



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:23 PM UTC

PDB ID : 3IAP / pdb_00003iap
Title : E. coli (lacZ) beta-galactosidase (E416Q)
Authors : Lo, S.; Dugdale, M.L.; Jeerh, N.; Ku, T.; Roth, N.J.; Huber, R.E.
Deposited on : 2009-07-14
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

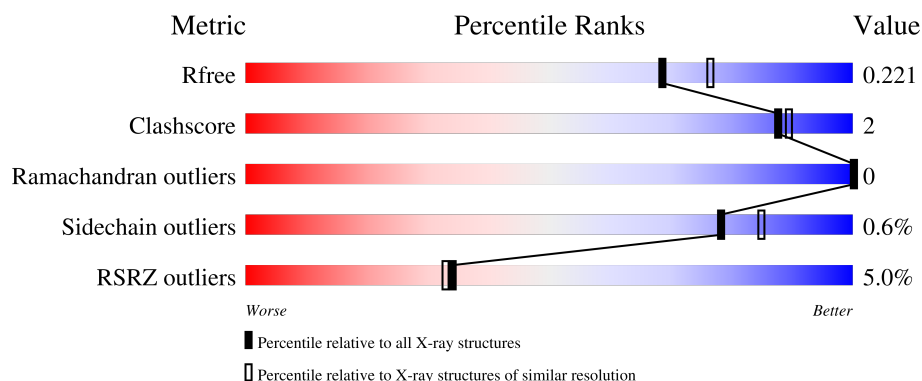
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	4% 93% 5%
1	B	1023	5% 94% 5%
1	C	1023	6% 94% 5%
1	D	1023	5% 93% 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BTB	C	6001	-	-	X	-
5	DMS	B	7030	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36912 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
			8125	5138	1441	1508	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8125	5138	1441	1508	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8125	5138	1441	1508	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8125	5138	1441	1508	38			

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	416	GLN	GLU	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	416	GLN	GLU	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	416	GLN	GLU	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	416	GLN	GLU	engineered mutation	UNP B8LFD6

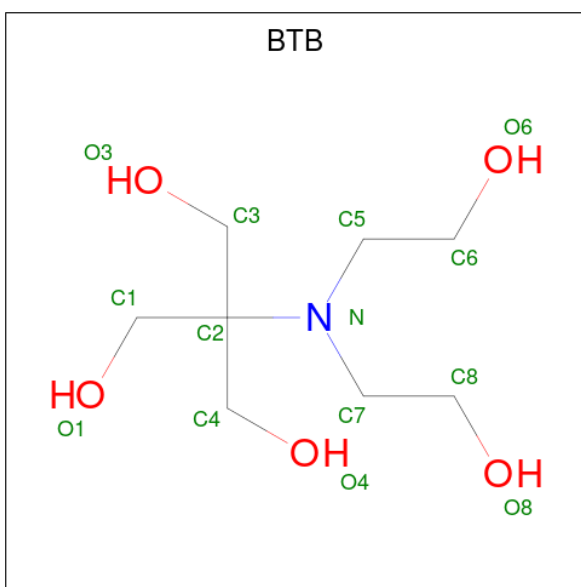
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

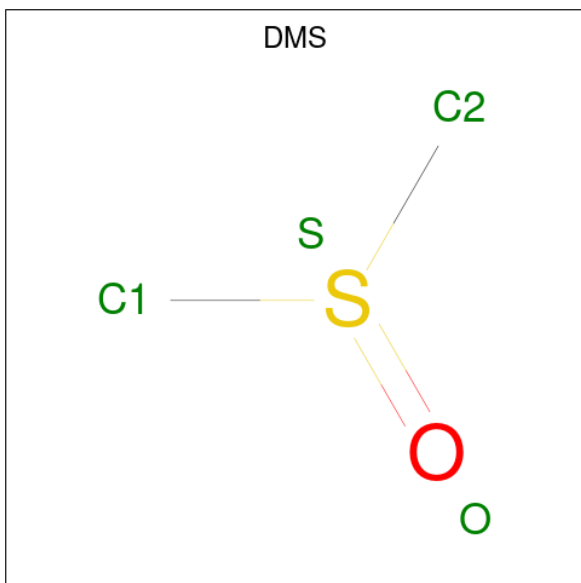
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

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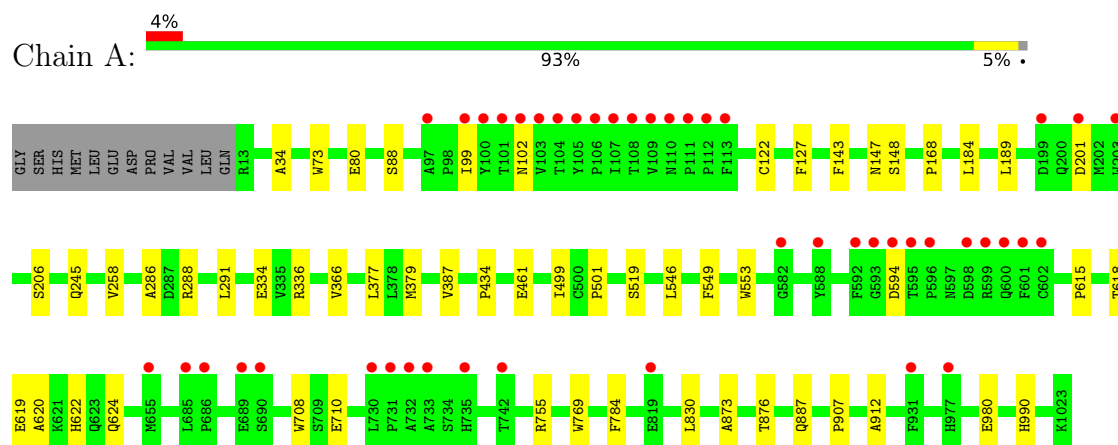
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1038	Total 1038	O 1038	0	0
6	B	974	Total 974	O 974	0	0
6	C	889	Total 889	O 889	0	0
6	D	931	Total 931	O 931	0	0

