52
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.92	0.52
1:B:542:ALA:HA	1:B:604:ASN:HA	1.91	0.52
1:B:595:THR:HA	1:B:596:PRO:C	2.29	0.52
1:A:873:ALA:O	1:A:876:THR:HG22	2.09	0.52
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.22	0.51
1:B:777:LEU:HD11	1:B:980:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ASN:HB3	1:A:1023:LYS:HZ2	1.75	0.51
1:B:863:GLN:HG2	1:B:1021:CYS:CB	2.38	0.51
1:C:251:ARG:HB2	1:C:254:LEU:HG	1.92	0.51
1:D:19:PRO:HD3	1:D:112:PRO:CB	2.41	0.51
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.45	0.51
1:B:369:GLU:HG3	1:B:397:LEU:HD21	1.93	0.51
1:C:240:LEU:C	1:C:240:LEU:HD23	2.31	0.51
1:C:237:ARG:HB3	1:C:237:ARG:HH11	1.75	0.51
1:D:105:TYR:CE1	1:D:199:ASP:HB2	2.45	0.51
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.93	0.51
1:B:427:THR:HG21	1:B:462:SER:HB3	1.93	0.51
1:B:937:LEU:HA	1:B:957:PHE:O	2.11	0.51
1:B:930:VAL:O	1:B:932:PRO:HD3	2.11	0.50
1:A:749:ILE:CD1	1:A:858:ILE:HD12	2.41	0.50
1:B:44:THR:OG1	1:B:46:ARG:HG3	2.11	0.50
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.11	0.50
1:D:595:THR:HA	1:D:596:PRO:C	2.32	0.50
1:A:688:PRO:HD3	1:A:694:LEU:HD11	1.92	0.50
1:B:464:HIS:HB2	1:B:489:GLY:HA3	1.92	0.50
1:D:881:ARG:HE	1:D:987:ASP:CG	2.14	0.50
1:B:416:GLU:HG3	1:B:460:ASN:O	2.12	0.50
1:B:615:PRO:O	1:B:618:THR:HG22	2.12	0.50
1:C:427:THR:HG21	1:C:462:SER:HB3	1.93	0.50
1:D:801:ILE:HD12	1:D:801:ILE:N	2.26	0.50
1:A:533:LEU:C	1:A:533:LEU:HD23	2.32	0.50
1:D:464:HIS:HB2	1:D:489:GLY:HA3	1.93	0.50
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.93	0.49
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.45	0.49
1:B:651:LEU:HD12	1:B:651:LEU:O	2.12	0.49
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.94	0.49
1:B:194:GLY:O	1:B:198:GLU:HG3	2.12	0.49
1:B:124:SER:HA	1:B:184:LEU:O	2.13	0.49
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.47	0.49
1:A:651:LEU:C	1:A:651:LEU:HD12	2.32	0.49
1:A:279:ILE:HD11	1:D:422:PRO:CG	2.42	0.49
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.95	0.49
1:B:354:VAL:HG22	1:B:355:ASN:O	2.13	0.48
1:A:438:GLU:HG2	1:A:442:ARG:HD2	1.94	0.48
1:A:833:ALA:HB1	1:A:858:ILE:O	2.12	0.48
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.95	0.48
1:C:630:ARG:HD3	1:C:637:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:890:GLN:NE2	1:D:947:GLY:HA3	2.27	0.48
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.94	0.48
1:A:573:GLN:HB2	1:A:602:CYS:O	2.13	0.48
1:C:738:PRO:HG2	1:C:858:ILE:O	2.14	0.48
1:A:887:GLN:NE2	1:A:980:GLU:O	2.44	0.48
1:B:842:TRP:HZ3	1:B:852:SER:HB3	1.79	0.48
1:C:546:LEU:HA	6:C:4132:HOH:O	2.13	0.48
1:A:292:ARG:C	1:A:293:LEU:HD12	2.33	0.48
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.43	0.48
1:C:830:LEU:CD2	1:D:830:LEU:HD21	2.44	0.48
1:B:748:CYS:C	1:B:749:ILE:HD12	2.34	0.48
1:A:755:ARG:HB2	1:A:769:TRP:HB2	1.96	0.48
1:C:615:PRO:O	1:C:618:THR:HG22	2.14	0.48
1:D:542:ALA:HA	1:D:604:ASN:HA	1.96	0.48
1:D:895:VAL:HG21	1:D:925:MET:HG3	1.96	0.48
1:A:833:ALA:HB2	1:A:859:ASP:HA	1.96	0.48
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.49	0.48
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.95	0.48
1:B:636:ILE:HD13	1:B:698:VAL:HG11	1.96	0.47
1:A:830:LEU:HD22	1:B:828:ASP:HB3	1.97	0.47
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.97	0.47
1:B:143:PHE:O	1:B:168:PRO:HA	2.14	0.47
1:C:38:ASN:OD1	1:C:41:GLU:HG3	2.14	0.47
1:D:942:ARG:HA	1:D:953:GLY:O	2.14	0.47
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.48	0.47
1:B:361:PRO:HB2	1:B:576:ILE:HG12	1.95	0.47
1:D:225:PHE:HA	1:D:243:GLU:O	2.14	0.47
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.49	0.47
1:C:828:ASP:HB3	1:D:830:LEU:HD22	1.95	0.47
1:D:836:ILE:O	1:D:855:THR:HA	2.14	0.47
1:A:815:HIS:HE1	1:A:877:PRO:O	1.97	0.47
1:B:656:VAL:HG21	1:B:685:LEU:CD1	2.44	0.47
1:B:661:LYS:O	1:B:663:LEU:HD22	2.15	0.47
1:A:570:TRP:O	1:A:607:VAL:HG22	2.14	0.47
1:A:836:ILE:O	1:A:855:THR:HA	2.15	0.47
1:B:147:ASN:HA	1:B:148:SER:HA	1.56	0.47
1:B:613:PRO:HB3	1:B:617:LEU:HD23	1.96	0.47
1:A:102:ASN:HD21	5:A:5130:DMS:C2	2.27	0.47
1:D:117:GLU:HG2	6:D:4257:HOH:O	2.15	0.47
1:D:794:GLY:HA2	1:D:998:SER:O	2.15	0.47
