



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:19 AM UTC

PDB ID : 3I3D / pdb_00003i3d
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (M542A) IN COMPLEX WITH IPTG
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 types of validation reports are described at

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

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

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

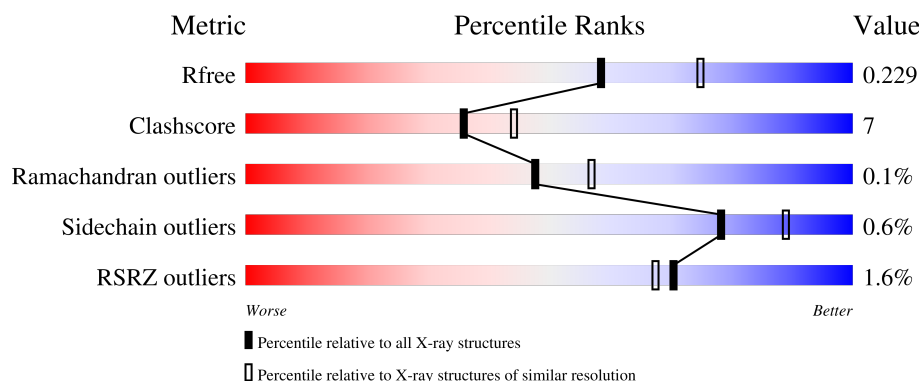
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	1023	0% 79% 19% ..
1	B	1023	2% 81% 17% ..
1	C	1023	0% 79% 19% ..
1	D	1023	2% 78% 19% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	C	9041	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36737 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:

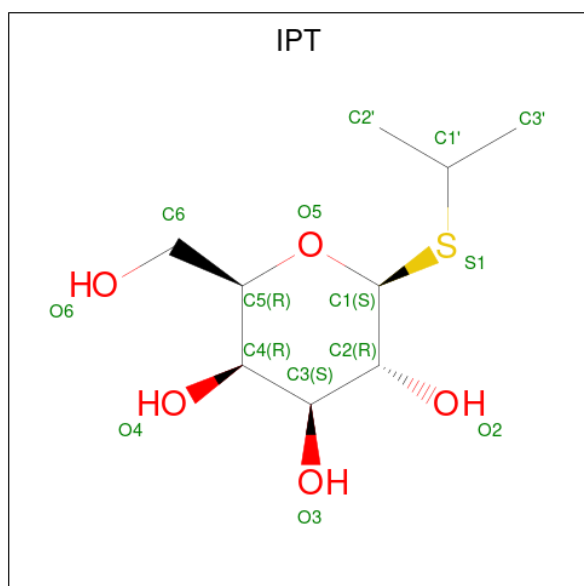
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP B8LFD6
A	2	SER	-	expression tag	UNP B8LFD6
A	3	HIS	-	expression tag	UNP B8LFD6
A	4	MET	-	expression tag	UNP B8LFD6
A	5	LEU	-	expression tag	UNP B8LFD6
A	6	GLU	-	expression tag	UNP B8LFD6
A	7	ASP	-	expression tag	UNP B8LFD6
A	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 1-methylethyl 1-thio-beta-D-galactopyranoside (CCD ID: IPT) (formula: $C_9H_{18}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			15	9	5	1		
2	A	1	Total	C	O	S	0	0
			15	9	5	1		
2	B	1	Total	C	O	S	0	0
			15	9	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	S	0	0
			15	9	5	1		
2	D	1	Total	C	O	S	0	0
			15	9	5	1		
2	D	1	Total	C	O	S	0	0
			15	9	5	1		

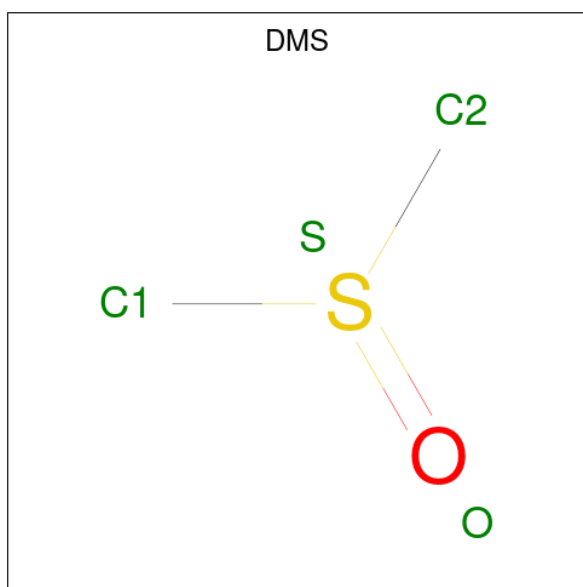
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Na	0	0
			4	4		
4	B	5	Total	Na	0	0
			5	5		
4	C	4	Total	Na	0	0
			4	4		
4	D	4	Total	Na	0	0
			4	4		

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



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

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

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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	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
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	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

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

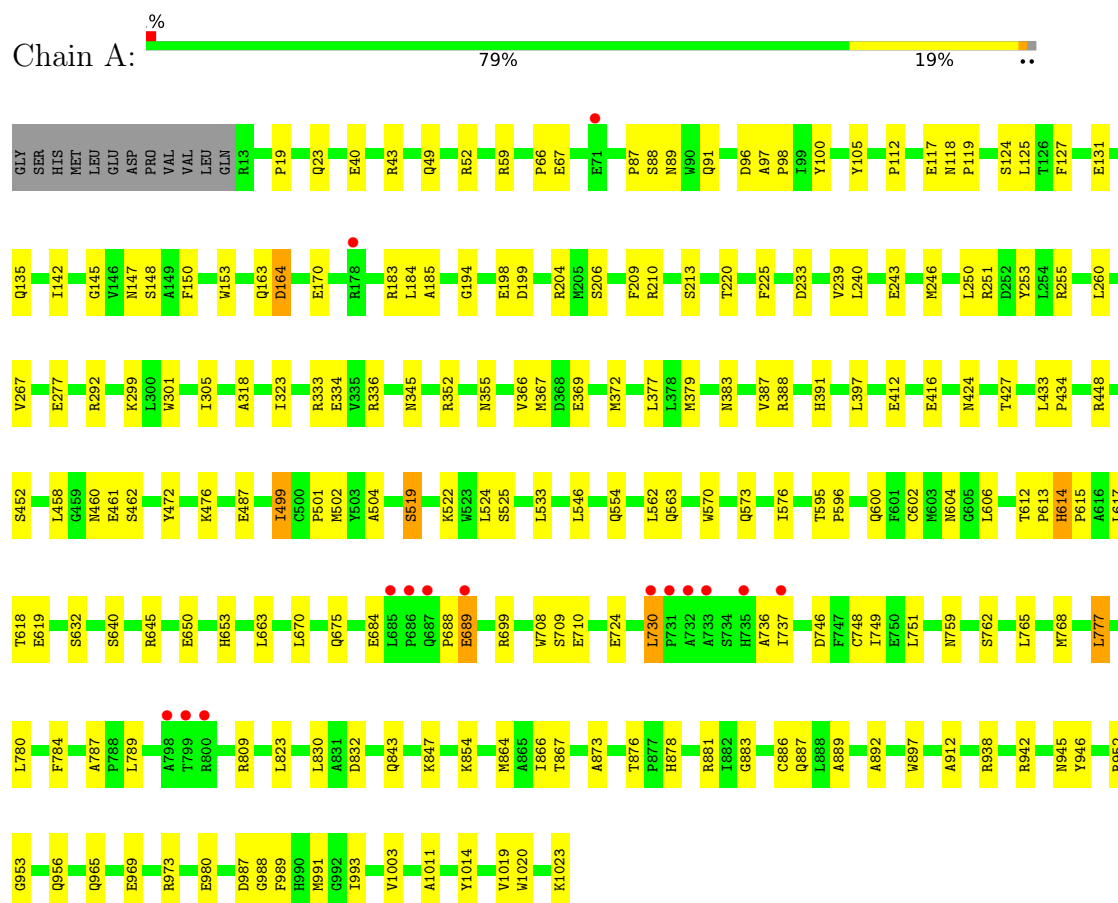
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	862	Total O 862 862	0	0
6	B	987	Total O 987 987	0	0
6	C	828	Total O 828 828	0	0
6	D	856	Total O 856 856	0	0

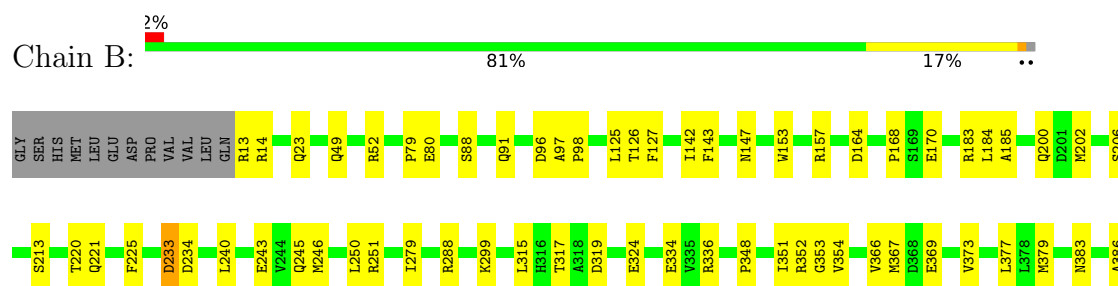
3 Residue-property plots

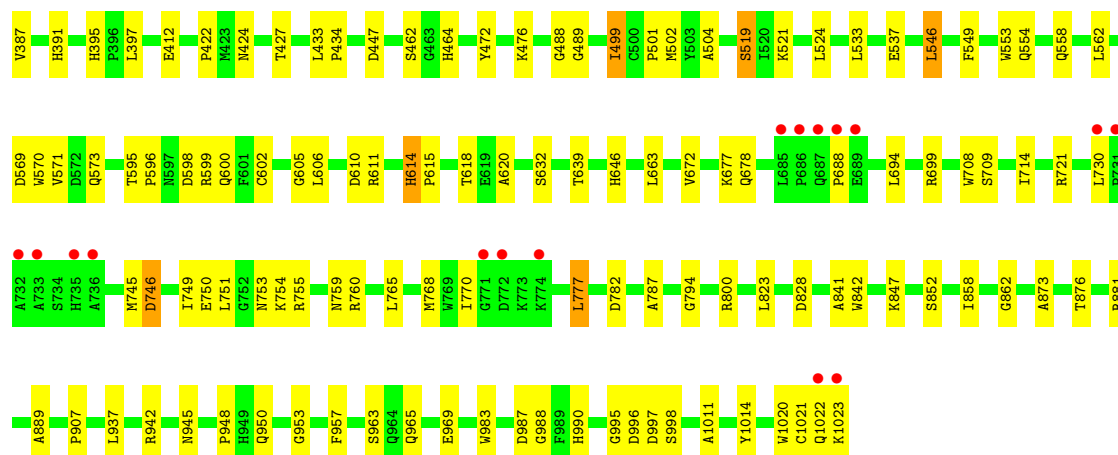
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

