



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:13 pm GMT

PDB ID : 3VD3
Title : E. coli (lacZ) beta-galactosidase (N460D)
Authors : Wheatley, R.W.; Kappelhoff, J.C.; Hahn, J.N.; Dugdale, M.L.; Dutkoski, M.J.;
Tamman, S.D.; Fraser, M.E.; Huber, R.E.
Deposited on : 2012-01-04
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28986

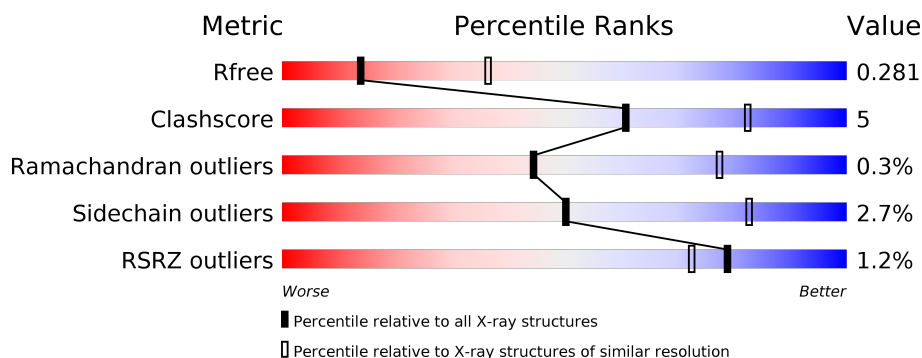
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1052	<div> <div>81%</div> <div>15%</div> <div>•</div> </div>
1	B	1052	<div> <div>80%</div> <div>15%</div> <div>•</div> </div>
1	C	1052	<div> <div>80%</div> <div>15%</div> <div>• •</div> </div>
1	D	1052	<div> <div>81%</div> <div>14%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	3001	-	-	-	X
2	MG	C	3001	-	-	-	X
2	MG	D	3001	-	-	-	X
4	DMS	A	8004	-	-	-	X
4	DMS	A	8005	-	-	-	X
4	DMS	A	8007	-	-	-	X
4	DMS	A	8009	-	-	-	X
4	DMS	B	8004	-	-	-	X
4	DMS	B	8008	-	-	-	X
4	DMS	B	8011	-	-	-	X
4	DMS	C	8003	-	-	-	X
4	DMS	C	8005	-	-	-	X
4	DMS	C	8010	-	-	-	X
4	DMS	C	8011	-	-	-	X
4	DMS	C	8012	-	-	-	X
4	DMS	D	8002	-	-	-	X
4	DMS	D	8003	-	-	-	X
4	DMS	D	8008	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33130 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
			8126	5138	1439	1511	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8126	5138	1439	1511	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8126	5138	1439	1511	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8126	5138	1439	1511	38			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	EXPRESSION TAG	UNP P00722
A	-27	GLY	-	EXPRESSION TAG	UNP P00722
A	-26	GLY	-	EXPRESSION TAG	UNP P00722
A	-25	SER	-	EXPRESSION TAG	UNP P00722
A	-24	HIS	-	EXPRESSION TAG	UNP P00722
A	-23	HIS	-	EXPRESSION TAG	UNP P00722
A	-22	HIS	-	EXPRESSION TAG	UNP P00722
A	-21	HIS	-	EXPRESSION TAG	UNP P00722
A	-20	HIS	-	EXPRESSION TAG	UNP P00722
A	-19	HIS	-	EXPRESSION TAG	UNP P00722
A	-18	GLY	-	EXPRESSION TAG	UNP P00722
A	-17	MET	-	EXPRESSION TAG	UNP P00722
A	-16	ALA	-	EXPRESSION TAG	UNP P00722
A	-15	SER	-	EXPRESSION TAG	UNP P00722
A	-14	MET	-	EXPRESSION TAG	UNP P00722
A	-13	THR	-	EXPRESSION TAG	UNP P00722
A	-12	GLY	-	EXPRESSION TAG	UNP P00722
A	-11	GLY	-	EXPRESSION TAG	UNP P00722
A	-10	GLN	-	EXPRESSION TAG	UNP P00722
A	-9	GLN	-	EXPRESSION TAG	UNP P00722
A	-8	MET	-	EXPRESSION TAG	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P00722
A	-6	ARG	-	EXPRESSION TAG	UNP P00722
A	-5	ASP	-	EXPRESSION TAG	UNP P00722
A	-4	LEU	-	EXPRESSION TAG	UNP P00722
A	-3	TYR	-	EXPRESSION TAG	UNP P00722
A	-2	ASP	-	EXPRESSION TAG	UNP P00722
A	-1	ASP	-	EXPRESSION TAG	UNP P00722
A	0	ASP	-	EXPRESSION TAG	UNP P00722
A	1	ASP	-	EXPRESSION TAG	UNP P00722
A	2	LYS	-	EXPRESSION TAG	UNP P00722
A	3	ASP	-	EXPRESSION TAG	UNP P00722
A	4	PRO	-	EXPRESSION TAG	UNP P00722
A	5	MET	-	EXPRESSION TAG	UNP P00722
A	6	ILE	-	EXPRESSION TAG	UNP P00722
A	7	ASP	-	EXPRESSION TAG	UNP P00722
A	8	PRO	-	EXPRESSION TAG	UNP P00722
A	460	ASP	ASN	ENGINEERED MUTATION	UNP P00722
B	-28	MET	-	EXPRESSION TAG	UNP P00722
B	-27	GLY	-	EXPRESSION TAG	UNP P00722
B	-26	GLY	-	EXPRESSION TAG	UNP P00722
B	-25	SER	-	EXPRESSION TAG	UNP P00722
B	-24	HIS	-	EXPRESSION TAG	UNP P00722
B	-23	HIS	-	EXPRESSION TAG	UNP P00722
B	-22	HIS	-	EXPRESSION TAG	UNP P00722
B	-21	HIS	-	EXPRESSION TAG	UNP P00722
B	-20	HIS	-	EXPRESSION TAG	UNP P00722
B	-19	HIS	-	EXPRESSION TAG	UNP P00722
B	-18	GLY	-	EXPRESSION TAG	UNP P00722
B	-17	MET	-	EXPRESSION TAG	UNP P00722
B	-16	ALA	-	EXPRESSION TAG	UNP P00722
B	-15	SER	-	EXPRESSION TAG	UNP P00722
B	-14	MET	-	EXPRESSION TAG	UNP P00722
B	-13	THR	-	EXPRESSION TAG	UNP P00722
B	-12	GLY	-	EXPRESSION TAG	UNP P00722
B	-11	GLY	-	EXPRESSION TAG	UNP P00722
B	-10	GLN	-	EXPRESSION TAG	UNP P00722
B	-9	GLN	-	EXPRESSION TAG	UNP P00722
B	-8	MET	-	EXPRESSION TAG	UNP P00722
B	-7	GLY	-	EXPRESSION TAG	UNP P00722
B	-6	ARG	-	EXPRESSION TAG	UNP P00722
B	-5	ASP	-	EXPRESSION TAG	UNP P00722
B	-4	LEU	-	EXPRESSION TAG	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	TYR	-	EXPRESSION TAG	UNP P00722
B	-2	ASP	-	EXPRESSION TAG	UNP P00722
B	-1	ASP	-	EXPRESSION TAG	UNP P00722
B	0	ASP	-	EXPRESSION TAG	UNP P00722
B	1	ASP	-	EXPRESSION TAG	UNP P00722
B	2	LYS	-	EXPRESSION TAG	UNP P00722
B	3	ASP	-	EXPRESSION TAG	UNP P00722
B	4	PRO	-	EXPRESSION TAG	UNP P00722
B	5	MET	-	EXPRESSION TAG	UNP P00722
B	6	ILE	-	EXPRESSION TAG	UNP P00722
B	7	ASP	-	EXPRESSION TAG	UNP P00722
B	8	PRO	-	EXPRESSION TAG	UNP P00722
B	460	ASP	ASN	ENGINEERED MUTATION	UNP P00722
C	-28	MET	-	EXPRESSION TAG	UNP P00722
C	-27	GLY	-	EXPRESSION TAG	UNP P00722
C	-26	GLY	-	EXPRESSION TAG	UNP P00722
C	-25	SER	-	EXPRESSION TAG	UNP P00722
C	-24	HIS	-	EXPRESSION TAG	UNP P00722
C	-23	HIS	-	EXPRESSION TAG	UNP P00722
C	-22	HIS	-	EXPRESSION TAG	UNP P00722
C	-21	HIS	-	EXPRESSION TAG	UNP P00722
C	-20	HIS	-	EXPRESSION TAG	UNP P00722
C	-19	HIS	-	EXPRESSION TAG	UNP P00722
C	-18	GLY	-	EXPRESSION TAG	UNP P00722
C	-17	MET	-	EXPRESSION TAG	UNP P00722
C	-16	ALA	-	EXPRESSION TAG	UNP P00722
C	-15	SER	-	EXPRESSION TAG	UNP P00722
C	-14	MET	-	EXPRESSION TAG	UNP P00722
C	-13	THR	-	EXPRESSION TAG	UNP P00722
C	-12	GLY	-	EXPRESSION TAG	UNP P00722
C	-11	GLY	-	EXPRESSION TAG	UNP P00722
C	-10	GLN	-	EXPRESSION TAG	UNP P00722
C	-9	GLN	-	EXPRESSION TAG	UNP P00722
C	-8	MET	-	EXPRESSION TAG	UNP P00722
C	-7	GLY	-	EXPRESSION TAG	UNP P00722
C	-6	ARG	-	EXPRESSION TAG	UNP P00722
C	-5	ASP	-	EXPRESSION TAG	UNP P00722
C	-4	LEU	-	EXPRESSION TAG	UNP P00722
C	-3	TYR	-	EXPRESSION TAG	UNP P00722
C	-2	ASP	-	EXPRESSION TAG	UNP P00722
C	-1	ASP	-	EXPRESSION TAG	UNP P00722
C	0	ASP	-	EXPRESSION TAG	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	EXPRESSION TAG	UNP P00722
C	2	LYS	-	EXPRESSION TAG	UNP P00722
C	3	ASP	-	EXPRESSION TAG	UNP P00722
C	4	PRO	-	EXPRESSION TAG	UNP P00722
C	5	MET	-	EXPRESSION TAG	UNP P00722
C	6	ILE	-	EXPRESSION TAG	UNP P00722
C	7	ASP	-	EXPRESSION TAG	UNP P00722
C	8	PRO	-	EXPRESSION TAG	UNP P00722
C	460	ASP	ASN	ENGINEERED MUTATION	UNP P00722
D	-28	MET	-	EXPRESSION TAG	UNP P00722
D	-27	GLY	-	EXPRESSION TAG	UNP P00722
D	-26	GLY	-	EXPRESSION TAG	UNP P00722
D	-25	SER	-	EXPRESSION TAG	UNP P00722
D	-24	HIS	-	EXPRESSION TAG	UNP P00722
D	-23	HIS	-	EXPRESSION TAG	UNP P00722
D	-22	HIS	-	EXPRESSION TAG	UNP P00722
D	-21	HIS	-	EXPRESSION TAG	UNP P00722
D	-20	HIS	-	EXPRESSION TAG	UNP P00722
D	-19	HIS	-	EXPRESSION TAG	UNP P00722
D	-18	GLY	-	EXPRESSION TAG	UNP P00722
D	-17	MET	-	EXPRESSION TAG	UNP P00722
D	-16	ALA	-	EXPRESSION TAG	UNP P00722
D	-15	SER	-	EXPRESSION TAG	UNP P00722
D	-14	MET	-	EXPRESSION TAG	UNP P00722
D	-13	THR	-	EXPRESSION TAG	UNP P00722
D	-12	GLY	-	EXPRESSION TAG	UNP P00722
D	-11	GLY	-	EXPRESSION TAG	UNP P00722
D	-10	GLN	-	EXPRESSION TAG	UNP P00722
D	-9	GLN	-	EXPRESSION TAG	UNP P00722
D	-8	MET	-	EXPRESSION TAG	UNP P00722
D	-7	GLY	-	EXPRESSION TAG	UNP P00722
D	-6	ARG	-	EXPRESSION TAG	UNP P00722
D	-5	ASP	-	EXPRESSION TAG	UNP P00722
D	-4	LEU	-	EXPRESSION TAG	UNP P00722
D	-3	TYR	-	EXPRESSION TAG	UNP P00722
D	-2	ASP	-	EXPRESSION TAG	UNP P00722
D	-1	ASP	-	EXPRESSION TAG	UNP P00722
D	0	ASP	-	EXPRESSION TAG	UNP P00722
D	1	ASP	-	EXPRESSION TAG	UNP P00722
D	2	LYS	-	EXPRESSION TAG	UNP P00722
D	3	ASP	-	EXPRESSION TAG	UNP P00722
D	4	PRO	-	EXPRESSION TAG	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
D	5	MET	-	EXPRESSION TAG	UNP P00722
D	6	ILE	-	EXPRESSION TAG	UNP P00722
D	7	ASP	-	EXPRESSION TAG	UNP P00722
D	8	PRO	-	EXPRESSION TAG	UNP P00722
D	460	ASP	ASN	ENGINEERED MUTATION	UNP P00722