1:C:738:PRO:HB2	1:C:834:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.97	0.47
1:D:636:ILE:HD11	1:D:682:LEU:HD11	1.97	0.47
1:C:368:ASP:OD2	1:C:370:GLN:HB3	2.15	0.46
1:C:764:PHE:CE2	1:C:781:ARG:NH1	2.82	0.46
1:D:128:ASN:HB3	1:D:180:GLY:O	2.15	0.46
1:A:542:ALA:HA	1:A:604:ASN:HA	1.98	0.46
1:B:13:ARG:NH1	1:C:13:ARG:HD2	2.30	0.46
1:C:416:GLU:HA	1:C:460:ASN:O	2.15	0.46
1:C:651:LEU:HD12	1:C:668:VAL:O	2.15	0.46
1:D:301:TRP:CH2	1:D:452:SER:HA	2.49	0.46
1:D:476:LYS:HD2	6:D:4195:HOH:O	2.14	0.46
1:B:693:GLN:OE1	1:B:724:GLU:HB2	2.15	0.46
1:B:777:LEU:CD1	1:B:980:GLU:HG2	2.44	0.46
1:C:573:GLN:HB2	1:C:602:CYS:O	2.15	0.46
1:C:595:THR:HA	1:C:596:PRO:C	2.36	0.46
1:D:784:PHE:HA	1:D:881:ARG:O	2.15	0.46
1:A:595:THR:HA	1:A:596:PRO:C	2.35	0.46
1:C:460:ASN:ND2	1:C:461:GLU:HG3	2.31	0.46
1:D:352:ARG:HG2	1:D:553:TRP:CH2	2.51	0.46
1:D:577:LYS:O	1:D:584:PRO:HA	2.15	0.46
1:A:794:GLY:HA2	1:A:998:SER:O	2.16	0.46
1:B:362:LEU:HD23	1:B:576:ILE:HB	1.97	0.46
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.51	0.46
1:A:945:ASN:HB3	1:A:1023:LYS:HZ3	1.81	0.46
1:B:246:MET:C	1:B:246:MET:SD	2.94	0.46
1:C:131:GLU:HG3	1:C:135:GLN:HG3	1.98	0.46
1:D:144:ASP:OD2	1:D:211:ASP:HB2	2.16	0.46
1:D:26:ARG:HD2	1:D:169:SER:HA	1.98	0.46
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.97	0.46
1:B:942:ARG:HA	1:B:953:GLY:O	2.16	0.46
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.51	0.45
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.97	0.45
1:C:606:LEU:O	1:C:614:HIS:HB2	2.16	0.45
1:C:693:GLN:OE1	1:C:724:GLU:HB2	2.16	0.45
1:A:390:SER:HA	1:A:391:HIS:HA	1.71	0.45
1:B:210:ARG:NH2	1:B:358:GLU:OE1	2.46	0.45
1:B:506:VAL:HG12	1:B:521:LYS:HE3	1.98	0.45
1:B:646:HIS:HB3	6:B:4983:HOH:O	2.15	0.45
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.99	0.45
1:D:598:ASP:OD1	1:D:797:GLU:HA	2.16	0.45
1:D:656:VAL:HG21	1:D:685:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:MET:CE	1:B:250:LEU:HD23	2.46	0.45
1:C:835:LEU:HD11	1:C:855:THR:HB	1.98	0.45
1:A:753:ASN:O	1:A:771:GLY:N	2.48	0.45
1:B:546:LEU:HA	6:B:4129:HOH:O	2.16	0.45
1:C:800:ARG:HG2	1:C:800:ARG:HH11	1.81	0.45
1:A:240:LEU:C	1:A:240:LEU:HD23	2.36	0.45
1:A:230:ARG:NH2	1:A:241:GLU:OE2	2.49	0.45
1:A:577:LYS:O	1:A:584:PRO:HA	2.17	0.45
1:B:801:ILE:O	1:B:803:PRO:HD3	2.17	0.45
1:D:390:SER:HA	1:D:391:HIS:HA	1.73	0.45
1:D:873:ALA:O	1:D:876:THR:HG22	2.17	0.45
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.98	0.45
1:B:505:ARG:O	1:B:519:SER:HA	2.16	0.45
1:B:533:LEU:HD23	1:B:533:LEU:C	2.37	0.45
1:B:610:ASP:O	1:B:611:ARG:HB2	2.16	0.45
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.98	0.45
1:C:830:LEU:HD21	1:D:830:LEU:HD21	1.99	0.45
1:D:19:PRO:HD3	1:D:112:PRO:HB3	1.98	0.45
1:A:797:GLU:C	1:A:799:THR:H	2.20	0.45
1:C:225:PHE:HA	1:C:243:GLU:O	2.16	0.45
1:A:658:LEU:HD22	1:A:688:PRO:HB2	1.99	0.45
1:D:368:ASP:OD2	1:D:370:GLN:HB3	2.17	0.45
1:D:756:TRP:CD2	1:D:858:ILE:HD13	2.52	0.45
1:A:964:GLN:O	1:A:968:MET:HB2	2.17	0.45
1:C:965:GLN:O	1:C:969:GLU:HG3	2.16	0.45
1:A:301:TRP:CH2	1:A:452:SER:HA	2.52	0.44
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.51	0.44
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.52	0.44
1:C:952:ARG:NH1	1:C:952:ARG:HB2	2.32	0.44
1:D:196:TYR:O	1:D:417:THR:HG22	2.17	0.44
1:A:687:GLN:CD	1:A:687:GLN:H	2.20	0.44
1:B:427:THR:O	1:B:467:ASN:HB2	2.17	0.44
1:D:147:ASN:HA	1:D:148:SER:HA	1.62	0.44
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.52	0.44
1:A:730:LEU:HD12	1:A:730:LEU:N	2.32	0.44
1:B:1020:TRP:HD1	1:B:1021:CYS:N	2.15	0.44
1:A:587:ALA:HB1	1:A:591:ASP:CB	2.47	0.44
1:D:577:LYS:HD3	1:D:585:TRP:CH2	2.52	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.61	0.44
1:B:40:GLU:OE2	1:B:43:ARG:NH2	2.50	0.44
1:C:143:PHE:O	1:C:168:PRO:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:HIS:HB3	1:C:699:ARG:NH2	2.32	0.44
1:D:688:PRO:HG3	1:D:694:LEU:HD21	2.00	0.44
1:D:755:ARG:HB2	1:D:769:TRP:HB2	2.00	0.44
1:A:370:GLN:HG3	6:A:4474:HOH:O	2.16	0.44
1:C:200:GLN:HA	1:C:416:GLU:OE1	2.17	0.44
1:A:369:GLU:HG3	1:A:397:LEU:HD21	2.00	0.44
1:A:422:PRO:CG	1:D:279:ILE:HD11	2.48	0.44
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.33	0.44