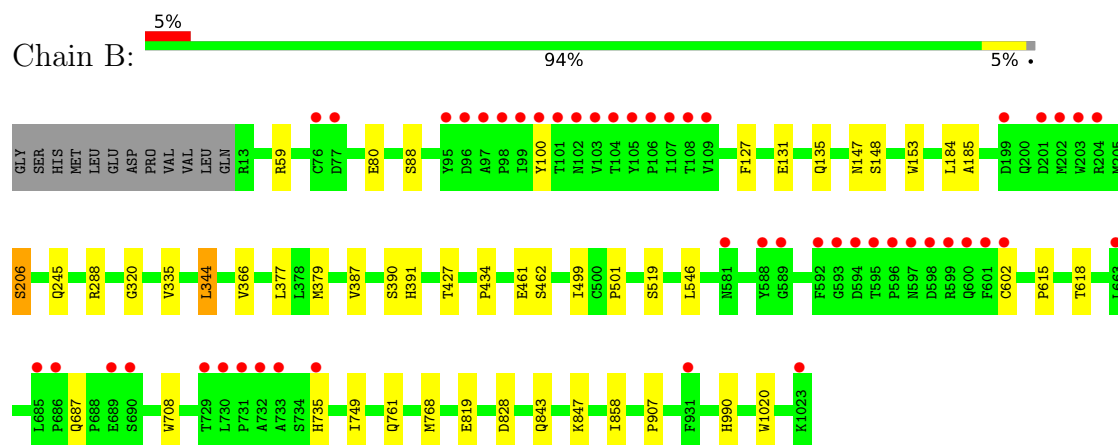
3 Residue-property plots

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

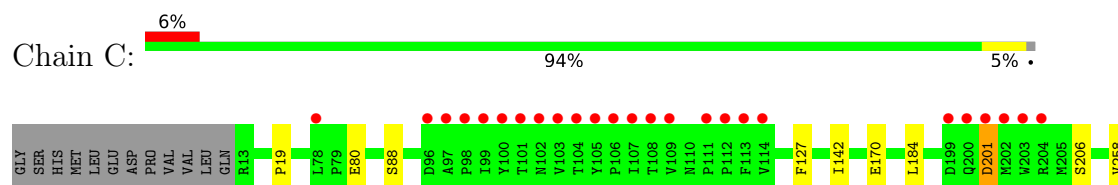
• Molecule 1: Beta-galactosidase

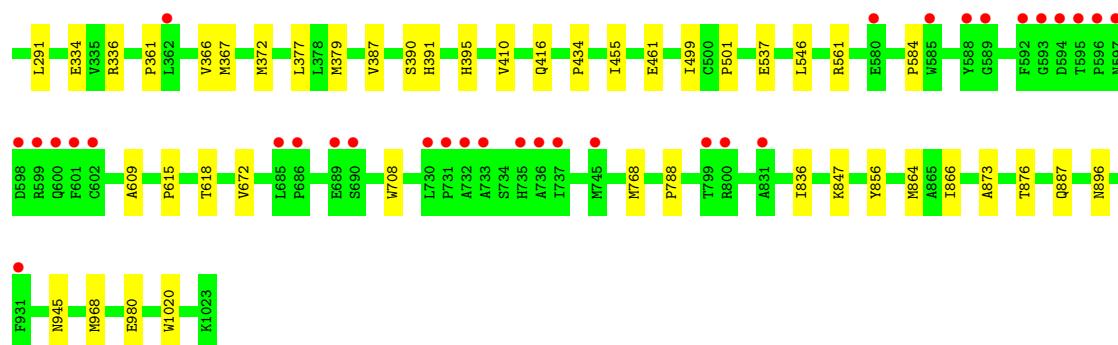


• Molecule 1: Beta-galactosidase

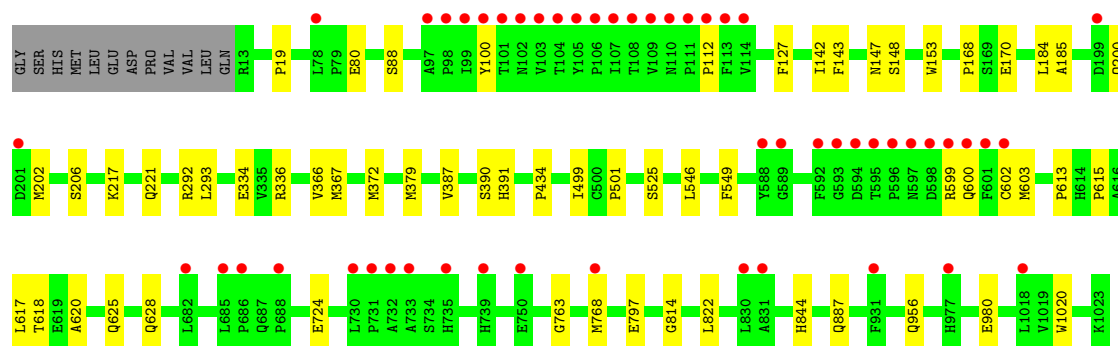


• Molecule 1: Beta-galactosidase





• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.23Å 162.34Å 202.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.38 – 2.00 53.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (53.38-2.00) 87.6 (53.38-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.181 , 0.220 0.181 , 0.221	Depositor DCC
R_{free} test set	4186 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36912	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 42.44 % 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 2.0401e-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: BTB, NA, DMS, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/8367	0.68	0/11415
1	B	0.43	0/8367	0.67	0/11415
1	C	0.42	0/8367	0.68	0/11415
1	D	0.43	0/8367	0.69	0/11415
All	All	0.43	0/33468	0.68	0/45660

There are no bond length outliers.

There are no bond angle outliers.

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	8125	0	7718	32	0
1	B	8125	0	7718	26	0
1	C	8125	0	7718	33	0
1	D	8125	0	7717	32	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	14	0	19	3	0
4	B	14	0	19	4	0
4	C	14	0	19	9	0
4	D	14	0	18	2	0
5	A	128	0	192	5	0
5	B	132	0	198	2	0
5	C	128	0	192	2	0
5	D	112	0	168	3	0
6	A	1038	0	0	0	0
6	B	974	0	0	0	0
6	C	889	0	0	0	0
6	D	931	0	0	0	0
All	All	36912	0	31696	127	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 2.

