



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:03 AM UTC

PDB ID : 3VD5 / pdb_00003vd5
Title : E. coli (lacZ) beta-galactosidase (N460S)
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 : 2.70 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

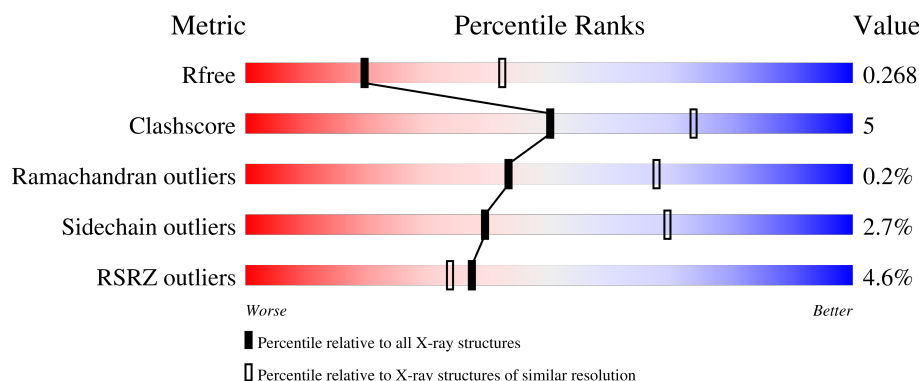
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

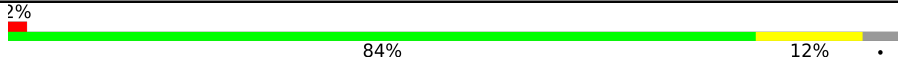
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	1052	
1	B	1052	
1	C	1052	
1	D	1052	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33647 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
			8124	5137	1439	1510	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8124	5137	1439	1510	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8124	5137	1439	1510	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8124	5137	1439	1510	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	SER	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	SER	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	SER	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	SER	ASN	engineered mutation	UNP P00722

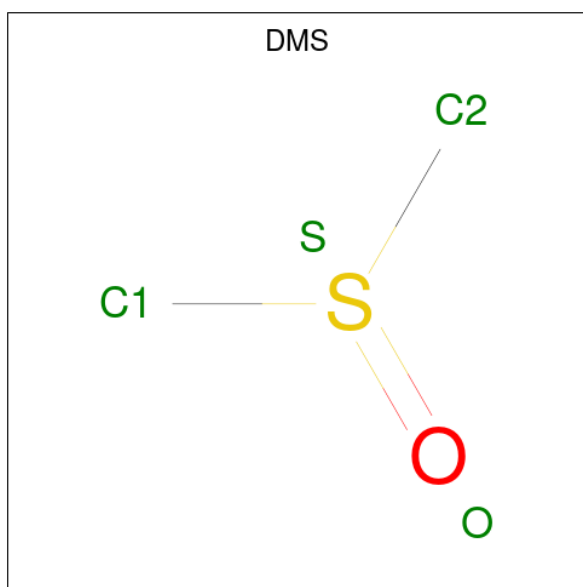
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: 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	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		

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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	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

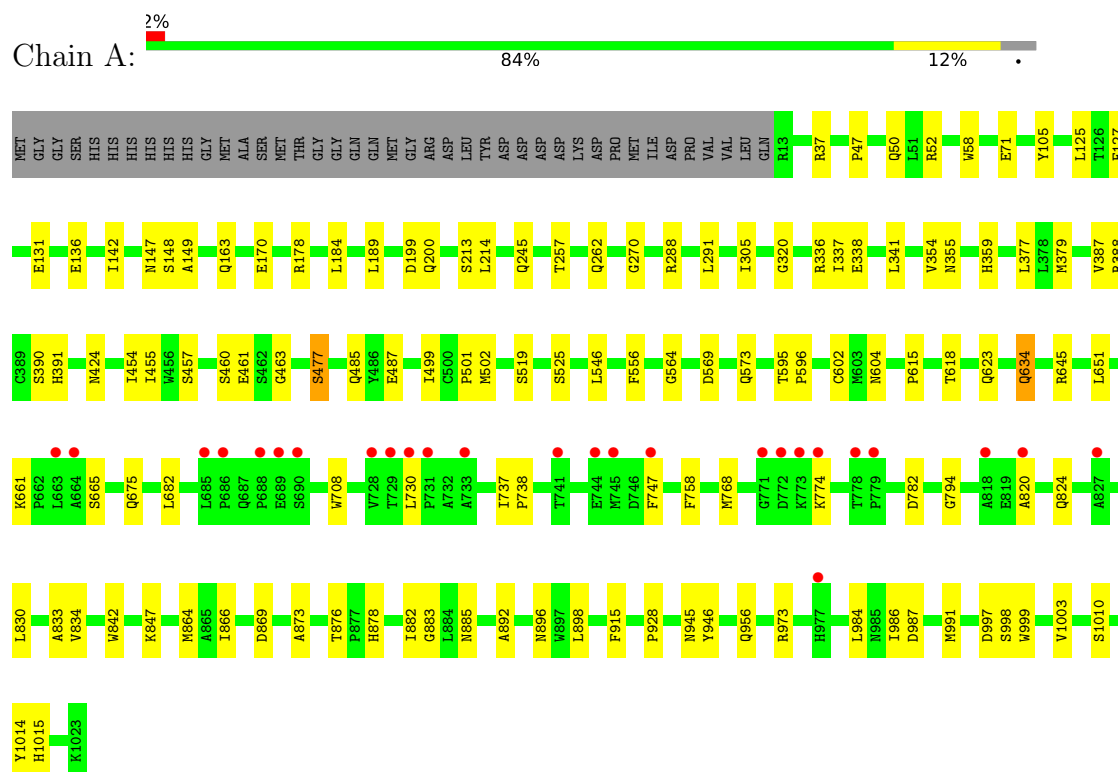
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total 314	O 314	0	0
5	C	204	Total 204	O 204	0	0
5	D	272	Total 272	O 272	0	0
5	B	246	Total 246	O 246	0	0

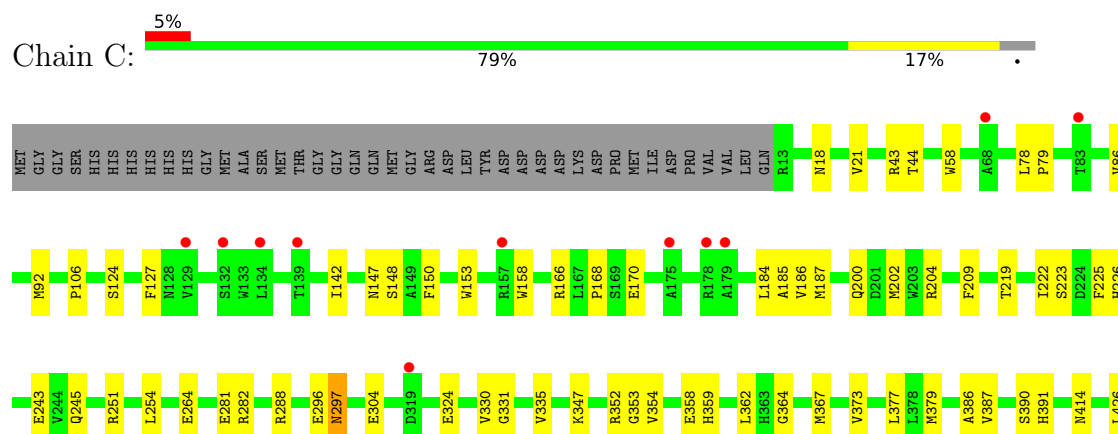
3 Residue-property plots [i](#)

