



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 08:41 AM EDT

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 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

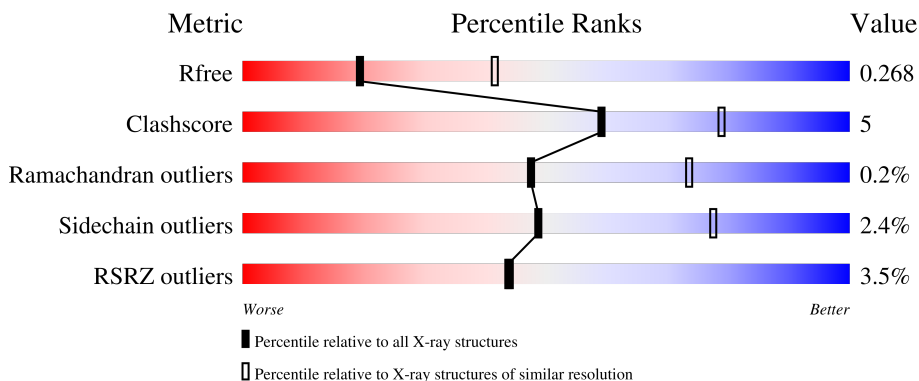
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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	 2% 86% 10% •
1	B	1052	 2% 82% 14% •
1	C	1052	 4% 81% 15% •
1	D	1052	 5% 81% 14% ••

2 Entry composition i

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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	B	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	A	3	Total Na 3 3	0	0
3	C	3	Total Na 3 3	0	0
3	D	2	Total Na 2 2	0	0
3	B	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	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	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		
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		

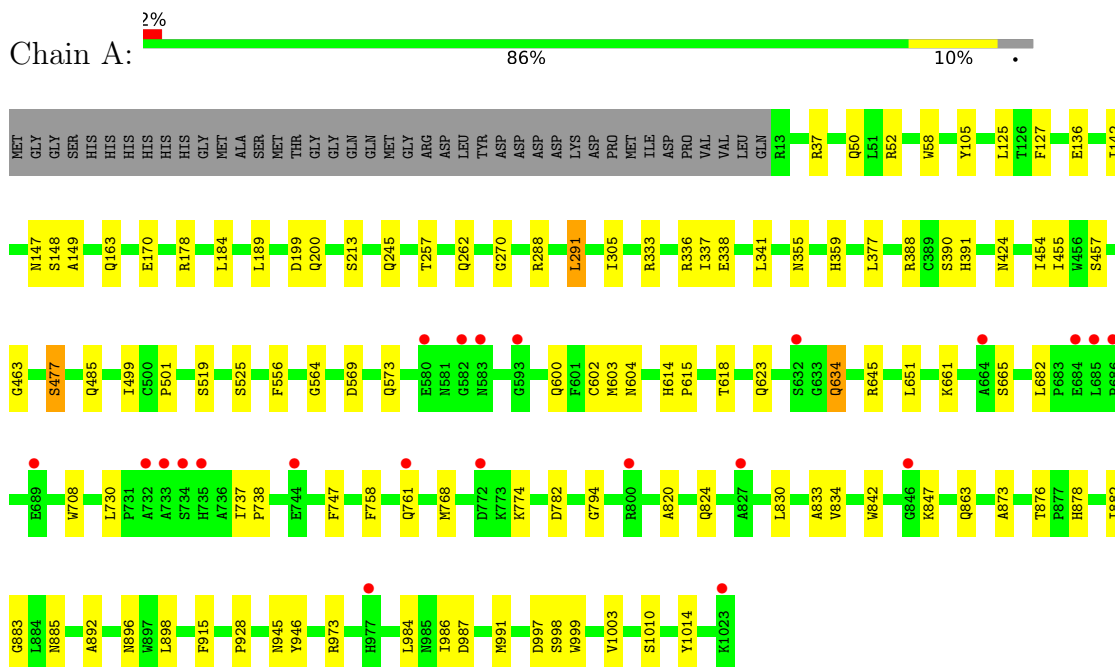
- Molecule 5 is water.