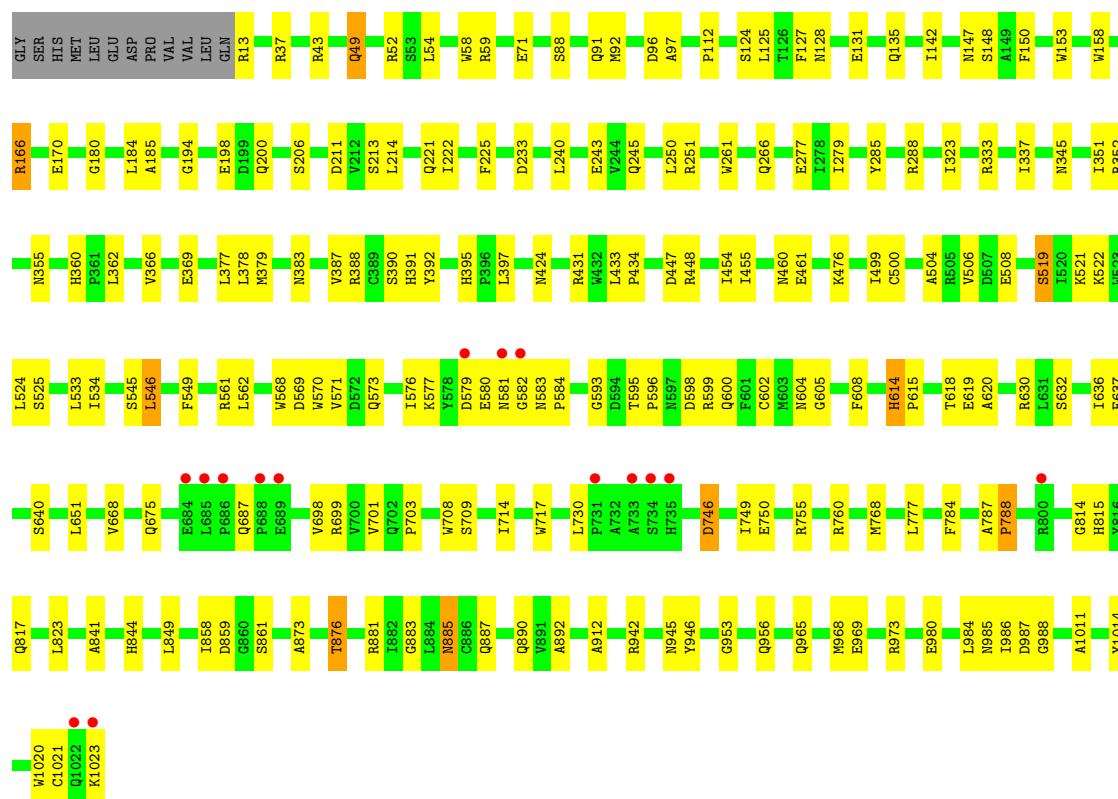
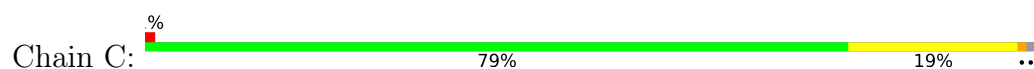


• Molecule 1: Beta-galactosidase

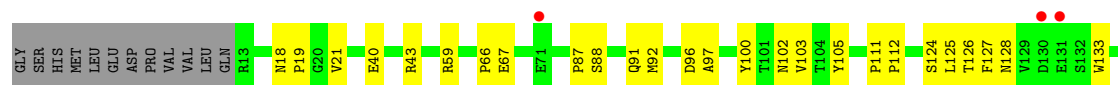
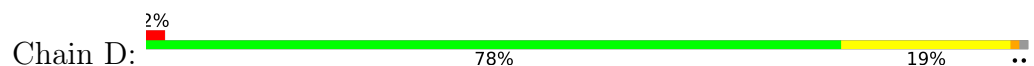




● Molecule 1: Beta-galactosidase



● 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	151.54Å 162.39Å 203.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.97 – 2.20 61.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.97-2.20) 99.9 (61.97-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.185 , 0.232 0.182 , 0.229	Depositor DCC
R_{free} test set	3625 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36737	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 40.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6394e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IPT, 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	0.34	0/8364	0.87	24/11412 (0.2%)
1	B	0.36	0/8364	0.88	25/11412 (0.2%)
1	C	0.36	0/8364	0.89	30/11412 (0.3%)
1	D	0.34	0/8364	0.87	25/11412 (0.2%)
All	All	0.35	0/33456	0.88	104/45648 (0.2%)