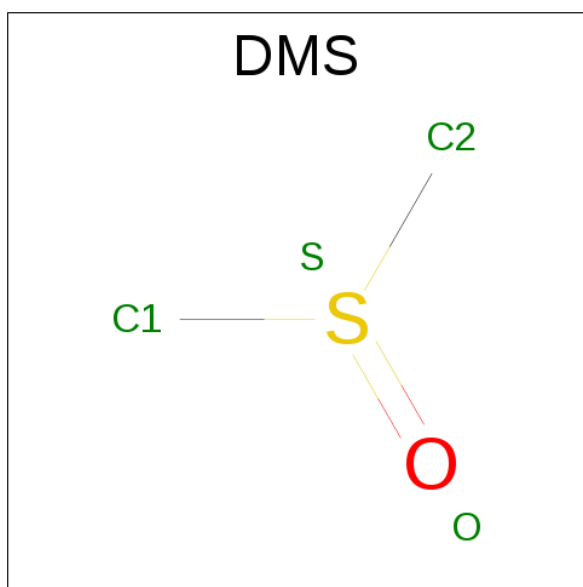
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	1	Total	Mg	0	0
			1	1		
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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

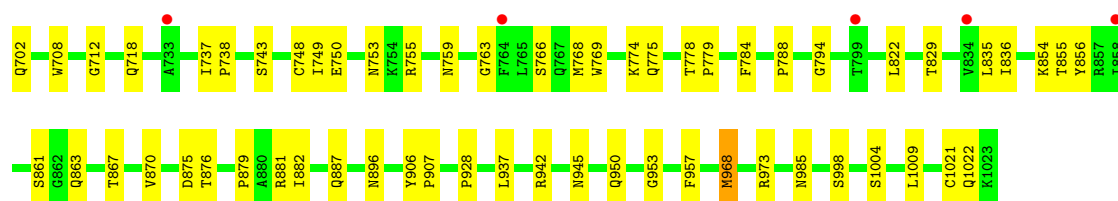
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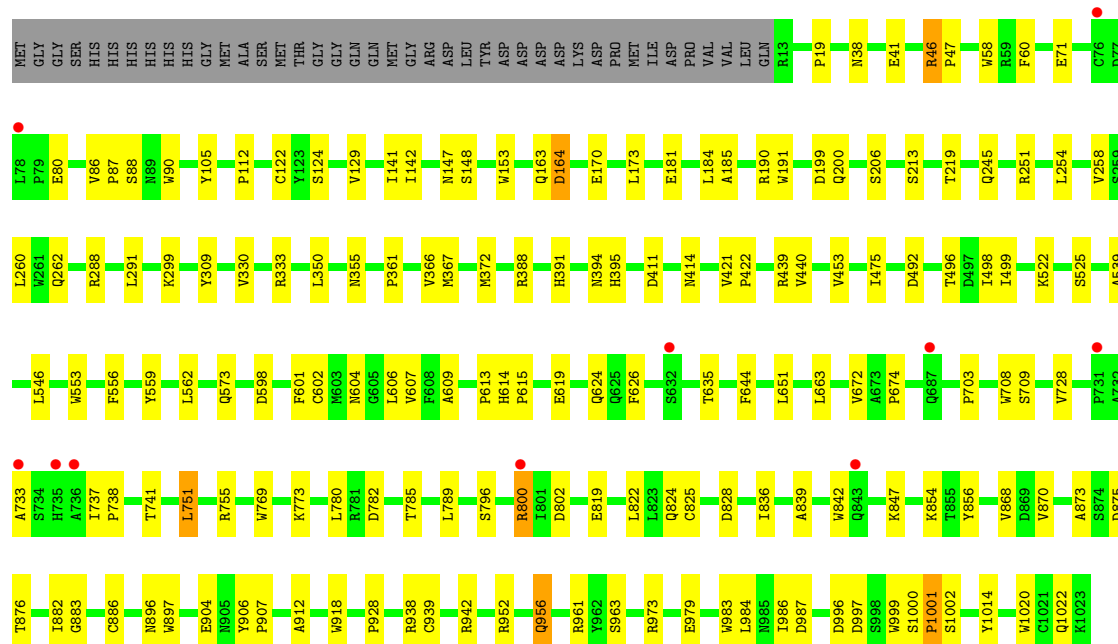
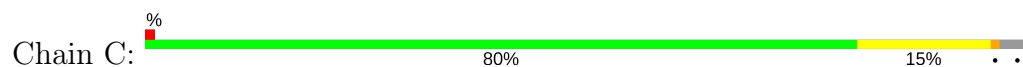
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2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