All (127) 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)
4:B:6001:BTB:H11	4:B:6001:BTB:H61	1.18	1.11
4:B:6001:BTB:H61	4:B:6001:BTB:C1	1.89	1.03
4:B:6001:BTB:H11	4:B:6001:BTB:C6	1.91	1.00
4:D:6001:BTB:H41	4:D:6001:BTB:H62	1.46	0.98
1:C:416:GLN:HE22	4:C:6001:BTB:H81	1.35	0.91
1:B:461:GLU:OE1	4:B:6001:BTB:H72	1.85	0.76
1:A:102:ASN:HA	1:A:201:ASP:HB2	1.72	0.72
1:C:416:GLN:HE22	4:C:6001:BTB:C8	2.06	0.68
4:D:6001:BTB:H41	4:D:6001:BTB:C6	2.22	0.66
1:C:416:GLN:NE2	4:C:6001:BTB:H81	2.11	0.63
1:A:830:LEU:HD22	1:B:828:ASP:HB3	1.82	0.62
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.83	0.61
1:A:461:GLU:OE1	4:A:6001:BTB:H11	2.01	0.60
1:D:292:ARG:HH12	5:D:7010:DMS:H13	1.67	0.60
1:D:379:MET:HE1	1:D:387:VAL:HB	1.85	0.58
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.87	0.57
1:D:599:ARG:HE	1:D:797:GLU:HG2	1.70	0.57
1:C:864:MET:HE3	1:C:866:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.41	0.56
4:C:6001:BTB:H71	4:C:6001:BTB:O4	2.05	0.55
1:C:768:MET:HE1	1:C:1020:TRP:CZ2	2.41	0.55
1:D:600:GLN:HB2	1:D:603:MET:HE2	1.89	0.54
1:C:887:GLN:NE2	1:C:980:GLU:O	2.37	0.54
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.42	0.54
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.42	0.54
1:A:379:MET:HE1	1:A:387:VAL:HB	1.91	0.52
1:C:461:GLU:OE1	4:C:6001:BTB:H31	2.09	0.52
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.91	0.51
1:D:367:MET:HB3	1:D:372:MET:HE2	1.93	0.50
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.46	0.50
1:D:88:SER:HA	1:D:366:VAL:HG21	1.91	0.50
1:B:147:ASN:HB3	1:B:206:SER:HA	1.94	0.50
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.94	0.50
1:B:59:ARG:HG2	5:B:7031:DMS:H13	1.94	0.49
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.40	0.49
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.77	0.49
1:D:147:ASN:HB3	1:D:206:SER:HA	1.93	0.49
1:B:88:SER:HA	1:B:366:VAL:HG21	1.94	0.49
1:A:88:SER:HA	1:A:366:VAL:HG21	1.95	0.49
1:A:147:ASN:HB3	1:A:206:SER:HA	1.93	0.49
1:A:873:ALA:O	1:A:876:THR:HG22	2.12	0.49
1:B:768:MET:HE1	1:B:1020:TRP:CZ2	2.48	0.49
1:B:379:MET:HE1	1:B:387:VAL:HB	1.95	0.49
1:C:367:MET:HB3	1:C:372:MET:HE3	1.96	0.48
1:D:147:ASN:HA	1:D:148:SER:HA	1.67	0.48
1:C:361:PRO:HB3	1:C:609:ALA:HB1	1.95	0.48
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.94	0.48
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.95	0.48
1:C:88:SER:HA	1:C:366:VAL:HG21	1.96	0.48
1:A:334:GLU:OE1	1:A:336:ARG:NH1	2.45	0.48
1:B:615:PRO:O	1:B:618:THR:HG22	2.14	0.47
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.80	0.47
1:C:201:ASP:OD1	4:C:6001:BTB:H71	2.14	0.47
1:D:625:GLN:HB2	5:D:7002:DMS:H21	1.96	0.47
1:C:615:PRO:O	1:C:618:THR:HG22	2.14	0.47
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.50	0.47
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.97	0.46
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.51	0.46
1:B:335:VAL:HG22	1:B:344:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.97	0.46
1:B:427:THR:HG21	1:B:462:SER:HB3	1.98	0.45
1:C:873:ALA:O	1:C:876:THR:HG22	2.16	0.45
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.98	0.45
1:C:561:ARG:HD3	1:D:525:SER:O	2.16	0.45
1:D:887:GLN:NE2	1:D:980:GLU:O	2.47	0.45
4:A:6001:BTB:H11	4:A:6001:BTB:H52	1.60	0.45
1:C:390:SER:HA	1:C:391:HIS:HA	1.75	0.45
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.52	0.45
1:A:34:ALA:HB2	5:A:7013:DMS:H23	1.99	0.45
1:A:99:ILE:HG23	1:A:594:ASP:HB2	1.99	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.68	0.45
1:C:537:GLU:OE1	4:C:6001:BTB:H32	2.17	0.45
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.00	0.44
1:B:390:SER:HA	1:B:391:HIS:HA	1.79	0.44
1:C:19:PRO:HG2	5:C:7034:DMS:H12	1.99	0.44
4:A:6001:BTB:H71	4:A:6001:BTB:H42	1.58	0.44
1:C:836:ILE:HB	1:C:856:TYR:HB2	1.99	0.44
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.53	0.44
1:D:628:GLN:OE1	5:D:7002:DMS:H23	2.17	0.44
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.99	0.43
1:D:217:LYS:HE3	1:D:221:GLN:HB2	2.00	0.43
1:D:763:GLY:HA3	1:D:822:LEU:HD13	2.00	0.43
1:A:434:PRO:HB3	1:D:434:PRO:HB3	2.01	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.43
1:C:201:ASP:HB3	4:C:6001:BTB:H72	1.99	0.43
1:A:258:VAL:HG23	1:A:291:LEU:HD13	2.00	0.43
1:A:553:TRP:CZ2	1:A:624:GLN:HG2	2.54	0.43
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.53	0.43
1:A:710:GLU:HG3	5:A:7010:DMS:H13	2.01	0.43
1:D:200:GLN:HB2	1:D:202:MET:HE2	2.00	0.43
1:B:907:PRO:HG2	1:B:990:HIS:O	2.19	0.43
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.01	0.42
1:D:143:PHE:O	1:D:168:PRO:HA	2.19	0.42
1:A:143:PHE:O	1:A:168:PRO:HA	2.19	0.42
1:A:619:GLU:HA	1:A:912:ALA:HB2	2.01	0.42
1:B:320:GLY:HA2	5:B:7006:DMS:O	2.20	0.42
1:D:613:PRO:HB3	1:D:617:LEU:HD23	2.00	0.42
1:B:434:PRO:HB3	1:C:434:PRO:HB3	2.01	0.42
1:D:390:SER:HA	1:D:391:HIS:HA	1.79	0.42
1:A:907:PRO:HG2	1:A:990:HIS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:HG23	1:C:291:LEU:HD13	2.02	0.42
1:D:142:ILE:HG23	1:D:170:GLU:HG2	2.02	0.42
1:B:749:ILE:HD13	1:B:858:ILE:HD12	2.02	0.41
1:C:896:ASN:HB3	1:C:945:ASN:HB2	2.02	0.41
1:A:615:PRO:O	1:A:618:THR:HG22	2.20	0.41
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.55	0.41
1:C:584:PRO:HB2	5:C:7009:DMS:H22	2.03	0.41
1:A:755:ARG:HB2	1:A:769:TRP:HB2	2.02	0.41
1:B:843:GLN:HA	1:B:847:LYS:O	2.20	0.41
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.55	0.41
1:A:784:PHE:HD1	5:A:7018:DMS:H22	1.84	0.41
1:C:847:LYS:NZ	1:D:724:GLU:O	2.53	0.41
1:D:768:MET:HE1	1:D:1020:TRP:CH2	2.55	0.41
1:B:131:GLU:HG3	1:B:135:GLN:HG3	2.01	0.41
1:C:788:PRO:HD2	1:C:968:MET:HG3	2.03	0.41
4:C:6001:BTB:H51	4:C:6001:BTB:H12	1.59	0.41
1:A:887:GLN:NE2	1:A:980:GLU:O	2.50	0.41
1:C:410:VAL:HG22	1:C:455:ILE:HB	2.03	0.41
1:D:19:PRO:HD3	1:D:112:PRO:CB	2.51	0.41
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.03	0.40
1:D:615:PRO:O	1:D:618:THR:HG22	2.21	0.40
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.56	0.40
1:A:102:ASN:HA	1:A:201:ASP:CB	2.47	0.40
1:A:622:HIS:CE1	5:A:7021:DMS:H22	2.56	0.40
1:A:286:ALA:HB2	5:A:7011:DMS:H13	2.04	0.40
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.47	0.40
1:C:379:MET:HE1	1:C:387:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	972 (96%)	37 (4%)	0	100	100
1	B	1009/1023 (99%)	977 (97%)	32 (3%)	0	100	100
1	C	1009/1023 (99%)	977 (97%)	32 (3%)	0	100	100
1	D	1009/1023 (99%)	973 (96%)	36 (4%)	0	100	100
All	All	4036/4092 (99%)	3899 (97%)	137 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	864/875 (99%)	860 (100%)	4 (0%)	81	87
1	B	864/875 (99%)	855 (99%)	9 (1%)	68	75
1	C	864/875 (99%)	859 (99%)	5 (1%)	78	85
1	D	864/875 (99%)	860 (100%)	4 (0%)	81	87
All	All	3456/3500 (99%)	3434 (99%)	22 (1%)	78	85

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

Mol	Chain	Res	Type
1	A	80	GLU
1	A	189	LEU
1	A	519	SER
1	A	546	LEU
1	B	80	GLU
1	B	206	SER
1	B	344	LEU
1	B	519	SER
1	B	546	LEU
1	B	687	GLN
1	B	735	HIS
1	B	761	GLN
1	B	819	GLU

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Mol	Chain	Res	Type
1	C	80	GLU
1	C	201	ASP
1	C	206	SER
1	C	546	LEU
1	C	672	VAL
1	D	80	GLU
1	D	293	LEU
1	D	546	LEU
1	D	956	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	262	GLN
1	A	394	ASN
1	A	485	GLN
1	A	510	GLN
1	A	634	GLN
1	A	903	GLN
1	A	1017	GLN
1	B	49	GLN
1	B	262	GLN
1	B	307	ASN
1	B	418	HIS
1	B	445	GLN
1	B	485	GLN
1	B	604	ASN
1	B	624	GLN
1	B	634	GLN
1	B	1017	GLN
1	C	102	ASN
1	C	363	HIS
1	C	416	GLN
1	C	418	HIS
1	C	485	GLN
1	C	510	GLN
1	C	634	GLN
1	C	739	HIS
1	D	128	ASN
1	D	445	GLN
1	D	485	GLN