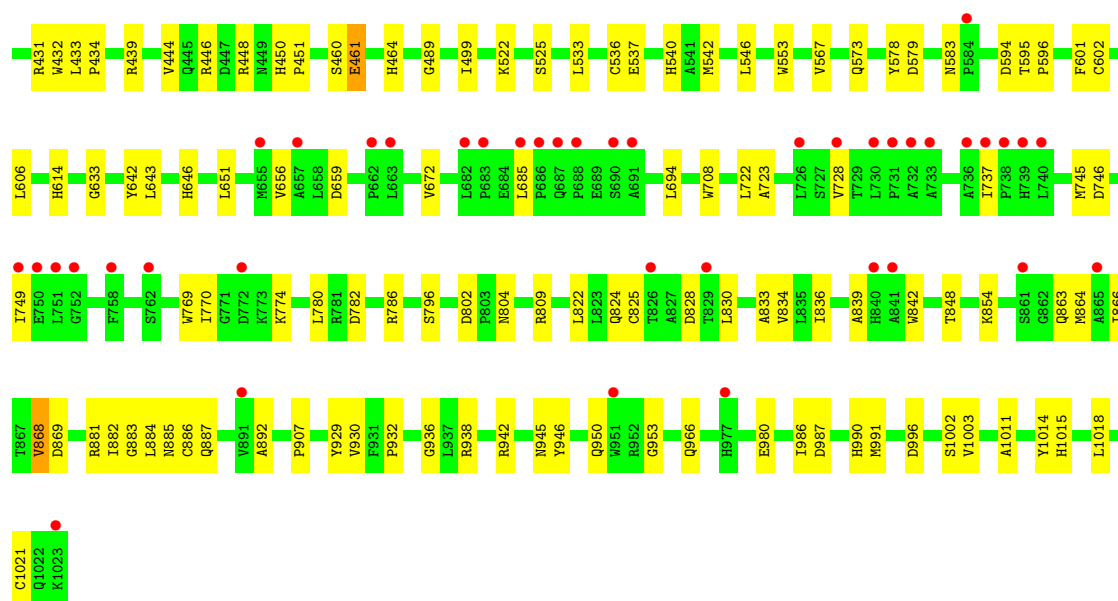
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Beta-galactosidase

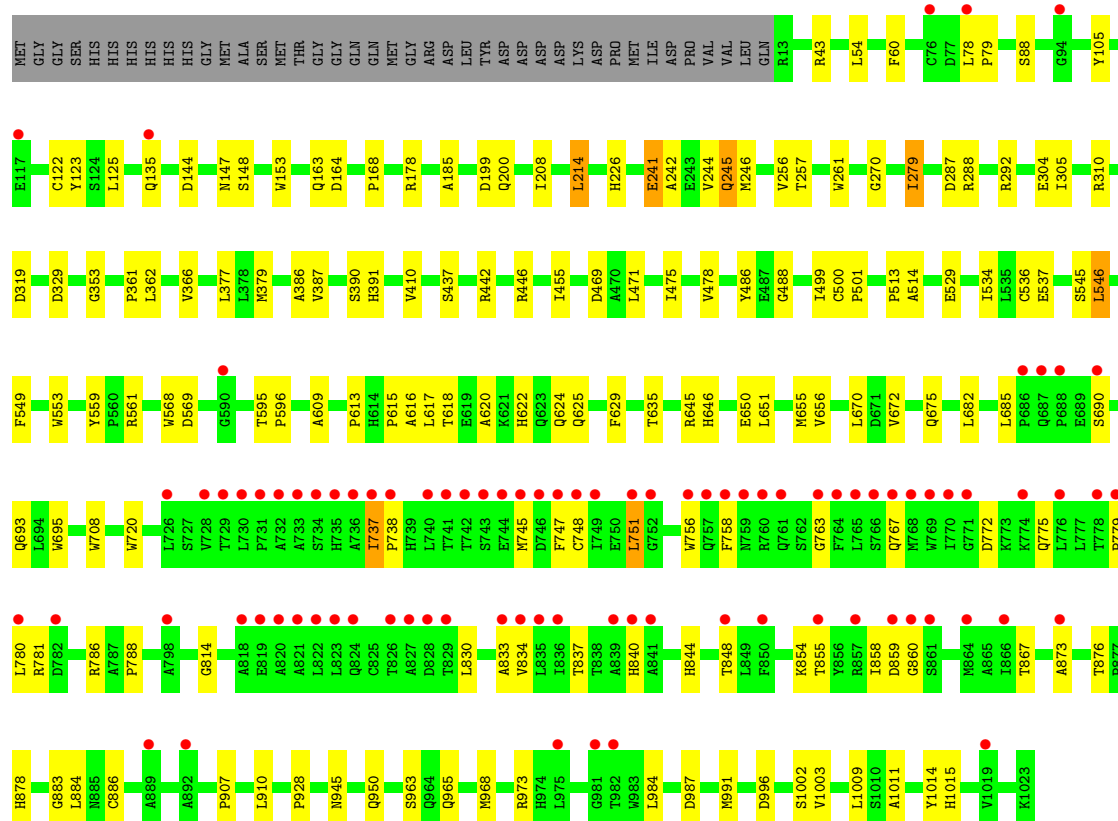
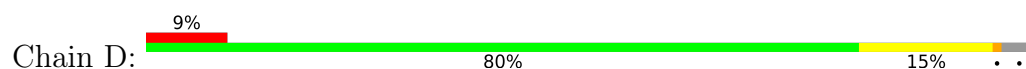


