



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:18 AM GMT

PDB ID : 3VD5
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 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/ValidationPDFNotes.html>

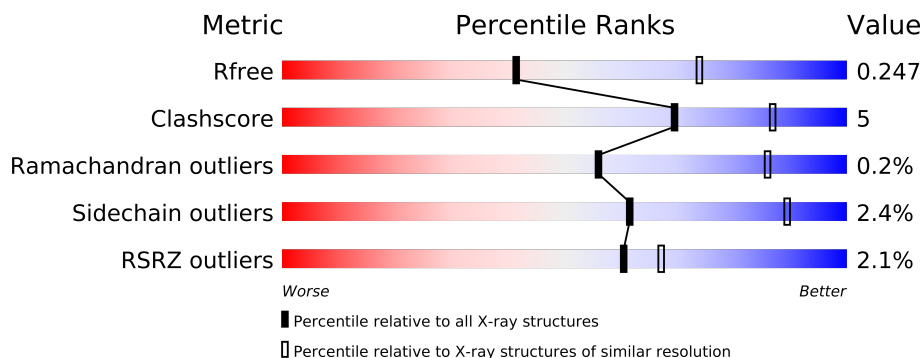
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1052	
1	B	1052	
1	C	1052	
1	D	1052	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	DMS	A	8001	-	X
4	DMS	A	8002	-	X
4	DMS	A	8003	-	X
4	DMS	A	8007	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	DMS	B	8003	-	X
4	DMS	C	8001	-	X
4	DMS	C	8002	-	X
4	DMS	C	8003	-	X
4	DMS	D	8002	-	X
4	DMS	D	8005	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33647 atoms, of which 0 are hydrogen and 0 are deuterium.

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

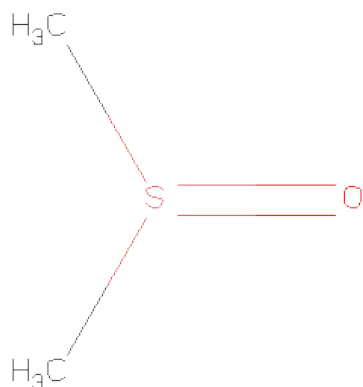
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- 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	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 C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is water.

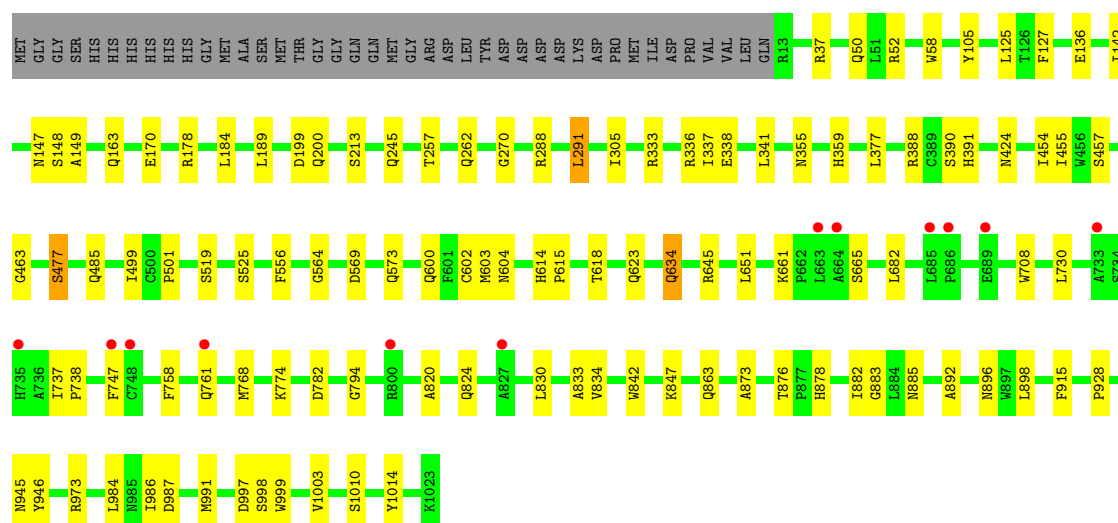
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	314	Total O 314 314	0	0
5	C	204	Total O 204 204	0	0
5	D	272	Total O 272 272	0	0
5	B	246	Total O 246 246	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