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Mol	Chain	Res	Type
1	D	885	ASN
1	D	945	ASN
1	D	950	GLN
1	D	974	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 153 ligands modelled in this entry, 24 are monoatomic - leaving 129 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DMS	A	7002	-	3,3,3	2.72	1 (33%)	3,3,3	0.45	0
5	DMS	A	7004	-	3,3,3	2.74	1 (33%)	3,3,3	0.51	0
5	DMS	A	7021	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
5	DMS	D	7005	-	3,3,3	2.64	1 (33%)	3,3,3	0.42	0
5	DMS	C	7008	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
5	DMS	D	7010	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
5	DMS	A	7029	-	3,3,3	2.72	1 (33%)	3,3,3	0.45	0
5	DMS	B	7020	-	3,3,3	2.72	1 (33%)	3,3,3	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	7026	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
5	DMS	B	7021	-	3,3,3	2.70	1 (33%)	3,3,3	0.50	0
5	DMS	A	7019	-	3,3,3	2.79	1 (33%)	3,3,3	0.66	0
5	DMS	D	7001	-	3,3,3	2.70	1 (33%)	3,3,3	0.54	0
5	DMS	D	7012	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0
5	DMS	D	7028	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
5	DMS	B	7014	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
5	DMS	C	7026	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
5	DMS	C	7028	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
5	DMS	D	7006	-	3,3,3	2.70	1 (33%)	3,3,3	0.51	0
5	DMS	A	7014	-	3,3,3	2.70	1 (33%)	3,3,3	0.37	0
5	DMS	A	7003	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
5	DMS	D	7027	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
5	DMS	A	7012	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
5	DMS	C	7015	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
5	DMS	D	7019	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
5	DMS	D	7022	-	3,3,3	2.72	1 (33%)	3,3,3	0.51	0
4	BTB	C	6001	-	13,13,13	0.57	0	7,16,16	0.69	0
5	DMS	D	7016	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
5	DMS	A	7007	-	3,3,3	2.72	1 (33%)	3,3,3	0.44	0
5	DMS	C	7024	-	3,3,3	2.69	1 (33%)	3,3,3	0.50	0
5	DMS	C	7017	3	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
5	DMS	C	7013	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
5	DMS	B	7028	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
5	DMS	A	7008	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
5	DMS	B	7025	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
5	DMS	A	7015	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
5	DMS	B	7008	-	3,3,3	2.72	1 (33%)	3,3,3	0.51	0
5	DMS	C	7010	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
5	DMS	C	7012	-	3,3,3	2.75	1 (33%)	3,3,3	0.54	0
5	DMS	A	7024	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
5	DMS	D	7015	-	3,3,3	2.74	1 (33%)	3,3,3	0.56	0
5	DMS	C	7011	-	3,3,3	2.75	1 (33%)	3,3,3	0.52	0
5	DMS	B	7033	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
5	DMS	A	7027	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	7013	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
5	DMS	A	7030	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
5	DMS	B	7029	-	3,3,3	2.70	1 (33%)	3,3,3	0.49	0
4	BTB	D	6001	3	13,13,13	0.90	0	7,16,16	0.83	0
5	DMS	A	7018	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
5	DMS	B	7016	3	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
5	DMS	C	7002	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
5	DMS	C	7023	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
5	DMS	D	7004	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
5	DMS	B	7001	-	3,3,3	2.69	1 (33%)	3,3,3	0.53	0
5	DMS	C	7001	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
5	DMS	B	7018	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
5	DMS	A	7011	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
4	BTB	B	6001	-	13,13,13	0.78	0	7,16,16	0.88	0
5	DMS	C	7006	-	3,3,3	2.73	1 (33%)	3,3,3	0.48	0
5	DMS	B	7011	-	3,3,3	2.71	1 (33%)	3,3,3	0.51	0
5	DMS	C	7005	-	3,3,3	2.70	1 (33%)	3,3,3	0.43	0
5	DMS	A	7017	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
5	DMS	C	7025	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
5	DMS	A	7016	-	3,3,3	2.75	1 (33%)	3,3,3	0.50	0
5	DMS	B	7026	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0
5	DMS	A	7001	-	3,3,3	2.68	1 (33%)	3,3,3	0.48	0
5	DMS	D	7020	-	3,3,3	2.70	1 (33%)	3,3,3	0.48	0
5	DMS	D	7018	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
5	DMS	C	7020	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
4	BTB	A	6001	3	13,13,13	0.46	0	7,16,16	0.22	0
5	DMS	C	7021	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
5	DMS	C	7022	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
5	DMS	A	7005	-	3,3,3	2.72	1 (33%)	3,3,3	0.60	0
5	DMS	D	7002	-	3,3,3	2.71	1 (33%)	3,3,3	0.52	0
5	DMS	D	7023	-	3,3,3	2.70	1 (33%)	3,3,3	0.47	0
5	DMS	C	7027	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
5	DMS	C	7018	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	D	7003	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
5	DMS	D	7024	-	3,3,3	2.71	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	7020	-	3,3,3	2.72	1 (33%)	3,3,3	0.47	0
5	DMS	D	7021	-	3,3,3	2.73	1 (33%)	3,3,3	0.56	0
5	DMS	B	7005	-	3,3,3	2.70	1 (33%)	3,3,3	0.43	0
5	DMS	B	7012	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
5	DMS	C	7034	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0
5	DMS	D	7013	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
5	DMS	B	7023	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
5	DMS	C	7004	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
5	DMS	A	7022	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
5	DMS	B	7027	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
5	DMS	B	7019	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
5	DMS	B	7022	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
5	DMS	C	7016	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
5	DMS	D	7009	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	B	7003	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
5	DMS	D	7007	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
5	DMS	A	7009	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
5	DMS	B	7024	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	A	7028	-	3,3,3	2.71	1 (33%)	3,3,3	0.51	0
5	DMS	B	7009	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
5	DMS	C	7014	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
5	DMS	A	7006	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	A	7031	-	3,3,3	2.73	1 (33%)	3,3,3	0.51	0
5	DMS	B	7017	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
5	DMS	D	7029	-	3,3,3	2.73	1 (33%)	3,3,3	0.54	0
5	DMS	B	7006	-	3,3,3	2.70	1 (33%)	3,3,3	0.47	0
5	DMS	B	7031	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
5	DMS	C	7029	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
5	DMS	B	7010	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
5	DMS	A	7023	-	3,3,3	2.76	1 (33%)	3,3,3	0.52	0
5	DMS	C	7030	-	3,3,3	2.72	1 (33%)	3,3,3	0.52	0
5	DMS	A	7010	-	3,3,3	2.71	1 (33%)	3,3,3	0.46	0
5	DMS	C	7031	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
5	DMS	B	7007	-	3,3,3	2.75	1 (33%)	3,3,3	0.51	0
5	DMS	D	7011	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	7032	-	3,3,3	2.74	1 (33%)	3,3,3	0.52	0
5	DMS	D	7025	-	3,3,3	2.70	1 (33%)	3,3,3	0.56	0
5	DMS	B	7002	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
5	DMS	B	7004	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
5	DMS	C	7003	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
5	DMS	D	7014	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
5	DMS	B	7032	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
5	DMS	B	7015	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
5	DMS	C	7019	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	B	7013	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
5	DMS	B	7030	-	3,3,3	2.73	1 (33%)	3,3,3	0.57	0
5	DMS	C	7009	-	3,3,3	2.72	1 (33%)	3,3,3	0.53	0
5	DMS	A	7025	-	3,3,3	2.73	1 (33%)	3,3,3	0.52	0
5	DMS	C	7007	-	3,3,3	2.74	1 (33%)	3,3,3	0.49	0
5	DMS	D	7017	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
5	DMS	A	7026	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	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
4	BTB	C	6001	-	-	10/21/21/21	-
4	BTB	B	6001	-	-	10/21/21/21	-
4	BTB	D	6001	3	-	4/21/21/21	-
4	BTB	A	6001	3	-	4/21/21/21	-