- Molecule 5 is water.

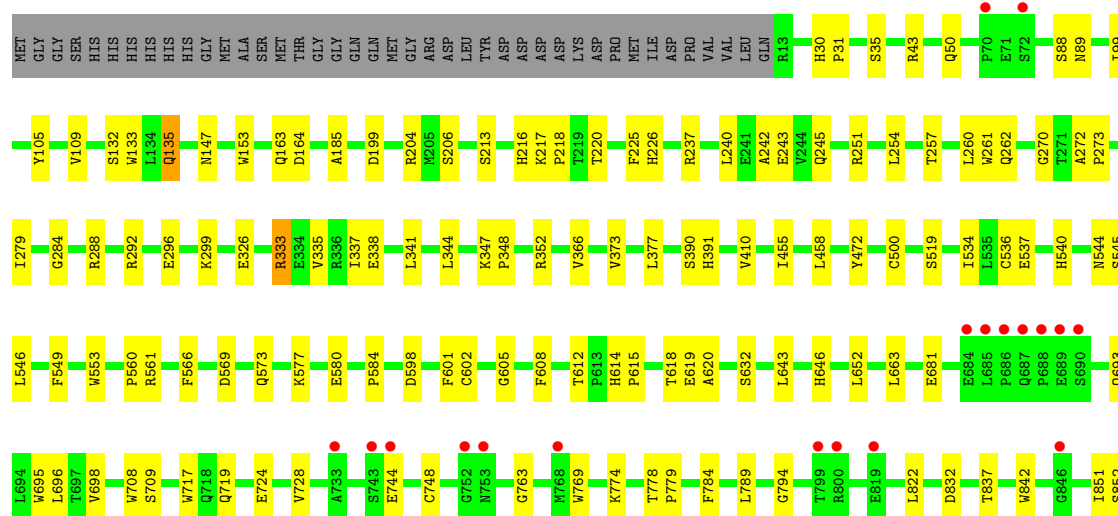
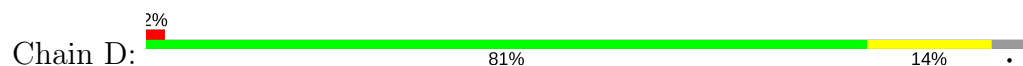
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total 112	O 112	0	0
5	B	110	Total 110	O 110	0	0
5	C	99	Total 99	O 99	0	0
5	D	106	Total 106	O 106	0	0



• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.14Å 151.65Å 131.33Å 90.00° 103.47° 90.00°	Depositor
Resolution (Å)	57.25 – 2.80 57.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.25-2.80) 88.0 (57.25-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.282 0.201 , 0.281	Depositor DCC
R_{free} test set	5235 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	33130	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NA, MG, DMS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/8368	0.57	0/11415
1	B	0.41	0/8368	0.57	0/11415
1	C	0.42	0/8368	0.57	0/11415
1	D	0.43	0/8368	0.57	0/11415
All	All	0.42	0/33472	0.57	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	8126	0	7714	86	0
1	B	8126	0	7714	86	0
1	C	8126	0	7714	82	0
1	D	8126	0	7714	81	0
2	A	1	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	3	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	3	0	0	0	0
3	D	2	0	0	0	0
4	A	48	0	72	0	0
4	B	44	0	66	0	0
4	C	48	0	72	2	0
4	D	40	0	60	1	0
5	A	112	0	0	5	0
5	B	110	0	0	3	0
5	C	99	0	0	1	0
5	D	106	0	0	6	0
All	All	33130	0	31126	331	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 5.