- Molecule 1: Beta-galactosidase

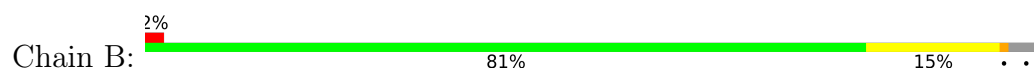


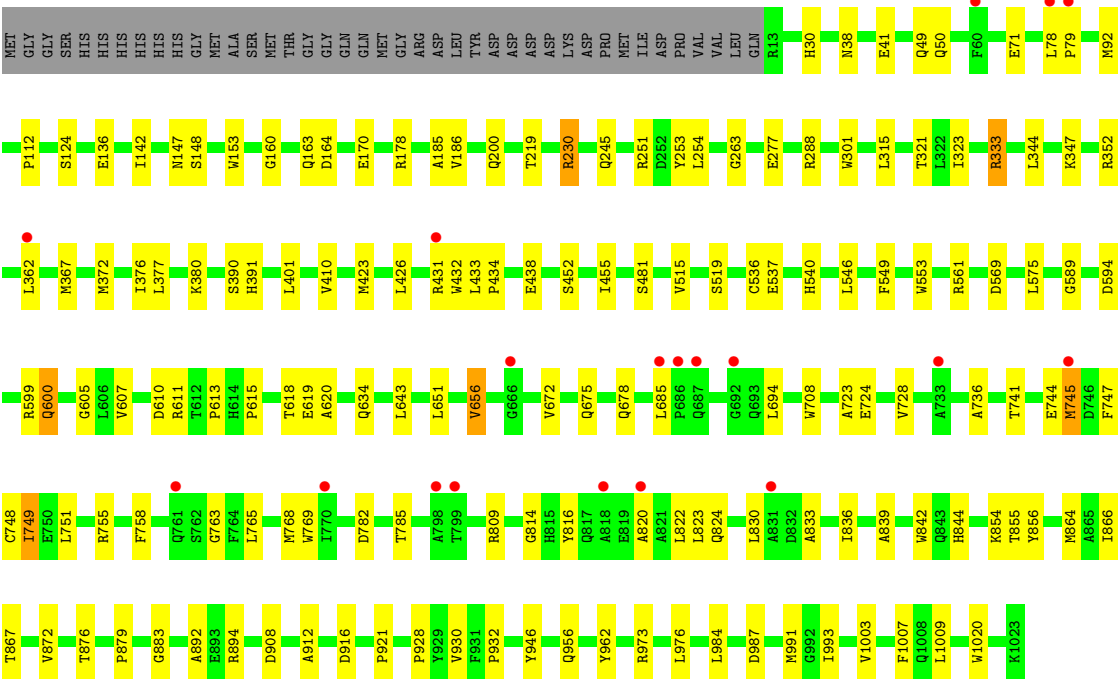


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.30Å 150.75Å 131.09Å 90.00° 104.06° 90.00°	Depositor
Resolution (Å)	54.58 – 2.70 54.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.58-2.70) 90.9 (54.58-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.203 , 0.276 0.194 , 0.268	Depositor DCC
R_{free} test set	5937 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	33647	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: DMS, NA, 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	0.49	0/8366	0.78	1/11412 (0.0%)
1	B	0.48	0/8366	0.76	1/11412 (0.0%)
1	C	0.46	0/8366	0.75	0/11412
1	D	0.49	0/8366	0.76	0/11412
All	All	0.48	0/33464	0.76	2/45648 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	GLY	N-CA-C	6.12	119.44	110.80
1	A	320	GLY	N-CA-C	5.20	120.92	114.37