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	7019	DMS	O-S	4.68	1.81	1.50
5	A	7023	DMS	O-S	4.64	1.80	1.50
5	C	7012	DMS	O-S	4.62	1.80	1.50
5	B	7007	DMS	O-S	4.62	1.80	1.50
5	A	7032	DMS	O-S	4.61	1.80	1.50
5	A	7004	DMS	O-S	4.61	1.80	1.50
5	A	7016	DMS	O-S	4.61	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	7015	DMS	O-S	4.61	1.80	1.50
5	B	7012	DMS	O-S	4.61	1.80	1.50
5	C	7011	DMS	O-S	4.61	1.80	1.50
5	C	7013	DMS	O-S	4.60	1.80	1.50
5	A	7013	DMS	O-S	4.60	1.80	1.50
5	D	7007	DMS	O-S	4.60	1.80	1.50
5	B	7030	DMS	O-S	4.60	1.80	1.50
5	C	7029	DMS	O-S	4.60	1.80	1.50
5	C	7007	DMS	O-S	4.60	1.80	1.50
5	C	7028	DMS	O-S	4.60	1.80	1.50
5	A	7009	DMS	O-S	4.60	1.80	1.50
5	D	7011	DMS	O-S	4.60	1.80	1.50
5	B	7019	DMS	O-S	4.60	1.80	1.50
5	A	7024	DMS	O-S	4.60	1.80	1.50
5	C	7015	DMS	O-S	4.60	1.80	1.50
5	A	7026	DMS	O-S	4.60	1.80	1.50
5	B	7010	DMS	O-S	4.59	1.80	1.50
5	D	7014	DMS	O-S	4.59	1.80	1.50
5	C	7016	DMS	O-S	4.59	1.80	1.50
5	D	7026	DMS	O-S	4.59	1.80	1.50
5	D	7027	DMS	O-S	4.59	1.80	1.50
5	A	7031	DMS	O-S	4.59	1.80	1.50
5	C	7020	DMS	O-S	4.59	1.80	1.50
5	B	7018	DMS	O-S	4.59	1.80	1.50
5	B	7004	DMS	O-S	4.59	1.80	1.50
5	B	7023	DMS	O-S	4.59	1.80	1.50
5	C	7006	DMS	O-S	4.59	1.80	1.50
5	C	7030	DMS	O-S	4.59	1.80	1.50
5	C	7021	DMS	O-S	4.59	1.80	1.50
5	B	7031	DMS	O-S	4.59	1.80	1.50
5	D	7013	DMS	O-S	4.58	1.80	1.50
5	D	7016	DMS	O-S	4.58	1.80	1.50
5	C	7023	DMS	O-S	4.58	1.80	1.50
5	D	7029	DMS	O-S	4.58	1.80	1.50
5	B	7024	DMS	O-S	4.58	1.80	1.50
5	A	7005	DMS	O-S	4.58	1.80	1.50
5	C	7026	DMS	O-S	4.58	1.80	1.50
5	C	7014	DMS	O-S	4.58	1.80	1.50
5	A	7025	DMS	O-S	4.58	1.80	1.50
5	B	7025	DMS	O-S	4.58	1.80	1.50
5	C	7034	DMS	O-S	4.58	1.80	1.50
5	C	7004	DMS	O-S	4.58	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	7015	DMS	O-S	4.58	1.80	1.50
5	A	7007	DMS	O-S	4.58	1.80	1.50
5	B	7032	DMS	O-S	4.58	1.80	1.50
5	A	7029	DMS	O-S	4.58	1.80	1.50
5	D	7017	DMS	O-S	4.58	1.80	1.50
5	B	7014	DMS	O-S	4.58	1.80	1.50
5	C	7008	DMS	O-S	4.58	1.80	1.50
5	A	7030	DMS	O-S	4.58	1.80	1.50
5	D	7002	DMS	O-S	4.58	1.80	1.50
5	D	7028	DMS	O-S	4.58	1.80	1.50
5	A	7006	DMS	O-S	4.58	1.80	1.50
5	A	7012	DMS	O-S	4.58	1.80	1.50
5	D	7021	DMS	O-S	4.58	1.80	1.50
5	B	7020	DMS	O-S	4.58	1.80	1.50
5	A	7015	DMS	O-S	4.58	1.80	1.50
5	C	7018	DMS	O-S	4.58	1.80	1.50
5	A	7027	DMS	O-S	4.58	1.80	1.50
5	A	7017	DMS	O-S	4.58	1.80	1.50
5	D	7018	DMS	O-S	4.58	1.80	1.50
5	D	7019	DMS	O-S	4.58	1.80	1.50
5	B	7033	DMS	O-S	4.57	1.80	1.50
5	B	7028	DMS	O-S	4.57	1.80	1.50
5	A	7008	DMS	O-S	4.57	1.80	1.50
5	A	7011	DMS	O-S	4.57	1.80	1.50
5	C	7031	DMS	O-S	4.57	1.80	1.50
5	C	7017	DMS	O-S	4.57	1.80	1.50
5	C	7027	DMS	O-S	4.57	1.80	1.50
5	B	7013	DMS	O-S	4.57	1.80	1.50
5	D	7022	DMS	O-S	4.57	1.80	1.50
5	A	7002	DMS	O-S	4.57	1.80	1.50
5	A	7020	DMS	O-S	4.57	1.80	1.50
5	B	7008	DMS	O-S	4.57	1.80	1.50
5	C	7009	DMS	O-S	4.57	1.80	1.50
5	C	7019	DMS	O-S	4.57	1.80	1.50
5	D	7010	DMS	O-S	4.56	1.80	1.50
5	B	7016	DMS	O-S	4.56	1.80	1.50
5	B	7027	DMS	O-S	4.56	1.80	1.50
5	A	7003	DMS	O-S	4.56	1.80	1.50
5	D	7009	DMS	O-S	4.56	1.80	1.50
5	B	7026	DMS	O-S	4.56	1.80	1.50
5	B	7017	DMS	O-S	4.56	1.80	1.50
5	C	7022	DMS	O-S	4.56	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	7010	DMS	O-S	4.56	1.80	1.50
5	C	7010	DMS	O-S	4.56	1.80	1.50
5	A	7028	DMS	O-S	4.56	1.80	1.50
5	B	7011	DMS	O-S	4.56	1.80	1.50
5	D	7024	DMS	O-S	4.55	1.80	1.50
5	C	7025	DMS	O-S	4.55	1.80	1.50
5	B	7003	DMS	O-S	4.55	1.80	1.50
5	D	7004	DMS	O-S	4.55	1.80	1.50
5	A	7014	DMS	O-S	4.55	1.80	1.50
5	C	7005	DMS	O-S	4.55	1.80	1.50
5	D	7006	DMS	O-S	4.55	1.80	1.50
5	B	7022	DMS	O-S	4.55	1.80	1.50
5	D	7003	DMS	O-S	4.54	1.80	1.50
5	B	7006	DMS	O-S	4.54	1.80	1.50
5	D	7012	DMS	O-S	4.54	1.80	1.50
5	D	7001	DMS	O-S	4.54	1.80	1.50
5	B	7029	DMS	O-S	4.54	1.80	1.50
5	B	7009	DMS	O-S	4.54	1.80	1.50
5	A	7022	DMS	O-S	4.53	1.80	1.50
5	C	7003	DMS	O-S	4.53	1.80	1.50
5	D	7020	DMS	O-S	4.53	1.80	1.50
5	B	7021	DMS	O-S	4.53	1.80	1.50
5	D	7023	DMS	O-S	4.53	1.80	1.50
5	B	7005	DMS	O-S	4.53	1.80	1.50
5	A	7018	DMS	O-S	4.52	1.80	1.50
5	D	7025	DMS	O-S	4.52	1.80	1.50
5	C	7024	DMS	O-S	4.52	1.80	1.50
5	B	7001	DMS	O-S	4.52	1.80	1.50
5	C	7001	DMS	O-S	4.51	1.80	1.50
5	A	7001	DMS	O-S	4.50	1.79	1.50
5	B	7002	DMS	O-S	4.50	1.79	1.50
5	C	7002	DMS	O-S	4.48	1.79	1.50
5	A	7021	DMS	O-S	4.47	1.79	1.50
5	D	7005	DMS	O-S	4.42	1.79	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	6001	BTB	N-C2-C4-O4