All (331) 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:B:573:GLN:HB2	1:B:602:CYS:O	1.82	0.79
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.67	0.76
1:D:832:ASP:HB3	5:D:4075:HOH:O	1.86	0.75
1:C:836:ILE:HB	1:C:856:TYR:HB2	1.68	0.75
1:A:809:ARG:HD2	5:A:4045:HOH:O	1.91	0.71
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.56	0.70
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.26	0.70
1:A:88:SER:HA	1:A:366:VAL:HG21	1.74	0.70
1:D:789:LEU:HD11	1:D:993:ILE:HG22	1.74	0.69
1:A:244:VAL:HG21	1:A:256:VAL:HG11	1.75	0.68
1:D:88:SER:HA	1:D:366:VAL:HG21	1.76	0.68
1:D:352:ARG:HG2	1:D:553:TRP:CH2	2.30	0.67
1:B:945:ASN:OD1	1:B:950:GLN:HG3	1.95	0.66
1:A:573:GLN:HB2	1:A:602:CYS:O	1.96	0.66
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.31	0.65
1:A:873:ALA:O	1:A:876:THR:HG22	1.96	0.64
1:B:854:LYS:HA	1:B:867:THR:O	1.98	0.64
1:A:136:GLU:HB2	5:A:4033:HOH:O	1.97	0.64
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.80	0.63
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.35	0.62
1:A:410:VAL:HG22	1:A:455:ILE:HB	1.81	0.61
1:A:895:VAL:HG21	1:A:925:MET:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:763:GLY:HA3	1:D:822:LEU:HD13	1.80	0.61
1:C:780:LEU:HD13	1:C:1020:TRP:HZ3	1.65	0.61
1:A:749:ILE:HD11	1:A:836:ILE:HD11	1.81	0.61
1:B:784:PHE:HA	1:B:881:ARG:O	2.00	0.61
1:D:939:CYS:HA	1:D:956:GLN:HB3	1.82	0.61
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.83	0.60
1:D:948:PRO:HB2	1:D:1022:GLN:HG2	1.82	0.60
1:C:651:LEU:HD23	1:C:703:PRO:HG3	1.82	0.60
1:C:782:ASP:HB2	1:C:842:TRP:CH2	2.36	0.59
1:A:36:TRP:CD1	1:A:48:SER:HB2	2.37	0.59
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.84	0.59
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.85	0.59
1:A:458:LEU:HD11	1:A:472:TYR:HB2	1.86	0.58
1:B:73:TRP:O	1:B:183:ARG:NH1	2.27	0.58
1:A:525:SER:O	1:B:561:ARG:HD3	2.03	0.58
1:C:573:GLN:HB2	1:C:602:CYS:O	2.05	0.56
1:B:163:GLN:O	1:B:164:ASP:CB	2.53	0.56
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.87	0.56
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.87	0.56
1:B:383:ASN:HB3	1:B:624:GLN:O	2.05	0.56
1:C:822:LEU:HD11	1:C:825:CYS:HB2	1.86	0.56
1:B:367:MET:HB3	1:B:372:MET:HE3	1.87	0.56
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.06	0.55
1:D:794:GLY:HA3	5:D:4049:HOH:O	2.06	0.55
1:A:335:VAL:HG22	1:A:344:LEU:HD12	1.88	0.55
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.07	0.55
1:C:258:VAL:HG23	1:C:291:LEU:HD23	1.89	0.55
1:D:632:SER:HB2	5:D:4021:HOH:O	2.06	0.55
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.89	0.55
1:C:38:ASN:HB3	1:C:41:GLU:HG3	1.89	0.55
1:C:58:TRP:CD1	1:C:86:VAL:HB	2.41	0.55
1:B:668:VAL:HG11	1:B:680:ILE:HG12	1.89	0.54
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.42	0.54
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.88	0.54
1:B:251:ARG:H	1:B:254:LEU:HD12	1.73	0.54
1:A:958:ASN:OD1	1:A:985:ASN:ND2	2.35	0.54
1:C:361:PRO:HD3	1:C:609:ALA:HB1	1.88	0.54
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.90	0.54
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.08	0.54
1:C:800:ARG:HG3	1:C:800:ARG:O	2.08	0.54
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:VAL:HG21	1:C:882:ILE:HG23	1.89	0.54
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.43	0.54
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.90	0.53
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.73	0.53
1:B:750:GLU:HG2	1:B:755:ARG:HG3	1.90	0.53
1:C:19:PRO:HD3	1:C:112:PRO:HB3	1.91	0.53
1:C:262:GLN:OE1	1:C:299:LYS:HD2	2.08	0.53
1:D:646:HIS:HB3	5:D:4019:HOH:O	2.08	0.53
1:A:395:HIS:ND1	1:A:396:PRO:HD2	2.23	0.53
1:B:367:MET:HB3	1:B:372:MET:CE	2.38	0.53
1:D:837:THR:HG23	1:D:855:THR:HG22	1.90	0.53
1:C:330:VAL:HG13	4:C:8001:DMS:H23	1.90	0.53
1:B:942:ARG:HA	1:B:953:GLY:O	2.08	0.53
1:D:794:GLY:HA2	1:D:998:SER:O	2.09	0.52
1:B:768:MET:HB2	1:B:775:GLN:HB2	1.92	0.52
1:A:613:PRO:HB3	1:A:617:LEU:CD2	2.40	0.52
1:B:427:THR:HG21	1:B:462:SER:HB3	1.91	0.52
1:D:942:ARG:HA	1:D:953:GLY:O	2.10	0.52
1:B:456:TRP:NE1	1:B:482:ARG:HD2	2.25	0.52
1:C:367:MET:HB3	1:C:372:MET:HE3	1.92	0.51
1:D:99:ILE:O	1:D:204:ARG:HG2	2.11	0.51
1:D:373:VAL:O	1:D:377:LEU:HG	2.10	0.51
1:B:226:HIS:CD2	1:B:448:ARG:HD3	2.45	0.51
1:C:882:ILE:HD13	1:C:1014:TYR:CD1	2.46	0.51
1:C:260:LEU:HD11	1:C:309:TYR:HB3	1.93	0.51
1:C:38:ASN:HB3	1:C:41:GLU:CG	2.41	0.51
1:B:879:PRO:O	1:B:1009:LEU:HD12	2.11	0.51
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.92	0.51
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.93	0.51
1:D:337:ILE:HA	1:D:341:LEU:O	2.11	0.51
1:A:881:ARG:HE	1:A:987:ASP:CG	2.15	0.51
1:B:256:VAL:O	1:B:271:THR:HA	2.11	0.51
1:A:1020:TRP:HD1	1:A:1021:CYS:N	2.08	0.51
1:A:610:ASP:O	1:A:611:ARG:HB2	2.11	0.51
1:B:257:THR:HA	1:B:270:GLY:O	2.11	0.51
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.92	0.51
1:A:414:ASN:O	1:A:439:ARG:HD3	2.11	0.50
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.93	0.50
1:A:146:VAL:HG22	1:A:208:ILE:HG12	1.92	0.50
1:A:854:LYS:HA	1:A:867:THR:O	2.12	0.50
1:B:607:VAL:HG12	1:B:613:PRO:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:PRO:O	1:B:618:THR:HG22	2.10	0.50
1:D:980:GLU:HA	5:D:4079:HOH:O	2.10	0.50
1:B:30:HIS:NE2	1:B:170:GLU:OE1	2.43	0.50
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.46	0.50
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.94	0.50
1:B:143:PHE:O	1:B:168:PRO:HA	2.11	0.50
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.92	0.50
1:D:784:PHE:HA	1:D:881:ARG:O	2.11	0.50
1:B:778:THR:HB	1:B:887:GLN:CB	2.42	0.50
1:A:341:LEU:HD13	1:A:348:PRO:HB3	1.94	0.49
1:D:279:ILE:HG12	1:D:284:GLY:HA2	1.94	0.49
1:A:696:LEU:HB2	1:A:722:LEU:HD11	1.94	0.49
1:B:147:ASN:HB3	1:B:206:SER:HA	1.94	0.49
1:D:778:THR:H	1:D:887:GLN:HB3	1.77	0.49
1:B:50:GLN:O	1:B:215:LEU:HA	2.11	0.49
1:B:672:VAL:HG22	1:B:678:GLN:HB2	1.93	0.49
1:C:147:ASN:HB3	1:C:206:SER:HA	1.94	0.49
1:D:133:TRP:HA	1:D:216:HIS:CE1	2.47	0.49
1:D:536:CYS:O	1:D:537:GLU:HG3	2.12	0.49
1:D:537:GLU:HA	1:D:566:PHE:O	2.12	0.49
1:B:17:GLU:HG2	1:B:114:VAL:HG22	1.95	0.48
1:D:237:ARG:HG2	1:D:296:GLU:OE1	2.13	0.48
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.47	0.48
1:C:124:SER:HA	1:C:184:LEU:O	2.13	0.48
1:C:606:LEU:O	1:C:614:HIS:HB2	2.13	0.48
1:A:333:ARG:HA	1:A:345:ASN:OD1	2.14	0.48
1:A:343:LEU:HA	1:A:347:LYS:O	2.13	0.48
1:C:847:LYS:NZ	1:C:875:ASP:OD2	2.44	0.48
1:D:333:ARG:HG2	1:D:333:ARG:NH1	2.28	0.48
1:C:163:GLN:O	1:C:164:ASP:HB3	2.13	0.48
1:C:88:SER:HA	1:C:366:VAL:HG21	1.95	0.48
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.96	0.48
1:D:598:ASP:O	1:D:601:PHE:HB2	2.13	0.48
1:A:114:VAL:HA	5:A:4077:HOH:O	2.13	0.48
1:D:573:GLN:HB2	1:D:602:CYS:O	2.13	0.48
1:C:897:TRP:CZ2	1:C:938:ARG:HG2	2.49	0.48
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.96	0.48
1:A:524:LEU:HD11	1:A:562:LEU:HG	1.96	0.47
1:A:907:PRO:HG2	1:A:990:HIS:O	2.14	0.47
1:A:147:ASN:ND2	1:A:205:MET:O	2.46	0.47
1:D:132:SER:HA	1:D:135:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:HG11	1:A:150:PHE:CD2	2.49	0.47
1:C:496:THR:OG1	1:C:498:ILE:O	2.31	0.47
1:D:842:TRP:HZ3	1:D:852:SER:HB3	1.79	0.47
1:B:875:ASP:OD2	1:B:875:ASP:N	2.43	0.47
1:C:440:VAL:HG13	1:C:475:ILE:HD11	1.96	0.47
1:D:226:HIS:O	1:D:242:ALA:HA	2.14	0.47
1:A:140:ARG:HG2	1:A:215:LEU:HB3	1.97	0.47
1:C:738:PRO:HG3	1:C:751:LEU:HD13	1.97	0.47
1:B:753:ASN:HA	5:B:4072:HOH:O	2.13	0.47
1:C:1000:SER:O	1:C:1001:PRO:C	2.53	0.47
1:C:824:GLN:HB3	1:C:839:ALA:HB3	1.96	0.47
1:A:245:GLN:HG2	1:A:288:ARG:CG	2.41	0.47
1:A:697:THR:HG23	1:A:719:GLN:HG3	1.96	0.47
1:D:347:LYS:HB3	1:D:643:LEU:HD22	1.97	0.46
1:C:626:PHE:CD1	4:C:8002:DMS:H22	2.50	0.46
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.96	0.46
1:B:390:SER:HA	1:B:391:HIS:HA	1.70	0.46
1:B:702:GLN:O	1:B:712:GLY:N	2.44	0.46
1:C:942:ARG:O	1:C:952:ARG:HA	2.16	0.46