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	8124	0	7715	64	0
1	B	8124	0	7715	86	0
1	C	8124	0	7715	102	0
1	D	8124	0	7715	93	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	32	0	48	5	0
4	B	16	0	24	2	0
4	C	24	0	36	2	0
4	D	24	0	36	3	0
5	A	314	0	0	1	0
5	B	246	0	0	1	0
5	C	204	0	0	2	0
5	D	272	0	0	4	0
All	All	33647	0	31004	334	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 (334) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.48	0.94
1:C:226:HIS:ND1	1:C:448:ARG:HD3	1.85	0.91
1:B:656:VAL:HG21	1:B:685:LEU:HD22	1.56	0.88
1:B:656:VAL:HG21	1:B:685:LEU:CD2	2.12	0.80
1:A:991:MET:HE3	1:A:1003:VAL:HG21	1.65	0.78
1:D:245:GLN:HG3	1:D:288:ARG:HG2	1.67	0.77
1:D:615:PRO:O	1:D:618:THR:HG22	1.88	0.73
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.72	0.70
1:B:38:ASN:OD1	1:B:41:GLU:HG2	1.92	0.69
1:C:331:GLY:H	4:C:8002:DMS:H22	1.57	0.69
1:C:828:ASP:HB3	1:D:830:LEU:HD22	1.75	0.68
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.76	0.68
1:D:241:GLU:HG3	1:D:292:ARG:HG2	1.77	0.66
1:A:615:PRO:O	1:A:618:THR:HG22	1.96	0.66
1:D:379:MET:HE1	1:D:387:VAL:HB	1.77	0.66
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.77	0.66
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.60	0.65
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:MET:HE1	1:A:387:VAL:HB	1.79	0.64
1:C:58:TRP:CD1	1:C:86:VAL:HB	2.33	0.64
1:C:991:MET:HE3	1:C:1003:VAL:HG21	1.80	0.63
1:B:883:GLY:HA3	1:B:987:ASP:HA	1.81	0.62
1:D:135:GLN:HG3	5:D:4006:HOH:O	1.99	0.62
1:B:112:PRO:HG3	1:B:431:ARG:HH22	1.65	0.61
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.65	0.61
1:C:830:LEU:HD12	1:C:833:ALA:HB3	1.83	0.61
1:C:451:PRO:HB3	4:C:8002:DMS:H23	1.82	0.61
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.84	0.60
1:B:672:VAL:HG22	1:B:678:GLN:HB2	1.84	0.59
1:A:896:ASN:HB3	1:A:945:ASN:HB2	1.85	0.59
1:C:942:ARG:HA	1:C:953:GLY:O	2.03	0.59
1:A:270:GLY:HA3	4:A:8004:DMS:H23	1.85	0.59
1:B:836:ILE:HB	1:B:856:TYR:HB2	1.84	0.59
1:D:928:PRO:HB2	1:D:973:ARG:HH11	1.68	0.59
1:D:779:PRO:O	1:D:781:ARG:HG3	2.03	0.58
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.84	0.58
1:A:47:PRO:HA	4:A:8005:DMS:H12	1.85	0.58
1:D:200:GLN:HG2	1:D:391:HIS:HB2	1.86	0.58
1:D:595:THR:HA	1:D:596:PRO:C	2.29	0.58
1:B:230:ARG:HH11	1:B:230:ARG:HG2	1.69	0.58
1:A:354:VAL:CG1	1:A:379:MET:HE3	2.34	0.57
1:C:347:LYS:HE3	1:C:643:LEU:HB3	1.86	0.57
1:B:991:MET:HE3	1:B:1003:VAL:HG21	1.85	0.57
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.86	0.57
1:B:367:MET:HB3	1:B:372:MET:HE2	1.87	0.56
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.04	0.56
1:D:786:ARG:NH2	1:D:991:MET:HE2	2.19	0.56
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.17	0.56
1:C:200:GLN:HB2	1:C:202:MET:HE2	1.88	0.56
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.88	0.56
1:C:354:VAL:HG23	1:C:567:VAL:HB	1.88	0.56
1:B:200:GLN:HG2	1:B:391:HIS:HB2	1.87	0.56
1:D:833:ALA:HB2	1:D:859:ASP:HB3	1.87	0.56
1:C:304:GLU:HG2	1:C:642:TYR:CD2	2.40	0.55
1:D:553:TRP:CZ2	1:D:624:GLN:HG2	2.42	0.55
1:B:251:ARG:H	1:B:254:LEU:HD12	1.71	0.55
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.41	0.55
1:D:656:VAL:HG21	1:D:685:LEU:HD22	1.87	0.55
1:A:623:GLN:NE2	4:A:8002:DMS:H12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:LEU:HD12	1:B:833:ALA:HB3	1.89	0.55
1:D:788:PRO:HD2	1:D:968:MET:HB2	1.89	0.55
1:A:882:ILE:HD13	1:A:1014:TYR:CD1	2.41	0.54
1:C:769:TRP:NE1	1:C:774:LYS:HG3	2.23	0.54
1:B:315:LEU:HG	1:B:323:ILE:HD12	1.89	0.54
1:B:749:ILE:N	1:B:749:ILE:HD13	2.23	0.54
1:B:615:PRO:O	1:B:618:THR:HG22	2.08	0.54
1:D:945:ASN:OD1	1:D:950:GLN:HG3	2.08	0.53
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.90	0.53
1:D:873:ALA:O	1:D:876:THR:HG22	2.09	0.53
1:C:304:GLU:HG2	1:C:642:TYR:HD2	1.73	0.53
1:D:780:LEU:HA	1:D:886:CYS:HB3	1.90	0.53
1:B:536:CYS:O	1:B:537:GLU:HG3	2.09	0.53
1:D:622:HIS:O	1:D:625:GLN:HG3	2.08	0.52
1:D:854:LYS:HA	1:D:867:THR:O	2.09	0.52
1:C:106:PRO:HG3	1:C:204:ARG:HG3	1.90	0.52
1:D:246:MET:HG3	1:D:287:ASP:O	2.09	0.52
1:A:525:SER:O	1:B:561:ARG:HD3	2.10	0.52
1:B:782:ASP:HB2	1:B:842:TRP:CZ2	2.45	0.52
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.45	0.52
1:D:682:LEU:HD13	1:D:685:LEU:HD21	1.91	0.52
1:A:730:LEU:HD11	1:B:823:LEU:O	2.10	0.51
1:D:867:THR:HG23	1:D:1015:HIS:CE1	2.45	0.51
1:B:814:GLY:HA3	1:B:844:HIS:CD2	2.44	0.51
1:A:52:ARG:O	1:A:213:SER:HB2	2.10	0.51
1:D:353:GLY:HA2	1:D:386:ALA:O	2.11	0.51
1:B:380:LYS:O	4:B:8002:DMS:H11	2.10	0.51
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.45	0.51
1:D:500:CYS:HA	1:D:534:ILE:O	2.11	0.51
1:B:694:LEU:HB2	1:B:723:ALA:O	2.11	0.51
1:B:92:MET:HE1	1:B:575:LEU:HD13	1.93	0.51
1:B:277:GLU:CD	1:B:277:GLU:H	2.19	0.51
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.76	0.51
1:B:768:MET:HE1	1:B:1020:TRP:CZ2	2.46	0.51
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.46	0.50
1:C:786:ARG:NH2	1:C:991:MET:HE2	2.26	0.50
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.93	0.50
1:D:168:PRO:O	1:D:442:ARG:NH2	2.45	0.50
1:D:54:LEU:HD11	1:D:214:LEU:HD13	1.92	0.50
1:C:150:PHE:HA	1:C:187:MET:O	2.12	0.50
1:C:525:SER:O	1:D:561:ARG:HD3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.94	0.49
1:C:43:ARG:HH12	1:C:264:GLU:CD	2.20	0.49
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.47	0.49
1:C:251:ARG:H	1:C:254:LEU:HD12	1.78	0.49
1:C:579:ASP:OD1	1:C:583:ASN:HB2	2.12	0.49
