Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 03:29 AM EDT

PDB ID	:	3VDA
Title	:	E. coli (lacZ) beta-galactosidase (N460T)
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	:	2.50 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 (i) 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 (i)) were used in the production of this report:

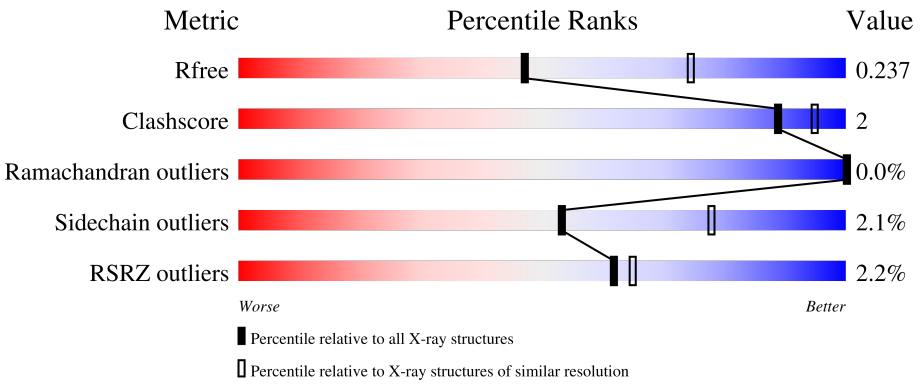
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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% 91% 5% •
1	B	1052	2% 91% 5% •
1	C	1052	2% 89% 7% •
1	D	1052	2% 90% 7% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34381 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
			Total	C	N	O	S			
1	A	1015	8156	5159	1444	1515	38	0	0	0
1	B	1015	8156	5159	1444	1515	38	0	0	0
1	C	1015	8156	5159	1444	1515	38	0	0	0
1	D	1015	8156	5159	1444	1515	38	0	0	0

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	THR	ASN	engineered mutation	UNP P00722
B	-28	MET	-	expression tag	UNP P00722
B	-27	GLY	-	expression tag	UNP P00722
B	-26	GLY	-	expression tag	UNP P00722
B	-25	SER	-	expression tag	UNP P00722
B	-24	HIS	-	expression tag	UNP P00722
B	-23	HIS	-	expression tag	UNP P00722
B	-22	HIS	-	expression tag	UNP P00722
B	-21	HIS	-	expression tag	UNP P00722
B	-20	HIS	-	expression tag	UNP P00722
B	-19	HIS	-	expression tag	UNP P00722
B	-18	GLY	-	expression tag	UNP P00722
B	-17	MET	-	expression tag	UNP P00722
B	-16	ALA	-	expression tag	UNP P00722
B	-15	SER	-	expression tag	UNP P00722
B	-14	MET	-	expression tag	UNP P00722
B	-13	THR	-	expression tag	UNP P00722
B	-12	GLY	-	expression tag	UNP P00722
B	-11	GLY	-	expression tag	UNP P00722
B	-10	GLN	-	expression tag	UNP P00722
B	-9	GLN	-	expression tag	UNP P00722
B	-8	MET	-	expression tag	UNP P00722
B	-7	GLY	-	expression tag	UNP P00722
B	-6	ARG	-	expression tag	UNP P00722
B	-5	ASP	-	expression tag	UNP P00722
B	-4	LEU	-	expression tag	UNP P00722

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	5	MET	-	expression tag	UNP P00722
D	6	ILE	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	460	THR	ASN	engineered mutation	UNP P00722

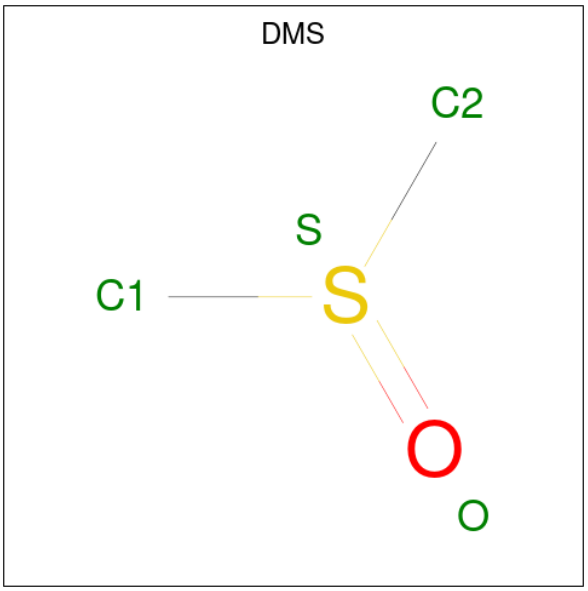
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	427	427	427	0	0