1:C:598:ASP:O	1:C:601:PHE:HB2	2.16	0.46
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.51	0.46
1:D:906:TYR:OH	1:D:934:GLU:HG3	2.16	0.46
1:B:610:ASP:O	1:B:611:ARG:HB2	2.16	0.46
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.97	0.46
1:A:706:THR:OG1	1:A:709:SER:OG	2.29	0.46
1:D:30:HIS:ND1	1:D:31:PRO:O	2.46	0.46
1:B:344:LEU:HD23	1:B:644:PHE:CZ	2.51	0.46
1:C:873:ALA:O	1:C:876:THR:HG22	2.16	0.46
1:A:227:VAL:HG13	1:A:240:LEU:HD21	1.98	0.46
1:D:163:GLN:O	1:D:164:ASP:HB3	2.16	0.46
1:D:220:THR:HG21	1:D:254:LEU:HD11	1.97	0.46
1:A:107:ILE:HB	5:A:4077:HOH:O	2.14	0.46
1:A:486:TYR:CZ	1:A:488:GLY:HA3	2.51	0.46
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.16	0.46
1:B:150:PHE:HA	1:B:187:MET:O	2.16	0.45
1:D:35:SER:O	1:D:50:GLN:HG3	2.16	0.45
1:C:728:VAL:HG12	1:D:851:ILE:HD11	1.98	0.45
1:C:782:ASP:OD1	1:C:854:LYS:NZ	2.45	0.45
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.51	0.45
1:B:749:ILE:HD11	1:B:836:ILE:HD11	1.97	0.45
1:B:861:SER:HB3	5:B:4061:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ASN:HB3	1:B:945:ASN:HB2	1.97	0.45
1:D:348:PRO:O	1:D:643:LEU:HD11	2.16	0.45
1:C:492:ASP:HB3	1:C:499:ILE:HG23	1.98	0.45
1:D:892:ALA:HB3	1:D:946:TYR:CZ	2.50	0.45
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.82	0.45
1:D:338:GLU:HB2	5:D:4031:HOH:O	2.15	0.45
1:B:755:ARG:HB3	1:B:769:TRP:HB2	1.99	0.45
1:A:240:LEU:HD23	1:A:241:GLU:N	2.32	0.45
1:A:390:SER:HB2	1:A:391:HIS:CE1	2.52	0.45
1:A:390:SER:HA	1:A:391:HIS:HA	1.74	0.45
1:C:367:MET:HB3	1:C:372:MET:CE	2.47	0.45
1:C:60:PHE:HA	1:C:122:CYS:O	2.17	0.45
1:D:43:ARG:HD2	1:D:261:TRP:CD2	2.52	0.45
1:B:58:TRP:CD1	1:B:86:VAL:HB	2.52	0.45
1:C:644:PHE:O	1:C:674:PRO:HG3	2.17	0.45
1:C:883:GLY:HA3	1:C:987:ASP:HA	1.99	0.44
1:D:410:VAL:HG22	1:D:455:ILE:HB	1.99	0.44
1:D:88:SER:HA	1:D:366:VAL:CG2	2.45	0.44
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.82	0.44
1:C:615:PRO:HB3	1:C:904:GLU:HB3	1.99	0.44
1:A:613:PRO:HB3	1:A:617:LEU:HD22	2.00	0.44
1:B:788:PRO:HD2	1:B:968:MET:HB2	1.98	0.44
1:B:456:TRP:CE2	1:B:482:ARG:HD2	2.53	0.44
1:B:766:SER:HA	1:B:779:PRO:HB3	1.99	0.44
1:D:335:VAL:HG22	1:D:344:LEU:HD12	1.99	0.44
1:D:698:VAL:O	1:D:717:TRP:HA	2.16	0.44
1:B:870:VAL:HG21	1:B:882:ILE:CG2	2.47	0.44
1:D:545:SER:O	1:D:909:ARG:HD3	2.18	0.44
1:D:789:LEU:HD21	1:D:934:GLU:HB3	2.00	0.44
1:A:770:ILE:HD13	1:A:1022:GLN:HG3	1.99	0.43
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.53	0.43
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.53	0.43
1:D:217:LYS:NZ	1:D:326:GLU:OE2	2.50	0.43
1:B:737:ILE:HD12	1:B:738:PRO:HD2	2.00	0.43
1:A:753:ASN:HB2	1:A:771:GLY:HA2	1.99	0.43
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.53	0.43
1:C:141:ILE:HB	1:C:173:LEU:HD11	1.99	0.43
1:C:553:TRP:CZ2	1:C:624:GLN:HG2	2.52	0.43
1:C:963:SER:HB3	1:C:983:TRP:CE2	2.53	0.43
1:D:693:GLN:HB2	1:D:724:GLU:HG3	2.01	0.43
1:A:256:VAL:HG23	1:A:274:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:THR:HG1	1:A:709:SER:HG	1.58	0.43
1:B:361:PRO:HB2	1:B:576:ILE:HG12	2.00	0.43
1:B:429:ASP:OD1	1:B:431:ARG:HG3	2.19	0.43
1:B:778:THR:HB	1:B:887:GLN:HB3	2.01	0.43
1:C:854:LYS:HG2	1:C:868:VAL:HG22	2.00	0.43
1:D:693:GLN:HG2	1:D:695:TRP:NE1	2.34	0.43
1:A:354:VAL:O	1:A:387:VAL:HG23	2.19	0.43
1:A:43:ARG:HH12	1:A:264:GLU:HG2	1.83	0.43
1:A:613:PRO:CB	1:A:617:LEU:HD23	2.49	0.43
1:B:390:SER:HB2	1:B:391:HIS:CE1	2.53	0.43
1:A:738:PRO:HG3	1:A:751:LEU:HD13	1.99	0.43
1:B:794:GLY:HA2	1:B:998:SER:O	2.19	0.43
1:C:522:LYS:HE3	1:D:560:PRO:HD3	2.00	0.43
1:D:778:THR:HA	1:D:779:PRO:HD3	1.85	0.43
1:B:474:TRP:CE2	1:B:478:VAL:HG21	2.54	0.43
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.54	0.43
1:D:608:PHE:CZ	1:D:614:HIS:HD2	2.37	0.43
1:D:544:ASN:HB3	1:D:789:LEU:HD13	2.01	0.43
1:A:260:LEU:HD11	1:A:309:TYR:HB3	2.00	0.43
1:A:147:ASN:HB3	1:A:206:SER:HA	2.00	0.42
1:A:454:ILE:HG13	1:A:455:ILE:HG13	2.01	0.42
1:B:505:ARG:O	1:B:519:SER:HA	2.19	0.42
1:D:225:PHE:HA	1:D:243:GLU:O	2.19	0.42
1:A:59:ARG:HB2	1:A:124:SER:OG	2.19	0.42
1:A:541:ALA:HB2	1:A:546:LEU:HD13	2.01	0.42
1:C:961:ARG:NH2	1:C:979:GLU:O	2.52	0.42
1:B:496:THR:OG1	1:B:498:ILE:O	2.35	0.42
1:B:906:TYR:HB3	1:B:907:PRO:HD2	2.02	0.42
1:C:755:ARG:HB3	1:C:769:TRP:HE3	1.84	0.42
1:D:240:LEU:HD13	1:D:260:LEU:HD22	2.01	0.42
1:A:226:HIS:CD2	1:A:448:ARG:HD3	2.55	0.42
1:B:235:PHE:HB3	1:B:300:LEU:HD11	2.01	0.42
1:D:500:CYS:HA	1:D:534:ILE:O	2.20	0.42
1:D:292:ARG:N	4:D:8004:DMS:O	2.50	0.42
1:D:927:THR:HA	1:D:928:PRO:HD3	1.91	0.42
1:D:972:HIS:HB2	1:D:975:LEU:HD12	2.01	0.42
1:B:249:GLU:OE2	1:B:251:ARG:HD3	2.19	0.42
1:C:350:LEU:HD11	1:C:556:PHE:HB3	2.01	0.42
1:C:896:ASN:HA	1:C:918:TRP:O	2.20	0.42
1:C:939:CYS:HA	1:C:956:GLN:HB3	2.02	0.42
1:A:1000:SER:O	1:A:1001:PRO:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:LEU:HD11	1:B:562:LEU:HG	2.01	0.42
1:B:937:LEU:HA	1:B:957:PHE:O	2.19	0.42
1:C:525:SER:O	1:D:561:ARG:HD3	2.20	0.42
1:D:272:ALA:HB1	1:D:273:PRO:HD2	2.02	0.42
1:D:569:ASP:O	1:D:605:GLY:HA2	2.20	0.42
1:A:931:PHE:HA	1:A:932:PRO:HD3	1.86	0.42
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.55	0.41
1:A:429:ASP:HA	1:A:430:PRO:HD2	1.89	0.41
1:B:545:SER:OG	1:B:546:LEU:N	2.52	0.41
1:B:957:PHE:HA	1:B:985:ASN:O	2.20	0.41
1:D:458:LEU:HD11	1:D:472:TYR:HB2	2.02	0.41
1:A:807:VAL:HG13	1:A:808:GLU:HG2	2.01	0.41
1:A:855:THR:OG1	1:A:867:THR:HB	2.20	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.76	0.41
1:B:559:TYR:HB2	1:B:562:LEU:HD12	2.02	0.41
1:C:414:ASN:O	1:C:439:ARG:HD3	2.20	0.41
1:C:997:ASP:HB2	1:C:999:TRP:CE2	2.55	0.41
1:A:824:GLN:O	1:A:838:THR:HA	2.20	0.41
1:C:142:ILE:HG21	5:C:4015:HOH:O	2.19	0.41
1:C:411:ASP:HB2	1:C:453:VAL:HG13	2.02	0.41
1:B:274:PHE:HA	1:B:289:VAL:HB	2.03	0.41
1:B:613:PRO:HB3	1:B:617:LEU:HD23	2.02	0.41
1:B:759:ASN:ND2	5:B:4104:HOH:O	2.54	0.41
1:C:147:ASN:OD1	1:C:148:SER:HB3	2.21	0.41
1:A:786:ARG:NH2	1:A:991:MET:HE2	2.35	0.41
1:B:957:PHE:CD1	1:B:957:PHE:C	2.94	0.41
1:C:251:ARG:H	1:C:254:LEU:HD12	1.85	0.41
1:C:421:VAL:HA	1:C:422:PRO:HA	1.94	0.41
1:D:218:PRO:HB2	1:D:220:THR:O	2.21	0.41
1:C:796:SER:HB2	1:C:802:ASP:HB3	2.03	0.41
1:A:58:TRP:O	1:A:83:THR:HA	2.21	0.41
1:A:957:PHE:HA	1:A:985:ASN:O	2.21	0.41
1:C:984:LEU:HD21	1:C:986:ILE:HD11	2.02	0.41
1:D:615:PRO:O	1:D:618:THR:HG22	2.21	0.41
1:A:33:PHE:HB3	1:A:326:GLU:OE2	2.20	0.41
1:A:523:TRP:CD1	1:A:526:LEU:HD12	2.55	0.41
1:A:600:GLN:HB2	1:A:603:MET:HE2	2.02	0.41
1:C:147:ASN:HA	1:C:148:SER:HA	1.67	0.41
1:D:257:THR:HA	1:D:270:GLY:O	2.21	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.76	0.41
1:A:568:TRP:HA	1:A:569:ASP:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.87	0.41
1:B:18:ASN:HA	1:B:19:PRO:HD2	1.93	0.41
1:C:372:MET:HE1	1:C:395:HIS:HB3	2.02	0.41
1:A:542:MET:HA	1:A:604:ASN:HA	2.03	0.40
1:B:835:LEU:HA	1:B:856:TYR:O	2.21	0.40
1:D:89:ASN:HA	1:D:206:SER:O	2.21	0.40
1:A:118:ASN:O	1:A:119:PRO:C	2.60	0.40
1:B:376:ILE:CD1	1:B:401:LEU:HB3	2.51	0.40
1:C:190:ARG:HG2	1:C:191:TRP:CE2	2.56	0.40
1:C:260:LEU:HD11	1:C:309:TYR:CB	2.51	0.40
1:C:46:ARG:HG3	1:C:47:PRO:HD2	2.03	0.40
1:D:262:GLN:NE2	1:D:299:LYS:HD2	2.36	0.40
1:A:107:ILE:HD12	5:A:4077:HOH:O	2.19	0.40
1:B:835:LEU:HD11	1:B:855:THR:HB	2.02	0.40
1:D:577:LYS:O	1:D:584:PRO:HA	2.21	0.40
1:D:696:LEU:O	1:D:719:GLN:HA	2.21	0.40
1:B:568:TRP:CG	1:B:569:ASP:HB3	2.56	0.40
1:C:780:LEU:HA	1:C:886:CYS:HB3	2.04	0.40
1:D:147:ASN:O	1:D:206:SER:HB2	2.21	0.40
1:A:421:VAL:HA	1:A:422:PRO:HA	1.97	0.40
1:B:246:MET:C	1:B:246:MET:SD	3.00	0.40
1:C:607:VAL:HG12	1:C:613:PRO:HA	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	1009/1052 (96%)	949 (94%)	58 (6%)	2 (0%)	51 83
1	B	1009/1052 (96%)	948 (94%)	57 (6%)	4 (0%)	38 72
1	C	1009/1052 (96%)	953 (94%)	52 (5%)	4 (0%)	38 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	1009/1052 (96%)	943 (94%)	65 (6%)	1 (0%)	55 86
All	All	4036/4208 (96%)	3793 (94%)	232 (6%)	11 (0%)	44 77