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.94	0.49
1:C:330:VAL:HG22	5:C:4081:HOH:O	2.12	0.49
1:A:782:ASP:OD1	1:A:842:TRP:HH2	1.96	0.49
1:C:694:LEU:HD12	1:C:723:ALA:HB3	1.93	0.49
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.48	0.49
1:A:487:GLU:OE1	1:A:502:MET:HE3	2.13	0.49
1:D:88:SER:HA	1:D:366:VAL:HG21	1.95	0.49
1:D:270:GLY:HA3	4:D:8002:DMS:H13	1.93	0.49
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.95	0.48
1:C:573:GLN:HB2	1:C:602:CYS:O	2.13	0.48
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.48	0.48
1:D:60:PHE:HA	1:D:122:CYS:O	2.14	0.48
1:D:471:LEU:O	1:D:475:ILE:HG13	2.13	0.48
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.13	0.48
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.96	0.48
1:B:908:ASP:OD1	1:B:993:ILE:HG12	2.13	0.48
1:C:883:GLY:HA3	1:C:987:ASP:HA	1.95	0.48
1:D:147:ASN:HA	1:D:148:SER:HA	1.58	0.48
1:A:747:PHE:HB2	1:A:758:PHE:HB2	1.96	0.48
1:C:854:LYS:HG2	1:C:868:VAL:HG13	1.96	0.48
1:A:457:SER:HA	1:A:485:GLN:O	2.13	0.47
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.95	0.47
1:C:373:VAL:O	1:C:377:LEU:HG	2.14	0.47
1:A:245:GLN:HG3	1:A:288:ARG:HG2	1.95	0.47
1:A:864:MET:HE3	1:A:866:ILE:HD11	1.96	0.47
1:B:607:VAL:HG12	1:B:613:PRO:HA	1.95	0.47
1:B:745:MET:HE3	1:B:745:MET:H	1.79	0.47
1:A:37:ARG:HG2	1:A:50:GLN:NE2	2.29	0.47
1:D:756:TRP:HB3	1:D:758:PHE:HE1	1.80	0.47
1:D:546:LEU:HD22	1:D:616:ALA:HB1	1.95	0.47
1:A:847:LYS:NZ	1:B:724:GLU:O	2.48	0.47
1:D:629:PHE:HB3	1:D:720:TRP:HH2	1.80	0.47
1:D:867:THR:HG23	1:D:1015:HIS:HE1	1.80	0.47
1:B:656:VAL:HG21	1:B:685:LEU:HD21	1.95	0.47
1:B:824:GLN:HB3	1:B:839:ALA:HB3	1.97	0.47
1:D:310:ARG:NH1	1:D:329:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.96	0.47
1:C:606:LEU:O	1:C:614:HIS:HB2	2.15	0.47
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.97	0.46
1:C:804:ASN:OD1	1:C:809:ARG:NH2	2.48	0.46
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.46
1:C:168:PRO:HD3	1:C:446:ARG:HH11	1.80	0.46
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.50	0.46
1:B:749:ILE:N	1:B:749:ILE:CD1	2.79	0.46
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.50	0.46
1:A:830:LEU:HD12	1:A:833:ALA:HB3	1.98	0.46
1:D:907:PRO:HA	1:D:910:LEU:HD23	1.97	0.46
1:C:769:TRP:HE1	1:C:774:LYS:HG3	1.80	0.46
1:D:410:VAL:HG22	1:D:455:ILE:HB	1.98	0.46
1:B:347:LYS:HB3	1:B:643:LEU:HD22	1.97	0.46
1:A:424:ASN:OD1	1:D:279:ILE:HD11	2.16	0.46
1:A:984:LEU:HD21	1:A:986:ILE:HD11	1.97	0.46
1:C:749:ILE:HD11	1:C:836:ILE:HD11	1.97	0.46
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.51	0.46
1:C:863:GLN:HG2	1:C:1021:CYS:CB	2.46	0.46
1:C:864:MET:HE3	1:C:866:ILE:HD11	1.97	0.46
1:D:257:THR:HA	1:D:270:GLY:O	2.16	0.46
1:A:573:GLN:HB2	1:A:602:CYS:O	2.16	0.45
1:D:499:ILE:HD11	1:D:529:GLU:CD	2.41	0.45
1:B:589:GLY:O	1:B:599:ARG:HA	2.16	0.45
1:B:820:ALA:HB2	1:B:842:TRP:NE1	2.30	0.45
1:C:225:PHE:HA	1:C:243:GLU:O	2.16	0.45
1:C:460:SER:O	1:C:461:GLU:C	2.59	0.45
1:D:613:PRO:HB3	1:D:617:LEU:HD23	1.99	0.45
1:D:693:GLN:HG2	1:D:695:TRP:NE1	2.31	0.45
1:D:786:ARG:HH21	1:D:991:MET:HE2	1.79	0.45
1:B:741:THR:HB	1:B:748:CYS:HB3	1.96	0.45
1:C:542:MET:HE3	1:C:601:PHE:HA	1.97	0.45
1:C:824:GLN:HB3	1:C:839:ALA:HB3	1.99	0.45
1:A:424:ASN:HB3	1:A:463:GLY:HA3	1.97	0.45
1:A:898:LEU:HG	1:A:915:PHE:CZ	2.51	0.45
1:D:244:VAL:HG21	1:D:256:VAL:HG11	1.98	0.45
1:B:163:GLN:O	1:B:164:ASP:HB3	2.17	0.45
1:C:166:ARG:HD3	1:C:209:PHE:HZ	1.81	0.45
1:D:163:GLN:O	1:D:164:ASP:HB3	2.15	0.45
1:D:996:ASP:HB2	1:D:1002:SER:HB2	1.98	0.45
1:B:251:ARG:HD2	1:B:253:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:MET:CE	1:D:387:VAL:HB	2.46	0.45
1:A:336:ARG:HH21	1:A:338:GLU:CD	2.24	0.45
1:B:30:HIS:HE2	1:B:170:GLU:CD	2.25	0.45
1:B:301:TRP:CH2	1:B:452:SER:HA	2.51	0.45
1:C:226:HIS:ND1	1:C:448:ARG:CD	2.70	0.45
1:C:431:ARG:NH1	5:C:4073:HOH:O	2.49	0.45
1:C:887:GLN:NE2	1:C:980:GLU:O	2.49	0.45
1:D:390:SER:HA	1:D:391:HIS:HA	1.69	0.45
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.51	0.45
1:B:410:VAL:HG22	1:B:455:ILE:HB	1.99	0.45
1:B:569:ASP:O	1:B:605:GLY:HA2	2.17	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.58	0.45
1:C:822:LEU:HD11	1:C:825:CYS:HB2	1.99	0.45
1:D:615:PRO:O	1:D:618:THR:CG2	2.62	0.45
1:B:376:ILE:HD13	1:B:401:LEU:HB3	1.99	0.45
1:A:149:ALA:HB2	1:A:163:GLN:HG2	1.99	0.44
1:A:595:THR:HA	1:A:596:PRO:C	2.42	0.44
1:C:153:TRP:CD1	1:C:158:TRP:HA	2.52	0.44
1:C:770:ILE:O	1:C:770:ILE:HG22	2.16	0.44
1:C:782:ASP:HA	1:C:884:LEU:HD23	1.98	0.44
1:D:292:ARG:O	4:D:8002:DMS:H12	2.17	0.44
1:B:610:ASP:O	1:B:611:ARG:HB2	2.18	0.44
1:C:882:ILE:O	1:C:882:ILE:HG22	2.18	0.44
1:C:945:ASN:OD1	1:C:950:GLN:HG3	2.17	0.44
1:C:656:VAL:HG21	1:C:685:LEU:HD22	2.00	0.44
1:B:277:GLU:HG3	5:B:4091:HOH:O	2.17	0.44
1:C:930:VAL:O	1:C:932:PRO:HD3	2.17	0.44
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.83	0.44
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.99	0.44
1:B:49:GLN:HB2	1:B:50:GLN:OE1	2.18	0.44
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.79	0.44
1:B:333:ARG:HG2	1:B:333:ARG:NH1	2.33	0.44
1:C:749:ILE:HG12	1:C:834:VAL:HG11	2.00	0.43
1:D:763:GLY:O	1:D:840:HIS:CE1	2.71	0.43
1:B:930:VAL:O	1:B:932:PRO:HD3	2.17	0.43
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.53	0.43
1:A:820:ALA:HB2	1:A:842:TRP:NE1	2.33	0.43
1:D:43:ARG:HD2	1:D:261:TRP:CD2	2.53	0.43
1:D:319:ASP:HB2	5:D:4088:HOH:O	2.18	0.43
1:A:200:GLN:HG2	1:A:391:HIS:HB2	1.99	0.43