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

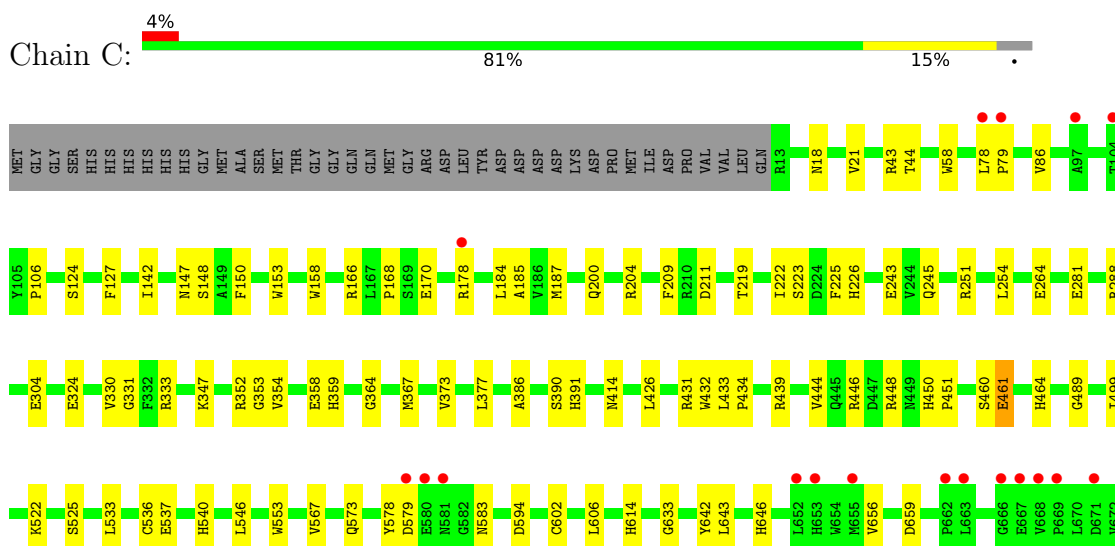
3 Residue-property plots [i](#)

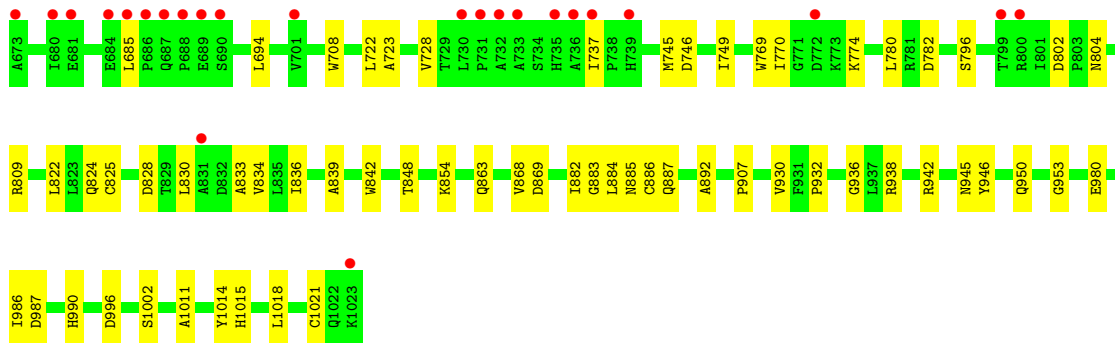
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