1:A:800:ARG:HG2	1:A:800:ARG:HH11	1.83	0.44
1:D:246:MET:SD	1:D:246:MET:C	2.96	0.44
1:A:249:GLU:CG	1:A:251:ARG:NE	2.79	0.44
1:B:546:LEU:HD22	1:B:616:ALA:HB1	1.99	0.44
1:C:131:GLU:HG3	1:C:135:GLN:CG	2.48	0.44
1:A:660:GLY:O	1:A:662:PRO:HD3	2.18	0.44
1:A:770:ILE:HG23	1:A:1022:GLN:OE1	2.17	0.44
1:A:920:LEU:HB3	1:A:921:PRO:HD2	2.00	0.44
1:C:505:ARG:O	1:C:519:SER:HA	2.17	0.44
1:D:610:ASP:O	1:D:611:ARG:HB2	2.18	0.44
1:A:802:ASP:O	1:A:808:GLU:HG3	2.18	0.43
1:A:945:ASN:OD1	1:A:1023:LYS:HD3	2.18	0.43
1:C:326:GLU:OE1	1:C:326:GLU:HA	2.18	0.43
1:A:842:TRP:HZ3	1:A:852:SER:HB3	1.82	0.43
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.17	0.43
1:C:525:SER:O	1:D:561:ARG:HD3	2.18	0.43
1:D:390:SER:HB2	1:D:391:HIS:CE1	2.54	0.43
1:A:610:ASP:O	1:A:611:ARG:HB2	2.18	0.43
1:B:824:GLN:HB3	1:B:839:ALA:HB3	2.00	0.43
1:D:240:LEU:HD23	1:D:240:LEU:C	2.38	0.43
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.18	0.43
1:B:147:ASN:HB3	1:B:206:SER:HA	2.01	0.43
1:B:833:ALA:HB1	1:B:858:ILE:O	2.19	0.43
1:C:777:LEU:HB2	1:C:887:GLN:HG2	2.00	0.43
1:D:673:ALA:HB1	1:D:674:PRO:HD2	2.00	0.43
1:D:687:GLN:H	1:D:687:GLN:CD	2.22	0.43
1:B:598:ASP:OD1	1:B:797:GLU:HA	2.17	0.43
1:D:568:TRP:HA	1:D:569:ASP:HA	1.78	0.43
1:C:59:ARG:HB2	1:C:124:SER:OG	2.19	0.43
1:D:524:LEU:HD11	1:D:562:LEU:HG	2.01	0.43
1:D:843:GLN:HA	1:D:847:LYS:O	2.18	0.43
1:A:634:GLN:HE21	1:A:684:GLU:HA	1.82	0.43
1:B:937:LEU:O	1:B:938:ARG:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:777:LEU:HD11	1:C:980:GLU:HG2	2.01	0.43
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.19	0.43
1:A:427:THR:O	1:A:467:ASN:HB2	2.19	0.43
1:B:19:PRO:HD3	1:B:112:PRO:CB	2.48	0.43
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.54	0.43
1:A:622:HIS:ND1	1:A:625:GLN:OE1	2.49	0.43
1:D:427:THR:O	1:D:467:ASN:HB2	2.18	0.43
1:B:788:PRO:HD2	1:B:968:MET:HG3	2.01	0.42
1:C:245:GLN:HG2	1:C:288:ARG:CG	2.48	0.42
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.53	0.42
1:B:657:ALA:HA	1:B:663:LEU:HD22	2.00	0.42
1:A:128:ASN:HA	1:A:180:GLY:O	2.19	0.42
1:A:256:VAL:HA	1:A:314:GLU:O	2.19	0.42
1:C:749:ILE:N	1:C:749:ILE:CD1	2.82	0.42
1:D:890:GLN:HB2	6:D:4659:HOH:O	2.18	0.42
1:B:638:VAL:O	1:B:677:LYS:HA	2.19	0.42
1:D:52:ARG:O	1:D:213:SER:HB2	2.19	0.42
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.54	0.42
1:A:173:LEU:O	1:A:177:LEU:HG	2.20	0.42
1:D:619:GLU:HA	1:D:912:ALA:HB2	2.01	0.42
1:A:225:PHE:HA	1:A:243:GLU:O	2.20	0.42
1:A:361:PRO:HB3	1:A:609:ALA:HB1	2.02	0.42
1:D:984:LEU:HD21	1:D:986:ILE:HD11	2.01	0.42
1:D:533:LEU:C	1:D:533:LEU:HD23	2.40	0.42
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.55	0.42
1:A:87:PRO:HA	1:A:208:ILE:O	2.20	0.42
1:D:340:GLY:O	1:D:561:ARG:HG2	2.20	0.42
1:A:618:THR:HG22	1:A:912:ALA:HB1	2.01	0.42
1:A:703:PRO:O	1:A:711:ALA:HB1	2.20	0.42
1:B:896:ASN:HB3	1:B:945:ASN:HB2	2.01	0.42
1:B:944:LEU:O	1:B:950:GLN:HA	2.20	0.42
1:C:661:LYS:HA	1:C:662:PRO:HD3	1.92	0.42
1:C:890:GLN:HE22	1:C:948:PRO:HD3	1.84	0.42
1:A:598:ASP:OD1	1:A:797:GLU:HA	2.20	0.41
1:B:815:HIS:HE1	1:B:877:PRO:O	2.02	0.41
1:A:433:LEU:N	1:A:434:PRO:CD	2.83	0.41
1:A:738:PRO:HD2	1:A:833:ALA:HA	2.03	0.41
1:A:773:LYS:HG2	1:A:774:LYS:O	2.20	0.41
1:B:581:ASN:HB2	1:B:583:ASN:ND2	2.35	0.41
1:C:105:TYR:CE1	1:C:199:ASP:HB2	2.54	0.41
1:B:105:TYR:CE1	1:B:199:ASP:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:VAL:CG1	1:B:521:LYS:HE3	2.50	0.41
1:B:634:GLN:HB2	1:B:681:GLU:OE2	2.21	0.41
1:B:658:LEU:HD22	1:B:688:PRO:HB2	2.02	0.41
1:C:19:PRO:HD3	1:C:112:PRO:CB	2.50	0.41
1:C:200:GLN:HG3	1:C:416:GLU:OE1	2.20	0.41
1:A:656:VAL:HG21	1:A:685:LEU:CD1	2.50	0.41
1:A:754:LYS:HA	1:A:769:TRP:O	2.19	0.41
1:B:128:ASN:HA	1:B:180:GLY:O	2.21	0.41
1:A:525:SER:O	1:B:561:ARG:HD3	2.21	0.41
1:B:390:SER:HA	1:B:391:HIS:HA	1.81	0.41
1:C:246:MET:SD	1:C:246:MET:C	2.99	0.41
1:C:784:PHE:HA	1:C:881:ARG:O	2.21	0.41
1:D:738:PRO:HG3	1:D:751:LEU:HD13	2.01	0.41
1:C:482:ARG:HA	1:C:483:PRO:HD3	1.97	0.41
1:C:952:ARG:HH11	1:C:952:ARG:CB	2.33	0.41
1:D:166:ARG:HG3	1:D:392:TYR:HB2	2.02	0.41
1:D:458:LEU:HD11	1:D:472:TYR:HB2	2.03	0.41
1:A:390:SER:HB2	1:A:391:HIS:CE1	2.56	0.41
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.56	0.41