1:C:414:ASN:O	1:C:439:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:HIS:O	1:D:242:ALA:HA	2.18	0.43
1:D:747:PHE:HB2	1:D:758:PHE:HB2	2.00	0.43
1:B:433:LEU:N	1:B:434:PRO:CD	2.80	0.43
1:B:872:VAL:HG11	1:B:879:PRO:HD3	2.01	0.43
1:A:460:SER:O	1:A:461:GLU:C	2.62	0.43
1:C:358:GLU:HG2	1:C:367:MET:HG3	2.01	0.43
1:A:305:ILE:HD11	1:A:645:ARG:HB3	2.00	0.43
1:C:444:VAL:O	1:C:448:ARG:HB3	2.18	0.43
1:C:595:THR:HA	1:C:596:PRO:C	2.44	0.43
1:C:390:SER:HB2	1:C:391:HIS:CE1	2.52	0.43
1:A:997:ASP:HB2	1:A:999:TRP:CE2	2.53	0.43
1:C:226:HIS:CE1	1:C:448:ARG:HH11	2.37	0.43
1:C:282:ARG:HG2	1:B:423:MET:HE2	2.01	0.43
1:A:354:VAL:HG12	1:A:379:MET:HE3	2.00	0.43
1:C:863:GLN:HG2	1:C:1021:CYS:HB3	2.00	0.43
1:B:894:ARG:NH1	1:B:921:PRO:HD3	2.33	0.43
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.54	0.43
1:D:446:ARG:HD2	5:D:4142:HOH:O	2.18	0.43
1:B:879:PRO:O	1:B:1009:LEU:HD12	2.18	0.43
1:C:78:LEU:HA	1:C:79:PRO:HD3	1.87	0.42
1:C:124:SER:HA	1:C:184:LEU:O	2.19	0.42
1:C:359:HIS:CD2	1:C:573:GLN:HA	2.54	0.42
1:A:634:GLN:HB2	1:A:682:LEU:HB2	2.01	0.42
1:A:869:ASP:CG	1:A:1015:HIS:HD1	2.27	0.42
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.54	0.42
1:D:991:MET:HE3	1:D:1003:VAL:HG21	2.01	0.42
1:B:736:ALA:HB1	1:B:751:LEU:HD11	2.00	0.42
1:C:147:ASN:HA	1:C:148:SER:HA	1.59	0.42
1:C:536:CYS:O	1:C:537:GLU:HG3	2.20	0.42
1:B:765:LEU:HD21	1:B:768:MET:HE2	2.02	0.42
1:A:454:ILE:HG13	1:A:455:ILE:HG13	2.01	0.42
1:C:881:ARG:HE	1:C:987:ASP:CG	2.26	0.42
1:A:359:HIS:CD2	1:A:573:GLN:HA	2.55	0.42
1:C:986:ILE:HG21	1:C:1018:LEU:HD11	2.02	0.42
1:D:125:LEU:HD11	4:D:8004:DMS:H13	2.00	0.42
1:B:854:LYS:HA	1:B:867:THR:O	2.20	0.42
1:A:794:GLY:HA2	1:A:998:SER:O	2.20	0.42
1:A:878:HIS:HD2	5:A:4165:HOH:O	2.01	0.42
1:C:222:ILE:N	1:C:324:GLU:OE1	2.49	0.42
1:C:996:ASP:HB2	1:C:1002:SER:HB2	2.02	0.42
1:D:304:GLU:C	1:D:305:ILE:HG13	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.01	0.42
1:B:481:SER:HA	4:B:8003:DMS:H11	2.01	0.42
1:A:355:ASN:O	1:A:569:ASP:HB2	2.19	0.42
1:C:907:PRO:HG2	1:C:990:HIS:O	2.20	0.42
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.84	0.42
1:C:281:GLU:HG3	1:B:515:VAL:HG21	2.02	0.42
1:C:353:GLY:HA2	1:C:386:ALA:O	2.20	0.42
1:C:522:LYS:HA	1:D:559:TYR:CE2	2.55	0.42
1:B:367:MET:HE2	1:B:367:MET:HA	2.02	0.42
1:B:744:GLU:HB3	1:B:745:MET:HE3	2.01	0.42
1:B:747:PHE:HB2	1:B:758:PHE:HB2	2.00	0.42
1:B:755:ARG:HB3	1:B:769:TRP:HB2	2.01	0.42
1:B:864:MET:HE3	1:B:866:ILE:HD11	2.02	0.42
1:C:499:ILE:O	1:C:533:LEU:HA	2.20	0.42
1:D:361:PRO:HB3	1:D:609:ALA:HB1	2.02	0.42
1:D:536:CYS:O	1:D:537:GLU:HG3	2.20	0.42
1:D:737:ILE:HA	1:D:738:PRO:HD3	1.89	0.42
1:B:599:ARG:HB2	1:B:600:GLN:NE2	2.35	0.42
1:A:291:LEU:HA	4:A:8004:DMS:O	2.20	0.41
1:A:477:SER:OG	1:D:469:ASP:OD2	2.38	0.41
1:C:92:MET:HE2	1:C:92:MET:HA	2.02	0.41
1:D:738:PRO:HB2	1:D:834:VAL:HG23	2.02	0.41
1:C:464:HIS:HB2	1:C:489:GLY:HA3	2.02	0.41
1:D:629:PHE:HB3	1:D:720:TRP:CH2	2.55	0.41
1:B:390:SER:HA	1:B:391:HIS:HA	1.74	0.41
1:D:437:SER:CB	1:D:471:LEU:HD21	2.49	0.41
1:D:844:HIS:HA	5:D:4126:HOH:O	2.19	0.41
1:C:18:ASN:ND2	1:C:21:VAL:HG23	2.35	0.41
1:B:78:LEU:HA	1:B:79:PRO:HD3	1.84	0.41
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.56	0.41
1:D:780:LEU:HD11	1:D:884:LEU:HD13	2.02	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.75	0.41
1:D:123:TYR:CE1	1:D:208:ILE:HG13	2.56	0.41
1:C:796:SER:HB2	1:C:802:ASP:HB3	2.03	0.41
1:C:830:LEU:HD23	1:D:830:LEU:HD21	2.03	0.41
1:C:929:TYR:O	1:C:930:VAL:C	2.64	0.41
1:D:78:LEU:HA	1:D:79:PRO:HD3	1.92	0.41
1:A:556:PHE:CD1	1:A:564:GLY:HA2	2.56	0.41
1:D:144:ASP:OD1	1:D:168:PRO:HB3	2.21	0.41
1:D:650:GLU:HB3	1:D:670:LEU:HD12	2.03	0.41
1:A:270:GLY:CA	4:A:8004:DMS:H23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:SER:HA	1:A:391:HIS:HA	1.71	0.41
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.56	0.41
1:C:594:ASP:OD1	1:C:594:ASP:N	2.43	0.41
1:D:751:LEU:HD11	1:D:860:GLY:HA2	2.03	0.41
1:B:426:LEU:HD22	1:B:432:TRP:CE2	2.56	0.41
1:B:748:CYS:C	1:B:749:ILE:HD13	2.46	0.41
1:C:200:GLN:CG	1:C:391:HIS:HB2	2.51	0.41
1:C:426:LEU:HD22	1:C:432:TRP:CE2	2.56	0.41
1:C:782:ASP:HB2	1:C:842:TRP:CZ2	2.56	0.41
1:A:257:THR:HA	1:A:270:GLY:O	2.21	0.40
1:A:337:ILE:HA	1:A:341:LEU:O	2.21	0.40
1:C:296:GLU:O	1:C:297:ASN:C	2.65	0.40
1:B:147:ASN:HA	1:B:148:SER:HA	1.70	0.40
1:A:58:TRP:CD1	1:A:125:LEU:HD13	2.55	0.40
1:D:568:TRP:HA	1:D:569:ASP:HA	1.91	0.40
1:C:379:MET:HE1	1:C:387:VAL:HB	2.02	0.40
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.03	0.40
1:D:767:GLN:OE1	1:D:775:GLN:N	2.47	0.40
1:B:785:THR:HB	1:B:816:TYR:CE2	2.56	0.40
1:B:962:TYR:CE2	1:B:976:LEU:HB3	2.57	0.40
1:A:883:GLY:HA3	1:A:987:ASP:HA	2.04	0.40
1:C:352:ARG:HG2	1:C:553:TRP:CH2	2.57	0.40
1:C:450:HIS:HA	1:C:451:PRO:HD2	1.97	0.40
1:C:936:GLY:O	1:C:938:ARG:NH1	2.51	0.40
1:D:963:SER:C	1:D:965:GLN:N	2.79	0.40
1:A:738:PRO:HB2	1:A:834:VAL:HG23	2.04	0.40
1:C:578:TYR:HA	1:C:583:ASN:O	2.22	0.40
1:C:869:ASP:OD2	1:C:1015:HIS:ND1	2.34	0.40
1:D:513:PRO:O	1:D:514:ALA:HB3	2.22	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%)	972 (96%)	37 (4%)	0	100	100
1	B	1009/1052 (96%)	965 (96%)	41 (4%)	3 (0%)	36	60
1	C	1009/1052 (96%)	947 (94%)	56 (6%)	6 (1%)	21	44
1	D	1009/1052 (96%)	935 (93%)	74 (7%)	0	100	100
All	All	4036/4208 (96%)	3819 (95%)	208 (5%)	9 (0%)	43	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	461	GLU
1	C	659	ASP
1	C	722	LEU
1	B	916	ASP
1	B	540	HIS
1	C	633	GLY
1	C	540	HIS
1	B	263	GLY
1	C	364	GLY