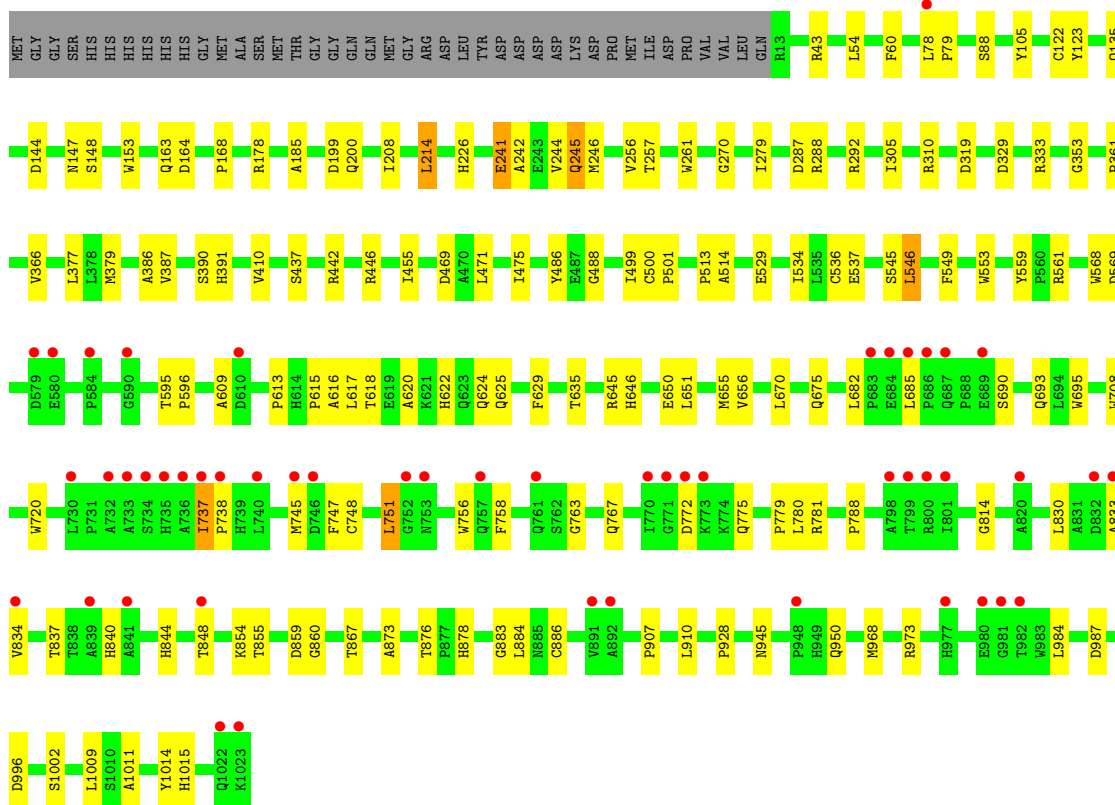
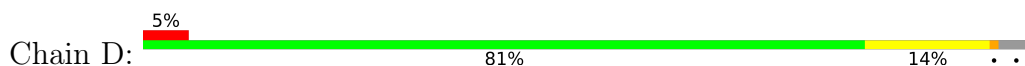


- Molecule 1: Beta-galactosidase

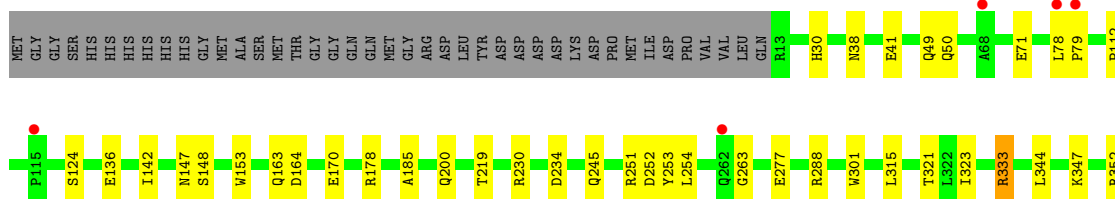
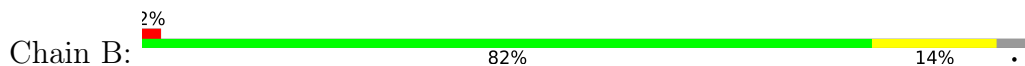