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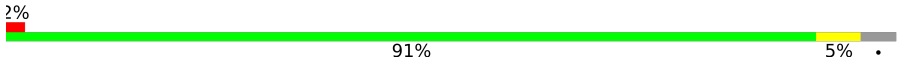
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	403	403	403	0	0
			Total	O		
5	C	389	389	389	0	0
			Total	O		
5	D	392	392	392	0	0

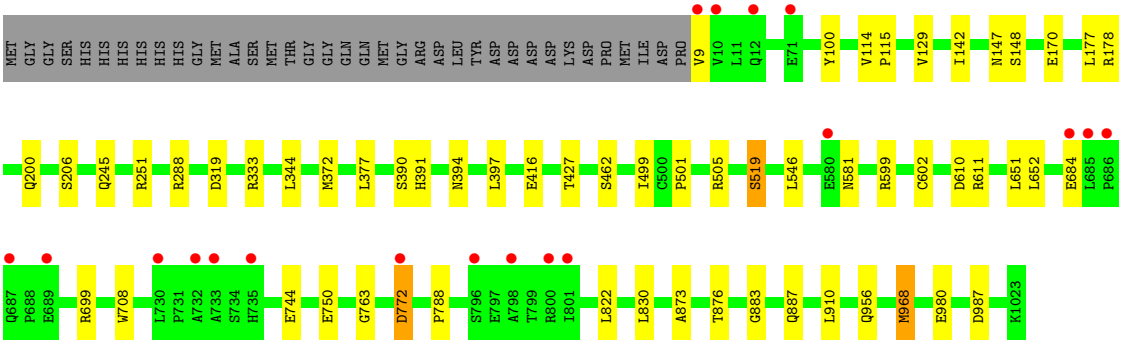
3 Residue-property plots (i)

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

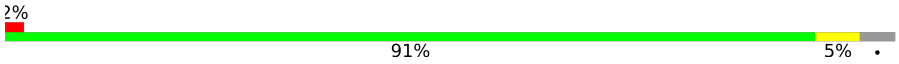
Chain A:

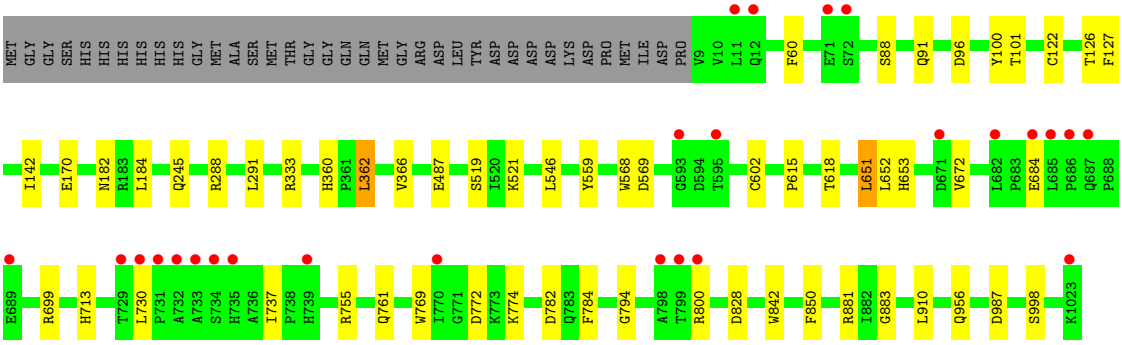




• Molecule 1: Beta-galactosidase

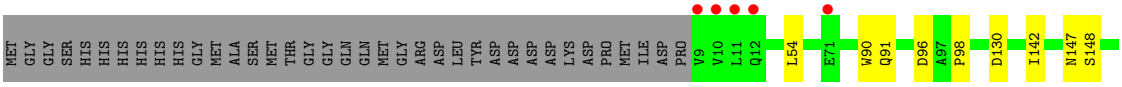
Chain B:

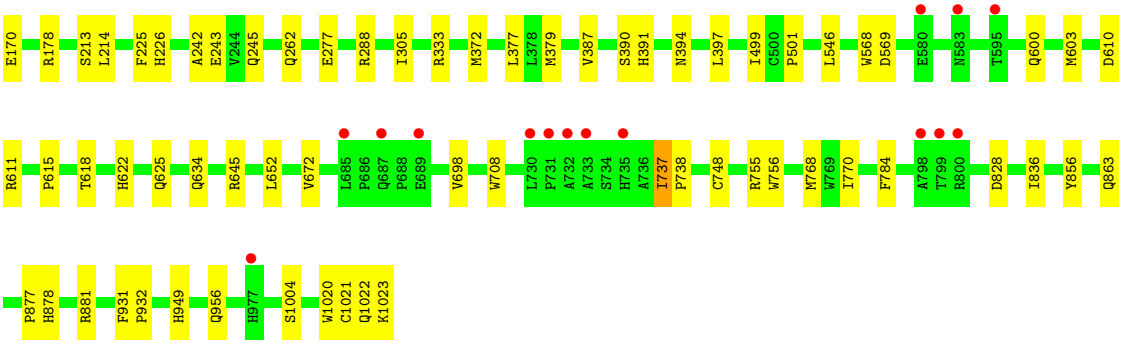




• Molecule 1: Beta-galactosidase

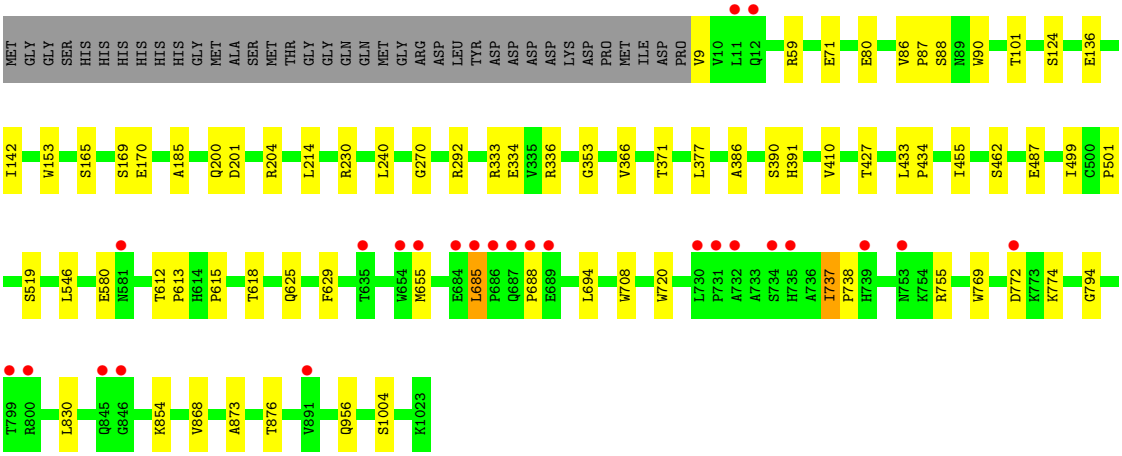
Chain C:





- Molecule 1: Beta-galactosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	152.60Å 164.69Å 203.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.05 – 2.50 46.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.05-2.50) 94.0 (46.05-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.174 , 0.237 0.178 , 0.237	Depositor DCC
R_{free} test set	2358 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34381	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4968e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, DMS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.46	0/8398	0.57	0/11457
1	B	0.47	0/8398	0.57	0/11457
1	C	0.46	0/8398	0.57	0/11457
1	D	0.45	0/8398	0.57	0/11457
All	All	0.46	0/33592	0.57	0/45828