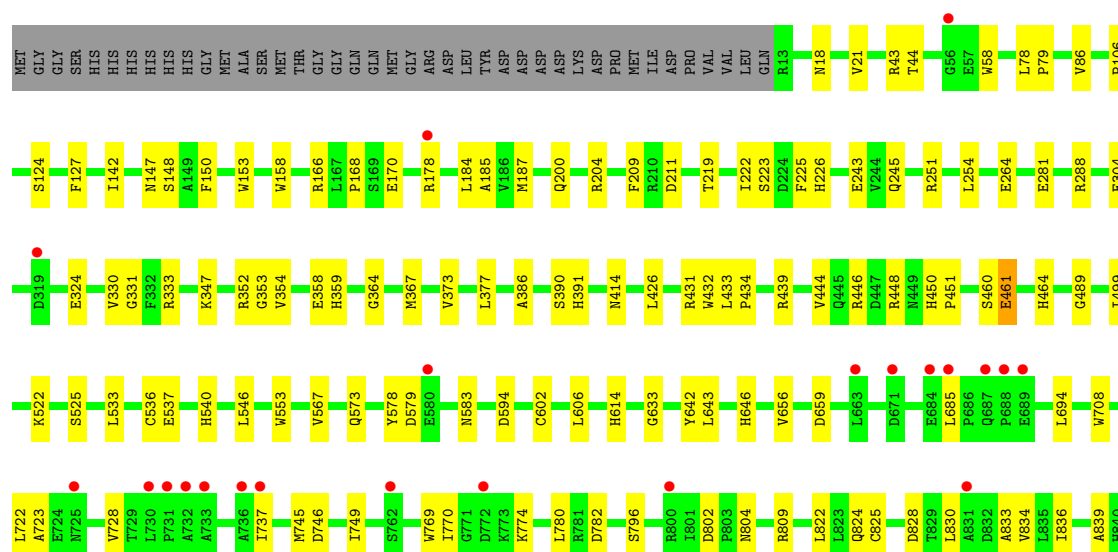
• Molecule 1: Beta-galactosidase

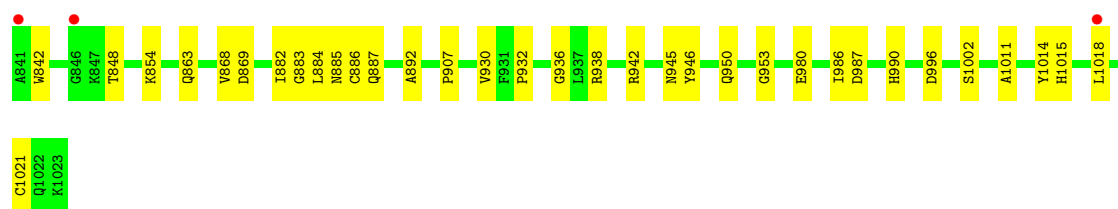
Chain A: 



• Molecule 1: Beta-galactosidase

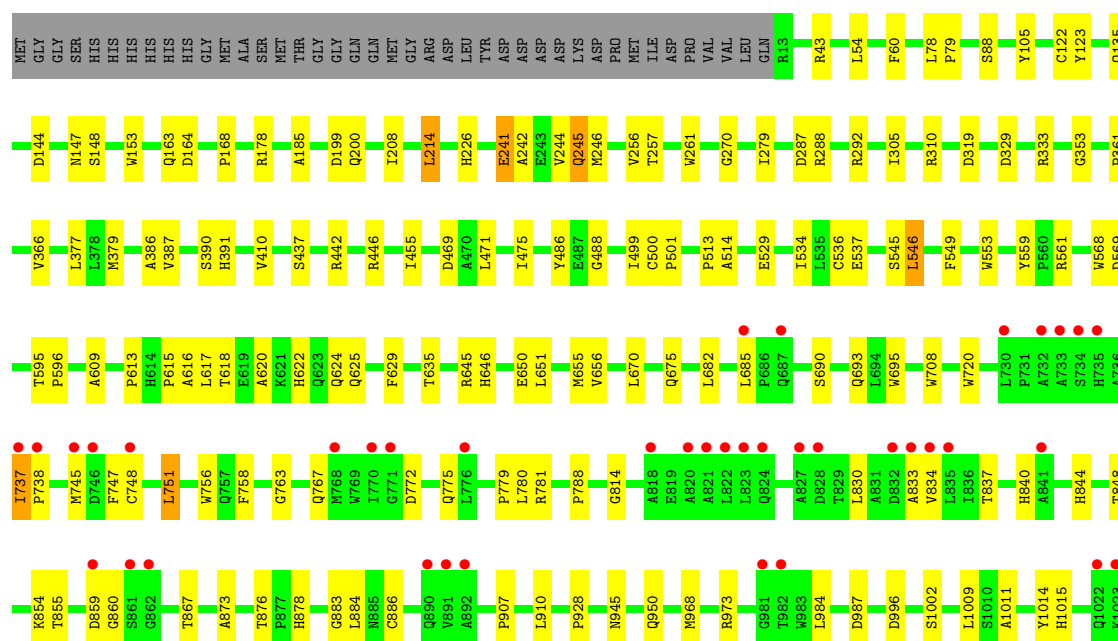
Chain C: 