1:B:223:SER:O	1:B:224:ASP:HB2	2.21	0.41
1:B:674:PRO:O	1:B:675:GLN:HB2	2.21	0.41
1:B:895:VAL:HG21	1:B:925:MET:HG3	2.03	0.41
1:D:863:GLN:NE2	1:D:952:ARG:NH2	2.67	0.41
1:A:126:THR:HA	1:A:182:ASN:O	2.21	0.41
1:A:292:ARG:HH12	5:A:5012:DMS:C1	2.34	0.41
1:A:335:VAL:HG22	1:A:344:LEU:HD12	2.03	0.41
1:A:587:ALA:HB1	1:A:591:ASP:HB2	2.03	0.41
1:A:793:ILE:HG22	1:A:795:VAL:HG22	2.03	0.41
6:A:4541:HOH:O	1:D:463:GLY:HA2	2.20	0.41
1:B:19:PRO:HD3	1:B:112:PRO:HB3	2.02	0.41
1:B:141:ILE:HB	1:B:173:LEU:HD11	2.03	0.41
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.56	0.41
1:C:638:VAL:O	1:C:677:LYS:HA	2.21	0.41
1:D:80:GLU:CD	1:D:80:GLU:H	2.25	0.41
1:D:482:ARG:HA	1:D:483:PRO:HD3	1.96	0.41
1:A:701:VAL:O	1:A:703:PRO:HD3	2.20	0.41
1:A:890:GLN:HG2	1:A:891:VAL:N	2.35	0.41
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.03	0.40
1:A:651:LEU:HD12	1:A:651:LEU:O	2.21	0.40
1:C:542:ALA:HA	1:C:604:ASN:HA	2.03	0.40
1:C:749:ILE:HD11	1:C:836:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:794:GLY:HA2	1:C:998:SER:O	2.21	0.40
1:C:802:ASP:O	1:C:808:GLU:HG3	2.21	0.40
1:A:896:ASN:HD21	1:A:917:ARG:HD2	1.86	0.40
1:A:900:LEU:CD1	1:A:910:LEU:HD22	2.51	0.40
1:B:163:GLN:O	1:B:164:ASP:HB3	2.21	0.40
1:B:251:ARG:HB2	1:B:254:LEU:HG	2.03	0.40
1:B:658:LEU:N	1:B:663:LEU:CD2	2.84	0.40
1:D:429:ASP:OD1	1:D:431:ARG:HG3	2.21	0.40
1:D:742:THR:HG22	1:D:743:SER:N	2.37	0.40
1:A:291:LEU:N	1:A:291:LEU:HD22	2.37	0.40
1:A:768:MET:HE3	1:A:1020:TRP:CZ2	2.56	0.40
1:B:847:LYS:HE2	1:B:848:THR:O	2.21	0.40
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.02	0.40
1:C:952:ARG:HB2	1:C:952:ARG:HH11	1.87	0.40
1:D:773:LYS:HA	1:D:773:LYS:HD2	1.94	0.40
1:A:59:ARG:HB2	1:A:124:SER:OG	2.21	0.40
1:A:87:PRO:HB2	1:A:209:PHE:C	2.42	0.40
1:A:88:SER:HA	1:A:366:VAL:CG2	2.48	0.40
1:A:533:LEU:HD23	1:A:534:ILE:N	2.36	0.40
1:A:742:THR:HG22	1:A:743:SER:N	2.36	0.40
1:C:533:LEU:HD23	1:C:534:ILE:N	2.36	0.40
1:C:546:LEU:HD22	1:C:616:ALA:HB1	2.04	0.40
1:B:372:MET:CE	1:B:397:LEU:HD23	2.52	0.40
1:B:789:LEU:HD11	1:B:993:ILE:HG22	2.03	0.40
6:B:4559:HOH:O	1:C:463:GLY:HA2	2.21	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	A	1009/1023 (99%)	963 (95%)	45 (4%)	1 (0%)	51 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1009/1023 (99%)	961 (95%)	48 (5%)	0	100	100
1	C	1009/1023 (99%)	962 (95%)	47 (5%)	0	100	100
1	D	1009/1023 (99%)	965 (96%)	43 (4%)	1 (0%)	51	60
All	All	4036/4092 (99%)	3851 (95%)	183 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	798	ALA
1	D	211	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	863/874 (99%)	858 (99%)	5 (1%)	86	93
1	B	863/874 (99%)	858 (99%)	5 (1%)	86	93
1	C	863/874 (99%)	857 (99%)	6 (1%)	84	91
1	D	863/874 (99%)	857 (99%)	6 (1%)	84	91
All	All	3452/3496 (99%)	3430 (99%)	22 (1%)	86	93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	GLU
1	A	333	ARG
1	A	519	SER
1	A	546	LEU
1	A	910	LEU
1	B	251	ARG
1	B	333	ARG
1	B	546	LEU
1	B	604	ASN

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Mol	Chain	Res	Type
1	B	956	GLN
1	C	112	PRO
1	C	333	ARG
1	C	344	LEU
1	C	546	LEU
1	C	773	LYS
1	C	804	ASN
1	D	76	CYS
1	D	333	ARG
1	D	546	LEU
1	D	655	MET
1	D	663	LEU
1	D	885	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	634	GLN
1	A	757	GLN
1	A	1017	GLN
1	B	262	GLN
1	B	583	ASN
1	B	804	ASN
1	B	965	GLN
1	C	817	GLN
1	C	863	GLN
1	D	675	GLN
1	D	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 157 ligands modelled in this entry, 27 are monoatomic - leaving 130 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	D	5027	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	D	5023	-	3,3,3	0.20	0	3,3,3	0.60	0
5	DMS	B	5001	-	3,3,3	0.25	0	3,3,3	0.60	0
5	DMS	D	5230	-	3,3,3	0.21	0	3,3,3	0.63	0
5	DMS	C	5001	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	B	5010	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	B	5005	-	3,3,3	0.22	0	3,3,3	0.60	0
2	149	D	2001	4	12,12,12	1.01	1 (8%)	15,17,17	0.84	0
5	DMS	B	5012	-	3,3,3	0.26	0	3,3,3	0.60	0