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8156	0	7754	25	0
1	B	8156	0	7754	25	0
1	C	8156	0	7754	35	0
1	D	8156	0	7754	35	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	28	0	42	0	0
4	B	32	0	48	0	0
4	C	28	0	42	1	0
4	D	40	0	60	4	0
5	A	427	0	0	1	0
5	B	403	0	0	2	0
5	C	389	0	0	3	0
5	D	392	0	0	6	0
All	All	34381	0	31208	119	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 2.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.60	0.84
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.67	0.76
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.69	0.74
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.69	0.74
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.72	0.70
1:B:91:GLN:HG3	1:B:96:ASP:OD1	1.96	0.65
1:C:54:LEU:HD11	1:C:214:LEU:HD13	1.81	0.63
1:B:755:ARG:HB3	1:B:769:TRP:HB2	1.80	0.62
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.82	0.61
1:C:770:ILE:HD11	1:C:1022:GLN:HG2	1.83	0.60
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.85	0.59
1:C:372:MET:HE3	1:C:397:LEU:HD23	1.85	0.59
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.83	0.58
1:A:9:VAL:HG12	1:D:9:VAL:HG12	1.87	0.57
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.87	0.55
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.89	0.55
1:D:487:GLU:HB3	5:D:4253:HOH:O	2.07	0.55
1:C:863:GLN:HG2	1:C:1021:CYS:HB3	1.90	0.53
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.43	0.53
1:A:788:PRO:HD2	1:A:968:MET:HB2	1.91	0.53
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.91	0.53
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:ALA:O	1:A:876:THR:HG22	2.09	0.52
1:D:88:SER:HA	1:D:366:VAL:HG21	1.92	0.51
1:A:887:GLN:NE2	1:A:980:GLU:O	2.44	0.51
1:D:427:THR:HG21	1:D:462:SER:HB3	1.93	0.50
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.12	0.50
1:D:270:GLY:HA3	4:D:8010:DMS:H13	1.94	0.50
1:B:487:GLU:HB3	5:B:4039:HOH:O	2.11	0.50
1:D:629:PHE:HB3	1:D:720:TRP:HH2	1.77	0.49
1:D:688:PRO:HG3	1:D:694:LEU:HD11	1.95	0.49
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.48	0.48
1:A:147:ASN:HA	1:A:148:SER:HA	1.62	0.48
1:D:292:ARG:O	4:D:8010:DMS:H11	2.13	0.48
1:D:755:ARG:HB3	1:D:769:TRP:HB2	1.96	0.48
1:B:794:GLY:HA2	1:B:998:SER:O	2.15	0.47
1:A:830:LEU:HD22	1:B:828:ASP:HB3	1.97	0.47
1:B:521:LYS:HG2	1:B:559:TYR:CZ	2.49	0.47
1:C:91:GLN:HB3	1:C:98:PRO:HD3	1.95	0.47
1:D:410:VAL:HG22	1:D:455:ILE:HB	1.96	0.47
1:D:655:MET:HB2	5:D:4353:HOH:O	2.13	0.47
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.50	0.47
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	2.33	0.46
1:D:615:PRO:O	1:D:618:THR:HG22	2.14	0.46
1:C:225:PHE:HA	1:C:243:GLU:O	2.15	0.46
1:A:427:THR:HG21	1:A:462:SER:HB3	1.98	0.46
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.51	0.46
4:C:8002:DMS:H21	5:C:4200:HOH:O	2.15	0.46
1:A:200:GLN:HA	1:A:416:GLU:OE1	2.16	0.46
1:D:136:GLU:HG2	5:D:4181:HOH:O	2.15	0.45
1:C:379:MET:CE	1:C:387:VAL:HB	2.47	0.45
1:D:101:THR:HG23	1:D:204:ARG:NH2	2.31	0.45
1:D:353:GLY:HA2	1:D:386:ALA:O	2.18	0.44
1:A:114:VAL:HB	1:A:115:PRO:CD	2.47	0.44
1:C:784:PHE:HA	1:C:881:ARG:O	2.18	0.44
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.98	0.44
1:D:873:ALA:O	1:D:876:THR:HG22	2.18	0.44