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%)	42	71
1	B	864/898 (96%)	836 (97%)	28 (3%)	34	64
1	C	864/898 (96%)	845 (98%)	19 (2%)	45	74
1	D	864/898 (96%)	838 (97%)	26 (3%)	36	66
All	All	3456/3592 (96%)	3361 (97%)	95 (3%)	39	69

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	131	GLU

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Mol	Chain	Res	Type
1	A	136	GLU
1	A	178	ARG
1	A	189	LEU
1	A	214	LEU
1	A	262	GLN
1	A	477	SER
1	A	519	SER
1	A	546	LEU
1	A	604	ASN
1	A	634	GLN
1	A	651	LEU
1	A	661	LYS
1	A	665	SER
1	A	675	GLN
1	A	737	ILE
1	A	768	MET
1	A	774	LYS
1	A	824	GLN
1	A	885	ASN
1	A	956	GLN
1	C	44	THR
1	C	186	VAL
1	C	219	THR
1	C	223	SER
1	C	297	ASN
1	C	335	VAL
1	C	362	LEU
1	C	546	LEU
1	C	646	HIS
1	C	651	LEU
1	C	672	VAL
1	C	728	VAL
1	C	737	ILE
1	C	745	MET
1	C	746	ASP
1	C	848	THR
1	C	868	VAL
1	C	885	ASN
1	C	966	GLN
1	D	178	ARG
1	D	214	LEU
1	D	241	GLU

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Mol	Chain	Res	Type
1	D	245	GLN
1	D	279	ILE
1	D	362	LEU
1	D	478	VAL
1	D	545	SER
1	D	546	LEU
1	D	635	THR
1	D	646	HIS
1	D	651	LEU
1	D	655	MET
1	D	672	VAL
1	D	675	GLN
1	D	690	SER
1	D	737	ILE
1	D	745	MET
1	D	748	CYS
1	D	751	LEU
1	D	772	ASP
1	D	837	THR
1	D	848	THR
1	D	855	THR
1	D	858	ILE
1	D	984	LEU
1	B	71	GLU
1	B	124	SER
1	B	136	GLU
1	B	178	ARG
1	B	186	VAL
1	B	219	THR
1	B	230	ARG
1	B	321	THR
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
1	B	438	GLU
1	B	519	SER
1	B	546	LEU
1	B	594	ASP
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	656	VAL