5	DMS	C	5012	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	D	5008	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	5024	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	B	5029	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	D	5012	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	A	5232	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	A	5129	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	A	5003	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	B	5002	-	3,3,3	0.20	0	3,3,3	0.58	0
5	DMS	C	5002	-	3,3,3	0.20	0	3,3,3	0.60	0
5	DMS	C	5030	-	3,3,3	0.27	0	3,3,3	0.63	0
5	DMS	D	5022	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	5013	-	3,3,3	0.25	0	3,3,3	0.60	0
5	DMS	C	5015	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	D	5016	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	B	5024	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	A	5011	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	B	5028	-	3,3,3	0.24	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	D	5006	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	A	5018	4	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	A	5022	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	A	5020	-	3,3,3	0.19	0	3,3,3	0.61	0
5	DMS	A	5014	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	A	5015	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	B	5025	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	C	5020	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	B	5015	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	C	5014	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	A	5023	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	D	5003	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	A	5006	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	C	5031	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	D	5011	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	A	5019	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	C	5006	-	3,3,3	0.26	0	3,3,3	0.63	0
2	149	A	2001	4	12,12,12	1.10	1 (8%)	15,17,17	0.80	0
5	DMS	C	5027	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	C	1024	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	A	5125	-	3,3,3	0.24	0	3,3,3	0.61	0
2	149	C	2001	4	12,12,12	1.16	2 (16%)	15,17,17	0.78	0
5	DMS	C	5021	4	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	A	5002	-	3,3,3	0.19	0	3,3,3	0.55	0
5	DMS	C	5010	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	D	5010	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	D	5007	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	A	5128	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	A	5010	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	A	5001	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	A	5127	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	B	5011	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	C	5134	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	A	5231	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	B	5013	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	A	5126	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	D	5025	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	B	5027	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	B	5003	-	3,3,3	0.24	0	3,3,3	0.63	0
2	149	B	2001	4	12,12,12	1.02	1 (8%)	15,17,17	0.77	0
5	DMS	B	5014	-	3,3,3	0.21	0	3,3,3	0.63	0
5	DMS	D	5017	-	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	D	5020	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	A	5004	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	B	5023	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	A	5017	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	B	5017	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	C	5016	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	D	5001	-	3,3,3	0.22	0	3,3,3	0.66	0
5	DMS	C	5018	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	D	5005	-	3,3,3	0.25	0	3,3,3	0.59	0
5	DMS	B	5021	4	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	A	5024	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	B	5004	-	3,3,3	0.20	0	3,3,3	0.59	0