4:D:8002:DMS:H11	5:D:4076:HOH:O	2.18	0.44
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.99	0.44
1:C:931:PHE:HA	1:C:932:PRO:HD3	1.78	0.44
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.81	0.44
1:B:615:PRO:O	1:B:618:THR:HG22	2.18	0.43
1:C:377:LEU:HD22	1:C:708:TRP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:GLN:HG2	1:D:391:HIS:HB2	1.99	0.43
1:D:737:ILE:HA	1:D:738:PRO:HD3	1.87	0.43
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.48	0.43
1:A:581:ASN:HB2	5:A:4192:HOH:O	2.18	0.43
1:B:782:ASP:HB2	1:B:842:TRP:CH2	2.53	0.43
1:C:828:ASP:HB3	1:D:830:LEU:HD22	2.00	0.43
1:B:784:PHE:HA	1:B:881:ARG:O	2.19	0.43
1:C:836:ILE:HB	1:C:856:TYR:HB2	2.00	0.43
1:C:622:HIS:O	1:C:625:GLN:HG3	2.19	0.43
1:B:651:LEU:HD12	1:B:651:LEU:C	2.39	0.43
1:A:772:ASP:OD1	1:A:772:ASP:N	2.51	0.43
1:B:651:LEU:HD11	1:B:653:HIS:CE1	2.54	0.43
1:D:270:GLY:CA	4:D:8010:DMS:H13	2.49	0.43
1:D:685:LEU:H	1:D:685:LEU:HG	1.42	0.43
1:D:854:LYS:HG2	1:D:868:VAL:HG22	2.01	0.43
1:A:390:SER:HA	1:A:391:HIS:HA	1.86	0.42
1:C:568:TRP:HA	1:C:569:ASP:HA	1.88	0.42
1:C:379:MET:HE1	1:C:387:VAL:HB	2.01	0.42
1:D:433:LEU:HB3	1:D:434:PRO:HD3	2.01	0.42
1:D:86:VAL:HG13	1:D:87:PRO:HA	2.01	0.42
1:A:129:VAL:HG21	1:A:177:LEU:HD22	2.02	0.42
1:C:737:ILE:HA	1:C:738:PRO:HD3	1.92	0.42
1:C:878:HIS:HD2	5:C:4072:HOH:O	2.02	0.42
1:C:147:ASN:HA	1:C:148:SER:HA	1.72	0.42
1:B:713:HIS:HE1	5:B:4262:HOH:O	2.02	0.42
1:B:883:GLY:HA3	1:B:987:ASP:HA	2.01	0.42
1:D:59:ARG:HB2	1:D:124:SER:OG	2.20	0.42
1:A:200:GLN:HG3	1:A:416:GLU:OE1	2.20	0.42
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.54	0.42
1:D:240:LEU:C	1:D:240:LEU:HD23	2.41	0.42
1:A:377:LEU:HD22	1:A:708:TRP:HA	2.02	0.41
1:C:600:GLN:HB2	1:C:603:MET:HE2	2.02	0.41
1:C:615:PRO:O	1:C:618:THR:HG22	2.20	0.41
1:A:505:ARG:O	1:A:519:SER:HA	2.21	0.41
1:B:88:SER:HA	1:B:366:VAL:HG21	2.02	0.41
1:C:610:ASP:O	1:C:611:ARG:HB2	2.20	0.41
1:C:748:CYS:HA	1:C:756:TRP:O	2.21	0.41
1:D:625:GLN:NE2	5:D:4062:HOH:O	2.52	0.41
1:B:730:LEU:H	1:B:730:LEU:HD12	1.86	0.41
1:C:226:HIS:O	1:C:242:ALA:HA	2.20	0.41
1:C:277:GLU:HG2	5:C:4075:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:O	1:A:206:SER:HB2	2.21	0.41
1:A:610:ASP:O	1:A:611:ARG:HB2	2.21	0.41
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.02	0.41
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.56	0.41
1:C:372:MET:CE	1:C:397:LEU:HD23	2.51	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.82	0.41
1:A:372:MET:HE3	1:A:397:LEU:HD23	2.01	0.41
1:A:883:GLY:HA3	1:A:987:ASP:HA	2.03	0.40
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.56	0.40
1:D:390:SER:HA	1:D:391:HIS:HA	1.75	0.40
1:B:60:PHE:HA	1:B:122:CYS:O	2.21	0.40
1:C:756:TRP:CD1	1:C:768:MET:HG2	2.56	0.40
1:B:126:THR:HA	1:B:182:ASN:O	2.21	0.40
1:D:794:GLY:HA3	5:D:4071:HOH:O	2.20	0.40
1:D:612:THR:HA	1:D:613:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1013/1052 (96%)	974 (96%)	39 (4%)	0	100	100
1	B	1013/1052 (96%)	967 (96%)	46 (4%)	0	100	100
1	C	1013/1052 (96%)	975 (96%)	38 (4%)	0	100	100
1	D	1013/1052 (96%)	976 (96%)	36 (4%)	1 (0%)	51	73
All	All	4052/4208 (96%)	3892 (96%)	159 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	201	ASP