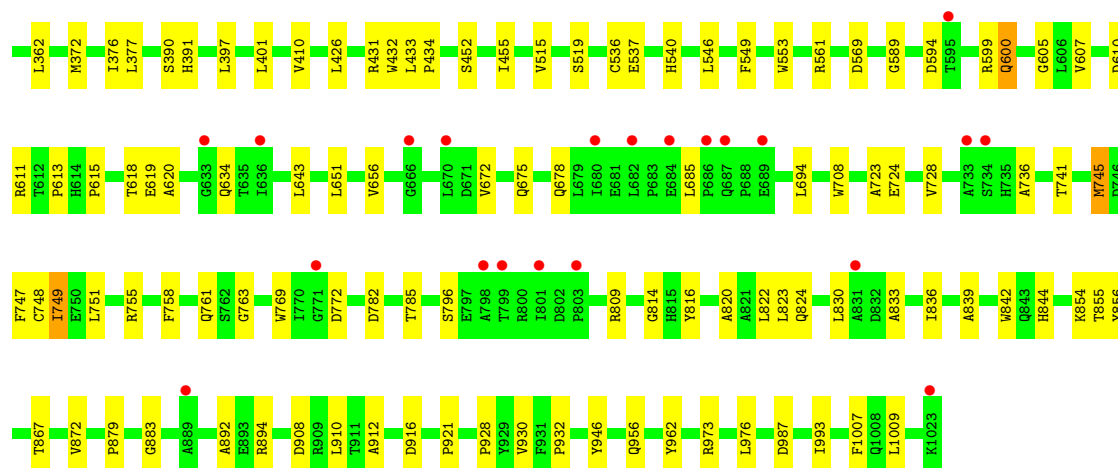


- Molecule 1: Beta-galactosidase



- 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) 91.0 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.026 for l,-k,h	Xtrriage
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

Xtrriage'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	0.40	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 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	55	0
1	B	8124	0	7715	75	0
1	C	8124	0	7715	90	0
1	D	8124	0	7715	85	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (296) 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: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	Interatomic distance (Å)	Clash overlap (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:HH11	1:B:230:ARG:HG2	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:892:ALA:HB3	1:A:946:TYR:CE1	2.45	0.51
1:A:623:GLN:NE2	4:A:8002:DMS:H11	2.25	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:333:ARG:HH11	1:B:333:ARG:HG2	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:C:525:SER:O	1:D:561:ARG:HD3	2.11	0.49
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.94	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:D:379:MET:HE1	1:D:387:VAL:HB	1.93	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:991:MET:CE	1:A:1003:VAL:HG21	2.43	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: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: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
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:B:277:GLU:CD	1:B:277:GLU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:863:GLN:HG2	1:C:1021:CYS:CB	2.46	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: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: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: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: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:379:MET:CE	1:D:387:VAL:HB	2.46	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
1:C:43:ARG:HH12	1:C:264:GLU:CD	2.20	0.45
4:C:8002:DMS:H21	5:C:4081:HOH:O	2.16	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: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:B:610:ASP:O	1:B:611:ARG:HB2	2.18	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:A:600:GLN:HB2	1:A:603:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:745:MET:HE3	1:B:745:MET:H	1.84	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:D:486:TYR:CE2	1:D:488:GLY:HA3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ILE:HG13	1:A:455:ILE:HG13	2.01	0.42
1:A:359:HIS:CD2	1:A:573:GLN:HA	2.55	0.42
1:C:331:GLY:H	4:C:8002:DMS:C2	2.30	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
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:499:ILE:HG22	1:D:501:PRO:HD3	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: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: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:336:ARG:HH21	1:A:338:GLU:CD	2.24	0.41
1:A:477:SER:OG	1:D:469:ASP:OD2	2.38	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:D:78:LEU:HA	1:D:79:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:499:ILE:HD11	1:D:529:GLU:CD	2.41	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: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: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: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: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
1:B:30:HIS:HE2	1:B:170:GLU:CD	2.25	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%)	41	66
1	C	1009/1052 (96%)	947 (94%)	56 (6%)	6 (1%)	25	50
1	D	1009/1052 (96%)	935 (93%)	74 (7%)	0	100	100
All	All	4036/4208 (96%)	3819 (95%)	208 (5%)	9 (0%)	47	73

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 [i](#)

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%)	50	78
1	B	864/898 (96%)	836 (97%)	28 (3%)	39	68
1	C	864/898 (96%)	850 (98%)	14 (2%)	62	85
1	D	864/898 (96%)	842 (98%)	22 (2%)	47	76
All	All	3456/3592 (96%)	3372 (98%)	84 (2%)	49	77