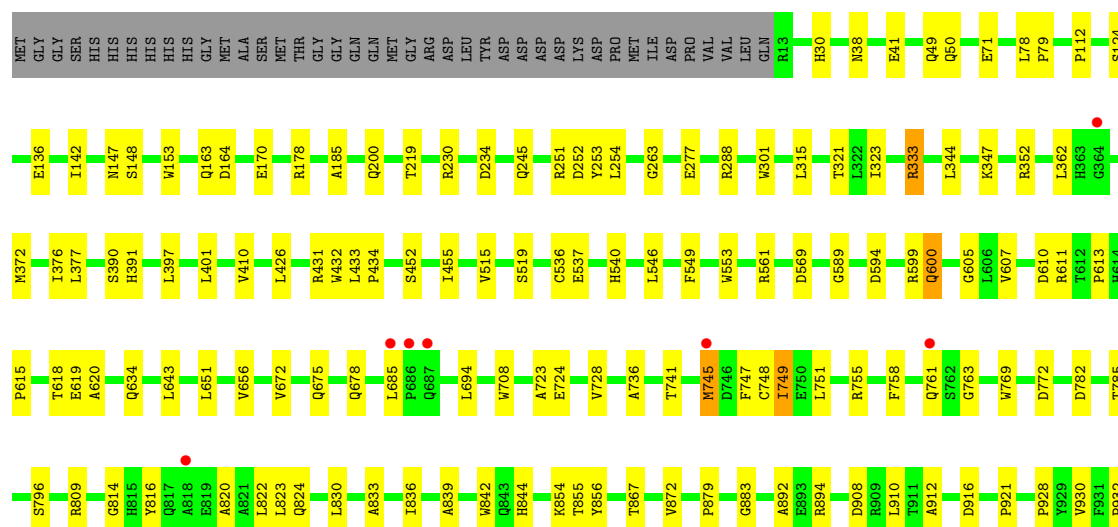
• Molecule 1: Beta-galactosidase

Chain D:



• Molecule 1: Beta-galactosidase

Chain B:





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) 81.2 (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	Depositor
R, R_{free}	0.203 , 0.276 0.217 , 0.247	Depositor DCC
R_{free} test set	5937 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 118682 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	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.