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	TRP	N-CA-C	8.19	120.12	111.03
1	B	988	GLY	N-CA-C	-7.85	102.08	113.86
1	C	614	HIS	N-CA-C	-7.75	99.98	110.36
1	D	570	TRP	N-CA-C	7.73	119.61	111.03
1	B	570	TRP	N-CA-C	7.70	119.57	111.03
1	C	988	GLY	N-CA-C	-7.50	102.61	113.86
1	B	614	HIS	N-CA-C	-7.35	100.51	110.36
1	C	570	TRP	N-CA-C	7.29	119.13	111.03
1	C	352	ARG	N-CA-C	-7.25	99.49	109.71
1	C	447	ASP	N-CA-C	7.16	122.19	113.17
1	C	97	ALA	N-CA-C	7.13	118.77	109.93
1	D	988	GLY	N-CA-C	-6.97	103.40	113.86
1	D	614	HIS	N-CA-C	-6.93	101.07	110.36
1	A	614	HIS	N-CA-C	-6.82	101.22	110.36
1	C	383	ASN	N-CA-C	6.67	120.78	112.24
1	A	383	ASN	N-CA-C	6.59	120.68	112.24
1	B	777	LEU	N-CA-C	-6.54	105.93	114.04
1	A	504	ALA	N-CA-C	-6.54	100.60	110.28
1	B	519	SER	N-CA-C	-6.42	101.19	110.24
1	C	746	ASP	N-CA-C	6.32	118.68	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ASP	N-CA-C	6.28	118.64	111.11
1	B	646	HIS	N-CA-C	-6.26	101.26	110.52
1	C	777	LEU	N-CA-C	-6.25	106.19	113.88
1	D	519	SER	N-CA-C	-6.21	101.48	110.24
1	A	519	SER	N-CA-C	-6.21	101.23	110.23
1	B	351	ILE	N-CA-C	6.20	116.43	108.12
1	D	746	ASP	N-CA-C	6.19	118.48	109.07
1	A	777	LEU	N-CA-C	-6.09	106.39	113.88
1	D	221	GLN	N-CA-C	6.08	118.42	109.24
1	D	97	ALA	N-CA-C	6.08	117.73	110.07
1	C	519	SER	N-CA-C	-6.00	101.78	110.24
1	B	383	ASN	N-CA-C	5.95	119.85	112.24
1	A	746	ASP	N-CA-C	5.91	118.05	109.07
1	D	209	PHE	N-CA-C	5.86	120.43	113.28
1	A	323	ILE	N-CA-C	-5.84	106.12	111.67
1	C	499	ILE	N-CA-C	-5.83	100.30	108.12
1	C	233	ASP	N-CA-C	5.82	118.38	111.33
1	C	37	ARG	N-CA-C	-5.82	105.37	112.88
1	D	777	LEU	N-CA-C	-5.79	106.56	113.97
1	D	771	GLY	N-CA-C	-5.77	104.42	111.35
1	D	571	VAL	N-CA-C	5.75	117.03	108.46
1	A	612	THR	N-CA-C	-5.75	102.53	109.83
1	B	97	ALA	N-CA-C	5.75	117.32	110.07
1	A	352	ARG	N-CA-C	-5.71	101.00	109.11
1	A	499	ILE	N-CA-C	-5.71	100.47	108.12
1	A	233	ASP	N-CA-C	5.70	118.23	111.33
1	C	504	ALA	N-CA-C	-5.70	101.20	110.20
1	D	504	ALA	N-CA-C	-5.68	101.87	110.28
1	C	166	ARG	N-CA-C	5.67	120.19	112.88
1	B	447	ASP	N-CA-C	5.66	120.30	113.17
1	B	504	ALA	N-CA-C	-5.64	101.93	110.28
1	D	352	ARG	N-CA-C	-5.63	101.77	109.71
1	D	545	SER	N-CA-C	5.61	115.81	108.07
1	A	97	ALA	N-CA-C	5.57	117.08	110.07
1	B	746	ASP	N-CA-C	5.56	117.53	109.07
1	C	876	THR	N-CA-C	-5.55	103.18	110.39
1	D	383	ASN	N-CA-C	5.53	119.32	112.24
1	D	506	VAL	N-CA-C	5.51	115.60	110.42
1	C	788	PRO	N-CA-C	5.51	120.24	111.26
1	B	395	HIS	N-CA-C	-5.51	102.65	109.64
1	C	222	ILE	N-CA-C	-5.51	99.81	108.23
1	A	878	HIS	CA-C-N	5.43	125.34	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	878	HIS	C-N-CA	5.43	125.34	119.85
1	C	448	ARG	N-CA-C	5.43	119.01	112.38
1	B	220	THR	N-CA-C	-5.43	99.67	108.41
1	D	612	THR	N-CA-C	-5.42	102.81	109.65
1	B	221	GLN	N-CA-C	5.42	117.42	109.24
1	D	150	PHE	N-CA-C	5.42	116.75	108.52
1	A	220	THR	N-CA-C	-5.41	99.71	108.41
1	D	499	ILE	N-CA-C	-5.40	100.89	108.12
1	B	98	PRO	N-CA-C	-5.39	102.68	111.68
1	D	646	HIS	N-CA-C	-5.34	102.62	110.52
1	D	233	ASP	N-CA-C	5.32	117.77	111.33
1	C	956	GLN	N-CA-C	-5.31	101.46	109.85
1	C	221	GLN	N-CA-C	5.31	117.05	109.14
1	B	787	ALA	N-CA-C	-5.28	100.33	109.58
1	C	351	ILE	N-CA-C	5.28	115.20	108.12
1	B	488	GLY	N-CA-C	5.28	118.00	111.93
1	B	499	ILE	N-CA-C	-5.28	101.05	108.12
1	A	89	ASN	N-CA-C	-5.24	100.70	109.24
1	C	150	PHE	N-CA-C	5.24	116.48	108.42
1	C	323	ILE	N-CA-C	-5.21	106.72	111.67
1	B	765	LEU	N-CA-C	-5.21	101.65	109.15
1	C	571	VAL	N-CA-C	5.20	116.21	108.46
1	C	395	HIS	N-CA-C	-5.17	103.21	109.57
1	A	563	GLN	N-CA-C	5.15	118.39	112.57
1	B	571	VAL	N-CA-C	5.14	116.11	108.46
1	A	150	PHE	N-CA-C	5.11	116.29	108.42
1	B	299	LYS	N-CA-C	-5.11	101.44	109.25
1	A	448	ARG	N-CA-C	5.09	118.59	112.38
1	B	315	LEU	N-CA-C	-5.09	100.94	109.24
1	A	525	SER	N-CA-C	5.09	118.52	112.72
1	D	770	ILE	N-CA-C	-5.08	98.77	109.34
1	C	787	ALA	N-CA-C	-5.08	100.69	109.58
1	A	787	ALA	N-CA-C	-5.07	100.71	109.58
1	D	220	THR	N-CA-C	-5.07	99.53	108.20
1	A	956	GLN	N-CA-C	-5.05	101.64	109.72
1	C	211	ASP	N-CA-C	5.05	116.80	110.24
1	B	554	GLN	N-CA-C	-5.05	105.86	111.36
1	A	98	PRO	N-CA-C	-5.04	103.27	111.68
1	C	593	GLY	N-CA-C	-5.03	108.77	115.40
1	C	545	SER	N-CA-C	5.02	115.00	108.07
1	D	510	GLN	CA-C-N	5.00	126.09	119.84
1	D	510	GLN	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8122	0	7711	122	0
1	B	8122	0	7711	115	0
1	C	8122	0	7710	120	0
1	D	8122	0	7712	131	0
2	A	30	0	35	0	0
2	B	15	0	17	0	0
2	C	15	0	17	0	0
2	D	30	0	35	0	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	4	0	0	0	0
4	B	5	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	136	0	204	7	0
5	B	164	0	246	8	0
5	C	168	0	252	12	0
5	D	128	0	192	5	0
6	A	862	0	0	12	0
6	B	987	0	0	7	0
6	C	828	0	0	9	0
6	D	856	0	0	6	0
All	All	36737	0	31842	475	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 (475) 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:D:142:ILE:HG12	1:D:170:GLU:HG2	1.50	0.92
1:B:770:ILE:HG21	1:B:1022:GLN:HE22	1.34	0.91
1:C:599:ARG:NH2	1:C:600:GLN:HE22	1.75	0.84
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.59	0.83
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.58	0.82
1:B:599:ARG:NH1	1:B:600:GLN:HE22	1.76	0.82
1:C:125:LEU:HA	5:C:9030:DMS:H22	1.63	0.80
1:B:770:ILE:HD13	1:B:1022:GLN:NE2	1.98	0.79
1:A:765:LEU:HD21	1:A:768:MET:HE2	1.65	0.77
1:A:292:ARG:HH12	5:A:9010:DMS:H13	1.49	0.76
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.68	0.76
1:C:337:ILE:H	5:C:9037:DMS:H12	1.50	0.76
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.67	0.74
1:A:689:GLU:CD	1:A:689:GLU:H	1.96	0.74
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.70	0.73
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.71	0.73
1:C:714:ILE:HG21	5:C:9041:DMS:H11	1.70	0.72
1:A:131:GLU:O	1:A:135:GLN:HG3	1.89	0.72
1:D:246:MET:HG2	6:D:4582:HOH:O	1.89	0.70
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.55	0.70
1:A:699:ARG:HD2	5:A:9036:DMS:H13	1.73	0.70
1:A:737:ILE:HD13	1:A:832:ASP:HA	1.73	0.70
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.73	0.70
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.75	0.69
1:C:749:ILE:HD12	1:C:858:ILE:HD12	1.74	0.69
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.28	0.69
1:D:88:SER:HA	1:D:366:VAL:HG21	1.75	0.69
1:D:965:GLN:O	1:D:969:GLU:HG3	1.93	0.69
1:C:88:SER:HA	1:C:366:VAL:HG21	1.76	0.68
1:D:651:LEU:HD23	1:D:653:HIS:HE2	1.57	0.68
1:B:615:PRO:O	1:B:618:THR:HG22	1.93	0.67
1:C:615:PRO:O	1:C:618:THR:HG22	1.95	0.67
1:D:599:ARG:HH11	1:D:797:GLU:CG	2.08	0.67
1:D:600:GLN:H	1:D:600:GLN:NE2	1.93	0.67
1:D:714:ILE:HB	5:D:9027:DMS:H22	1.77	0.67
1:D:748:CYS:HB2	6:D:4906:HOH:O	1.94	0.66
1:A:59:ARG:HB2	1:A:124:SER:OG	1.96	0.66
1:B:770:ILE:HG21	1:B:1022:GLN:NE2	2.07	0.66
1:C:699:ARG:HD2	5:C:9041:DMS:H13	1.78	0.66
1:B:88:SER:HA	1:B:366:VAL:HG21	1.78	0.65
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.32	0.64
1:A:379:MET:HE1	1:A:387:VAL:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:GLN:HB2	1:C:602:CYS:O	1.97	0.64