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	164	ASP
1	B	461	GLU
1	A	541	ALA
1	C	733	ALA
1	B	540	HIS
1	C	164	ASP
1	D	109	VAL
1	A	539	ALA
1	C	539	ALA
1	B	633	GLY
1	C	1001	PRO

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	864/898 (96%)	842 (98%)	22 (2%)	53 84
1	B	864/898 (96%)	841 (97%)	23 (3%)	50 83
1	C	864/898 (96%)	836 (97%)	28 (3%)	44 78
1	D	864/898 (96%)	843 (98%)	21 (2%)	54 85
All	All	3456/3592 (96%)	3362 (97%)	94 (3%)	50 83

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	49	GLN
1	A	131	GLU

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Mol	Chain	Res	Type
1	A	195	SER
1	A	213	SER
1	A	333	ARG
1	A	519	SER
1	A	595	THR
1	A	604	ASN
1	A	655	MET
1	A	663	LEU
1	A	681	GLU
1	A	737	ILE
1	A	745	MET
1	A	782	ASP
1	A	800	ARG
1	A	817	GLN
1	A	850	PHE
1	A	910	LEU
1	A	916	ASP
1	A	924	ASP
1	A	956	GLN
1	B	13	ARG
1	B	80	GLU
1	B	126	THR
1	B	186	VAL
1	B	252	ASP
1	B	269	SER
1	B	333	ARG
1	B	344	LEU
1	B	394	ASN
1	B	481	SER
1	B	519	SER
1	B	535	LEU
1	B	546	LEU
1	B	663	LEU
1	B	718	GLN
1	B	743	SER
1	B	748	CYS
1	B	774	LYS
1	B	829	THR
1	B	876	THR
1	B	968	MET
1	B	1004	SER
1	B	1022	GLN