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Mol	Chain	Res	Type	Atoms
4	B	6001	BTB	N-C2-C4-O4
4	B	6001	BTB	C6-C5-N-C2
4	C	6001	BTB	O1-C1-C2-C4
4	C	6001	BTB	O1-C1-C2-N
4	C	6001	BTB	N-C2-C3-O3
4	C	6001	BTB	C6-C5-N-C7
4	D	6001	BTB	N-C2-C4-O4
4	D	6001	BTB	C6-C5-N-C2
4	C	6001	BTB	N-C7-C8-O8
4	B	6001	BTB	N-C5-C6-O6
4	C	6001	BTB	N-C5-C6-O6
4	B	6001	BTB	N-C7-C8-O8
4	A	6001	BTB	N-C5-C6-O6
4	C	6001	BTB	C1-C2-C3-O3
4	D	6001	BTB	N-C7-C8-O8
4	A	6001	BTB	C1-C2-C4-O4
4	B	6001	BTB	C4-C2-C3-O3
4	C	6001	BTB	O1-C1-C2-C3
4	B	6001	BTB	C8-C7-N-C2
4	D	6001	BTB	C8-C7-N-C2
4	B	6001	BTB	N-C2-C3-O3
4	B	6001	BTB	C1-C2-N-C7
4	C	6001	BTB	C1-C2-N-C5
4	C	6001	BTB	C3-C2-N-C5
4	B	6001	BTB	C3-C2-C4-O4
4	A	6001	BTB	C1-C2-C3-O3
4	B	6001	BTB	C3-C2-N-C7

There are no ring outliers.