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	868/898 (97%)	849 (98%)	19 (2%)	52	77
1	B	868/898 (97%)	849 (98%)	19 (2%)	52	77
1	C	868/898 (97%)	852 (98%)	16 (2%)	59	81
1	D	868/898 (97%)	850 (98%)	18 (2%)	53	78
All	All	3472/3592 (97%)	3400 (98%)	72 (2%)	53	78

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ARG
1	A	251	ARG
1	A	319	ASP
1	A	333	ARG
1	A	344	LEU
1	A	394	ASN
1	A	519	SER
1	A	546	LEU
1	A	599	ARG
1	A	651	LEU
1	A	652	LEU
1	A	684	GLU
1	A	699	ARG
1	A	744	GLU
1	A	750	GLU
1	A	772	ASP
1	A	910	LEU
1	A	956	GLN
1	A	968	MET
1	B	101	THR
1	B	291	LEU

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Mol	Chain	Res	Type
1	B	333	ARG
1	B	362	LEU
1	B	519	SER
1	B	546	LEU
1	B	651	LEU
1	B	652	LEU
1	B	672	VAL
1	B	684	GLU
1	B	699	ARG
1	B	737	ILE
1	B	761	GLN
1	B	772	ASP
1	B	774	LYS
1	B	800	ARG
1	B	850	PHE
1	B	910	LEU
1	B	956	GLN
1	C	90	TRP
1	C	130	ASP
1	C	178	ARG
1	C	213	SER
1	C	262	GLN
1	C	333	ARG
1	C	394	ASN
1	C	546	LEU
1	C	634	GLN
1	C	672	VAL
1	C	737	ILE
1	C	755	ARG
1	C	877	PRO
1	C	956	GLN
1	C	1004	SER
1	C	1023	LYS
1	D	71	GLU
1	D	80	GLU
1	D	90	TRP
1	D	165	SER
1	D	169	SER
1	D	214	LEU
1	D	230	ARG
1	D	333	ARG
1	D	371	THR