1:D:147:ASN:HB3	1:D:206:SER:HA	1.80	0.64
1:A:864:MET:HE3	1:A:866:ILE:HD11	1.77	0.64
1:B:379:MET:HE1	1:B:387:VAL:HB	1.77	0.64
1:A:965:GLN:O	1:A:969:GLU:HG3	1.97	0.64
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.63	0.64
1:C:59:ARG:HG2	5:C:9030:DMS:H23	1.79	0.64
1:D:18:ASN:ND2	1:D:21:VAL:HG23	2.13	0.64
1:B:79:PRO:HG2	1:B:80:GLU:OE2	1.97	0.64
1:A:88:SER:HA	1:A:366:VAL:HG21	1.80	0.63
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.34	0.63
1:B:663:LEU:HD21	1:B:688:PRO:HB3	1.80	0.63
1:C:788:PRO:HD2	1:C:968:MET:HG3	1.79	0.63
1:C:431:ARG:HB2	6:C:4908:HOH:O	1.99	0.63
1:D:355:ASN:OD1	1:D:388:ARG:HD3	1.99	0.63
1:B:751:LEU:HD23	1:B:862:GLY:HA2	1.81	0.62
1:D:246:MET:HE3	6:D:4582:HOH:O	1.99	0.62
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.00	0.62
1:D:91:GLN:HG3	1:D:96:ASP:OD1	1.99	0.62
1:B:397:LEU:HD11	5:B:9021:DMS:H13	1.82	0.62
1:C:131:GLU:O	1:C:135:GLN:HG3	1.99	0.62
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.48	0.61
1:D:333:ARG:HG3	1:D:333:ARG:HH11	1.65	0.61
1:B:157:ARG:HD3	6:B:5057:HOH:O	2.00	0.61
1:A:277:GLU:H	1:A:277:GLU:CD	2.08	0.60
1:B:965:GLN:O	1:B:969:GLU:HG3	2.02	0.60
1:B:533:LEU:HD23	1:B:533:LEU:C	2.27	0.60
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.01	0.60
1:D:615:PRO:O	1:D:618:THR:HG22	2.01	0.60
1:D:991:MET:HE3	1:D:1003:VAL:HG21	1.82	0.60
1:A:777:LEU:HG	1:A:889:ALA:HA	1.84	0.60
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.37	0.60
1:D:246:MET:SD	1:D:246:MET:C	2.86	0.59
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.84	0.59
1:A:823:LEU:O	1:B:730:LEU:HD21	2.01	0.59
1:C:580:GLU:C	1:C:582:GLY:H	2.11	0.59
1:C:749:ILE:CD1	1:C:858:ILE:HD12	2.32	0.59
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.85	0.59
1:A:730:LEU:HD12	1:A:730:LEU:N	2.17	0.58
1:B:721:ARG:HH12	5:B:9030:DMS:H22	1.68	0.58
1:A:369:GLU:HG3	1:A:397:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:PHE:HA	1:D:243:GLU:O	2.05	0.57
1:D:749:ILE:HD12	1:D:749:ILE:N	2.19	0.57
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.68	0.56
1:B:250:LEU:O	1:B:251:ARG:HD2	2.04	0.56
1:C:128:ASN:HA	1:C:180:GLY:O	2.05	0.56
1:C:369:GLU:HG3	1:C:397:LEU:HD21	1.87	0.56
1:D:379:MET:HE1	1:D:387:VAL:HB	1.87	0.56
1:A:749:ILE:HD12	1:A:749:ILE:N	2.21	0.56
1:C:250:LEU:O	1:C:251:ARG:HD2	2.05	0.56
1:A:117:GLU:HG2	6:A:4260:HOH:O	2.06	0.56
1:B:595:THR:HA	1:B:596:PRO:C	2.30	0.56
1:D:748:CYS:C	1:D:749:ILE:HD12	2.31	0.56
1:C:379:MET:HE1	1:C:387:VAL:HB	1.88	0.56
1:C:1023:LYS:HE3	6:C:4959:HOH:O	2.05	0.56
1:A:595:THR:HA	1:A:596:PRO:C	2.30	0.56
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.87	0.55
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.88	0.55
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.88	0.55
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.89	0.55
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.87	0.55
1:C:823:LEU:HD11	1:C:841:ALA:HB2	1.88	0.55
1:A:615:PRO:O	1:A:618:THR:HG22	2.07	0.55
1:B:599:ARG:NH1	1:B:600:GLN:NE2	2.52	0.55
1:D:66:PRO:HG2	1:D:67:GLU:OE1	2.07	0.55
1:A:487:GLU:OE1	1:A:502:MET:HE3	2.07	0.55
1:C:58:TRP:HA	5:C:9030:DMS:H21	1.88	0.55
1:A:684:GLU:HG2	6:A:4957:HOH:O	2.07	0.54
1:C:887:GLN:NE2	1:C:980:GLU:O	2.41	0.54
1:C:476:LYS:HA	6:C:4199:HOH:O	2.07	0.54
1:A:830:LEU:HD22	1:B:828:ASP:HB3	1.90	0.54
1:B:746:ASP:OD1	1:B:759:ASN:HA	2.07	0.54
1:B:126:THR:H	5:B:9040:DMS:H11	1.71	0.54
1:A:730:LEU:HD12	1:A:730:LEU:H	1.72	0.54
1:B:354:VAL:CG1	1:B:379:MET:HE3	2.38	0.54
1:C:750:GLU:HG3	1:C:755:ARG:HG2	1.89	0.54
1:B:745:MET:HE3	6:B:5037:HOH:O	2.07	0.54
1:B:749:ILE:HD12	1:B:858:ILE:HD12	1.89	0.54
1:B:945:ASN:OD1	1:B:950:GLN:HG3	2.08	0.54
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.06	0.54
1:A:748:CYS:C	1:A:749:ILE:HD12	2.33	0.53
1:C:533:LEU:C	1:C:533:LEU:HD23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.43	0.53
1:C:984:LEU:HD21	1:C:986:ILE:HD11	1.89	0.53
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.91	0.53
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.41	0.53
1:C:598:ASP:C	1:C:599:ARG:HG2	2.33	0.53
1:A:40:GLU:OE2	1:A:43:ARG:NH2	2.42	0.53
1:C:965:GLN:O	1:C:969:GLU:HG3	2.08	0.53
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.89	0.53
1:C:730:LEU:HD12	1:C:730:LEU:N	2.23	0.53
1:A:246:MET:HG3	6:A:4958:HOH:O	2.09	0.52
1:B:688:PRO:HD3	1:B:694:LEU:HD11	1.89	0.52
1:D:599:ARG:HH11	1:D:797:GLU:HG3	1.75	0.52
1:B:714:ILE:HG21	5:B:9043:DMS:H11	1.90	0.52
1:B:598:ASP:C	1:B:599:ARG:HG2	2.33	0.52
1:C:568:TRP:HE1	1:C:604:ASN:ND2	2.07	0.52
1:D:362:LEU:HD13	1:D:576:ILE:HD12	1.90	0.52
1:A:991:MET:HE3	1:A:1003:VAL:HG21	1.92	0.52
1:B:573:GLN:HB2	1:B:602:CYS:O	2.10	0.52
1:C:714:ILE:HG21	5:C:9041:DMS:C1	2.36	0.52
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.45	0.51
1:B:942:ARG:HA	1:B:953:GLY:O	2.10	0.51
1:D:613:PRO:HB3	1:D:617:LEU:HD23	1.92	0.51
1:D:801:ILE:HG23	1:D:808:GLU:HG3	1.93	0.51
1:B:873:ALA:O	1:B:876:THR:HG22	2.09	0.51
1:A:472:TYR:O	1:A:476:LYS:HG2	2.10	0.51
1:C:362:LEU:CD2	1:C:576:ILE:HD12	2.40	0.51
1:A:125:LEU:HD21	5:A:9029:DMS:H21	1.93	0.51
1:A:554:GLN:HG2	6:A:4411:HOH:O	2.10	0.51
1:D:391:HIS:HD2	1:D:412:GLU:OE2	1.93	0.51
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.10	0.51
1:A:689:GLU:CD	1:A:689:GLU:N	2.65	0.51
1:D:333:ARG:HG3	1:D:333:ARG:NH1	2.25	0.51
1:D:887:GLN:NE2	1:D:980:GLU:O	2.42	0.51
1:D:809:ARG:HD2	6:D:4569:HOH:O	2.10	0.51
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.76	0.51
1:D:573:GLN:HB2	1:D:602:CYS:O	2.11	0.51
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.46	0.50
1:B:768:MET:HE1	1:B:1020:TRP:CZ2	2.46	0.50
1:D:133:TRP:HE1	5:D:5030:DMS:H11	1.75	0.50
1:A:334:GLU:OE1	1:A:336:ARG:NH1	2.44	0.50
1:A:573:GLN:HB2	1:A:602:CYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ALA:HB1	1:A:751:LEU:HD11	1.93	0.50
1:C:945:ASN:CG	1:C:1023:LYS:HE2	2.37	0.50
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.93	0.50
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.92	0.50
1:D:675:GLN:HG3	6:D:4699:HOH:O	2.12	0.50
1:B:749:ILE:CD1	1:B:858:ILE:HD12	2.41	0.50
1:C:194:GLY:O	1:C:198:GLU:HG3	2.10	0.50
1:D:59:ARG:HB2	1:D:124:SER:OG	2.11	0.50
1:D:595:THR:HA	1:D:596:PRO:C	2.37	0.50
1:A:367:MET:HB3	1:A:372:MET:HE2	1.94	0.50
1:A:653:HIS:HB3	6:A:4887:HOH:O	2.10	0.50
1:B:13:ARG:CZ	1:C:13:ARG:HG3	2.42	0.50
1:D:128:ASN:OD1	1:D:181:GLU:HG2	2.11	0.50
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.42	0.50
1:D:976:LEU:HD12	5:D:9015:DMS:H22	1.93	0.50
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.94	0.50
1:D:701:VAL:O	1:D:703:PRO:HD3	2.11	0.50
1:C:687:GLN:OE1	1:C:687:GLN:HA	2.11	0.50
1:A:147:ASN:HB3	1:A:206:SER:HA	1.94	0.49
1:D:672:VAL:HG22	1:D:678:GLN:HB2	1.93	0.49
1:A:239:VAL:HG23	5:A:9018:DMS:H11	1.94	0.49
1:B:147:ASN:HB3	1:B:206:SER:HA	1.94	0.49
1:C:599:ARG:NH2	1:C:600:GLN:NE2	2.52	0.49
1:A:873:ALA:O	1:A:876:THR:HG22	2.12	0.49