15 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	7021	DMS	1	0
5	D	7010	DMS	1	0
4	C	6001	BTB	9	0
5	A	7013	DMS	1	0
4	D	6001	BTB	2	0
5	A	7018	DMS	1	0
5	A	7011	DMS	1	0
4	B	6001	BTB	4	0
4	A	6001	BTB	3	0
5	D	7002	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	7034	DMS	1	0
5	B	7006	DMS	1	0
5	B	7031	DMS	1	0
5	A	7010	DMS	1	0
5	C	7009	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%)	-0.16	45 (4%) 38 37	6, 18, 50, 88	0
1	B	1011/1023 (98%)	-0.06	49 (4%) 35 34	6, 19, 50, 97	0
1	C	1011/1023 (98%)	0.04	57 (5%) 30 29	8, 21, 51, 89	0
1	D	1011/1023 (98%)	-0.05	51 (5%) 34 33	7, 19, 54, 92	0
All	All	4044/4092 (98%)	-0.06	202 (4%) 34 33	6, 19, 51, 97	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	TYR	8.7
1	A	107	ILE	8.3
1	B	105	TYR	8.2
1	D	106	PRO	8.1
1	A	105	TYR	7.5
1	B	103	VAL	7.3
1	A	103	VAL	7.3
1	D	107	ILE	7.3
1	B	107	ILE	7.1
1	C	105	TYR	7.0
1	D	600	GLN	7.0
1	B	102	ASN	6.9
1	B	99	ILE	6.9
1	C	103	VAL	6.7
1	C	106	PRO	6.5
1	B	108	THR	6.5
1	D	103	VAL	6.4
1	D	105	TYR	6.3
1	B	104	THR	6.1
1	C	107	ILE	6.0
1	A	102	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	106	PRO	5.8
1	C	102	ASN	5.6
1	D	102	ASN	5.6
1	D	588	TYR	5.6
1	D	109	VAL	5.6
1	B	101	THR	5.6
1	B	601	PHE	5.5
1	C	201	ASP	5.5
1	B	201	ASP	5.5
1	A	106	PRO	5.4
1	C	100	TYR	5.4
1	A	600	GLN	5.2
1	D	594	ASP	5.1
1	A	108	THR	5.1
1	D	100	TYR	5.0
1	B	600	GLN	5.0
1	C	101	THR	5.0
1	D	592	PHE	4.9
1	A	109	VAL	4.9
1	D	101	THR	4.9
1	D	595	THR	4.8
1	A	588	TYR	4.7
1	D	108	THR	4.7
1	B	731	PRO	4.7
1	B	199	ASP	4.5
1	D	201	ASP	4.5
1	C	109	VAL	4.5
1	D	99	ILE	4.4
1	B	593	GLY	4.4
1	A	101	THR	4.3
1	D	593	GLY	4.3
1	C	104	THR	4.3
1	D	104	THR	4.3
1	B	109	VAL	4.3
1	B	595	THR	4.3
1	C	599	ARG	4.3
1	A	596	PRO	4.2
1	C	108	THR	4.2
1	D	601	PHE	4.2
1	A	104	THR	4.2
1	A	595	THR	4.2
1	B	598	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	732	ALA	4.2
1	B	592	PHE	4.1
1	C	601	PHE	4.1
1	C	595	THR	4.1
1	A	100	TYR	4.1
1	C	600	GLN	4.0
1	B	931	PHE	4.0
1	A	99	ILE	4.0
1	C	731	PRO	3.9
1	B	686	PRO	3.9
1	C	737	ILE	3.9
1	B	732	ALA	3.8
1	D	599	ARG	3.8
1	D	596	PRO	3.8
1	C	594	ASP	3.8
1	C	596	PRO	3.8
1	C	99	ILE	3.7
1	C	733	ALA	3.7
1	D	97	ALA	3.7
1	B	730	LEU	3.7
1	B	602	CYS	3.6
1	A	201	ASP	3.6
1	D	730	LEU	3.6
1	C	588	TYR	3.6
1	A	601	PHE	3.5
1	B	596	PRO	3.5
1	D	733	ALA	3.5
1	B	589	GLY	3.5
1	D	589	GLY	3.5
1	B	98	PRO	3.4
1	D	931	PHE	3.4
1	D	199	ASP	3.4
1	B	689	GLU	3.4
1	C	931	PHE	3.4
1	D	598	ASP	3.4
1	A	931	PHE	3.4
1	B	594	ASP	3.3
1	C	685	LEU	3.3
1	C	592	PHE	3.2
1	A	599	ARG	3.2
1	D	686	PRO	3.2
1	A	592	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	735	HIS	3.2
1	D	98	PRO	3.2
1	D	688	PRO	3.2
1	D	685	LEU	3.1
1	C	689	GLU	3.1
1	B	202	MET	3.1
1	B	733	ALA	3.1
1	A	598	ASP	3.1
1	C	202	MET	3.1
1	A	733	ALA	3.0
1	B	588	TYR	3.0
1	A	594	ASP	3.0
1	B	599	ARG	3.0
1	D	112	PRO	3.0
1	B	597	ASN	2.9
1	B	203	TRP	2.9
1	B	97	ALA	2.9
1	A	685	LEU	2.9
1	B	76	CYS	2.8
1	A	689	GLU	2.8
1	C	200	GLN	2.8
1	C	199	ASP	2.8
1	D	602	CYS	2.8
1	C	730	LEU	2.7
1	C	362	LEU	2.7
1	D	111	PRO	2.7
1	A	735	HIS	2.7
1	A	686	PRO	2.7
1	A	690	SER	2.7
1	D	597	ASN	2.6
1	A	113	PHE	2.6
1	A	730	LEU	2.6
1	C	686	PRO	2.6
1	A	593	GLY	2.6
1	B	735	HIS	2.6
1	C	736	ALA	2.6
1	A	111	PRO	2.6
1	C	745	MET	2.5
1	B	95	TYR	2.5
1	A	732	ALA	2.5
1	C	96	ASP	2.5
1	C	598	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	731	PRO	2.5
1	C	98	PRO	2.5
1	D	768	MET	2.4
1	C	735	HIS	2.4
1	C	585	TRP	2.4
1	A	97	ALA	2.4
1	D	732	ALA	2.4
1	A	742	THR	2.4
1	C	78	LEU	2.4
1	A	977	HIS	2.4
1	C	112	PRO	2.4
1	C	597	ASN	2.3
1	C	203	TRP	2.3
1	A	199	ASP	2.3
1	B	96	ASP	2.3
1	D	113	PHE	2.3
1	A	203	TRP	2.3
1	D	1018	LEU	2.3
1	C	799	THR	2.3
1	B	581	ASN	2.3
1	A	112	PRO	2.2
1	C	589	GLY	2.2
1	C	593	GLY	2.2
1	C	690	SER	2.2
1	A	110	ASN	2.2
1	A	819	GLU	2.2
1	B	663	LEU	2.2
1	D	739	HIS	2.2
1	B	204	ARG	2.2
1	D	731	PRO	2.2
1	A	582	GLY	2.2
1	B	77	ASP	2.2
1	C	111	PRO	2.1
1	C	800	ARG	2.1
1	B	1023	LYS	2.1
1	C	580	GLU	2.1
1	D	750	GLU	2.1
1	D	114	VAL	2.1
1	C	114	VAL	2.1
1	C	97	ALA	2.1
1	B	690	SER	2.1
1	D	78	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	602	CYS	2.1
1	B	729	THR	2.1
1	C	831	ALA	2.1
1	B	685	LEU	2.0
1	D	682	LEU	2.0
1	D	110	ASN	2.0
1	A	602	CYS	2.0
1	C	204	ARG	2.0
1	D	977	HIS	2.0
1	C	113	PHE	2.0
1	A	655	MET	2.0
1	D	831	ALA	2.0
1	D	830	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	7008	4/4	0.48	0.36	134,134,134,134	0
5	DMS	C	7020	4/4	0.54	0.23	141,141,141,142	0
5	DMS	C	7015	4/4	0.57	0.30	100,100,100,101	0
5	DMS	B	7019	4/4	0.60	0.31	64,65,65,66	0
4	BTB	D	6001	14/14	0.60	0.39	77,83,85,85	0
5	DMS	D	7019	4/4	0.63	0.33	114,114,115,115	0
5	DMS	D	7013	4/4	0.64	0.26	87,87,87,87	0
3	NA	B	3104	1/1	0.66	0.34	87,87,87,87	0
5	DMS	A	7019	4/4	0.68	0.29	55,55,56,57	0
5	DMS	D	7028	4/4	0.69	0.25	76,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BTB	C	6001	14/14	0.70	0.21	43,45,47,52	0
5	DMS	B	7010	4/4	0.70	0.26	67,67,67,68	0
5	DMS	B	7012	4/4	0.70	0.28	76,76,76,77	0
5	DMS	C	7017	4/4	0.70	0.27	69,70,70,70	0
5	DMS	B	7025	4/4	0.71	0.36	131,131,131,131	0
5	DMS	B	7016	4/4	0.71	0.32	85,85,85,85	0
5	DMS	C	7021	4/4	0.72	0.33	93,93,93,93	0
4	BTB	A	6001	14/14	0.72	0.21	31,48,54,55	0
5	DMS	B	7031	4/4	0.73	0.31	77,77,78,78	0
3	NA	D	3102	1/1	0.73	0.16	44,44,44,44	0
5	DMS	B	7030	4/4	0.73	0.41	91,91,91,91	0
3	NA	D	3103	1/1	0.74	0.27	83,83,83,83	0
5	DMS	C	7034	4/4	0.75	0.28	74,75,75,75	0
5	DMS	B	7014	4/4	0.76	0.22	84,84,84,85	0
5	DMS	A	7012	4/4	0.76	0.28	89,89,89,89	0
5	DMS	B	7018	4/4	0.76	0.25	75,75,75,76	0
4	BTB	B	6001	14/14	0.76	0.39	107,108,108,108	0