5	DMS	C	5003	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	A	5016	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	B	5016	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	D	5229	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	B	5019	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	5008	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	C	5019	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	D	5004	-	3,3,3	0.18	0	3,3,3	0.61	0
5	DMS	D	5026	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	A	5012	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	B	5009	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	C	5028	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	B	5008	-	3,3,3	0.19	0	3,3,3	0.61	0
5	DMS	B	5133	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	A	5008	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	C	5009	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	D	5013	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	B	5018	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	D	5021	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	B	5026	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	5023	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	C	5007	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	C	5032	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	A	5130	-	3,3,3	0.15	0	3,3,3	0.59	0
5	DMS	C	5017	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	B	5020	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	D	5018	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	D	5028	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	A	5009	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	B	5007	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	C	5022	-	3,3,3	0.21	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	D	5014	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	D	5002	-	3,3,3	0.18	0	3,3,3	0.54	0
5	DMS	C	5004	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	D	5009	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	D	5015	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	B	5132	-	3,3,3	0.19	0	3,3,3	0.60	0
5	DMS	A	5007	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	B	5131	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	C	5033	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	C	5025	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	A	5005	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	B	5006	-	3,3,3	0.27	0	3,3,3	0.60	0
5	DMS	C	5011	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	B	5034	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	D	5019	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	C	5005	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	B	5022	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	D	5024	-	3,3,3	0.23	0	3,3,3	0.64	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	D	2001	4	-	1/2/22/22	0/1/1/1
2	149	A	2001	4	-	1/2/22/22	0/1/1/1
2	149	C	2001	4	-	1/2/22/22	0/1/1/1
2	149	B	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	A	2001	149	O5-C1	2.86	1.39	1.34
2	C	2001	149	O5-C1	2.73	1.38	1.34
2	B	2001	149	O5-C1	2.66	1.38	1.34
2	D	2001	149	O5-C1	2.65	1.38	1.34
2	C	2001	149	O5-C5	2.06	1.49	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	149	O5-C5-C6-O6
2	D	2001	149	O5-C5-C6-O6
2	B	2001	149	O5-C5-C6-O6
2	A	2001	149	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5030	DMS	1	0
5	A	5012	DMS	1	0
5	A	5130	DMS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.33	29 (2%)	51	49	7, 20, 41, 66	0
1	B	1011/1023 (98%)	-0.42	25 (2%)	57	55	5, 18, 39, 66	0
1	C	1011/1023 (98%)	-0.46	22 (2%)	62	59	6, 17, 37, 73	0
1	D	1011/1023 (98%)	-0.43	24 (2%)	59	56	6, 18, 38, 66	0
All	All	4044/4092 (98%)	-0.41	100 (2%)	57	55	5, 18, 39, 73	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	6.4
1	D	732	ALA	6.2
1	A	732	ALA	6.0
1	B	732	ALA	6.0
1	C	732	ALA	5.9
1	C	800	ARG	5.7
1	A	799	THR	5.4
1	C	735	HIS	5.3
1	C	801	ILE	5.3
1	D	689	GLU	5.3
1	D	801	ILE	5.3
1	C	689	GLU	5.2
1	C	733	ALA	5.2
1	A	795	VAL	5.1
1	C	731	PRO	4.9
1	D	731	PRO	4.8