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.46	0.49
1:B:948:PRO:HB2	1:B:1022:GLN:HE21	1.78	0.49
1:C:873:ALA:O	1:C:876:THR:HG22	2.13	0.49
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.48	0.49
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.95	0.49
1:C:525:SER:O	1:D:561:ARG:HD3	2.13	0.49
1:C:973:ARG:HH12	5:C:9042:DMS:H22	1.76	0.49
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.48	0.49
1:A:145:GLY:N	1:A:210:ARG:HB2	2.27	0.49
1:B:639:THR:OG1	1:B:677:LYS:HE2	2.11	0.49
1:D:599:ARG:HH21	1:D:599:ARG:HG3	1.78	0.49
1:C:378:LEU:HG	6:C:4885:HOH:O	2.13	0.49
1:C:630:ARG:NH1	1:C:637:GLU:OE1	2.46	0.49
1:D:505:ARG:HG3	1:D:510:GLN:NE2	2.28	0.49
1:D:930:VAL:O	1:D:932:PRO:HD3	2.13	0.49
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.48	0.48
1:A:367:MET:HA	1:A:367:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASP:OD1	1:B:234:ASP:N	2.46	0.48
1:B:730:LEU:N	1:B:730:LEU:HD12	2.29	0.48
1:D:942:ARG:HA	1:D:953:GLY:O	2.13	0.48
1:A:427:THR:HG21	1:A:462:SER:HB3	1.94	0.48
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.43	0.48
1:B:245:GLN:HG2	1:B:288:ARG:CG	2.36	0.48
1:C:52:ARG:O	1:C:213:SER:HB2	2.13	0.48
1:D:472:TYR:O	1:D:476:LYS:HG2	2.12	0.48
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.49	0.48
1:C:942:ARG:HA	1:C:953:GLY:O	2.14	0.48
1:D:249:GLU:OE2	1:D:251:ARG:HD3	2.14	0.48
1:D:579:ASP:OD2	1:D:583:ASN:HB2	2.13	0.48
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.95	0.48
1:B:143:PHE:O	1:B:168:PRO:HA	2.14	0.47
1:B:391:HIS:HD2	1:B:412:GLU:OE2	1.97	0.47
1:B:768:MET:HE1	1:B:1020:TRP:CH2	2.48	0.47
1:D:742:THR:HG22	1:D:743:SER:N	2.28	0.47
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.96	0.47
1:C:147:ASN:HB3	1:C:206:SER:HA	1.97	0.47
1:D:600:GLN:H	1:D:600:GLN:HE21	1.62	0.47
1:A:225:PHE:HA	1:A:243:GLU:O	2.15	0.47
1:A:240:LEU:C	1:A:240:LEU:HD23	2.40	0.47
1:A:600:GLN:CD	1:A:600:GLN:H	2.22	0.47
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.96	0.47
1:C:632:SER:HB3	5:C:9021:DMS:H12	1.96	0.47
1:A:52:ARG:O	1:A:213:SER:HB2	2.15	0.47
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.97	0.47
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.50	0.47
1:D:40:GLU:OE2	1:D:43:ARG:NH2	2.46	0.47
1:D:369:GLU:O	1:D:373:VAL:HG23	2.15	0.47
1:A:460:ASN:ND2	1:A:461:GLU:HG3	2.29	0.47
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.50	0.47
1:B:225:PHE:HA	1:B:243:GLU:O	2.15	0.47
1:B:422:PRO:HG3	1:C:285:TYR:CE1	2.50	0.47
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.49	0.47
1:D:124:SER:HA	1:D:184:LEU:O	2.15	0.46
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.46
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.51	0.46
1:A:204:ARG:HB3	6:A:4190:HOH:O	2.15	0.46
1:D:87:PRO:HB2	1:D:209:PHE:C	2.41	0.46
1:D:102:ASN:HD22	5:D:5025:DMS:H12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:GLU:O	1:B:847:LYS:NZ	2.48	0.46
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.98	0.46
1:D:291:LEU:HD22	1:D:291:LEU:N	2.30	0.46
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.98	0.46
1:D:945:ASN:OD1	1:D:950:GLN:HG3	2.16	0.46
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.50	0.46
1:D:103:VAL:HG22	1:D:418:HIS:CE1	2.51	0.46
1:A:809:ARG:HD2	6:A:4560:HOH:O	2.15	0.46
1:C:71:GLU:CD	1:C:71:GLU:H	2.24	0.46
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.97	0.46
1:D:223:SER:O	1:D:224:ASP:HB2	2.14	0.46
1:D:369:GLU:HG3	1:D:397:LEU:HD21	1.98	0.46
1:A:299:LYS:HD2	6:A:4789:HOH:O	2.15	0.46
1:D:554:GLN:HG2	6:D:4923:HOH:O	2.16	0.46
1:C:454:ILE:HG13	1:C:455:ILE:HG13	1.98	0.45
1:C:640:SER:O	1:C:675:GLN:HA	2.16	0.45
1:A:897:TRP:CZ2	1:A:938:ARG:HG2	2.51	0.45
1:A:945:ASN:HB3	1:A:1023:LYS:CE	2.46	0.45
1:A:973:ARG:HD2	5:A:9034:DMS:H21	1.99	0.45
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.34	0.45
1:B:546:LEU:HA	6:B:4127:HOH:O	2.17	0.45
1:C:524:LEU:HD11	1:C:562:LEU:HG	1.98	0.45
1:C:579:ASP:OD2	1:C:583:ASN:HB3	2.17	0.45
1:A:606:LEU:O	1:A:614:HIS:HB2	2.17	0.45
1:B:240:LEU:C	1:B:240:LEU:HD23	2.42	0.45
1:B:52:ARG:O	1:B:213:SER:HB2	2.17	0.45
1:B:770:ILE:HD13	1:B:1022:GLN:CD	2.40	0.45
1:A:710:GLU:HG3	5:A:9022:DMS:H11	1.99	0.45
1:C:240:LEU:C	1:C:240:LEU:HD23	2.41	0.45
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.51	0.45
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.51	0.45
1:A:391:HIS:HD2	1:A:412:GLU:OE2	2.00	0.45
1:A:768:MET:HB3	6:A:4985:HOH:O	2.16	0.45
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.48	0.45
1:B:427:THR:HG21	1:B:462:SER:HB3	1.98	0.45
1:C:54:LEU:HD11	1:C:214:LEU:HG	1.99	0.45
1:C:595:THR:HA	1:C:596:PRO:C	2.41	0.45
1:C:546:LEU:HA	6:C:4128:HOH:O	2.17	0.45
1:D:851:ILE:HB	1:D:871:GLU:HB2	1.99	0.45
1:C:59:ARG:HB2	1:C:124:SER:OG	2.17	0.45
1:B:464:HIS:HB2	1:B:489:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:LYS:HD2	1:D:558:GLN:HG2	1.99	0.44
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.15	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.60	0.44
1:A:199:ASP:C	1:A:416:GLU:HG2	2.42	0.44
1:B:125:LEU:HD12	5:B:9040:DMS:S	2.56	0.44
1:B:881:ARG:HE	1:B:987:ASP:CG	2.25	0.44
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.52	0.44
1:D:125:LEU:O	1:D:183:ARG:HA	2.18	0.44
1:D:373:VAL:O	1:D:377:LEU:HG	2.17	0.44
1:D:427:THR:HG21	1:D:462:SER:HB3	1.99	0.44
1:D:598:ASP:C	1:D:599:ARG:HG2	2.42	0.44
1:A:87:PRO:HB2	1:A:209:PHE:C	2.43	0.44
1:A:663:LEU:HD21	1:A:688:PRO:HB3	1.98	0.44
1:A:945:ASN:OD1	1:A:1023:LYS:HE2	2.17	0.44
1:B:279:ILE:HD11	1:C:424:ASN:OD1	2.17	0.44
1:C:561:ARG:HD3	1:D:525:SER:O	2.18	0.44
1:C:701:VAL:O	1:C:703:PRO:HD3	2.18	0.44
1:D:995:GLY:O	1:D:996:ASP:C	2.61	0.44
1:A:301:TRP:CH2	1:A:452:SER:HA	2.53	0.44
1:A:784:PHE:HA	1:A:881:ARG:O	2.17	0.44
1:C:890:GLN:HB2	6:C:4427:HOH:O	2.17	0.44
1:D:391:HIS:CD2	1:D:412:GLU:OE2	2.71	0.44
1:B:907:PRO:HG2	1:B:990:HIS:O	2.18	0.44
1:C:49:GLN:H	1:C:49:GLN:HG2	1.64	0.44
1:C:580:GLU:C	1:C:582:GLY:N	2.76	0.44
1:D:663:LEU:HD21	1:D:688:PRO:HB3	1.98	0.44
1:A:524:LEU:HD11	1:A:562:LEU:HG	1.99	0.44
1:A:883:GLY:HA3	1:A:987:ASP:HA	2.00	0.44
1:B:699:ARG:HD3	5:B:9043:DMS:H21	1.99	0.44
1:D:674:PRO:O	1:D:675:GLN:HB2	2.17	0.44
1:A:942:ARG:HA	1:A:953:GLY:O	2.17	0.44
1:B:246:MET:C	1:B:246:MET:SD	3.00	0.44
1:D:19:PRO:HD3	1:D:112:PRO:CB	2.48	0.44
1:D:688:PRO:HD3	1:D:694:LEU:HD11	1.99	0.44
1:B:424:ASN:OD1	1:C:279:ILE:HD11	2.18	0.44
1:C:266:GLN:O	5:C:9019:DMS:H22	2.18	0.44
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.00	0.44
1:D:163:GLN:O	1:D:164:ASP:HB3	2.18	0.44
1:D:348:PRO:HD3	5:D:9025:DMS:H12	2.00	0.44
1:A:424:ASN:OD1	1:D:279:ILE:HD11	2.18	0.43
1:D:240:LEU:HD23	1:D:240:LEU:C	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:LEU:O	1:D:614:HIS:HB2	2.18	0.43
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.53	0.43
1:B:348:PRO:HG2	6:B:4322:HOH:O	2.18	0.43
1:B:753:ASN:OD1	1:B:754:LYS:HG3	2.19	0.43
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.99	0.43
1:C:883:GLY:HA3	1:C:987:ASP:HA	2.00	0.43