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
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

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Mol	Chain	Res	Type
1	D	651	LEU
1	D	655	MET
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	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

Sometimes 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
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 [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 monosaccharides 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	B	8002	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
4	DMS	A	8002	-	3,3,3	2.55	1 (33%)	3,3,3	0.43	0
4	DMS	A	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	B	8001	-	3,3,3	2.69	1 (33%)	3,3,3	0.63	0
4	DMS	C	8003	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
4	DMS	A	8008	-	3,3,3	2.67	1 (33%)	3,3,3	0.58	0
4	DMS	D	8005	-	3,3,3	2.58	1 (33%)	3,3,3	0.59	0
4	DMS	D	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.47	0
4	DMS	C	8002	-	3,3,3	2.67	1 (33%)	3,3,3	0.62	0
4	DMS	D	8004	-	3,3,3	2.64	1 (33%)	3,3,3	0.55	0
4	DMS	D	8006	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
4	DMS	B	8003	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
4	DMS	D	8002	-	3,3,3	2.61	1 (33%)	3,3,3	0.38	0
4	DMS	C	8004	-	3,3,3	2.62	1 (33%)	3,3,3	0.49	0
4	DMS	A	8005	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	0
4	DMS	A	8006	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
4	DMS	A	8001	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
4	DMS	B	8004	-	3,3,3	1.66	1 (33%)	3,3,3	0.36	0
4	DMS	A	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.70	0
4	DMS	C	8005	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
4	DMS	C	8006	-	3,3,3	2.74	1 (33%)	3,3,3	0.66	0
4	DMS	A	8003	-	3,3,3	2.65	1 (33%)	3,3,3	0.70	0
4	DMS	D	8001	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
4	DMS	C	8001	-	3,3,3	2.66	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	4.57	1.81	1.50
4	C	8006	DMS	O-S	4.57	1.81	1.50
4	A	8006	DMS	O-S	4.56	1.81	1.50
4	A	8005	DMS	O-S	4.54	1.80	1.50
4	D	8006	DMS	O-S	4.53	1.80	1.50
4	D	8003	DMS	O-S	4.51	1.80	1.50
4	C	8002	DMS	O-S	4.50	1.80	1.50
4	D	8001	DMS	O-S	4.50	1.80	1.50
4	B	8001	DMS	O-S	4.49	1.80	1.50
4	C	8005	DMS	O-S	4.48	1.80	1.50
4	A	8008	DMS	O-S	4.47	1.80	1.50
4	C	8003	DMS	O-S	4.46	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8003	DMS	O-S	4.46	1.80	1.50
4	B	8003	DMS	O-S	4.45	1.80	1.50
4	C	8001	DMS	O-S	4.45	1.80	1.50
4	B	8002	DMS	O-S	4.44	1.80	1.50
4	D	8004	DMS	O-S	4.43	1.80	1.50