5 Model quality

5.1 Standard geometry

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	0.40	0/8366	0.56	1/11412 (0.0%)
1	B	0.38	0/8366	0.55	0/11412
1	C	0.37	0/8366	0.53	0/11412
1	D	0.39	0/8366	0.55	0/11412
All	All	0.39	0/33464	0.55	1/45648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	LEU	CA-CB-CG	5.33	127.57	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8124	0	7715	55	0
1	B	8124	0	7715	75	0
1	C	8124	0	7715	90	0
1	D	8124	0	7715	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	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	2	0
4	B	16	0	24	0	0
4	C	24	0	36	3	0
4	D	24	0	36	0	0
5	A	314	0	0	1	0
5	B	246	0	0	1	0
5	C	204	0	0	3	0
5	D	272	0	0	4	0
All	All	33647	0	31004	296	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (296) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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: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: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: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
1:C:58:TRP:CD1	1:C:86:VAL:HB	2.33	0.64
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:331:GLY:H	4:C:8002:DMS:H22	1.66	0.60
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: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:D:200:GLN:HG2	1:D:391:HIS:HB2	1.86	0.58
1:B:230:ARG:HG2	1:B:230:ARG:HH11	1.69	0.58
1:C:347:LYS:HE3	1:C:643:LEU:HB3	1.86	0.57
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.86	0.57
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.04	0.56
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.17	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: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:553:TRP:CZ2	1:D:624:GLN:HG2	2.42	0.55
1:D:656:VAL:HG21	1:D:685:LEU:HD22	1.87	0.55
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:595:THR:HA	1:D:596:PRO:C	2.29	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:B:372:MET:HE3	1:B:397:LEU:HD23	1.90	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:854:LYS:HA	1:D:867:THR:O	2.09	0.52
1:D:246:MET:HG3	1:D:287:ASP:O	2.09	0.52
1:C:106:PRO:HG3	1:C:204:ARG:HG3	1.90	0.52
1:B:782:ASP:HB2	1:B:842:TRP:CZ2	2.45	0.52
1:A:525:SER:O	1:B:561:ARG:HD3	2.10	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: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:730:LEU:HD11	1:B:823:LEU:O	2.10	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: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:A:623:GLN:NE2	4:A:8002:DMS:H11	2.25	0.51
1:B:694:LEU:HB2	1:B:723:ALA:O	2.11	0.51
1:B:333:ARG:HG2	1:B:333:ARG:HH11	1.76	0.51
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.46	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:D:153:TRP:HB2	1:D:185:ALA:HB3	1.94	0.49
1:C:525:SER:O	1:D:561:ARG:HD3	2.11	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:D:379:MET:HE1	1:D:387:VAL:HB	1.93	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:C:694:LEU:HD12	1:C:723:ALA:HB3	1.93	0.49
1:A:782:ASP:OD1	1:A:842:TRP:HH2	1.96	0.49
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.48	0.49
1:D:88:SER:HA	1:D:366:VAL:HG21	1.95	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:878:HIS:HB3	1:D:1009:LEU:O	2.13	0.48
1:A:991:MET:HE3	1:A:1003:VAL:HG21	1.94	0.48
1:D:471:LEU:O	1:D:475:ILE:HG13	2.13	0.48
1:B:908:ASP:OD1	1:B:993:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.96	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:991:MET:CE	1:A:1003:VAL:HG21	2.43	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:C:373:VAL:O	1:C:377:LEU:HG	2.14	0.47
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:A:245:GLN:HG3	1:A:288:ARG:HG2	1.95	0.47
1:B:607:VAL:HG12	1:B:613:PRO:HA	1.95	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:B:656:VAL:HG21	1:B:685:LEU:HD21	1.95	0.47
1:D:867:THR:HG23	1:D:1015:HIS:HE1	1.80	0.47
1:A:847:LYS:NZ	1:B:724:GLU:O	2.48	0.47
1:B:824:GLN:HB3	1:B:839:ALA:HB3	1.97	0.47
1:D:629:PHE:HB3	1:D:720:TRP:HH2	1.80	0.47
1:D:310:ARG:NH1	1:D:329:ASP:OD1	2.46	0.47
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:C:168:PRO:HD3	1:C:446:ARG:HH11	1.80	0.46
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.46
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.50	0.46
1:B:749:ILE:CD1	1:B:749:ILE:N	2.79	0.46
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.50	0.46
1:D:907:PRO:HA	1:D:910:LEU:HD23	1.97	0.46
1:A:830:LEU:HD12	1:A:833:ALA:HB3	1.98	0.46
1:B:277:GLU:H	1:B:277:GLU:CD	2.19	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:D:257:THR:HA	1:D:270:GLY:O	2.16	0.46
1:C:863:GLN:HG2	1:C:1021:CYS:CB	2.46	0.46
1:B:820:ALA:HB2	1:B:842:TRP:NE1	2.30	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:573:GLN:HB2	1:A:602:CYS:O	2.16	0.45
1:B:589:GLY:O	1:B:599:ARG:HA	2.16	0.45
1:C:225:PHE:HA	1:C:243:GLU:O	2.16	0.45
1:D:693:GLN:HG2	1:D:695:TRP:NE1	2.31	0.45
1:D:613:PRO:HB3	1:D:617:LEU:HD23	1.99	0.45
1:B:741:THR:HB	1:B:748:CYS:HB3	1.96	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:B:163:GLN:O	1:B:164:ASP:HB3	2.17	0.45
1:D:244:VAL:HG21	1:D:256:VAL:HG11	1.98	0.45
1:A:898:LEU:HG	1:A:915:PHE:CZ	2.51	0.45
1:B:251:ARG:HD2	1:B:253:TYR:CE2	2.52	0.45
1:D:379:MET:CE	1:D:387:VAL:HB	2.46	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
4:C:8002:DMS:H21	5:C:4081:HOH:O	2.16	0.45