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Mol	Chain	Res	Type
1	C	46	ARG
1	C	71	GLU
1	C	80	GLU
1	C	90	TRP
1	C	129	VAL
1	C	181	GLU
1	C	213	SER
1	C	219	THR
1	C	333	ARG
1	C	394	ASN
1	C	546	LEU
1	C	604	ASN
1	C	635	THR
1	C	663	LEU
1	C	672	VAL
1	C	737	ILE
1	C	741	THR
1	C	751	LEU
1	C	773	LYS
1	C	785	THR
1	C	789	LEU
1	C	800	ARG
1	C	819	GLU
1	C	828	ASP
1	C	956	GLN
1	C	996	ASP
1	C	1002	SER
1	C	1022	GLN
1	D	135	GLN
1	D	213	SER
1	D	251	ARG
1	D	333	ARG
1	D	519	SER
1	D	540	HIS
1	D	546	LEU
1	D	580	GLU
1	D	612	THR
1	D	652	LEU
1	D	663	LEU
1	D	681	GLU
1	D	728	VAL
1	D	744	GLU

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Mol	Chain	Res	Type
1	D	748	CYS
1	D	769	TRP
1	D	774	LYS
1	D	956	GLN
1	D	966	GLN
1	D	970	THR
1	D	986	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	634	GLN
1	A	704	ASN
1	B	221	GLN
1	B	394	ASN
1	B	624	GLN
1	B	718	GLN
1	B	890	GLN
1	C	221	GLN
1	C	704	ASN
1	C	804	ASN
1	C	824	GLN
1	C	956	GLN
1	C	1022	GLN
1	D	93	HIS
1	D	135	GLN
1	D	381	GLN
1	D	510	GLN
1	D	614	HIS
1	D	804	ASN
1	D	956	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 19 are monoatomic - leaving 45 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
4	DMS	A	8001	-	3,3,3	2.61	1 (33%)	3,3,3	0.51	0
4	DMS	A	8002	-	3,3,3	2.64	1 (33%)	3,3,3	0.70	0
4	DMS	A	8003	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
4	DMS	A	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.48	0
4	DMS	A	8005	-	3,3,3	2.67	1 (33%)	3,3,3	0.65	0
4	DMS	A	8006	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
4	DMS	A	8007	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
4	DMS	A	8008	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
4	DMS	A	8009	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
4	DMS	A	8010	-	3,3,3	2.67	1 (33%)	3,3,3	0.63	0
4	DMS	A	8011	-	3,3,3	2.70	1 (33%)	3,3,3	0.55	0
4	DMS	A	8012	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
4	DMS	B	8001	-	3,3,3	2.62	1 (33%)	3,3,3	0.60	0
4	DMS	B	8002	-	3,3,3	2.64	1 (33%)	3,3,3	0.56	0
4	DMS	B	8003	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
4	DMS	B	8004	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
4	DMS	B	8005	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
4	DMS	B	8006	-	3,3,3	2.66	1 (33%)	3,3,3	0.63	0
4	DMS	B	8007	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
4	DMS	B	8008	-	3,3,3	2.64	1 (33%)	3,3,3	0.55	0
4	DMS	B	8009	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
4	DMS	B	8010	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	B	8011	-	3,3,3	2.65	1 (33%)	3,3,3	0.59	0
4	DMS	C	8001	-	3,3,3	2.53	1 (33%)	3,3,3	0.44	0
4	DMS	C	8002	-	3,3,3	2.73	1 (33%)	3,3,3	0.84	0
4	DMS	C	8003	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
4	DMS	C	8004	-	3,3,3	2.58	1 (33%)	3,3,3	0.46	0
4	DMS	C	8005	-	3,3,3	2.71	1 (33%)	3,3,3	0.62	0
4	DMS	C	8006	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
4	DMS	C	8007	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	0
4	DMS	C	8008	-	3,3,3	2.59	1 (33%)	3,3,3	0.59	0
4	DMS	C	8009	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
4	DMS	C	8010	-	3,3,3	2.66	1 (33%)	3,3,3	0.78	0
4	DMS	C	8011	-	3,3,3	2.64	1 (33%)	3,3,3	0.44	0
4	DMS	C	8012	-	3,3,3	2.69	1 (33%)	3,3,3	0.56	0
4	DMS	D	8001	-	3,3,3	2.66	1 (33%)	3,3,3	0.60	0
4	DMS	D	8002	-	3,3,3	2.61	1 (33%)	3,3,3	0.52	0
4	DMS	D	8003	-	3,3,3	2.60	1 (33%)	3,3,3	0.54	0
4	DMS	D	8004	-	3,3,3	2.56	1 (33%)	3,3,3	0.67	0
4	DMS	D	8005	-	3,3,3	2.66	1 (33%)	3,3,3	0.61	0
4	DMS	D	8006	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
4	DMS	D	8007	-	3,3,3	2.72	1 (33%)	3,3,3	0.78	0
4	DMS	D	8008	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
4	DMS	D	8009	-	3,3,3	2.60	1 (33%)	3,3,3	0.48	0
4	DMS	D	8010	-	3,3,3	2.67	1 (33%)	3,3,3	0.63	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	DMS	A	8001	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8002	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8003	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8004	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8005	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8006	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8007	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	A	8008	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8009	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8010	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8011	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8012	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8001	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8002	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8003	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8004	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8005	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8006	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8007	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8008	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8009	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8010	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8011	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8001	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8002	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8003	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8004	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8005	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8006	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8007	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8008	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8009	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8010	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8011	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8012	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8001	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8002	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8003	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8004	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8005	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8006	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8007	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8008	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8009	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8010	-	-	0/0/0/0	0/0/0/0