1:A:377:LEU:CD2	1:A:708:TRP:HA	2.46	0.43
1:C:277:GLU:HG2	6:C:4755:HOH:O	2.19	0.43
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.54	0.43
1:A:250:LEU:O	1:A:251:ARG:HD3	2.19	0.43
1:A:576:ILE:HD11	6:A:4214:HOH:O	2.18	0.43
1:B:354:VAL:HG12	1:B:379:MET:HE3	2.01	0.43
1:B:672:VAL:HG22	1:B:678:GLN:HB2	1.99	0.43
1:C:784:PHE:HA	1:C:881:ARG:O	2.18	0.43
1:A:194:GLY:O	1:A:198:GLU:HG3	2.19	0.43
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.00	0.43
1:B:377:LEU:HD22	1:B:708:TRP:HA	2.00	0.43
1:B:391:HIS:CD2	1:B:412:GLU:OE2	2.71	0.43
1:C:717:TRP:HB3	5:C:9041:DMS:H12	2.00	0.43
1:D:533:LEU:C	1:D:533:LEU:HD23	2.44	0.43
1:D:937:LEU:HD12	1:D:957:PHE:C	2.43	0.43
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.18	0.43
1:C:147:ASN:HA	1:C:148:SER:HA	1.64	0.43
1:C:225:PHE:HA	1:C:243:GLU:O	2.18	0.43
1:B:200:GLN:HB2	1:B:202:MET:HE2	1.99	0.43
1:D:194:GLY:O	1:D:198:GLU:HG3	2.19	0.43
1:A:163:GLN:O	1:A:164:ASP:HB3	2.19	0.43
1:C:333:ARG:HA	1:C:345:ASN:OD1	2.18	0.43
1:D:67:GLU:OE1	1:D:67:GLU:N	2.51	0.43
1:A:613:PRO:HB3	1:A:617:LEU:HD23	2.01	0.43
1:B:794:GLY:HA2	1:B:998:SER:O	2.19	0.43
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.53	0.43
1:C:390:SER:HA	1:C:391:HIS:HA	1.79	0.43
1:D:92:MET:HA	1:D:92:MET:HE2	2.01	0.43
1:D:663:LEU:CD2	1:D:688:PRO:HB3	2.49	0.43
1:C:460:ASN:ND2	1:C:461:GLU:HG3	2.34	0.42
1:C:508:GLU:OE2	5:C:9006:DMS:H21	2.19	0.42
1:D:730:LEU:N	1:D:730:LEU:HD12	2.34	0.42
1:A:19:PRO:HD3	1:A:112:PRO:CB	2.49	0.42
1:A:391:HIS:HE1	6:A:4865:HOH:O	2.02	0.42
1:A:533:LEU:C	1:A:533:LEU:HD23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:GLU:HB3	1:A:670:LEU:HD12	2.02	0.42
1:A:945:ASN:HB3	1:A:1023:LYS:NZ	2.34	0.42
1:C:153:TRP:CD1	1:C:158:TRP:HA	2.55	0.42
1:C:651:LEU:HD12	1:C:668:VAL:O	2.19	0.42
1:C:885:ASN:HB2	1:C:985:ASN:OD1	2.20	0.42
1:D:390:SER:HA	1:D:391:HIS:HA	1.75	0.42
1:A:49:GLN:HG2	6:A:4609:HOH:O	2.18	0.42
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.54	0.42
1:D:319:ASP:OD1	1:D:319:ASP:N	2.39	0.42
1:D:854:LYS:HA	1:D:867:THR:O	2.19	0.42
1:A:305:ILE:HD11	1:A:645:ARG:HB3	2.01	0.42
1:C:506:VAL:HG12	1:C:521:LYS:HE3	2.00	0.42
1:D:751:LEU:HD23	1:D:862:GLY:HA2	2.01	0.42
1:A:251:ARG:HG3	1:A:253:TYR:CZ	2.54	0.42
1:C:569:ASP:O	1:C:605:GLY:HA2	2.20	0.42
1:D:111:PRO:HA	1:D:112:PRO:HA	1.77	0.42
1:A:333:ARG:HA	1:A:345:ASN:OD1	2.20	0.42
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.54	0.42
1:B:823:LEU:HD11	1:B:841:ALA:HB2	2.02	0.42
1:B:1023:LYS:HA	6:B:4995:HOH:O	2.19	0.42
1:D:147:ASN:HA	1:D:148:SER:HA	1.62	0.42
1:A:260:LEU:O	1:A:267:VAL:HG22	2.20	0.42
1:B:125:LEU:O	1:B:183:ARG:HA	2.20	0.42
1:B:995:GLY:O	1:B:996:ASP:C	2.61	0.42
1:B:472:TYR:O	1:B:476:LYS:HG2	2.20	0.42
1:B:606:LEU:O	1:B:614:HIS:HB2	2.19	0.42
1:B:1020:TRP:HD1	1:B:1021:CYS:N	2.16	0.42
1:A:640:SER:O	1:A:675:GLN:HA	2.20	0.42
1:A:759:ASN:HB3	1:A:762:SER:OG	2.19	0.42
1:B:13:ARG:O	1:B:14:ARG:C	2.62	0.42
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.55	0.42
1:A:843:GLN:HA	1:A:847:LYS:O	2.19	0.41
1:B:782:ASP:HB2	1:B:842:TRP:CH2	2.55	0.41
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.55	0.41
1:D:126:THR:HA	1:D:182:ASN:O	2.20	0.41
1:D:650:GLU:HB3	1:D:670:LEU:HD12	2.02	0.41
1:B:610:ASP:O	1:B:611:ARG:HB2	2.20	0.41
1:D:937:LEU:HA	1:D:957:PHE:O	2.19	0.41
1:A:125:LEU:O	1:A:183:ARG:HA	2.19	0.41
1:A:255:ARG:HG3	1:A:318:ALA:HA	2.01	0.41
1:B:373:VAL:O	1:B:377:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ARG:HD2	1:C:261:TRP:CE3	2.55	0.41
1:A:522:LYS:HD2	1:B:558:GLN:HG2	2.01	0.41
1:A:854:LYS:HA	1:A:867:THR:O	2.21	0.41
1:B:49:GLN:HG3	6:B:4927:HOH:O	2.21	0.41
1:C:814:GLY:HA3	1:C:844:HIS:CG	2.56	0.41
1:D:143:PHE:O	1:D:168:PRO:HA	2.20	0.41
1:D:873:ALA:O	1:D:876:THR:HG22	2.21	0.41
1:D:965:GLN:HA	1:D:968:MET:HE2	2.02	0.41
1:A:887:GLN:NE2	1:A:980:GLU:O	2.53	0.41
1:B:23:GLN:C	1:B:23:GLN:CD	2.89	0.41
1:B:708:TRP:CZ2	5:B:9003:DMS:H23	2.56	0.41
1:C:433:LEU:N	1:C:434:PRO:CD	2.84	0.41
1:D:995:GLY:C	1:D:997:ASP:N	2.78	0.41
1:B:569:ASP:O	1:B:605:GLY:HA2	2.21	0.41
1:B:937:LEU:HD12	1:B:957:PHE:C	2.46	0.41
1:D:910:LEU:HD12	1:D:910:LEU:C	2.46	0.41
1:B:800:ARG:HH11	1:B:800:ARG:HG3	1.86	0.41
1:C:124:SER:HA	1:C:184:LEU:O	2.20	0.41
1:C:521:LYS:HE2	6:C:4418:HOH:O	2.19	0.41
1:D:233:ASP:OD1	1:D:234:ASP:N	2.54	0.41
1:B:353:GLY:HA2	1:B:386:ALA:O	2.21	0.41
1:B:502:MET:HB2	1:B:537:GLU:HB2	2.03	0.41
1:C:92:MET:HE2	1:C:92:MET:HA	2.03	0.41
1:C:636:ILE:HD13	1:C:698:VAL:HG11	2.01	0.41
1:D:863:GLN:HG2	1:D:1021:CYS:CB	2.50	0.41
1:A:23:GLN:C	1:A:23:GLN:CD	2.88	0.41
1:A:66:PRO:HG2	1:A:67:GLU:OE1	2.21	0.41
1:A:632:SER:HB3	5:A:9020:DMS:H12	2.03	0.41
1:B:632:SER:HB2	5:B:9025:DMS:H23	2.02	0.41
1:B:777:LEU:HG	1:B:889:ALA:HA	2.02	0.41
1:C:96:ASP:OD1	1:C:96:ASP:C	2.64	0.41
1:C:500:CYS:HA	1:C:534:ILE:O	2.21	0.41
1:C:568:TRP:HA	1:C:569:ASP:HA	1.81	0.41
1:D:354:VAL:CG1	1:D:379:MET:HE3	2.51	0.41
1:C:815:HIS:CD2	1:C:849:LEU:HD13	2.56	0.41
1:D:148:SER:HA	1:D:165:SER:OG	2.21	0.41
1:D:801:ILE:HD12	1:D:801:ILE:N	2.36	0.41
1:A:737:ILE:HG23	1:A:737:ILE:O	2.21	0.40
1:C:577:LYS:O	1:C:584:PRO:HA	2.21	0.40
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.38	0.40
1:D:460:ASN:ND2	1:D:461:GLU:HG3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:GLU:OE1	1:D:502:MET:HE3	2.21	0.40
1:D:746:ASP:HA	1:D:760:ARG:HG3	2.03	0.40
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.56	0.40
1:A:952:ARG:NH2	1:A:1019:VAL:HG11	2.36	0.40
1:B:521:LYS:HE2	6:B:4415:HOH:O	2.21	0.40
1:C:859:ASP:OD1	1:C:861:SER:OG	2.38	0.40
1:D:237:ARG:HD2	1:D:296:GLU:OE1	2.20	0.40
1:A:458:LEU:HD11	1:A:472:TYR:HB2	2.03	0.40
1:A:988:GLY:C	1:A:989:PHE:CD1	2.99	0.40
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.56	0.40
1:B:750:GLU:HG3	1:B:755:ARG:HG2	2.02	0.40
1:B:842:TRP:HZ3	1:B:852:SER:HB3	1.86	0.40
1:D:742:THR:CG2	1:D:743:SER:N	2.84	0.40
1:B:366:VAL:O	1:B:367:MET:HE2	2.20	0.40
1:B:524:LEU:HD11	1:B:562:LEU:HG	2.03	0.40
1:C:749:ILE:O	1:C:755:ARG:HA	2.22	0.40
1:C:817:GLN:HG2	6:C:4333:HOH:O	2.20	0.40
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.57	0.40
1:A:118:ASN:O	1:A:119:PRO:C	2.64	0.40
1:B:369:GLU:HG3	1:B:397:LEU:HD21	2.04	0.40
1:B:995:GLY:C	1:B:997:ASP:N	2.79	0.40
1:D:542:ALA:HA	1:D:604:ASN:HA	2.03	0.40
1:D:820:ALA:HB2	1:D:842:TRP:CE2	2.56	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%)	966 (96%)	42 (4%)	1 (0%)	48 57
1	B	1009/1023 (99%)	966 (96%)	42 (4%)	1 (0%)	48 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1009/1023 (99%)	970 (96%)	38 (4%)	1 (0%)	48	57
1	D	1009/1023 (99%)	968 (96%)	40 (4%)	1 (0%)	48	57
All	All	4036/4092 (99%)	3870 (96%)	162 (4%)	4 (0%)	48	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	581	ASN
1	A	164	ASP
1	B	164	ASP
1	D	164	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%)	78	89
1	B	863/874 (99%)	860 (100%)	3 (0%)	86	93
1	C	863/874 (99%)	858 (99%)	5 (1%)	78	89
1	D	863/874 (99%)	854 (99%)	9 (1%)	68	81
All	All	3452/3496 (99%)	3430 (99%)	22 (1%)	78	89