1:C:43:ARG:HH12	1:C:264:GLU:CD	2.20	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:D:390:SER:HA	1:D:391:HIS:HA	1.69	0.45
1:B:569:ASP:O	1:B:605:GLY:HA2	2.17	0.45
1:C:887:GLN:NE2	1:C:980:GLU:O	2.49	0.45
1:C:431:ARG:NH1	5:C:4073:HOH:O	2.49	0.45
1:B:410:VAL:HG22	1:B:455:ILE:HB	1.99	0.45
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.51	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:C:822:LEU:HD11	1:C:825:CYS:HB2	1.99	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.58	0.45
1:C:153:TRP:CD1	1:C:158:TRP:HA	2.52	0.44
1:A:149:ALA:HB2	1:A:163:GLN:HG2	1.99	0.44
1:C:782:ASP:HA	1:C:884:LEU:HD23	1.98	0.44
1:B:610:ASP:O	1:B:611:ARG:HB2	2.18	0.44
1:C:770:ILE:O	1:C:770:ILE:HG22	2.16	0.44
1:C:882:ILE:HG22	1:C:882:ILE:O	2.18	0.44
1:C:945:ASN:OD1	1:C:950:GLN:HG3	2.17	0.44
1:B:277:GLU:HG3	5:B:4091:HOH:O	2.17	0.44
1:A:600:GLN:HB2	1:A:603:MET:HE2	1.98	0.44
1:C:656:VAL:HG21	1:C:685:LEU:HD22	2.00	0.44
1:C:930:VAL:O	1:C:932:PRO:HD3	2.17	0.44
1:B:230:ARG:NH1	1:B:230:ARG:CG	2.79	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:333:ARG:NH1	1:B:333:ARG:HG2	2.33	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: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:820:ALA:HB2	1:A:842:TRP:NE1	2.33	0.43
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.53	0.43
1:D:319:ASP:HB2	5:D:4088:HOH:O	2.18	0.43
1:D:43:ARG:HD2	1:D:261:TRP:CD2	2.53	0.43
1:D:747:PHE:HB2	1:D:758:PHE:HB2	2.00	0.43
1:C:414:ASN:O	1:C:439:ARG:HD3	2.18	0.43
1:B:433:LEU:N	1:B:434:PRO:CD	2.80	0.43
1:D:226:HIS:O	1:D:242:ALA:HA	2.18	0.43
1:A:200:GLN:HG2	1:A:391:HIS:HB2	1.99	0.43
1:B:872:VAL:HG11	1:B:879:PRO:HD3	2.01	0.43
1:C:358:GLU:HG2	1:C:367:MET:HG3	2.01	0.43
1:C:444:VAL:O	1:C:448:ARG:HB3	2.18	0.43
1:A:305:ILE:HD11	1:A:645:ARG:HB3	2.00	0.43
1:C:390:SER:HB2	1:C:391:HIS:CE1	2.52	0.43
1:C:226:HIS:CE1	1:C:448:ARG:HH11	2.37	0.43
1:A:997:ASP:HB2	1:A:999:TRP:CE2	2.53	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:B:879:PRO:O	1:B:1009:LEU:HD12	2.18	0.43
1:B:745:MET:HE3	1:B:745:MET:H	1.84	0.43
1:D:446:ARG:HD2	5:D:4142:HOH:O	2.18	0.43
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.54	0.43
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:C:78:LEU:HA	1:C:79:PRO:HD3	1.87	0.42
1:B:736:ALA:HB1	1:B:751:LEU:HD11	2.00	0.42
1:A:634:GLN:HB2	1:A:682:LEU:HB2	2.01	0.42
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.54	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:A:454:ILE:HG13	1:A:455:ILE:HG13	2.01	0.42
1:C:331:GLY:H	4:C:8002:DMS:C2	2.30	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:B:854:LYS:HA	1:B:867:THR:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:222:ILE:N	1:C:324:GLU:OE1	2.49	0.42
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.01	0.42
1:C:996:ASP:HB2	1:C:1002:SER:HB2	2.02	0.42
1:A:878:HIS:HD2	5:A:4165:HOH:O	2.01	0.42
1:A:794:GLY:HA2	1:A:998:SER:O	2.20	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:C:281:GLU:HG3	1:B:515:VAL:HG21	2.02	0.42
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.84	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: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:599:ARG:HB2	1:B:600:GLN:NE2	2.35	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:C:499:ILE:O	1:C:533:LEU:HA	2.20	0.42
1:D:738:PRO:HB2	1:D:834:VAL:HG23	2.02	0.41
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:A:336:ARG:HH21	1:A:338:GLU:CD	2.24	0.41
1:B:390:SER:HA	1:B:391:HIS:HA	1.74	0.41
1:D:629:PHE:HB3	1:D:720:TRP:CH2	2.55	0.41
1:C:464:HIS:HB2	1:C:489:GLY:HA3	2.02	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:D:780:LEU:HD11	1:D:884:LEU:HD13	2.02	0.41
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.56	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:830:LEU:HD23	1:D:830:LEU:HD21	2.03	0.41
1:D:78:LEU:HA	1:D:79:PRO:HD3	1.92	0.41
1:C:796:SER:HB2	1:C:802:ASP:HB3	2.03	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:556:PHE:CD1	1:A:564:GLY:HA2	2.56	0.41
1:C:460:SER:O	1:C:461:GLU:C	2.59	0.41
1:A:390:SER:HA	1:A:391:HIS:HA	1.71	0.41
1:D:499:ILE:HD11	1:D:529:GLU:CD	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.56	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:C:594:ASP:OD1	1:C:594:ASP:N	2.43	0.41
1:C:200:GLN:CG	1:C:391:HIS:HB2	2.51	0.41
1:C:782:ASP:HB2	1:C:842:TRP:CZ2	2.56	0.41
1:C:426:LEU:HD22	1:C:432:TRP:CE2	2.56	0.41
1:A:257:THR:HA	1:A:270:GLY:O	2.21	0.40
1:B:147:ASN:HA	1:B:148:SER:HA	1.70	0.40
1:A:337:ILE:HA	1:A:341:LEU:O	2.21	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:D:767:GLN:OE1	1:D:775:GLN:N	2.47	0.40
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.03	0.40
1:B:962:TYR:CE2	1:B:976:LEU:HB3	2.57	0.40
1:B:785:THR:HB	1:B:816:TYR:CE2	2.56	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: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:578:TYR:HA	1:C:583:ASN:O	2.22	0.40
1:B:30:HIS:HE2	1:B:170:GLU:CD	2.25	0.40
1:A:738:PRO:HB2	1:A:834:VAL:HG23	2.04	0.40
1:D:513:PRO:O	1:D:514:ALA:HB3	2.22	0.40
1:C:869:ASP:OD2	1:C:1015:HIS:ND1	2.34	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%)	50	82
1	C	1009/1052 (96%)	947 (94%)	56 (6%)	6 (1%)	33	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1009/1052 (96%)	935 (93%)	74 (7%)	0	100	100
All	All	4036/4208 (96%)	3819 (95%)	208 (5%)	9 (0%)	56	86