5	DMS	B	7015	4/4	0.77	0.27	75,75,75,76	0
5	DMS	C	7024	4/4	0.77	0.32	83,83,83,83	0
5	DMS	C	7026	4/4	0.77	0.37	92,92,92,92	0
5	DMS	A	7026	4/4	0.77	0.29	84,85,85,85	0
5	DMS	C	7019	4/4	0.77	0.33	112,112,113,113	0
5	DMS	A	7024	4/4	0.77	0.33	86,86,86,87	0
5	DMS	A	7008	4/4	0.78	0.26	60,61,62,62	0
5	DMS	D	7016	4/4	0.78	0.31	93,94,94,94	0
5	DMS	C	7011	4/4	0.78	0.28	49,50,50,50	0
5	DMS	D	7024	4/4	0.78	0.29	67,68,68,68	0
5	DMS	A	7003	4/4	0.78	0.27	84,84,85,85	0
5	DMS	C	7029	4/4	0.79	0.27	76,76,76,77	0
5	DMS	D	7009	4/4	0.79	0.25	75,75,75,75	0
5	DMS	C	7009	4/4	0.79	0.29	86,86,86,86	0
3	NA	C	3103	1/1	0.79	0.16	42,42,42,42	0
5	DMS	C	7012	4/4	0.79	0.25	59,59,59,60	0
5	DMS	B	7026	4/4	0.79	0.30	82,83,83,83	0
5	DMS	A	7025	4/4	0.79	0.23	65,66,66,67	0
5	DMS	A	7015	4/4	0.80	0.26	57,58,58,59	0
3	NA	C	3104	1/1	0.81	0.19	59,59,59,59	0
5	DMS	A	7009	4/4	0.81	0.25	61,61,62,62	0
5	DMS	A	7031	4/4	0.81	0.21	73,73,73,73	0
5	DMS	D	7017	4/4	0.81	0.30	93,93,93,93	0
5	DMS	B	7021	4/4	0.81	0.29	68,68,68,68	0
5	DMS	C	7016	4/4	0.81	0.23	70,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	7032	4/4	0.81	0.27	69,69,69,70	0
5	DMS	D	7011	4/4	0.82	0.20	63,63,63,63	0
5	DMS	A	7006	4/4	0.82	0.37	100,101,101,101	0
5	DMS	A	7018	4/4	0.82	0.24	57,57,58,59	0
5	DMS	B	7008	4/4	0.82	0.23	75,75,75,75	0
5	DMS	B	7032	4/4	0.82	0.20	55,56,56,57	0
5	DMS	D	7004	4/4	0.82	0.22	43,43,44,44	0
5	DMS	B	7033	4/4	0.82	0.22	54,54,55,56	0
5	DMS	D	7014	4/4	0.83	0.21	67,67,67,67	0
5	DMS	B	7020	4/4	0.83	0.30	96,96,96,96	0
5	DMS	C	7014	4/4	0.83	0.25	67,67,67,67	0
5	DMS	B	7013	4/4	0.83	0.25	70,70,70,70	0
2	MG	D	3002	1/1	0.83	0.13	51,51,51,51	0
5	DMS	A	7011	4/4	0.83	0.20	58,58,58,58	0
5	DMS	B	7011	4/4	0.84	0.20	69,69,69,69	0
5	DMS	D	7018	4/4	0.84	0.22	62,63,63,63	0
5	DMS	C	7030	4/4	0.84	0.27	68,68,68,68	0
5	DMS	D	7021	4/4	0.84	0.25	80,80,80,80	0
5	DMS	A	7020	4/4	0.84	0.19	48,48,48,49	0
5	DMS	D	7027	4/4	0.84	0.21	55,56,57,58	0
5	DMS	A	7013	4/4	0.84	0.22	59,59,60,60	0
5	DMS	D	7029	4/4	0.84	0.20	78,78,78,78	0
3	NA	D	3104	1/1	0.85	0.12	32,32,32,32	0
5	DMS	D	7026	4/4	0.85	0.26	73,74,74,74	0
5	DMS	A	7016	4/4	0.85	0.19	53,54,54,54	0
3	NA	B	3103	1/1	0.85	0.11	34,34,34,34	0
5	DMS	D	7023	4/4	0.85	0.17	42,42,42,42	0
5	DMS	A	7028	4/4	0.86	0.19	57,58,58,58	0
5	DMS	A	7004	4/4	0.86	0.18	59,59,60,60	0
5	DMS	B	7028	4/4	0.86	0.15	63,63,63,63	0
5	DMS	C	7031	4/4	0.86	0.16	52,53,53,53	0
5	DMS	A	7017	4/4	0.86	0.20	66,66,66,66	0
5	DMS	B	7024	4/4	0.87	0.19	59,59,60,60	0
3	NA	C	3102	1/1	0.87	0.10	44,44,44,44	0
5	DMS	A	7023	4/4	0.87	0.17	32,32,33,35	0
5	DMS	B	7027	4/4	0.87	0.22	57,57,57,57	0
5	DMS	A	7007	4/4	0.87	0.21	49,49,49,50	0
3	NA	B	3102	1/1	0.87	0.09	47,47,47,47	0
5	DMS	C	7004	4/4	0.88	0.19	44,45,45,46	0
5	DMS	B	7029	4/4	0.88	0.21	63,63,63,63	0
5	DMS	C	7018	4/4	0.88	0.19	62,62,62,63	0
5	DMS	D	7020	4/4	0.88	0.18	57,57,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	7014	4/4	0.88	0.19	41,44,44,44	0
2	MG	A	3002	1/1	0.88	0.12	42,42,42,42	0
5	DMS	B	7004	4/4	0.88	0.16	46,46,47,47	0
5	DMS	C	7023	4/4	0.88	0.18	66,66,67,67	0
3	NA	A	3102	1/1	0.88	0.10	41,41,41,41	0
5	DMS	D	7015	4/4	0.88	0.17	46,47,48,48	0
2	MG	C	3002	1/1	0.88	0.10	55,55,55,55	0
5	DMS	D	7025	4/4	0.89	0.19	55,56,56,56	0
5	DMS	C	7013	4/4	0.89	0.14	58,58,59,59	0
5	DMS	A	7027	4/4	0.89	0.15	51,51,51,52	0
5	DMS	C	7006	4/4	0.89	0.16	45,46,46,46	0
5	DMS	C	7022	4/4	0.89	0.23	68,69,69,69	0
5	DMS	A	7002	4/4	0.90	0.15	41,42,43,43	0
3	NA	A	3103	1/1	0.90	0.09	31,31,31,31	0
5	DMS	B	7022	4/4	0.90	0.19	60,60,60,61	0
5	DMS	B	7023	4/4	0.90	0.17	66,66,67,67	0
5	DMS	C	7025	4/4	0.91	0.16	51,51,51,51	0
5	DMS	D	7012	4/4	0.91	0.13	45,46,46,46	0
5	DMS	B	7006	4/4	0.91	0.18	58,58,58,59	0
5	DMS	C	7027	4/4	0.91	0.16	54,55,55,55	0
5	DMS	C	7007	4/4	0.91	0.16	35,35,35,37	0
5	DMS	B	7017	4/4	0.91	0.17	50,50,50,50	0
3	NA	A	3104	1/1	0.91	0.10	50,50,50,50	0
5	DMS	A	7005	4/4	0.91	0.18	43,44,44,45	0
5	DMS	A	7021	4/4	0.91	0.18	36,37,37,38	0
3	NA	C	3101	1/1	0.92	0.05	17,17,17,17	0
5	DMS	B	7009	4/4	0.92	0.14	37,38,38,39	0
5	DMS	C	7010	4/4	0.92	0.13	43,43,43,43	0
5	DMS	D	7002	4/4	0.92	0.17	37,37,39,40	0
5	DMS	A	7030	4/4	0.92	0.17	59,60,60,61	0
5	DMS	D	7006	4/4	0.92	0.16	52,52,52,53	0
5	DMS	D	7022	4/4	0.92	0.14	46,47,47,48	0
5	DMS	D	7010	4/4	0.93	0.14	48,49,49,49	0
5	DMS	B	7002	4/4	0.93	0.13	33,34,35,35	0
5	DMS	C	7028	4/4	0.94	0.15	40,41,41,42	0
5	DMS	C	7002	4/4	0.94	0.11	27,30,30,31	0
5	DMS	D	7007	4/4	0.94	0.12	32,32,33,33	0
2	MG	C	3001	1/1	0.94	0.09	19,19,19,19	0
3	NA	D	3101	1/1	0.94	0.05	15,15,15,15	0
5	DMS	A	7029	4/4	0.94	0.13	41,42,42,42	0
3	NA	A	3101	1/1	0.95	0.04	11,11,11,11	0
2	MG	B	3002	1/1	0.95	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	7005	4/4	0.95	0.11	38,38,39,39	0
5	DMS	A	7010	4/4	0.95	0.11	48,49,49,49	0
5	DMS	C	7005	4/4	0.95	0.11	38,38,38,38	0
5	DMS	B	7007	4/4	0.95	0.13	32,32,33,33	0
3	NA	B	3101	1/1	0.95	0.04	13,13,13,13	0
5	DMS	C	7003	4/4	0.96	0.09	30,30,30,31	0
2	MG	B	3001	1/1	0.96	0.09	21,21,21,21	0
5	DMS	B	7003	4/4	0.96	0.10	36,36,36,36	0
5	DMS	A	7022	4/4	0.97	0.09	27,28,28,29	0
5	DMS	D	7005	4/4	0.97	0.09	31,31,32,32	0
2	MG	D	3001	1/1	0.97	0.07	18,18,18,18	0
2	MG	A	3001	1/1	0.97	0.07	18,18,18,18	0
5	DMS	D	7003	4/4	0.97	0.08	27,28,28,29	0
5	DMS	D	7001	4/4	0.98	0.07	20,20,22,23	0
5	DMS	B	7001	4/4	0.98	0.07	20,20,20,21	0
5	DMS	A	7001	4/4	0.98	0.06	17,17,17,20	0
5	DMS	C	7001	4/4	0.98	0.06	19,19,20,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.