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Mol	Chain	Res	Type
1	D	519	SER
1	D	546	LEU
1	D	580	GLU
1	D	685	LEU
1	D	737	ILE
1	D	772	ASP
1	D	774	LYS
1	D	956	GLN
1	D	1004	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	878	HIS
1	B	878	HIS
1	C	49	GLN
1	C	50	GLN
1	C	394	ASN
1	C	1008	GLN
1	D	163	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 50 ligands modelled in this entry, 18 are monoatomic - leaving 32 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	8002	-	3,3,3	2.67	1 (33%)	3,3,3	0.45	0
4	DMS	B	8007	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
4	DMS	C	8007	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
4	DMS	B	8002	-	3,3,3	2.59	1 (33%)	3,3,3	0.74	0
4	DMS	A	8006	-	3,3,3	2.58	1 (33%)	3,3,3	0.34	0
4	DMS	B	8001	-	3,3,3	2.56	1 (33%)	3,3,3	0.72	0
4	DMS	A	8003	-	3,3,3	2.65	1 (33%)	3,3,3	0.63	0
4	DMS	D	8007	-	3,3,3	2.62	1 (33%)	3,3,3	0.66	0
4	DMS	D	8010	-	3,3,3	2.62	1 (33%)	3,3,3	0.40	0
4	DMS	B	8005	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	0
4	DMS	B	8003	-	3,3,3	2.64	1 (33%)	3,3,3	0.56	0
4	DMS	C	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.51	0
4	DMS	A	8004	-	3,3,3	2.69	1 (33%)	3,3,3	0.65	0
4	DMS	D	8006	-	3,3,3	2.67	1 (33%)	3,3,3	0.65	0
4	DMS	C	8001	-	3,3,3	2.54	1 (33%)	3,3,3	0.58	0
4	DMS	B	8004	-	3,3,3	2.68	1 (33%)	3,3,3	0.73	0
4	DMS	D	8009	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
4	DMS	A	8001	-	3,3,3	2.58	1 (33%)	3,3,3	0.79	0
4	DMS	D	8003	-	3,3,3	2.66	1 (33%)	3,3,3	0.36	0
4	DMS	B	8008	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
4	DMS	C	8002	-	3,3,3	2.63	1 (33%)	3,3,3	0.58	0
4	DMS	D	8001	-	3,3,3	2.62	1 (33%)	3,3,3	0.55	0
4	DMS	C	8006	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
4	DMS	A	8005	-	3,3,3	2.60	1 (33%)	3,3,3	0.60	0
4	DMS	B	8006	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
4	DMS	D	8002	-	3,3,3	2.60	1 (33%)	3,3,3	0.67	0
4	DMS	C	8005	-	3,3,3	2.61	1 (33%)	3,3,3	0.45	0
4	DMS	C	8004	-	3,3,3	2.70	1 (33%)	3,3,3	0.76	0
4	DMS	D	8005	-	3,3,3	2.66	1 (33%)	3,3,3	0.61	0
4	DMS	D	8008	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DMS	A	8007	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
4	DMS	D	8004	-	3,3,3	2.71	1 (33%)	3,3,3	0.69	0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8004	DMS	O-S	4.53	1.80	1.50
4	B	8006	DMS	O-S	4.52	1.80	1.50
4	C	8003	DMS	O-S	4.51	1.80	1.50
4	A	8004	DMS	O-S	4.51	1.80	1.50
4	C	8004	DMS	O-S	4.50	1.80	1.50
4	A	8002	DMS	O-S	4.50	1.80	1.50
4	B	8004	DMS	O-S	4.49	1.80	1.50
4	D	8008	DMS	O-S	4.48	1.80	1.50
4	B	8008	DMS	O-S	4.48	1.80	1.50
4	D	8003	DMS	O-S	4.48	1.80	1.50
4	D	8006	DMS	O-S	4.46	1.80	1.50
4	D	8005	DMS	O-S	4.46	1.80	1.50
4	D	8009	DMS	O-S	4.45	1.80	1.50
4	C	8006	DMS	O-S	4.45	1.80	1.50
4	A	8003	DMS	O-S	4.44	1.80	1.50
4	B	8003	DMS	O-S	4.42	1.80	1.50
4	D	8010	DMS	O-S	4.41	1.80	1.50
4	C	8002	DMS	O-S	4.41	1.80	1.50
4	C	8007	DMS	O-S	4.40	1.80	1.50
4	A	8007	DMS	O-S	4.40	1.79	1.50
4	B	8007	DMS	O-S	4.39	1.79	1.50
4	D	8001	DMS	O-S	4.39	1.79	1.50
4	D	8007	DMS	O-S	4.38	1.79	1.50
4	C	8005	DMS	O-S	4.37	1.79	1.50
4	D	8002	DMS	O-S	4.35	1.79	1.50
4	B	8002	DMS	O-S	4.34	1.79	1.50
4	B	8005	DMS	O-S	4.33	1.79	1.50
4	A	8005	DMS	O-S	4.33	1.79	1.50
4	A	8001	DMS	O-S	4.33	1.79	1.50
4	A	8006	DMS	O-S	4.32	1.79	1.50
4	B	8001	DMS	O-S	4.29	1.79	1.50
4	C	8001	DMS	O-S	4.24	1.78	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	D	8010	DMS	3	0
4	C	8002	DMS	1	0
4	D	8002	DMS	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	1015/1052 (96%)	-0.24	19 (1%)	66	69	28, 41, 64, 96	0
1	B	1015/1052 (96%)	-0.15	26 (2%)	56	59	25, 42, 66, 109	0
1	C	1015/1052 (96%)	-0.17	20 (1%)	65	68	27, 42, 66, 99	0
1	D	1015/1052 (96%)	-0.17	25 (2%)	57	61	26, 42, 66, 101	0
All	All	4060/4208 (96%)	-0.18	90 (2%)	62	65	25, 42, 66, 109	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	732	ALA	5.4