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Mol	Chain	Res	Type
1	B	675	GLN
1	B	728	VAL
1	B	745	MET
1	B	749	ILE
1	B	809	ARG
1	B	855	THR
1	B	876	THR
1	B	956	GLN
1	B	984	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	128	ASN
1	A	226	HIS
1	A	266	GLN
1	A	307	ASN
1	A	374	GLN
1	A	624	GLN
1	A	702	GLN
1	A	718	GLN
1	A	843	GLN
1	A	950	GLN
1	C	135	GLN
1	C	245	GLN
1	C	266	GLN
1	C	445	GLN
1	C	623	GLN
1	C	693	GLN
1	C	739	HIS
1	C	783	GLN
1	C	824	GLN
1	C	878	HIS
1	C	885	ASN
1	D	89	ASN
1	D	128	ASN
1	D	294	ASN
1	D	540	HIS
1	D	622	HIS
1	D	646	HIS
1	D	675	GLN

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Mol	Chain	Res	Type
1	D	704	ASN
1	D	783	GLN
1	D	903	GLN
1	D	990	HIS
1	B	445	GLN
1	B	628	GLN
1	B	757	GLN
1	B	775	GLN
1	B	817	GLN
1	B	844	HIS
1	B	945	ASN
1	B	950	GLN
1	B	1015	HIS
1	B	1022	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 43 ligands modelled in this entry, 19 are monoatomic - leaving 24 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	C	8004	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
4	DMS	D	8004	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
4	DMS	C	8002	-	3,3,3	2.73	1 (33%)	3,3,3	0.64	0
4	DMS	A	8007	-	3,3,3	2.79	1 (33%)	3,3,3	0.72	0
4	DMS	D	8006	-	3,3,3	2.77	1 (33%)	3,3,3	0.54	0
4	DMS	B	8002	-	3,3,3	2.71	1 (33%)	3,3,3	0.52	0
4	DMS	B	8003	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
4	DMS	A	8008	-	3,3,3	2.73	1 (33%)	3,3,3	0.59	0
4	DMS	D	8002	-	3,3,3	2.67	1 (33%)	3,3,3	0.40	0
4	DMS	C	8006	-	3,3,3	2.80	1 (33%)	3,3,3	0.68	0
4	DMS	A	8003	-	3,3,3	2.71	1 (33%)	3,3,3	0.72	0
4	DMS	B	8001	-	3,3,3	2.75	1 (33%)	3,3,3	0.65	0
4	DMS	A	8006	-	3,3,3	2.79	1 (33%)	3,3,3	0.66	0
4	DMS	A	8005	-	3,3,3	2.76	1 (33%)	3,3,3	0.60	0
4	DMS	A	8001	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
4	DMS	C	8003	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
4	DMS	A	8002	-	3,3,3	2.61	1 (33%)	3,3,3	0.44	0
4	DMS	A	8004	-	3,3,3	2.67	1 (33%)	3,3,3	0.69	0
4	DMS	D	8005	-	3,3,3	2.64	1 (33%)	3,3,3	0.61	0
4	DMS	B	8004	-	3,3,3	1.69	1 (33%)	3,3,3	0.37	0
4	DMS	C	8001	-	3,3,3	2.72	1 (33%)	3,3,3	0.63	0
4	DMS	D	8003	-	3,3,3	2.75	1 (33%)	3,3,3	0.48	0
4	DMS	D	8001	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
4	DMS	C	8005	-	3,3,3	2.74	1 (33%)	3,3,3	0.61	0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8007	DMS	O-S	4.68	1.81	1.50
4	C	8006	DMS	O-S	4.68	1.81	1.50
4	A	8006	DMS	O-S	4.67	1.81	1.50
4	A	8005	DMS	O-S	4.65	1.80	1.50
4	D	8006	DMS	O-S	4.64	1.80	1.50
4	D	8003	DMS	O-S	4.62	1.80	1.50
4	C	8002	DMS	O-S	4.61	1.80	1.50
4	D	8001	DMS	O-S	4.61	1.80	1.50
4	B	8001	DMS	O-S	4.60	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8005	DMS	O-S	4.59	1.80	1.50
4	A	8008	DMS	O-S	4.58	1.80	1.50
4	C	8003	DMS	O-S	4.57	1.80	1.50
4	A	8003	DMS	O-S	4.56	1.80	1.50
4	B	8003	DMS	O-S	4.56	1.80	1.50
4	C	8001	DMS	O-S	4.55	1.80	1.50
4	B	8002	DMS	O-S	4.55	1.80	1.50
4	D	8004	DMS	O-S	4.54	1.80	1.50
4	C	8004	DMS	O-S	4.52	1.80	1.50
4	A	8001	DMS	O-S	4.52	1.80	1.50
4	D	8002	DMS	O-S	4.51	1.80	1.50
4	A	8004	DMS	O-S	4.46	1.79	1.50
4	A	8002	DMS	O-S	4.41	1.79	1.50
4	D	8005	DMS	O-S	4.41	1.79	1.50
4	B	8004	DMS	O-S	2.88	1.69	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	8004	DMS	1	0
4	C	8002	DMS	2	0
4	B	8002	DMS	1	0
4	B	8003	DMS	1	0
4	D	8002	DMS	2	0
4	A	8005	DMS	1	0
4	A	8002	DMS	1	0
4	A	8004	DMS	3	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%)	0.05	26 (2%) 57 54	24, 43, 79, 114	0
1	B	1011/1052 (96%)	0.27	19 (1%) 66 63	28, 51, 75, 111	0
1	C	1011/1052 (96%)	0.50	52 (5%) 33 29	30, 56, 87, 123	0
1	D	1011/1052 (96%)	0.43	90 (8%) 15 13	27, 48, 94, 127	0
All	All	4044/4208 (96%)	0.32	187 (4%) 37 34	24, 50, 84, 127	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	737	ILE	5.3
1	D	770	ILE	4.8
1	D	740	LEU	4.5
1	D	745	MET	4.4
1	D	771	GLY	4.2
1	D	742	THR	4.2
1	A	689	GLU	4.1
1	D	758	PHE	4.1
1	C	730	LEU	4.1
1	D	732	ALA	3.8
1	D	861	SER	3.8
1	D	834	VAL	3.7
1	C	865	ALA	3.6
1	D	767	GLN	3.5
1	D	839	ALA	3.5
1	D	744	GLU	3.5
1	D	769	TRP	3.5
1	D	835	LEU	3.5
1	C	739	HIS	3.5
1	C	688	PRO	3.5
1	D	117	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	663	LEU	3.4
1	D	733	ALA	3.4
1	A	688	PRO	3.4
1	D	738	PRO	3.4
1	D	860	GLY	3.4
1	A	733	ALA	3.3
1	B	692	GLY	3.3
1	B	733	ALA	3.3
1	A	772	ASP	3.3
1	C	772	ASP	3.3
1	D	757	GLN	3.3
1	D	822	LEU	3.3
1	D	820	ALA	3.3
1	D	747	PHE	3.3
1	D	829	THR	3.2
1	D	827	ALA	3.2
1	D	686	PRO	3.1
1	A	663	LEU	3.1
1	C	732	ALA	3.1
1	D	736	ALA	3.1
1	D	748	CYS	3.1
1	C	690	SER	3.0
1	D	828	ASP	3.0
1	C	829	THR	3.0
1	D	981	GLY	3.0
1	C	175	ALA	3.0
1	D	735	HIS	2.9
1	B	820	ALA	2.9
1	C	740	LEU	2.9
1	C	758	PHE	2.9
1	D	798	ALA	2.9
1	C	736	ALA	2.9
1	C	737	ILE	2.8
1	C	319	ASP	2.8
1	D	741	THR	2.8
1	D	841	ALA	2.8
1	A	686	PRO	2.8
1	D	756	TRP	2.8
1	A	747	PHE	2.8
1	D	765	LEU	2.8
1	C	733	ALA	2.8
1	D	833	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	731	PRO	2.7
1	D	836	ILE	2.7
1	A	731	PRO	2.7
1	B	686	PRO	2.7
1	A	730	LEU	2.7
1	D	818	ALA	2.7
1	D	826	THR	2.7
1	D	760	ARG	2.7
1	D	821	ALA	2.7
1	C	584	PRO	2.7
1	D	768	MET	2.7
1	D	94	GLY	2.7
1	A	664	ALA	2.7
1	A	774	LYS	2.7
1	C	662	PRO	2.7
1	D	823	LEU	2.6
1	D	857	ARG	2.6
1	A	827	ALA	2.6
1	C	68	ALA	2.6
1	C	129	VAL	2.6
1	D	774	LYS	2.6
1	C	686	PRO	2.6
1	D	731	PRO	2.6
1	D	855	THR	2.6
1	C	1023	LYS	2.6
1	C	179	ALA	2.6
1	D	759	ASN	2.6
1	B	799	THR	2.5
1	B	818	ALA	2.5
1	D	729	THR	2.5
1	D	982	THR	2.5
1	C	841	ALA	2.5
1	D	687	GLN	2.5
1	B	745	MET	2.5
1	C	132	SER	2.5
1	D	766	SER	2.5
1	D	782	ASP	2.5
1	B	362	LEU	2.5
1	A	729	THR	2.5
1	B	687	GLN	2.5
1	D	778	THR	2.4
1	C	749	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	770	ILE	2.4
1	D	850	PHE	2.4
1	C	685	LEU	2.4
1	D	749	ILE	2.4
1	B	685	LEU	2.4
1	D	840	HIS	2.4
1	A	685	LEU	2.4
1	D	730	LEU	2.4
1	D	889	ALA	2.4
1	A	744	GLU	2.4
1	D	752	GLY	2.4
1	C	738	PRO	2.3
1	C	687	GLN	2.3
1	D	763	GLY	2.3
1	A	728	VAL	2.3
1	C	657	ALA	2.3
1	B	831	ALA	2.3
1	C	83	THR	2.3
1	C	683	PRO	2.3
1	D	728	VAL	2.3
1	D	776	LEU	2.3
1	C	977	HIS	2.3
1	C	752	GLY	2.3
1	C	655	MET	2.3
1	D	690	SER	2.3
1	D	761	GLN	2.3
1	D	824	GLN	2.3
1	D	873	ALA	2.2
1	C	178	ARG	2.2
1	D	688	PRO	2.2
1	B	79	PRO	2.2
1	C	726	LEU	2.2
1	C	951	TRP	2.2
1	C	728	VAL	2.2
1	B	761	GLN	2.2
1	D	590	GLY	2.2
1	C	751	LEU	2.2
1	C	139	THR	2.2
1	A	779	PRO	2.2
1	A	690	SER	2.2
1	B	78	LEU	2.2
1	A	745	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	820	ALA	2.2
1	C	682	LEU	2.2
1	D	726	LEU	2.2
1	D	780	LEU	2.2
1	B	666	GLY	2.2
1	D	746	ASP	2.2
1	C	826	THR	2.1
1	C	861	SER	2.1
1	D	734	SER	2.1
1	D	866	ILE	2.1
1	D	764	PHE	2.1
1	B	60	PHE	2.1
1	C	157	ARG	2.1
1	B	431	ARG	2.1
1	D	779	PRO	2.1
1	C	691	ALA	2.1
1	D	892	ALA	2.1
1	A	778	THR	2.1
1	D	848	THR	2.1
1	C	891	VAL	2.1
1	D	1019	VAL	2.1
1	D	819	GLU	2.1
1	B	798	ALA	2.1
1	A	773	LYS	2.1
1	A	741	THR	2.1
1	D	864	MET	2.1
1	D	859	ASP	2.0
1	C	750	GLU	2.0
1	C	762	SER	2.0
1	C	134	LEU	2.0
1	D	135	GLN	2.0
1	D	975	LEU	2.0
1	A	977	HIS	2.0
1	C	840	HIS	2.0
1	D	76	CYS	2.0
1	A	818	ALA	2.0
1	D	743	SER	2.0
1	D	78	LEU	2.0
1	D	751	LEU	2.0
1	A	771	GLY	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
4	DMS	C	8001	4/4	0.81	0.24	75,77,79,80	0
4	DMS	C	8003	4/4	0.81	0.26	83,84,85,86	0
4	DMS	A	8008	4/4	0.84	0.21	81,82,83,86	0
4	DMS	C	8006	4/4	0.84	0.20	65,65,66,70	0
4	DMS	C	8005	4/4	0.87	0.20	63,64,64,65	0
3	NA	D	3101	1/1	0.88	0.17	55,55,55,55	0
4	DMS	B	8003	4/4	0.89	0.16	63,65,67,68	0
3	NA	C	3103	1/1	0.90	0.12	62,62,62,62	0
4	DMS	B	8004	4/4	0.90	0.17	43,46,46,46	0
3	NA	C	3101	1/1	0.91	0.10	57,57,57,57	0
4	DMS	D	8006	4/4	0.91	0.14	58,60,62,65	0
3	NA	B	3103	1/1	0.92	0.08	58,58,58,58	0
4	DMS	B	8001	4/4	0.92	0.16	64,66,67,70	0
3	NA	A	3103	1/1	0.92	0.13	59,59,59,59	0
4	DMS	D	8004	4/4	0.92	0.15	74,75,76,76	0
3	NA	B	3101	1/1	0.93	0.08	55,55,55,55	0
4	DMS	D	8003	4/4	0.94	0.16	66,67,68,69	0
4	DMS	A	8004	4/4	0.94	0.15	60,61,63,64	0
4	DMS	C	8004	4/4	0.94	0.16	53,54,55,56	0
2	MG	C	3001	1/1	0.95	0.07	42,42,42,42	0
4	DMS	C	8002	4/4	0.95	0.13	49,53,53,55	0
4	DMS	A	8005	4/4	0.95	0.12	56,56,57,60	0
3	NA	D	3102	1/1	0.95	0.06	34,34,34,34	0
4	DMS	A	8001	4/4	0.96	0.16	71,71,72,74	0
4	DMS	D	8005	4/4	0.96	0.14	53,56,57,61	0
3	NA	B	3102	1/1	0.96	0.08	35,35,35,35	0
3	NA	C	3102	1/1	0.96	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	D	8001	4/4	0.96	0.11	56,56,56,58	0
4	DMS	A	8007	4/4	0.96	0.13	57,58,59,67	0
2	MG	B	3002	1/1	0.97	0.08	56,56,56,56	0
3	NA	A	3101	1/1	0.97	0.05	51,51,51,51	0
4	DMS	A	8006	4/4	0.97	0.10	56,58,59,63	0
2	MG	C	3002	1/1	0.97	0.08	54,54,54,54	0
2	MG	D	3002	1/1	0.97	0.04	42,42,42,42	0
4	DMS	B	8002	4/4	0.97	0.08	58,59,61,62	0
4	DMS	A	8002	4/4	0.97	0.12	53,53,53,54	0
4	DMS	D	8002	4/4	0.97	0.11	58,62,62,63	0
2	MG	B	3001	1/1	0.98	0.04	50,50,50,50	0
2	MG	A	3002	1/1	0.99	0.05	43,43,43,43	0
2	MG	D	3001	1/1	0.99	0.03	39,39,39,39	0
2	MG	A	3001	1/1	0.99	0.02	51,51,51,51	0
4	DMS	A	8003	4/4	0.99	0.06	44,45,47,47	0
3	NA	A	3102	1/1	0.99	0.02	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.