All (45) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8001	DMS	O-S	4.24	1.79	1.50
4	D	8004	DMS	O-S	4.26	1.79	1.50
4	C	8004	DMS	O-S	4.31	1.79	1.50
4	C	8008	DMS	O-S	4.32	1.79	1.50
4	D	8003	DMS	O-S	4.36	1.79	1.50
4	D	8009	DMS	O-S	4.36	1.79	1.50
4	A	8004	DMS	O-S	4.37	1.79	1.50
4	D	8002	DMS	O-S	4.38	1.80	1.50
4	A	8001	DMS	O-S	4.39	1.80	1.50
4	B	8001	DMS	O-S	4.39	1.80	1.50
4	B	8008	DMS	O-S	4.41	1.80	1.50
4	D	8008	DMS	O-S	4.41	1.80	1.50
4	B	8005	DMS	O-S	4.41	1.80	1.50
4	B	8002	DMS	O-S	4.42	1.80	1.50
4	B	8010	DMS	O-S	4.42	1.80	1.50
4	B	8007	DMS	O-S	4.43	1.80	1.50
4	C	8011	DMS	O-S	4.43	1.80	1.50
4	A	8003	DMS	O-S	4.44	1.80	1.50
4	A	8002	DMS	O-S	4.44	1.80	1.50
4	B	8011	DMS	O-S	4.44	1.80	1.50
4	C	8010	DMS	O-S	4.45	1.80	1.50
4	D	8005	DMS	O-S	4.45	1.80	1.50
4	A	8009	DMS	O-S	4.45	1.80	1.50
4	D	8010	DMS	O-S	4.46	1.80	1.50
4	C	8003	DMS	O-S	4.46	1.80	1.50
4	A	8010	DMS	O-S	4.46	1.80	1.50
4	B	8006	DMS	O-S	4.46	1.80	1.50
4	C	8006	DMS	O-S	4.46	1.80	1.50
4	B	8003	DMS	O-S	4.47	1.80	1.50
4	B	8009	DMS	O-S	4.48	1.80	1.50
4	D	8001	DMS	O-S	4.49	1.80	1.50
4	C	8009	DMS	O-S	4.49	1.80	1.50
4	A	8012	DMS	O-S	4.49	1.80	1.50
4	A	8005	DMS	O-S	4.49	1.80	1.50
4	A	8008	DMS	O-S	4.50	1.80	1.50
4	A	8006	DMS	O-S	4.50	1.80	1.50
4	C	8012	DMS	O-S	4.51	1.80	1.50
4	A	8011	DMS	O-S	4.52	1.80	1.50
4	C	8007	DMS	O-S	4.52	1.80	1.50
4	D	8006	DMS	O-S	4.53	1.81	1.50
4	A	8007	DMS	O-S	4.55	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8005	DMS	O-S	4.55	1.81	1.50
4	D	8007	DMS	O-S	4.55	1.81	1.50
4	B	8004	DMS	O-S	4.57	1.81	1.50
4	C	8002	DMS	O-S	4.59	1.81	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8001	DMS	1	0
4	C	8002	DMS	1	0
4	D	8004	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	1011/1052 (96%)	-0.54	8 (0%) 86 81	8, 25, 52, 91	0
1	B	1011/1052 (96%)	-0.43	10 (0%) 82 77	9, 31, 52, 90	0
1	C	1011/1052 (96%)	-0.41	10 (0%) 82 77	13, 30, 54, 92	0
1	D	1011/1052 (96%)	-0.39	21 (2%) 64 54	6, 28, 61, 96	0
All	All	4044/4208 (96%)	-0.44	49 (1%) 79 72	6, 28, 55, 96	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	688	PRO	6.9
1	A	581	ASN	5.4
1	D	687	GLN	5.2
1	A	580	GLU	4.1
1	D	686	PRO	4.0
1	D	689	GLU	3.9
1	D	744	GLU	3.9
1	A	686	PRO	3.8
1	B	799	THR	3.7
1	D	70	PRO	3.7
1	B	858	ILE	3.6
1	D	819	GLU	3.3
1	C	735	HIS	3.3
1	D	684	GLU	3.2
1	C	632	SER	3.2
1	A	689	GLU	2.8
1	C	78	LEU	2.8
1	C	76	CYS	2.7
1	C	731	PRO	2.7
1	D	891	VAL	2.7
1	D	743	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	732	ALA	2.6
1	D	72	SER	2.6
1	A	685	LEU	2.5
1	B	733	ALA	2.5
1	B	253	TYR	2.5
1	C	800	ARG	2.5
1	D	753	ASN	2.5
1	D	733	ALA	2.4
1	B	834	VAL	2.4
1	D	690	SER	2.4
1	D	768	MET	2.4
1	B	764	PHE	2.4
1	D	977	HIS	2.3
1	B	683	PRO	2.3
1	D	800	ARG	2.3
1	C	736	ALA	2.3
1	D	685	LEU	2.3
1	D	846	GLY	2.2
1	C	733	ALA	2.2
1	A	735	HIS	2.2
1	D	799	THR	2.1
1	D	752	GLY	2.1
1	C	843	GLN	2.1
1	B	687	GLN	2.1
1	A	1023	LYS	2.0
1	B	698	VAL	2.0
1	C	687	GLN	2.0
1	B	680	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	DMS	A	8007	4/4	0.50	0.40	8.60	82,82,83,87	0
4	DMS	C	8003	4/4	0.95	0.26	3.78	77,77,77,77	0
4	DMS	B	8004	4/4	0.90	0.22	3.70	67,67,67,68	0
4	DMS	C	8012	4/4	0.96	0.22	3.64	65,66,66,66	0
4	DMS	D	8002	4/4	0.96	0.20	3.33	40,43,45,47	0
4	DMS	C	8010	4/4	0.93	0.22	3.33	53,54,54,58	0
4	DMS	A	8005	4/4	0.92	0.25	3.26	62,63,64,66	0
4	DMS	A	8004	4/4	0.97	0.27	3.21	41,44,44,44	0
4	DMS	A	8009	4/4	0.96	0.18	3.18	62,63,64,65	0
4	DMS	D	8003	4/4	0.98	0.18	3.16	26,30,31,38	0
4	DMS	D	8008	4/4	0.97	0.30	3.08	57,57,58,58	0
2	MG	C	3001	1/1	0.94	0.24	3.01	43,43,43,43	0
2	MG	B	3001	1/1	0.96	0.23	2.91	45,45,45,45	0
4	DMS	C	8011	4/4	0.98	0.24	2.47	46,47,47,48	0
4	DMS	B	8011	4/4	0.93	0.24	2.31	70,71,72,72	0
4	DMS	B	8008	4/4	0.96	0.18	2.21	54,55,55,56	0
2	MG	D	3001	1/1	0.90	0.15	2.19	47,47,47,47	0
4	DMS	C	8005	4/4	0.94	0.20	2.03	54,54,56,58	0
4	DMS	D	8005	4/4	0.93	0.20	1.92	49,51,52,53	0
4	DMS	A	8002	4/4	0.97	0.19	1.77	27,29,29,35	0
4	DMS	D	8001	4/4	0.97	0.17	1.65	37,38,38,39	0
4	DMS	A	8003	4/4	0.97	0.14	1.59	32,32,33,34	0
4	DMS	C	8009	4/4	0.95	0.21	1.44	49,50,51,51	0
4	DMS	A	8001	4/4	0.98	0.16	1.42	31,34,34,37	0
3	NA	A	3102	1/1	0.96	0.17	1.40	15,15,15,15	0
4	DMS	B	8010	4/4	0.96	0.20	1.32	47,48,49,49	0
3	NA	A	3103	1/1	0.95	0.19	1.23	35,35,35,35	0
3	NA	C	3102	1/1	0.97	0.16	0.99	23,23,23,23	0
4	DMS	C	8002	4/4	0.90	0.18	0.98	37,38,38,39	0
4	DMS	B	8007	4/4	0.97	0.19	0.89	53,55,55,56	0
4	DMS	C	8001	4/4	0.96	0.20	0.56	34,38,38,40	0
4	DMS	B	8001	4/4	0.96	0.17	0.54	36,36,37,38	0
4	DMS	C	8004	4/4	0.97	0.14	0.38	27,27,27,28	0
4	DMS	D	8009	4/4	0.95	0.18	0.11	62,62,63,65	0
4	DMS	B	8003	4/4	0.95	0.17	0.03	46,46,48,48	0
4	DMS	B	8002	4/4	0.96	0.12	0.02	42,44,47,47	0
4	DMS	B	8005	4/4	0.95	0.17	-0.28	83,83,83,83	0
3	NA	D	3102	1/1	0.98	0.14	-0.28	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DMS	D	8004	4/4	0.97	0.17	-0.29	24,25,25,28	0
4	DMS	C	8007	4/4	0.95	0.14	-0.51	43,43,44,48	0
2	MG	D	3002	1/1	0.98	0.12	-1.00	31,31,31,31	0
3	NA	B	3104	1/1	0.94	0.09	-1.06	38,38,38,38	0
4	DMS	D	8006	4/4	0.98	0.13	-1.10	30,32,33,35	0
2	MG	A	3001	1/1	0.90	0.12	-1.15	42,42,42,42	0
3	NA	D	3101	1/1	0.91	0.11	-1.40	36,36,36,36	0
2	MG	C	3002	1/1	0.95	0.11	-1.46	29,29,29,29	0
3	NA	B	3103	1/1	0.92	0.08	-1.56	41,41,41,41	0
3	NA	B	3101	1/1	0.93	0.07	-1.81	24,24,24,24	0
3	NA	A	3101	1/1	0.97	0.08	-2.05	26,26,26,26	0
2	MG	B	3002	1/1	0.90	0.06	-2.59	33,33,33,33	0
3	NA	B	3102	1/1	0.99	0.08	-2.94	18,18,18,18	0
3	NA	C	3101	1/1	0.99	0.07	-7.04	30,30,30,30	0
4	DMS	C	8006	4/4	0.88	0.33	-	82,83,83,83	0
4	DMS	C	8008	4/4	0.98	0.34	-	29,29,30,30	0
4	DMS	B	8009	4/4	0.96	0.18	-	63,65,65,66	0
4	DMS	D	8010	4/4	0.76	0.31	-	68,69,70,72	0
4	DMS	A	8010	4/4	0.92	0.28	-	56,59,60,61	0
4	DMS	A	8011	4/4	0.94	0.20	-	56,57,57,61	0
4	DMS	A	8008	4/4	0.93	0.27	-	62,64,64,65	0
4	DMS	A	8012	4/4	0.92	0.20	-	56,56,56,57	0
3	NA	C	3105	1/1	0.91	0.19	-	38,38,38,38	0
4	DMS	D	8007	4/4	0.94	0.15	-	39,40,45,46	0
4	DMS	B	8006	4/4	0.95	0.15	-	52,52,52,55	0
4	DMS	A	8006	4/4	0.94	0.14	-	40,44,46,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.