1	B	731	PRO	5.1
1	B	732	ALA	4.9
1	A	735	HIS	4.4
1	D	735	HIS	4.3
1	A	686	PRO	4.2
1	A	733	ALA	4.1
1	D	685	LEU	4.0
1	D	730	LEU	3.9
1	C	733	ALA	3.8
1	D	689	GLU	3.8
1	D	686	PRO	3.7
1	D	687	GLN	3.6
1	B	730	LEU	3.4
1	B	685	LEU	3.4
1	B	686	PRO	3.3
1	B	735	HIS	3.3
1	B	1023	LYS	3.3
1	B	684	GLU	3.2
1	D	11	LEU	3.1
1	B	12	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	687	GLN	3.0
1	B	72	SER	3.0
1	C	799	THR	3.0
1	A	689	GLU	3.0
1	C	689	GLU	3.0
1	D	654	TRP	2.9
1	A	800	ARG	2.9
1	A	9	VAL	2.8
1	D	846	GLY	2.8
1	A	798	ALA	2.7
1	B	799	THR	2.7
1	A	772	ASP	2.7
1	D	655	MET	2.7
1	D	739	HIS	2.7
1	C	580	GLU	2.7
1	B	733	ALA	2.7
1	C	595	THR	2.7
1	B	689	GLU	2.7
1	A	71	GLU	2.7
1	D	731	PRO	2.7
1	D	845	GLN	2.7
1	D	799	THR	2.6
1	D	800	ARG	2.6
1	B	739	HIS	2.6
1	C	798	ALA	2.6
1	C	730	LEU	2.6
1	C	732	ALA	2.6
1	B	687	GLN	2.5
1	C	685	LEU	2.5
1	B	729	THR	2.5
1	B	71	GLU	2.5
1	C	977	HIS	2.5
1	C	800	ARG	2.5
1	D	581	ASN	2.5
1	A	685	LEU	2.5
1	B	593	GLY	2.4
1	C	583	ASN	2.4
1	B	770	ILE	2.4
1	C	731	PRO	2.4
1	D	12	GLN	2.4
1	A	684	GLU	2.4
1	A	10	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	9	VAL	2.4
1	C	12	GLN	2.4
1	A	580	GLU	2.4
1	C	71	GLU	2.4
1	D	734	SER	2.3
1	B	11	LEU	2.3
1	C	10	VAL	2.3
1	B	800	ARG	2.3
1	D	684	GLU	2.3
1	B	734	SER	2.2
1	D	891	VAL	2.2
1	A	801	ILE	2.2
1	C	11	LEU	2.2
1	B	671	ASP	2.2
1	D	753	ASN	2.2
1	A	796	SER	2.2
1	B	595	THR	2.2
1	B	682	LEU	2.2
1	D	732	ALA	2.2
1	A	730	LEU	2.2
1	C	735	HIS	2.1
1	D	772	ASP	2.1
1	C	687	GLN	2.1
1	D	635	THR	2.1
1	D	688	PRO	2.1
1	B	798	ALA	2.0
1	A	12	GLN	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 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
4	DMS	B	8004	4/4	0.86	0.26	67,70,71,71	0
2	MG	B	3002	1/1	0.88	0.08	46,46,46,46	0
4	DMS	C	8004	4/4	0.88	0.17	75,76,76,78	0
4	DMS	D	8004	4/4	0.88	0.18	76,77,77,80	0
4	DMS	A	8004	4/4	0.90	0.27	77,78,79,79	0
3	NA	D	3103	1/1	0.90	0.12	51,51,51,51	0
4	DMS	C	8007	4/4	0.91	0.19	71,73,74,74	0
4	DMS	A	8007	4/4	0.91	0.24	74,75,78,78	0
2	MG	D	3002	1/1	0.92	0.08	45,45,45,45	0
4	DMS	C	8006	4/4	0.93	0.21	82,82,82,83	0
4	DMS	B	8007	4/4	0.93	0.26	72,72,73,74	0
3	NA	D	3101	1/1	0.93	0.09	43,43,43,43	0
4	DMS	B	8006	4/4	0.94	0.16	62,64,64,67	0
3	NA	A	3102	1/1	0.94	0.06	36,36,36,36	0
4	DMS	A	8006	4/4	0.94	0.24	65,67,69,69	0
4	DMS	D	8005	4/4	0.94	0.22	75,75,76,78	0
4	DMS	D	8009	4/4	0.94	0.15	72,73,74,76	0
3	NA	B	3102	1/1	0.95	0.10	31,31,31,31	0
4	DMS	D	8002	4/4	0.95	0.19	68,68,69,71	0
4	DMS	B	8008	4/4	0.95	0.14	48,49,50,51	0
4	DMS	B	8005	4/4	0.95	0.22	69,71,72,72	0
4	DMS	D	8006	4/4	0.95	0.14	78,79,80,81	0
4	DMS	A	8005	4/4	0.95	0.28	55,58,59,60	0
4	DMS	C	8005	4/4	0.96	0.19	67,68,68,69	0
2	MG	A	3002	1/1	0.96	0.06	39,39,39,39	0
3	NA	A	3101	1/1	0.96	0.13	41,41,41,41	0
4	DMS	A	8001	4/4	0.96	0.22	52,54,55,56	0
4	DMS	A	8003	4/4	0.96	0.17	52,53,54,55	0
4	DMS	B	8001	4/4	0.96	0.18	47,48,50,51	0
4	DMS	C	8001	4/4	0.96	0.21	50,52,54,55	0
4	DMS	D	8008	4/4	0.96	0.15	61,61,62,64	0
4	DMS	B	8002	4/4	0.96	0.21	51,52,53,53	0
4	DMS	B	8003	4/4	0.97	0.14	56,57,57,58	0
4	DMS	A	8002	4/4	0.97	0.14	48,49,50,52	0
4	DMS	D	8003	4/4	0.97	0.17	55,55,57,57	0
4	DMS	C	8002	4/4	0.97	0.15	56,56,58,59	0
4	DMS	C	8003	4/4	0.97	0.18	64,65,65,66	0
2	MG	D	3001	1/1	0.97	0.12	39,39,39,39	0
3	NA	C	3101	1/1	0.97	0.07	44,44,44,44	0
3	NA	C	3102	1/1	0.97	0.06	33,33,33,33	0
3	NA	D	3102	1/1	0.98	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	B	3101	1/1	0.98	0.12	44,44,44,44	0
2	MG	A	3001	1/1	0.98	0.10	39,39,39,39	0
2	MG	C	3002	1/1	0.98	0.06	44,44,44,44	0
2	MG	B	3001	1/1	0.98	0.08	39,39,39,39	0
4	DMS	D	8007	4/4	0.98	0.18	62,65,65,67	0
3	NA	A	3103	1/1	0.98	0.13	41,41,41,41	0
4	DMS	D	8001	4/4	0.98	0.15	51,51,51,53	0
4	DMS	D	8010	4/4	0.98	0.21	54,55,56,61	0
2	MG	C	3001	1/1	0.99	0.07	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.