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

Mol	Chain	Res	Type
1	A	519	SER
1	A	546	LEU
1	A	604	ASN
1	A	689	GLU
1	A	730	LEU
1	B	324	GLU
1	B	519	SER
1	B	546	LEU

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Mol	Chain	Res	Type
1	C	49	GLN
1	C	112	PRO
1	C	519	SER
1	C	546	LEU
1	C	885	ASN
1	D	319	ASP
1	D	333	ARG
1	D	478	VAL
1	D	546	LEU
1	D	600	GLN
1	D	604	ASN
1	D	663	LEU
1	D	672	VAL
1	D	885	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	128	ASN
1	A	226	HIS
1	A	294	ASN
1	A	365	GLN
1	A	374	GLN
1	A	391	HIS
1	A	510	GLN
1	A	583	ASN
1	A	702	GLN
1	A	804	ASN
1	A	844	HIS
1	A	845	GLN
1	A	950	GLN
1	B	25	ASN
1	B	50	GLN
1	B	135	GLN
1	B	365	GLN
1	B	391	HIS
1	B	485	GLN
1	B	702	GLN
1	B	704	ASN
1	B	863	GLN
1	B	1022	GLN

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Mol	Chain	Res	Type
1	C	262	GLN
1	C	266	GLN
1	C	294	ASN
1	C	445	GLN
1	C	485	GLN
1	C	554	GLN
1	C	558	GLN
1	C	600	GLN
1	C	634	GLN
1	C	725	ASN
1	C	757	GLN
1	C	844	HIS
1	C	1022	GLN
1	D	18	ASN
1	D	221	GLN
1	D	266	GLN
1	D	374	GLN
1	D	391	HIS
1	D	485	GLN
1	D	583	ASN
1	D	600	GLN
1	D	624	GLN
1	D	634	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 185 ligands modelled in this entry, 30 are monoatomic - leaving 155 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	9008	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	A	9018	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	B	9004	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	D	9022	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	A	9022	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	A	9009	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	D	9017	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	A	9032	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	C	9008	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	A	9013	-	3,3,3	0.25	0	3,3,3	0.63	0
2	IPT	A	2002	-	15,15,15	0.94	1 (6%)	18,21,21	0.70	0
5	DMS	D	9013	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	A	9010	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	D	9007	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	A	9007	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	C	9034	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	C	9037	-	3,3,3	0.21	0	3,3,3	0.66	0
5	DMS	D	9004	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	D	9023	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	D	9027	-	3,3,3	0.17	0	3,3,3	0.61	0
5	DMS	B	9024	-	3,3,3	0.25	0	3,3,3	0.60	0
5	DMS	A	9006	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	A	9001	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	D	9010	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	C	9015	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	A	9020	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	C	9029	-	3,3,3	0.27	0	3,3,3	0.64	0
5	DMS	C	9022	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	C	9042	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	B	9022	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	C	9017	4	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	C	9038	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	B	9017	4	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	C	9016	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	B	9030	-	3,3,3	0.22	0	3,3,3	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	9035	-	3,3,3	0.28	0	3,3,3	0.66	0
5	DMS	D	9020	-	3,3,3	0.27	0	3,3,3	0.64	0
5	DMS	D	5030	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	B	9025	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	B	9014	-	3,3,3	0.24	0	3,3,3	0.62	0
2	IPT	D	2001	4	15,15,15	0.87	1 (6%)	18,21,21	0.67	0
5	DMS	A	9005	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	C	9028	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	D	9028	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	A	9003	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	C	9023	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	B	9027	-	3,3,3	0.29	0	3,3,3	0.59	0
5	DMS	B	9040	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	C	9043	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	B	9011	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	A	9011	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	B	9012	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	D	9009	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	C	9004	-	3,3,3	0.20	0	3,3,3	0.64	0
5	DMS	D	9018	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	C	9021	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	B	9013	-	3,3,3	0.25	0	3,3,3	0.65	0
5	DMS	C	9036	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	B	9041	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	D	9003	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	D	5028	-	3,3,3	0.28	0	3,3,3	0.65	0
2	IPT	C	2001	4	15,15,15	0.93	1 (6%)	18,21,21	0.66	0
5	DMS	A	9030	-	3,3,3	0.23	0	3,3,3	0.62	0
2	IPT	B	2001	4	15,15,15	0.92	1 (6%)	18,21,21	0.72	0
2	IPT	D	2002	-	15,15,15	0.98	1 (6%)	18,21,21	0.76	0
5	DMS	C	9040	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	A	9015	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	A	9024	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	C	9010	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	B	9029	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	B	9042	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	C	9009	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	B	9038	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	A	9026	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	A	9019	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	A	9034	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	C	9018	-	3,3,3	0.22	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	B	9018	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	C	9031	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	C	9033	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	C	9007	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	D	9014	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	C	9041	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	D	9015	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	B	9043	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	C	9001	-	3,3,3	0.23	0	3,3,3	0.66	0
5	DMS	B	9023	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	A	9012	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	B	9037	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	D	9005	-	3,3,3	0.24	0	3,3,3	0.57	0
5	DMS	A	9014	-	3,3,3	0.20	0	3,3,3	0.63	0
5	DMS	D	9019	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	C	9019	-	3,3,3	0.20	0	3,3,3	0.60	0
5	DMS	D	5027	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	B	9021	-	3,3,3	0.25	0	3,3,3	0.65	0
5	DMS	A	9036	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	B	9006	-	3,3,3	0.27	0	3,3,3	0.66	0
5	DMS	B	9016	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	C	9020	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	D	9011	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	B	9020	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	B	9005	-	3,3,3	0.26	0	3,3,3	0.60	0
5	DMS	B	9034	-	3,3,3	0.22	0	3,3,3	0.65	0
5	DMS	D	9006	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	B	9008	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	C	9003	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	A	9008	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	C	9013	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	9032	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	B	9010	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	C	9039	-	3,3,3	0.23	0	3,3,3	0.65	0
5	DMS	C	9011	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	D	9002	-	3,3,3	0.18	0	3,3,3	0.63	0
5	DMS	C	9002	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	A	9004	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	C	9005	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	A	9017	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	9027	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	A	9016	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	D	9024	-	3,3,3	0.24	0	3,3,3	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	9019	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	A	9033	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	B	9007	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	C	9024	-	3,3,3	0.27	0	3,3,3	0.63	0
5	DMS	A	9029	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	D	5026	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	A	9023	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	B	9009	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	A	9031	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	B	9001	-	3,3,3	0.20	0	3,3,3	0.62	0
5	DMS	D	9025	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	D	9026	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	C	9025	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	A	9028	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	C	9030	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	D	5025	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	B	9015	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	B	9036	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	D	9012	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	C	9006	-	3,3,3	0.24	0	3,3,3	0.62	0
2	IPT	A	2001	4	15,15,15	0.86	1 (6%)	18,21,21	0.69	0
5	DMS	B	9003	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	A	9035	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	B	9026	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	A	9021	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	D	9001	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	B	9032	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	B	9039	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	C	9035	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	C	9044	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	B	9002	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	A	9002	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	C	9014	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	B	9033	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	D	9016	-	3,3,3	0.23	0	3,3,3	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IPT	D	2001	4	-	3/6/26/26	0/1/1/1
2	IPT	A	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	C	2001	4	-	1/6/26/26	0/1/1/1
2	IPT	B	2001	4	-	1/6/26/26	0/1/1/1
2	IPT	D	2002	-	-	3/6/26/26	0/1/1/1
2	IPT	A	2001	4	-	1/6/26/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	IPT	O5-C1	2.69	1.46	1.42
2	B	2001	IPT	O5-C1	2.67	1.46	1.42
2	D	2002	IPT	O5-C1	2.66	1.46	1.42
2	C	2001	IPT	O5-C1	2.65	1.46	1.42
2	D	2001	IPT	O5-C1	2.46	1.46	1.42
2	A	2001	IPT	O5-C1	2.35	1.46	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2002	IPT	C2'-C1'-S1-C1
2	B	2001	IPT	O5-C5-C6-O6
2	C	2001	IPT	O5-C5-C6-O6
2	A	2001	IPT	O5-C5-C6-O6
2	D	2002	IPT	C4-C5-C6-O6
2	D	2001	IPT	O5-C5-C6-O6
2	D	2001	IPT	C2'-C1'-S1-C1
2	D	2001	IPT	C3'-C1'-S1-C1
2	D	2002	IPT	O5-C5-C6-O6