4	C	8004	DMS	O-S	4.41	1.80	1.50
4	A	8001	DMS	O-S	4.41	1.80	1.50
4	D	8002	DMS	O-S	4.40	1.80	1.50
4	A	8004	DMS	O-S	4.36	1.79	1.50
4	A	8002	DMS	O-S	4.31	1.79	1.50
4	D	8005	DMS	O-S	4.31	1.79	1.50
4	B	8004	DMS	O-S	2.81	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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8002	DMS	1	0
4	A	8004	DMS	1	0
4	C	8002	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%)	-0.17	22 (2%) 62 63	24, 43, 79, 114	0
1	B	1011/1052 (96%)	-0.04	26 (2%) 56 57	28, 51, 75, 111	0
1	C	1011/1052 (96%)	0.08	42 (4%) 36 35	30, 56, 87, 123	0
1	D	1011/1052 (96%)	0.06	51 (5%) 28 27	27, 48, 94, 127	0
All	All	4044/4208 (96%)	-0.02	141 (3%) 44 44	24, 50, 84, 127	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	GLU	6.5
1	D	732	ALA	5.5
1	D	833	ALA	5.5
1	C	685	LEU	5.4
1	D	771	GLY	5.0
1	C	689	GLU	4.9
1	D	770	ILE	4.8
1	D	745	MET	4.8
1	D	737	ILE	4.8
1	A	685	LEU	4.5
1	A	733	ALA	4.5
1	D	733	ALA	4.4
1	C	687	GLN	4.3
1	C	800	ARG	4.3
1	B	686	PRO	4.2
1	A	686	PRO	4.1
1	C	671	ASP	4.1
1	C	731	PRO	4.0
1	B	799	THR	4.0
1	B	733	ALA	4.0
1	D	735	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	3.9
1	C	732	ALA	3.8
1	C	673	ALA	3.8
1	D	798	ALA	3.8
1	A	583	ASN	3.6
1	C	580	GLU	3.6
1	B	687	GLN	3.5
1	C	739	HIS	3.5
1	C	831	ALA	3.4
1	C	684	GLU	3.3
1	D	948	PRO	3.3
1	C	733	ALA	3.3
1	B	666	GLY	3.2
1	C	737	ILE	3.2
1	A	800	ARG	3.2
1	B	682	LEU	3.2
1	D	761	GLN	3.2
1	D	832	ASP	3.1
1	D	982	THR	3.1
1	D	730	LEU	3.1
1	A	977	HIS	3.1
1	D	689	GLU	3.1
1	B	831	ALA	3.0
1	C	666	GLY	3.0
1	D	685	LEU	2.9
1	A	734	SER	2.9
1	D	734	SER	2.9
1	C	667	GLU	2.9
1	D	738	PRO	2.9
1	A	732	ALA	2.9
1	C	772	ASP	2.9
1	D	981	GLY	2.8
1	C	78	LEU	2.8
1	C	736	ALA	2.8
1	D	740	LEU	2.8
1	D	736	ALA	2.8
1	D	580	GLU	2.8
1	B	684	GLU	2.8
1	C	579	ASP	2.8
1	C	669	PRO	2.7
1	D	892	ALA	2.7
1	C	681	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	761	GLN	2.7
1	D	772	ASP	2.7
1	B	636	ILE	2.7
1	C	655	MET	2.7
1	D	977	HIS	2.7
1	D	1023	LYS	2.7
1	B	79	PRO	2.7
1	B	68	ALA	2.7
1	A	1023	LYS	2.6
1	D	891	VAL	2.6
1	D	753	ASN	2.6
1	B	1023	LYS	2.6
1	C	690	SER	2.6
1	B	595	THR	2.6
1	B	633	GLY	2.6
1	B	78	LEU	2.6
1	D	746	ASP	2.5
1	D	834	VAL	2.5
1	B	689	GLU	2.5
1	D	848	THR	2.5
1	C	668	VAL	2.5
1	A	846	GLY	2.5
1	C	1023	LYS	2.5
1	A	772	ASP	2.5
1	C	686	PRO	2.5
1	D	683	PRO	2.5
1	C	663	LEU	2.5
1	D	839	ALA	2.5
1	C	688	PRO	2.5
1	A	827	ALA	2.5
1	C	104	THR	2.4
1	D	820	ALA	2.4
1	D	841	ALA	2.4
1	D	801	ILE	2.4
1	B	680	ILE	2.4
1	D	773	LYS	2.4
1	B	734	SER	2.4
1	C	799	THR	2.4
1	D	78	LEU	2.4
1	B	262	GLN	2.3
1	C	79	PRO	2.3
1	D	752	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	653	HIS	2.3