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%)	844 (98%)	20 (2%)	63	90
1	B	864/898 (96%)	836 (97%)	28 (3%)	51	82
1	C	864/898 (96%)	850 (98%)	14 (2%)	75	94
1	D	864/898 (96%)	842 (98%)	22 (2%)	60	89
All	All	3456/3592 (96%)	3372 (98%)	84 (2%)	61	89

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	178	ARG
1	A	189	LEU
1	A	262	GLN
1	A	333	ARG
1	A	477	SER

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Mol	Chain	Res	Type
1	A	519	SER
1	A	604	ASN
1	A	614	HIS
1	A	634	GLN
1	A	651	LEU
1	A	661	LYS
1	A	665	SER
1	A	737	ILE
1	A	761	GLN
1	A	768	MET
1	A	774	LYS
1	A	824	GLN
1	A	863	GLN
1	A	885	ASN
1	C	44	THR
1	C	178	ARG
1	C	211	ASP
1	C	219	THR
1	C	223	SER
1	C	333	ARG
1	C	546	LEU
1	C	646	HIS
1	C	728	VAL
1	C	737	ILE
1	C	745	MET
1	C	746	ASP
1	C	848	THR
1	C	885	ASN
1	D	178	ARG
1	D	214	LEU
1	D	241	GLU
1	D	245	GLN
1	D	333	ARG
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	675	GLN
1	D	690	SER
1	D	737	ILE

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Mol	Chain	Res	Type
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	984	LEU
1	B	71	GLU
1	B	124	SER
1	B	136	GLU
1	B	178	ARG
1	B	219	THR
1	B	234	ASP
1	B	252	ASP
1	B	321	THR
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
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	675	GLN
1	B	728	VAL
1	B	745	MET
1	B	749	ILE
1	B	761	GLN
1	B	772	ASP
1	B	796	SER
1	B	809	ARG
1	B	855	THR
1	B	910	LEU
1	B	956	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	A	307	ASN