1	A	1023	LYS	4.8
1	B	733	ALA	4.8
1	B	686	PRO	4.7
1	B	731	PRO	4.7
1	A	730	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	735	HIS	4.4
1	A	800	ARG	4.3
1	C	799	THR	4.3
1	B	689	GLU	4.3
1	D	734	SER	4.2
1	A	734	SER	4.2
1	A	689	GLU	4.2
1	B	687	GLN	4.2
1	A	686	PRO	4.0
1	B	580	GLU	4.0
1	A	731	PRO	3.9
1	B	800	ARG	3.9
1	A	687	GLN	3.8
1	A	684	GLU	3.8
1	A	580	GLU	3.7
1	D	687	GLN	3.7
1	C	745	MET	3.7
1	A	801	ILE	3.7
1	C	772	ASP	3.7
1	D	730	LEU	3.6
1	D	800	ARG	3.6
1	A	733	ALA	3.5
1	C	730	LEU	3.5
1	C	580	GLU	3.5
1	D	684	GLU	3.5
1	B	684	GLU	3.4
1	D	772	ASP	3.4
1	D	580	GLU	3.4
1	C	687	GLN	3.3
1	D	733	ALA	3.2
1	A	771	GLY	3.2
1	B	1023	LYS	3.2
1	C	734	SER	3.1
1	C	744	GLU	3.1
1	B	730	LEU	3.0
1	A	71	GLU	3.0
1	B	745	MET	2.9
1	A	76	CYS	2.9
1	D	686	PRO	2.8
1	B	690	SER	2.8
1	D	1023	LYS	2.8
1	B	734	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1022	GLN	2.7
1	B	801	ILE	2.7
1	D	845	GLN	2.7
1	B	799	THR	2.7
1	A	1022	GLN	2.6
1	A	729	THR	2.6
1	D	831	ALA	2.6
1	D	799	THR	2.6
1	C	686	PRO	2.5
1	B	772	ASP	2.5
1	A	819	GLU	2.5
1	C	684	GLU	2.5
1	A	581	ASN	2.5
1	D	581	ASN	2.5
1	C	1023	LYS	2.4
1	A	49	GLN	2.4
1	B	735	HIS	2.4
1	C	817	GLN	2.4
1	B	581	ASN	2.3
1	D	1022	GLN	2.3
1	C	795	VAL	2.3
1	A	79	PRO	2.2
1	A	178	ARG	2.2
1	B	688	PRO	2.2
1	D	79	PRO	2.2
1	D	795	VAL	2.2
1	B	846	GLY	2.2
1	A	582	GLY	2.2
1	C	729	THR	2.2
1	D	832	ASP	2.2
1	B	1022	GLN	2.2
1	B	795	VAL	2.1
1	A	249	GLU	2.1
1	B	744	GLU	2.1
1	B	819	GLU	2.0
1	D	71	GLU	2.0
1	A	772	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	D	5007	4/4	0.50	0.33	86,87,87,87	0
5	DMS	B	5017	4/4	0.60	0.34	74,74,74,75	0
5	DMS	D	5026	4/4	0.61	0.28	113,113,113,113	0
5	DMS	B	5013	4/4	0.64	0.32	109,109,109,109	0
5	DMS	D	5015	4/4	0.65	0.28	78,79,79,79	0
5	DMS	C	5012	4/4	0.65	0.35	97,97,97,97	0
5	DMS	D	5023	4/4	0.67	0.31	81,82,82,82	0
5	DMS	D	5024	4/4	0.69	0.28	85,85,86,86	0
5	DMS	C	5024	4/4	0.71	0.25	66,66,66,67	0
5	DMS	C	5016	4/4	0.74	0.25	68,68,69,69	0
5	DMS	B	5007	4/4	0.78	0.22	75,75,76,76	0
5	DMS	A	5010	4/4	0.78	0.30	71,71,71,72	0
5	DMS	C	5028	4/4	0.78	0.24	84,85,85,85	0
5	DMS	C	5014	4/4	0.78	0.26	65,65,66,66	0
5	DMS	A	5232	4/4	0.80	0.22	58,58,58,59	0
5	DMS	D	5229	4/4	0.81	0.23	67,67,69,69	0
5	DMS	B	5026	4/4	0.82	0.20	55,55,55,56	0
5	DMS	C	5020	4/4	0.82	0.21	68,68,68,69	0
5	DMS	C	5009	4/4	0.82	0.24	90,90,90,91	0
5	DMS	B	5015	4/4	0.82	0.18	59,59,60,60	0
5	DMS	A	5019	4/4	0.82	0.27	84,84,84,84	0
5	DMS	B	5025	4/4	0.83	0.23	70,70,70,72	0
5	DMS	D	5017	4/4	0.83	0.22	70,70,71,72	0
5	DMS	A	5024	4/4	0.83	0.29	79,79,79,79	0
5	DMS	B	5006	4/4	0.84	0.23	63,63,64,64	0
5	DMS	C	5017	4/4	0.85	0.16	65,65,66,67	0
5	DMS	C	5018	4/4	0.85	0.21	66,67,67,67	0
5	DMS	C	1024	4/4	0.86	0.20	63,64,64,65	0
5	DMS	A	5007	4/4	0.86	0.22	65,66,66,66	0
5	DMS	D	5013	4/4	0.86	0.39	87,87,87,88	0
5	DMS	D	5230	4/4	0.86	0.18	54,54,54,55	0
5	DMS	A	5017	4/4	0.87	0.25	59,59,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	3003	1/1	0.87	0.13	59,59,59,59	0
5	DMS	A	5015	4/4	0.87	0.24	65,65,65,66	0
3	MG	A	1024	1/1	0.88	0.06	44,44,44,44	0
5	DMS	A	5016	4/4	0.88	0.20	57,57,57,58	0
5	DMS	D	5021	4/4	0.88	0.18	83,83,83,83	0
5	DMS	C	5015	4/4	0.88	0.24	56,57,57,57	0
5	DMS	D	5010	4/4	0.89	0.25	71,71,71,72	0
5	DMS	A	5128	4/4	0.89	0.27	54,54,55,55	0
5	DMS	C	5021	4/4	0.89	0.21	60,60,60,61	0
5	DMS	A	5231	4/4	0.89	0.18	57,57,57,58	0
5	DMS	D	5018	4/4	0.89	0.18	71,71,71,72	0
5	DMS	D	5020	4/4	0.89	0.19	65,66,66,66	0
5	DMS	B	5028	4/4	0.89	0.19	53,53,54,55	0
5	DMS	C	5030	4/4	0.89	0.17	62,63,63,64	0
5	DMS	A	5004	4/4	0.89	0.17	57,57,58,59	0
5	DMS	C	5031	4/4	0.89	0.24	69,69,70,70	0
5	DMS	D	5028	4/4	0.89	0.19	63,63,63,63	0
5	DMS	C	5032	4/4	0.89	0.19	61,62,62,63	0
5	DMS	A	5125	4/4	0.89	0.26	72,72,72,73	0
5	DMS	A	5009	4/4	0.90	0.19	44,45,46,47	0
5	DMS	D	5022	4/4	0.90	0.16	62,62,62,63	0
5	DMS	B	5022	4/4	0.90	0.28	89,89,89,90	0
5	DMS	B	5010	4/4	0.90	0.14	72,72,73,73	0
5	DMS	A	5002	4/4	0.90	0.17	45,46,46,47	0
5	DMS	A	5022	4/4	0.90	0.27	65,65,66,66	0
5	DMS	C	5033	4/4	0.90	0.17	58,58,59,60	0
5	DMS	C	5134	4/4	0.90	0.22	40,41,41,43	0
5	DMS	C	5027	4/4	0.91	0.22	65,66,66,66	0
5	DMS	B	5018	4/4	0.91	0.15	45,46,46,48	0