1	A	582	GLY	2.2
1	D	684	GLU	2.2
1	B	889	ALA	2.2
1	B	771	GLY	2.2
1	B	801	ILE	2.2
1	D	579	ASP	2.2
1	B	670	LEU	2.2
1	A	684	GLU	2.2
1	C	680	ILE	2.2
1	C	581	ASN	2.2
1	C	178	ARG	2.2
1	D	1022	GLN	2.2
1	B	803	PRO	2.2
1	D	799	THR	2.2
1	D	757	GLN	2.2
1	C	97	ALA	2.2
1	C	735	HIS	2.2
1	B	115	PRO	2.2
1	A	632	SER	2.1
1	D	590	GLY	2.1
1	D	687	GLN	2.1
1	D	800	ARG	2.1
1	A	593	GLY	2.1
1	D	584	PRO	2.1
1	D	980	GLU	2.1
1	C	652	LEU	2.1
1	A	744	GLU	2.1
1	D	610	ASP	2.1
1	C	701	VAL	2.1
1	A	664	ALA	2.1
1	A	580	GLU	2.1
1	C	662	PRO	2.0
1	D	686	PRO	2.0
1	B	798	ALA	2.0
1	C	730	LEU	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 [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
3	NA	D	3101	1/1	0.75	0.18	55,55,55,55	0
3	NA	C	3101	1/1	0.79	0.11	57,57,57,57	0
3	NA	C	3103	1/1	0.80	0.14	62,62,62,62	0
3	NA	B	3101	1/1	0.80	0.12	55,55,55,55	0
2	MG	B	3001	1/1	0.88	0.06	50,50,50,50	0
4	DMS	C	8001	4/4	0.88	0.24	75,77,79,80	0
3	NA	C	3102	1/1	0.90	0.14	41,41,41,41	0
4	DMS	C	8003	4/4	0.91	0.30	83,84,85,86	0
2	MG	C	3002	1/1	0.93	0.10	54,54,54,54	0
3	NA	B	3102	1/1	0.93	0.15	35,35,35,35	0
3	NA	A	3103	1/1	0.93	0.12	59,59,59,59	0
3	NA	D	3102	1/1	0.93	0.15	34,34,34,34	0
2	MG	C	3001	1/1	0.94	0.09	42,42,42,42	0
4	DMS	A	8007	4/4	0.95	0.16	57,58,59,67	0
4	DMS	A	8008	4/4	0.95	0.14	81,82,83,86	0
2	MG	D	3002	1/1	0.95	0.09	42,42,42,42	0
3	NA	B	3103	1/1	0.95	0.23	58,58,58,58	0
4	DMS	C	8005	4/4	0.95	0.21	63,64,64,65	0
4	DMS	C	8006	4/4	0.95	0.27	65,65,66,70	0
4	DMS	D	8006	4/4	0.95	0.15	58,60,62,65	0
4	DMS	B	8003	4/4	0.95	0.15	63,65,67,68	0
4	DMS	B	8004	4/4	0.95	0.15	43,46,46,46	0
2	MG	B	3002	1/1	0.96	0.06	56,56,56,56	0
2	MG	D	3001	1/1	0.96	0.08	39,39,39,39	0
4	DMS	D	8005	4/4	0.96	0.20	53,56,57,61	0
4	DMS	A	8001	4/4	0.96	0.22	71,71,72,74	0
4	DMS	C	8002	4/4	0.96	0.20	49,53,53,55	0
4	DMS	A	8004	4/4	0.96	0.27	60,61,63,64	0
3	NA	A	3101	1/1	0.97	0.10	51,51,51,51	0
4	DMS	C	8004	4/4	0.97	0.18	53,54,55,56	0
4	DMS	B	8001	4/4	0.97	0.14	64,66,67,70	0
4	DMS	B	8002	4/4	0.97	0.18	58,59,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DMS	D	8003	4/4	0.97	0.15	66,67,68,69	0
4	DMS	D	8004	4/4	0.97	0.19	74,75,76,76	0
4	DMS	A	8006	4/4	0.98	0.14	56,58,59,63	0
3	NA	A	3102	1/1	0.98	0.10	34,34,34,34	0
4	DMS	A	8002	4/4	0.98	0.20	53,53,53,54	0
2	MG	A	3002	1/1	0.98	0.08	43,43,43,43	0
4	DMS	D	8001	4/4	0.98	0.22	56,56,56,58	0
4	DMS	D	8002	4/4	0.98	0.30	58,62,62,63	0
4	DMS	A	8005	4/4	0.98	0.12	56,56,57,60	0
4	DMS	A	8003	4/4	0.99	0.17	44,45,47,47	0
2	MG	A	3001	1/1	0.99	0.05	51,51,51,51	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.