There are no ring outliers.

25 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	9018	DMS	1	0
5	A	9022	DMS	1	0
5	A	9010	DMS	1	0
5	C	9037	DMS	1	0
5	D	9027	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	9020	DMS	1	0
5	C	9042	DMS	1	0
5	B	9030	DMS	1	0
5	D	5030	DMS	1	0
5	B	9025	DMS	1	0
5	B	9040	DMS	2	0
5	C	9021	DMS	1	0
5	A	9034	DMS	1	0
5	C	9041	DMS	4	0
5	D	9015	DMS	1	0
5	B	9043	DMS	2	0
5	C	9019	DMS	1	0
5	B	9021	DMS	1	0
5	A	9036	DMS	1	0
5	A	9029	DMS	1	0
5	D	9025	DMS	1	0
5	C	9030	DMS	3	0
5	D	5025	DMS	1	0
5	C	9006	DMS	1	0
5	B	9003	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%)	-0.27	15 (1%) 72 69	5, 19, 40, 70	0
1	B	1011/1023 (98%)	-0.45	16 (1%) 70 67	6, 15, 37, 71	0
1	C	1011/1023 (98%)	-0.50	15 (1%) 72 69	5, 14, 33, 68	0
1	D	1011/1023 (98%)	-0.31	18 (1%) 67 64	7, 19, 38, 71	0
All	All	4044/4092 (98%)	-0.38	64 (1%) 70 67	5, 17, 37, 71	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	PRO	4.0
1	A	71	GLU	3.8
1	D	689	GLU	3.8
1	A	685	LEU	3.7
1	B	1023	LYS	3.6
1	B	1022	GLN	3.5
1	C	1022	GLN	3.4
1	D	730	LEU	3.4
1	B	688	PRO	3.4
1	B	685	LEU	3.3
1	C	1023	LYS	3.2
1	B	730	LEU	3.2
1	B	689	GLU	3.2
1	D	735	HIS	3.1
1	C	731	PRO	3.1
1	B	732	ALA	3.1
1	D	688	PRO	3.1
1	D	686	PRO	3.1
1	A	735	HIS	3.0
1	A	689	GLU	3.0
1	C	689	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	799	THR	3.0
1	A	686	PRO	3.0
1	C	581	ASN	3.0
1	D	131	GLU	2.9
1	B	733	ALA	2.9
1	C	686	PRO	2.9
1	A	737	ILE	2.9
1	C	688	PRO	2.8
1	B	686	PRO	2.8
1	C	800	ARG	2.8
1	A	687	GLN	2.7
1	B	687	GLN	2.7
1	B	774	LYS	2.6
1	A	178	ARG	2.6
1	B	772	ASP	2.6
1	C	735	HIS	2.6
1	A	730	LEU	2.5
1	C	685	LEU	2.5
1	D	732	ALA	2.5
1	D	685	LEU	2.5
1	A	731	PRO	2.5
1	D	748	CYS	2.5
1	D	687	GLN	2.4
1	A	798	ALA	2.4
1	C	684	GLU	2.4
1	A	733	ALA	2.3
1	B	735	HIS	2.3
1	D	634	GLN	2.3
1	D	684	GLU	2.3
1	A	732	ALA	2.3
1	C	733	ALA	2.3
1	C	582	GLY	2.2
1	A	800	ARG	2.2
1	D	71	GLU	2.2
1	D	1023	LYS	2.2
1	C	579	ASP	2.1
1	D	130	ASP	2.1
1	D	734	SER	2.1
1	B	771	GLY	2.1
1	C	734	SER	2.0
1	D	800	ARG	2.0
1	B	736	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	731	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	9040	4/4	0.64	0.28	56,56,56,59	0
5	DMS	B	9020	4/4	0.68	0.35	92,93,93,93	0
5	DMS	B	9043	4/4	0.69	0.29	68,69,69,70	0
5	DMS	C	9037	4/4	0.69	0.31	67,67,67,70	0
5	DMS	A	9024	4/4	0.69	0.38	92,93,93,93	0
5	DMS	B	9019	4/4	0.70	0.29	92,92,92,93	0
5	DMS	D	9008	4/4	0.70	0.33	85,85,86,86	0
3	MG	B	3004	1/1	0.71	0.16	64,64,64,64	0
5	DMS	B	9017	4/4	0.71	0.25	72,73,73,74	0
5	DMS	D	9022	4/4	0.72	0.31	82,82,82,83	0
5	DMS	B	9034	4/4	0.74	0.30	79,80,80,81	0
5	DMS	B	9035	4/4	0.75	0.30	58,59,59,60	0
5	DMS	A	9032	4/4	0.75	0.26	86,86,87,87	0
5	DMS	D	5030	4/4	0.75	0.26	68,68,69,69	0
5	DMS	D	9028	4/4	0.75	0.28	70,70,71,71	0
5	DMS	A	9013	4/4	0.76	0.25	73,73,73,73	0
5	DMS	A	9036	4/4	0.76	0.30	64,65,65,66	0
5	DMS	D	5025	4/4	0.76	0.34	96,96,97,97	0
5	DMS	D	5026	4/4	0.76	0.30	79,79,79,80	0
5	DMS	B	9025	4/4	0.76	0.26	71,71,71,72	0
3	MG	D	3004	1/1	0.76	0.16	60,60,60,60	0
5	DMS	B	9013	4/4	0.77	0.25	64,64,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	9017	4/4	0.77	0.22	70,70,70,70	0
5	DMS	C	9033	4/4	0.77	0.23	72,72,72,72	0
5	DMS	C	9034	4/4	0.77	0.21	70,71,71,71	0
5	DMS	B	9036	4/4	0.77	0.21	52,53,53,54	0
5	DMS	B	9041	4/4	0.77	0.24	72,72,72,73	0
5	DMS	C	9039	4/4	0.78	0.25	71,72,72,73	0
5	DMS	D	9026	4/4	0.78	0.22	76,76,77,77	0
5	DMS	D	9027	4/4	0.78	0.33	81,82,82,83	0
3	MG	A	3004	1/1	0.78	0.14	56,56,56,56	0
5	DMS	C	9021	4/4	0.79	0.23	68,69,69,69	0
5	DMS	A	9031	4/4	0.79	0.22	83,83,83,83	0
5	DMS	D	9024	4/4	0.79	0.23	81,81,81,81	0
5	DMS	B	9030	4/4	0.80	0.26	89,89,89,89	0
5	DMS	C	9031	4/4	0.81	0.22	64,65,65,66	0
5	DMS	A	9021	4/4	0.81	0.21	69,69,69,69	0
5	DMS	B	9039	4/4	0.81	0.22	63,63,63,64	0
5	DMS	C	9035	4/4	0.81	0.23	60,61,62,62	0
5	DMS	C	9041	4/4	0.82	0.25	56,56,57,57	0
5	DMS	A	9020	4/4	0.82	0.25	80,81,81,82	0
5	DMS	D	9011	4/4	0.82	0.20	67,67,67,67	0
5	DMS	D	9014	4/4	0.82	0.20	69,70,70,70	0
5	DMS	A	9035	4/4	0.82	0.20	62,62,62,62	0
5	DMS	A	9023	4/4	0.82	0.28	91,92,92,92	0
5	DMS	D	9018	4/4	0.83	0.21	55,57,57,57	0
5	DMS	B	9040	4/4	0.83	0.20	45,45,46,47	0
5	DMS	A	9015	4/4	0.83	0.32	81,81,81,81	0
5	DMS	C	9043	4/4	0.84	0.21	65,66,66,66	0
5	DMS	B	9037	4/4	0.84	0.22	71,72,72,72	0
5	DMS	C	9023	4/4	0.84	0.25	74,75,75,75	0
5	DMS	B	9021	4/4	0.84	0.26	61,61,61,61	0
5	DMS	A	9018	4/4	0.84	0.23	70,70,70,71	0
5	DMS	D	9019	4/4	0.84	0.19	60,60,61,62	0
5	DMS	C	9019	4/4	0.84	0.22	50,50,51,52	0
5	DMS	D	9017	4/4	0.85	0.32	91,92,92,92	0
5	DMS	B	9038	4/4	0.85	0.23	60,61,61,61	0
5	DMS	D	5027	4/4	0.85	0.22	54,55,56,56	0
5	DMS	A	9028	4/4	0.85	0.18	55,55,56,57	0
5	DMS	D	9020	4/4	0.85	0.20	60,61,62,62	0
5	DMS	D	9013	4/4	0.85	0.22	76,76,77,77	0
5	DMS	B	9014	4/4	0.85	0.23	62,62,62,63	0
5	DMS	A	9030	4/4	0.86	0.20	62,63,63,63	0
5	DMS	B	9042	4/4	0.86	0.25	72,72,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	9044	4/4	0.86	0.25	81,81,81,82	0
5	DMS	C	9032	4/4	0.86	0.20	52,54,54,55	0
2	IPT	D	2002	15/15	0.87	0.14	26,29,31,32	0
5	DMS	C	9036	4/4	0.87	0.19	66,68,68,68	0
5	DMS	B	9008	4/4	0.87	0.21	55,56,56,56	0
5	DMS	C	9008	4/4	0.87	0.19	57,58,58,59	0
5	DMS	C	9015	4/4	0.87	0.20	64,65,65,66	0
5	DMS	C	9027	4/4	0.88	0.18	55,56,57,57	0
5	DMS	C	9038	4/4	0.88	0.17	62,62,62,63	0
5	DMS	B	9016	4/4	0.88	0.18	56,57,58,58	0
4	NA	B	3105	1/1	0.88	0.11	42,42,42,42	0
5	DMS	B	9018	4/4	0.88	0.20	63,63,63,64	0
5	DMS	D	9025	4/4	0.88	0.20	65,66,66,66	0
5	DMS	A	9012	4/4	0.88	0.21	73,73,74,74	0
5	DMS	A	9026	4/4	0.88	0.22	67,68,68,69	0
5	DMS	A	9016	4/4	0.88	0.21	72,72,72,73	0
5	DMS	A	9011	4/4	0.89	0.17	62,63,63,63	0
5	DMS	C	9006	4/4	0.89	0.17	40,41,41,42	0
5	DMS	C	9042	4/4	0.89	0.17	43,45,45,47	0
5	DMS	B	9024	4/4	0.89	0.19	54,54,54,54	0
5	DMS	B	9011	4/4	0.89	0.18	38,41,41,41	0
5	DMS	C	9016	4/4	0.89	0.16	53,54,54,55	0
5	DMS	B	9012	4/4	0.89	0.16	63,63,63,64	0
5	DMS	B	9032	4/4	0.89	0.18	44,44,45,45	0
5	DMS	C	9020	4/4	0.89	0.14	60,61,61,61	0
5	DMS	D	9015	4/4	0.89	0.20	74,74,74,74	0
5	DMS	A	9034	4/4	0.89	0.19	64,65,65,65	0
5	DMS	B	9006	4/4	0.89	0.18	48,48,48,49	0
5	DMS	C	9014	4/4	0.90	0.18	65,65,66,66	0
5	DMS	C	9030	4/4	0.90	0.17	49,50,50,50	0
5	DMS	A	9007	4/4	0.90	0.20	59,59,60,60	0
5	DMS	B	9015	4/4	0.90	0.16	58,58,59,59	0
5	DMS	C	9022	4/4	0.90	0.17	56,57,57,57	0
5	DMS	A	9017	4/4	0.90	0.16	53,53,53,54	0
5	DMS	C	9025	4/4	0.90	0.19	57,58,58,58	0
5	DMS	B	9023	4/4	0.91	0.14	52,52,52,52	0
5	DMS	A	9008	4/4	0.91	0.16	48,49,49,50	0
5	DMS	C	9018	4/4	0.91	0.16	47,48,49,49	0
5	DMS	D	9012	4/4	0.91	0.15	54,55,55,55	0
3	MG	C	3004	1/1	0.91	0.08	49,49,49,49	0
5	DMS	B	9026	4/4	0.91	0.15	61,61,62,62	0
3	MG	B	3005	1/1	0.91	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	D	9023	4/4	0.92	0.15	52,53,53,54	0
5	DMS	B	9027	4/4	0.92	0.13	30,30,31,34	0
4	NA	D	3103	1/1	0.92	0.10	34,34,34,34	0
5	DMS	B	9007	4/4	0.92	0.13	33,33,35,37	0
5	DMS	A	9019	4/4	0.92	0.14	46,46,47,47	0
5	DMS	D	5028	4/4	0.92	0.16	40,40,40,42	0
5	DMS	C	9024	4/4	0.92	0.17	53,54,54,54	0
2	IPT	A	2002	15/15	0.92	0.09	19,25,27,27	15
5	DMS	D	9007	4/4	0.92	0.15	48,48,48,49	0
2	IPT	A	2001	15/15	0.92	0.10	19,22,29,30	0
5	DMS	A	9022	4/4	0.92	0.15	48,49,49,51	0
4	NA	D	3104	1/1	0.93	0.08	33,33,33,33	0
5	DMS	B	9029	4/4	0.93	0.17	59,59,59,60	0
5	DMS	A	9004	4/4	0.93	0.12	38,39,40,41	0
5	DMS	C	9029	4/4	0.93	0.15	57,58,58,59	0
5	DMS	C	9004	4/4	0.93	0.15	49,49,50,51	0
4	NA	C	3103	1/1	0.93	0.08	33,33,33,33	0
5	DMS	B	9033	4/4	0.93	0.14	46,47,47,47	0
5	DMS	C	9011	4/4	0.93	0.12	40,40,40,42	0
5	DMS	C	9013	4/4	0.93	0.13	56,56,57,57	0
5	DMS	D	9006	4/4	0.93	0.14	48,49,50,51	0
5	DMS	B	9022	4/4	0.93	0.13	53,53,53,53	0
5	DMS	A	9033	4/4	0.94	0.12	44,45,45,46	0
2	IPT	C	2001	15/15	0.94	0.09	15,18,24,25	0
5	DMS	A	9029	4/4	0.94	0.13	47,47,47,47	0
2	IPT	D	2001	15/15	0.94	0.09	20,25,29,29	0
4	NA	C	3104	1/1	0.94	0.06	30,30,30,30	0
5	DMS	A	9006	4/4	0.94	0.14	56,57,57,58	0
5	DMS	A	9014	4/4	0.95	0.11	49,50,50,51	0
5	DMS	B	9005	4/4	0.95	0.11	26,27,27,29	0
2	IPT	B	2001	15/15	0.95	0.08	14,18,21,23	0
5	DMS	C	9007	4/4	0.95	0.11	42,42,42,42	0
5	DMS	A	9003	4/4	0.95	0.11	29,31,32,32	0
5	DMS	C	9009	4/4	0.95	0.12	31,32,32,33	0
4	NA	B	3103	1/1	0.95	0.07	39,39,39,39	0
5	DMS	C	9028	4/4	0.95	0.12	40,41,43,43	0
5	DMS	A	9002	4/4	0.96	0.10	24,25,25,26	0
5	DMS	C	9002	4/4	0.96	0.08	17,19,21,24	0
5	DMS	A	9010	4/4	0.96	0.10	43,44,45,45	0
5	DMS	D	9010	4/4	0.96	0.11	37,38,38,40	0
5	DMS	C	9005	4/4	0.96	0.09	25,27,28,30	0
4	NA	B	3104	1/1	0.96	0.05	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	D	3101	1/1	0.96	0.04	24,24,24,24	0
4	NA	A	3103	1/1	0.96	0.06	31,31,31,31	0
3	MG	A	3002	1/1	0.96	0.04	18,18,18,18	0
5	DMS	D	9016	4/4	0.96	0.10	45,46,46,48	0
5	DMS	D	9002	4/4	0.96	0.10	26,26,29,29	0
5	DMS	D	9003	4/4	0.96	0.12	36,36,37,37	0
5	DMS	D	9004	4/4	0.96	0.12	27,29,30,31	0
5	DMS	B	9002	4/4	0.97	0.09	22,24,25,26	0
5	DMS	B	9004	4/4	0.97	0.09	28,29,30,31	0
4	NA	A	3104	1/1	0.97	0.06	29,29,29,29	0
5	DMS	D	9009	4/4	0.97	0.10	42,42,42,42	0
3	MG	D	3002	1/1	0.97	0.06	19,19,19,19	0
3	MG	C	3001	1/1	0.97	0.03	12,12,12,12	0
4	NA	A	3101	1/1	0.97	0.04	27,27,27,27	0
5	DMS	B	9009	4/4	0.97	0.09	35,36,36,36	0
3	MG	A	3001	1/1	0.97	0.02	14,14,14,14	0
3	MG	D	3001	1/1	0.98	0.02	17,17,17,17	0
5	DMS	C	9010	4/4	0.98	0.07	34,34,35,35	0
5	DMS	A	9005	4/4	0.98	0.06	29,29,29,30	0
5	DMS	B	9010	4/4	0.98	0.07	32,32,33,34	0
5	DMS	D	9001	4/4	0.98	0.07	20,22,22,24	0
5	DMS	C	9003	4/4	0.98	0.07	28,28,29,29	0
5	DMS	B	9003	4/4	0.98	0.08	28,29,30,31	0
4	NA	A	3102	1/1	0.98	0.02	9,9,9,9	0
5	DMS	D	9005	4/4	0.98	0.07	28,28,28,29	0
4	NA	B	3102	1/1	0.98	0.02	13,13,13,13	0
4	NA	D	3102	1/1	0.98	0.06	12,12,12,12	0
5	DMS	A	9009	4/4	0.98	0.07	36,36,37,37	0
5	DMS	A	9001	4/4	0.99	0.04	16,17,18,19	0
4	NA	C	3101	1/1	0.99	0.03	18,18,18,18	0
4	NA	C	3102	1/1	0.99	0.03	15,15,15,15	0
5	DMS	C	9001	4/4	0.99	0.05	13,15,16,18	0
3	MG	B	3001	1/1	0.99	0.01	12,12,12,12	0
5	DMS	B	9001	4/4	0.99	0.04	15,17,18,18	0
3	MG	C	3002	1/1	0.99	0.08	11,11,11,11	0
4	NA	B	3101	1/1	1.00	0.02	15,15,15,15	0
3	MG	B	3002	1/1	1.00	0.09	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.