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Mol	Chain	Res	Type
1	C	245	GLN
1	C	623	GLN
1	C	878	HIS
1	D	418	HIS
1	D	540	HIS
1	B	93	HIS
1	B	1015	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	8001	-	3,3,3	2.62	1 (33%)	3,3,3	0.54	0
4	DMS	A	8002	-	3,3,3	2.56	1 (33%)	3,3,3	0.38	0
4	DMS	A	8003	-	3,3,3	2.65	1 (33%)	3,3,3	0.64	0
4	DMS	A	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.61	0
4	DMS	A	8005	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	A	8006	-	3,3,3	2.72	1 (33%)	3,3,3	0.58	0
4	DMS	A	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.64	0
4	DMS	A	8008	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
4	DMS	B	8001	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
4	DMS	B	8002	-	3,3,3	2.65	1 (33%)	3,3,3	0.45	0
4	DMS	B	8003	-	3,3,3	2.66	1 (33%)	3,3,3	0.44	0
4	DMS	B	8004	-	3,3,3	1.67	1 (33%)	3,3,3	0.33	0
4	DMS	C	8001	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
4	DMS	C	8002	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
4	DMS	C	8003	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
4	DMS	C	8004	-	3,3,3	2.62	1 (33%)	3,3,3	0.45	0
4	DMS	C	8005	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0
4	DMS	C	8006	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
4	DMS	D	8001	-	3,3,3	2.69	1 (33%)	3,3,3	0.50	0
4	DMS	D	8002	-	3,3,3	2.61	1 (33%)	3,3,3	0.34	0
4	DMS	D	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.42	0
4	DMS	D	8004	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
4	DMS	D	8005	-	3,3,3	2.58	1 (33%)	3,3,3	0.53	0
4	DMS	D	8006	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	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
4	DMS	A	8008	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8007	DMS	O-S	4.58	1.81	1.50
4	C	8006	DMS	O-S	4.58	1.81	1.50
4	A	8006	DMS	O-S	4.57	1.81	1.50
4	A	8005	DMS	O-S	4.55	1.80	1.50
4	D	8006	DMS	O-S	4.54	1.80	1.50
4	D	8003	DMS	O-S	4.52	1.80	1.50
4	D	8001	DMS	O-S	4.52	1.80	1.50
4	C	8002	DMS	O-S	4.52	1.80	1.50
4	B	8001	DMS	O-S	4.51	1.80	1.50
4	C	8005	DMS	O-S	4.49	1.80	1.50
4	A	8008	DMS	O-S	4.49	1.80	1.50
4	C	8003	DMS	O-S	4.47	1.80	1.50
4	A	8003	DMS	O-S	4.47	1.80	1.50
4	B	8003	DMS	O-S	4.46	1.80	1.50
4	C	8001	DMS	O-S	4.46	1.80	1.50
4	B	8002	DMS	O-S	4.45	1.80	1.50
4	D	8004	DMS	O-S	4.44	1.80	1.50
4	C	8004	DMS	O-S	4.42	1.80	1.50
4	A	8001	DMS	O-S	4.42	1.80	1.50
4	D	8002	DMS	O-S	4.41	1.80	1.50
4	A	8004	DMS	O-S	4.37	1.79	1.50
4	A	8002	DMS	O-S	4.32	1.79	1.50
4	D	8005	DMS	O-S	4.32	1.79	1.50
4	B	8004	DMS	O-S	2.83	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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.01	12 (1%) 75 81	24, 43, 79, 114	0
1	B	1011/1052 (96%)	0.08	8 (0%) 83 87	28, 51, 75, 111	0
1	C	1011/1052 (96%)	0.20	25 (2%) 54 61	30, 56, 87, 123	0
1	D	1011/1052 (96%)	0.20	39 (3%) 37 42	27, 48, 94, 127	0
All	All	4044/4208 (96%)	0.12	84 (2%) 60 67	24, 50, 84, 127	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	GLU	5.6
1	D	737	ILE	5.1
1	D	771	GLY	4.8
1	D	738	PRO	4.7
1	D	770	ILE	4.6
1	D	730	LEU	4.6
1	D	776	LEU	4.6
1	D	745	MET	4.3
1	A	733	ALA	4.1
1	C	663	LEU	3.7
1	A	685	LEU	3.6
1	C	687	GLN	3.6
1	C	732	ALA	3.6
1	D	818	ALA	3.6