5	DMS	B	5132	4/4	0.91	0.15	58,58,59,59	0
5	DMS	D	5004	4/4	0.91	0.17	52,52,53,54	0
5	DMS	D	5019	4/4	0.91	0.22	56,57,57,57	0
5	DMS	C	5022	4/4	0.91	0.18	65,65,65,66	0
5	DMS	A	5006	4/4	0.91	0.16	57,58,58,58	0
5	DMS	A	5020	4/4	0.92	0.15	56,57,57,58	0
5	DMS	A	5014	4/4	0.92	0.21	49,51,51,51	0
5	DMS	A	5127	4/4	0.92	0.26	51,53,53,53	0
5	DMS	B	5021	4/4	0.92	0.32	66,66,66,67	0
5	DMS	C	5004	4/4	0.92	0.16	36,37,39,39	0
5	DMS	C	5006	4/4	0.92	0.16	56,57,58,58	0
5	DMS	B	5004	4/4	0.92	0.15	51,52,53,53	0
5	DMS	A	5008	4/4	0.93	0.14	48,49,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	B	5009	4/4	0.93	0.18	39,40,41,41	0
5	DMS	D	5012	4/4	0.93	0.18	53,53,53,54	0
3	MG	A	3005	1/1	0.93	0.12	70,70,70,70	0
5	DMS	B	5019	4/4	0.93	0.16	60,60,60,61	0
5	DMS	D	5016	4/4	0.93	0.18	43,44,44,45	0
5	DMS	D	5027	4/4	0.93	0.23	75,75,76,76	0
5	DMS	B	5029	4/4	0.93	0.13	57,57,58,59	0
5	DMS	B	5020	4/4	0.93	0.28	67,68,68,68	0
4	NA	B	3103	1/1	0.93	0.10	23,23,23,23	0
4	NA	D	3104	1/1	0.94	0.16	29,29,29,29	0
5	DMS	B	5133	4/4	0.94	0.11	70,70,70,71	0
5	DMS	D	5014	4/4	0.94	0.20	58,59,60,60	0
5	DMS	C	5003	4/4	0.94	0.13	36,37,38,39	0
5	DMS	A	5023	4/4	0.94	0.12	60,61,61,62	0
5	DMS	B	5003	4/4	0.94	0.14	39,40,41,41	0
5	DMS	C	5008	4/4	0.94	0.17	55,55,55,55	0
5	DMS	D	5009	4/4	0.94	0.16	44,45,45,46	0
4	NA	C	3104	1/1	0.94	0.13	32,32,32,32	0
5	DMS	A	5018	4/4	0.95	0.21	55,55,55,56	0
5	DMS	B	5034	4/4	0.95	0.16	45,46,46,48	0
5	DMS	C	5002	4/4	0.95	0.12	32,33,34,35	0
5	DMS	B	5002	4/4	0.95	0.14	38,38,40,41	0
5	DMS	C	5019	4/4	0.95	0.19	51,52,52,52	0
4	NA	A	3103	1/1	0.95	0.09	39,39,39,39	0
2	149	A	2001	12/12	0.95	0.12	11,13,18,18	0
5	DMS	C	5007	4/4	0.95	0.14	38,39,41,42	0
4	NA	C	3102	1/1	0.95	0.08	14,14,14,14	0
5	DMS	A	5130	4/4	0.95	0.11	27,27,29,31	0
5	DMS	B	5131	4/4	0.95	0.15	58,58,58,59	0
5	DMS	C	5013	4/4	0.95	0.17	38,40,40,40	0
5	DMS	A	5012	4/4	0.95	0.14	46,46,47,47	0
5	DMS	B	5008	4/4	0.96	0.13	40,41,41,42	0
2	149	D	2001	12/12	0.96	0.10	8,13,15,20	0
4	NA	A	3104	1/1	0.96	0.05	28,28,28,28	0
5	DMS	A	5126	4/4	0.96	0.18	45,46,46,47	0
5	DMS	B	5014	4/4	0.96	0.15	40,40,41,42	0
5	DMS	B	5027	4/4	0.96	0.18	52,52,52,52	0
5	DMS	D	5002	4/4	0.96	0.14	30,31,32,32	0
2	149	B	2001	12/12	0.96	0.10	11,13,16,17	0
5	DMS	B	5016	4/4	0.96	0.19	41,42,42,42	0
5	DMS	D	5008	4/4	0.96	0.15	44,45,45,46	0
5	DMS	D	5025	4/4	0.96	0.12	40,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	C	5023	4/4	0.96	0.11	47,47,48,48	0
5	DMS	A	5003	4/4	0.96	0.11	38,38,38,39	0
5	DMS	C	5025	4/4	0.96	0.11	55,55,55,56	0
5	DMS	A	5129	4/4	0.96	0.17	60,61,61,61	0
3	MG	D	3002	1/1	0.96	0.08	23,23,23,23	0
5	DMS	A	5011	4/4	0.97	0.09	39,39,40,41	0
4	NA	B	3104	1/1	0.97	0.12	31,31,31,31	0
4	NA	C	3101	1/1	0.97	0.07	13,13,13,13	0
5	DMS	B	5005	4/4	0.97	0.11	34,36,37,38	0
3	MG	D	3001	1/1	0.97	0.07	13,13,13,13	0
5	DMS	A	5005	4/4	0.97	0.11	32,32,33,34	0
4	NA	C	3103	1/1	0.97	0.09	29,29,29,29	0
2	149	C	2001	12/12	0.97	0.09	9,12,13,15	0
5	DMS	B	5023	4/4	0.97	0.17	41,42,42,43	0
5	DMS	B	5024	4/4	0.97	0.12	62,62,62,62	0
4	NA	D	3101	1/1	0.97	0.07	12,12,12,12	0
5	DMS	B	5012	4/4	0.97	0.12	37,37,38,39	0
5	DMS	C	5011	4/4	0.97	0.12	41,41,41,42	0
4	NA	D	3103	1/1	0.97	0.07	33,33,33,33	0
4	NA	A	3101	1/1	0.97	0.07	13,13,13,13	0
4	NA	D	3102	1/1	0.98	0.04	16,16,16,16	0
4	NA	B	3102	1/1	0.98	0.06	16,16,16,16	0
5	DMS	B	5011	4/4	0.98	0.12	28,28,29,29	0
3	MG	A	3002	1/1	0.98	0.06	19,19,19,19	0
5	DMS	C	5005	4/4	0.98	0.10	36,36,37,38	0
5	DMS	B	5001	4/4	0.98	0.07	19,21,23,24	0
5	DMS	D	5001	4/4	0.98	0.07	21,21,22,24	0
5	DMS	A	5001	4/4	0.98	0.08	22,22,24,24	0
5	DMS	D	5003	4/4	0.98	0.09	32,33,33,33	0
3	MG	B	3001	1/1	0.98	0.04	15,15,15,15	0
5	DMS	D	5005	4/4	0.98	0.11	27,27,28,29	0
5	DMS	D	5006	4/4	0.98	0.10	30,32,33,33	0
3	MG	B	3002	1/1	0.98	0.05	19,19,19,19	0
4	NA	A	3102	1/1	0.98	0.04	21,21,21,21	0
3	MG	A	3001	1/1	0.98	0.06	17,17,17,17	0
3	MG	C	3002	1/1	0.98	0.05	17,17,17,17	0
5	DMS	D	5011	4/4	0.98	0.10	32,32,33,34	0
4	NA	B	3101	1/1	0.98	0.07	15,15,15,15	0
5	DMS	C	5010	4/4	0.99	0.10	34,35,35,36	0
3	MG	C	3001	1/1	0.99	0.03	12,12,12,12	0
5	DMS	C	5001	4/4	0.99	0.07	23,25,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.