1	B	687	GLN	3.6
1	D	827	ALA	3.5
1	C	689	GLU	3.5
1	D	732	ALA	3.5
1	D	892	ALA	3.4
1	D	1022	GLN	3.4
1	D	735	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	981	GLY	3.3
1	B	818	ALA	3.3
1	C	731	PRO	3.2
1	C	846	GLY	3.2
1	D	685	LEU	3.1
1	D	821	ALA	3.1
1	A	686	PRO	3.1
1	B	686	PRO	3.0
1	C	772	ASP	3.0
1	D	833	ALA	2.9
1	D	834	VAL	2.9
1	A	664	ALA	2.9
1	C	684	GLU	2.9
1	D	768	MET	2.9
1	D	1023	LYS	2.8
1	C	178	ARG	2.8
1	D	835	LEU	2.8
1	D	982	THR	2.8
1	D	861	SER	2.8
1	C	737	ILE	2.8
1	C	1018	LEU	2.7
1	D	890	GLN	2.7
1	C	736	ALA	2.6
1	D	733	ALA	2.6
1	D	734	SER	2.6
1	D	687	GLN	2.5
1	D	820	ALA	2.5
1	D	746	ASP	2.5
1	C	319	ASP	2.5
1	D	841	ALA	2.5
1	C	725	ASN	2.5
1	D	823	LEU	2.5
1	C	733	ALA	2.4
1	A	748	CYS	2.4
1	C	800	ARG	2.4
1	C	56	GLY	2.3
1	B	1023	LYS	2.3
1	D	828	ASP	2.3
1	B	364	GLY	2.3
1	A	663	LEU	2.3
1	C	685	LEU	2.3
1	D	862	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	891	VAL	2.2
1	C	580	GLU	2.2
1	B	761	GLN	2.2
1	A	747	PHE	2.2
1	D	824	GLN	2.2
1	D	859	ASP	2.2
1	C	688	PRO	2.2
1	D	822	LEU	2.2
1	C	762	SER	2.1
1	A	735	HIS	2.1
1	A	827	ALA	2.1
1	B	745	MET	2.1
1	C	730	LEU	2.1
1	C	841	ALA	2.0
1	B	685	LEU	2.0
1	A	761	GLN	2.0
1	A	800	ARG	2.0
1	C	671	ASP	2.0
1	D	832	ASP	2.0
1	C	831	ALA	2.0
1	D	748	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	DMS	D	8005	4/4	0.24	9.18	53,56,57,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DMS	A	8002	4/4	0.25	6.20	53,53,53,54	0
4	DMS	A	8001	4/4	0.26	5.51	71,71,72,74	0
4	DMS	A	8007	4/4	0.22	5.46	57,58,59,67	0
4	DMS	C	8001	4/4	0.26	3.16	75,77,79,80	0
4	DMS	C	8003	4/4	0.22	3.10	83,84,85,86	0
4	DMS	D	8002	4/4	0.21	2.80	58,62,62,63	0
4	DMS	A	8003	4/4	0.22	2.54	44,45,47,47	0
4	DMS	C	8002	4/4	0.22	2.49	49,53,53,55	0
4	DMS	B	8003	4/4	0.20	2.03	63,65,67,68	0
4	DMS	A	8004	4/4	0.22	1.64	60,61,63,64	0
4	DMS	C	8005	4/4	0.21	1.52	63,64,64,65	0
4	DMS	D	8003	4/4	0.21	1.42	66,67,68,69	0
3	NA	D	3101	1/1	0.20	1.29	55,55,55,55	0
4	DMS	B	8004	4/4	0.20	1.23	43,46,46,46	0
4	DMS	C	8004	4/4	0.19	0.81	53,54,55,56	0
4	DMS	B	8002	4/4	0.17	0.72	58,59,61,62	0
4	DMS	D	8004	4/4	0.21	0.61	74,75,76,76	0
4	DMS	D	8001	4/4	0.21	0.58	56,56,56,58	0
4	DMS	A	8006	4/4	0.19	-0.08	56,58,59,63	0
4	DMS	D	8006	4/4	0.17	-0.12	58,60,62,65	0
4	DMS	A	8008	4/4	0.15	-0.44	81,82,83,86	0
3	NA	A	3103	1/1	0.15	-0.87	59,59,59,59	0
4	DMS	B	8001	4/4	0.15	-0.89	64,66,67,70	0
3	NA	B	3103	1/1	0.12	-1.02	58,58,58,58	0
3	NA	B	3102	1/1	0.11	-1.61	35,35,35,35	0
3	NA	D	3102	1/1	0.11	-1.93	34,34,34,34	0
4	DMS	C	8006	4/4	0.13	-2.17	65,65,66,70	0
2	MG	C	3001	1/1	0.08	-2.33	42,42,42,42	0
3	NA	A	3101	1/1	0.11	-2.46	51,51,51,51	0
3	NA	B	3101	1/1	0.09	-2.48	55,55,55,55	0
4	DMS	A	8005	4/4	0.12	-2.50	56,56,57,60	0
2	MG	C	3002	1/1	0.10	-2.51	54,54,54,54	0
3	NA	C	3101	1/1	0.08	-2.55	57,57,57,57	0
3	NA	C	3102	1/1	0.11	-3.06	41,41,41,41	0
2	MG	B	3001	1/1	0.10	-3.17	50,50,50,50	0
2	MG	D	3001	1/1	0.07	-3.60	39,39,39,39	0
3	NA	C	3103	1/1	0.08	-3.94	62,62,62,62	0
2	MG	A	3002	1/1	0.06	-4.29	43,43,43,43	0
2	MG	D	3002	1/1	0.06	-4.67	42,42,42,42	0
3	NA	A	3102	1/1	0.09	-4.69	34,34,34,34	0
2	MG	B	3002	1/1	0.06	-4.91	56,56,56,56	0
2	MG	A	3001	1/1	0.05	-6.86	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.