



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:39 PM UTC

PDB ID : 3VD7 / pdb_00003vd7
Title : E. coli (lacZ) beta-galactosidase (N460S) in complex with galactotetrazole
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 : 2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

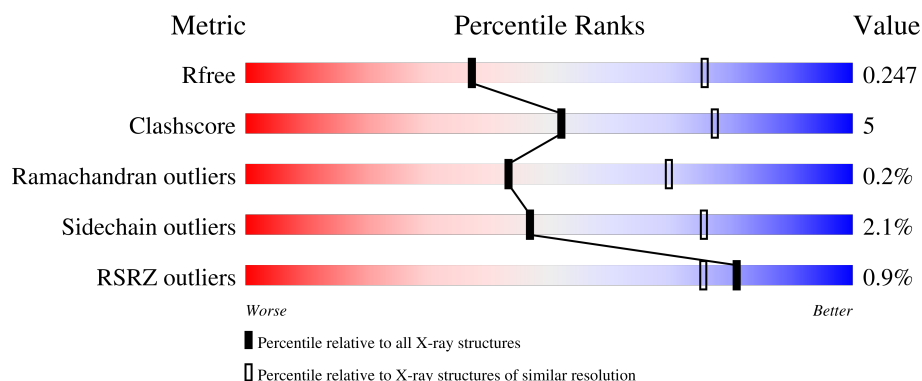
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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% 84% 12% .
1	B	1052	% 82% 13% ..
1	C	1052	81% 15% .
1	D	1052	82% 14% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	D	8001	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33041 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	B	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			

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
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	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
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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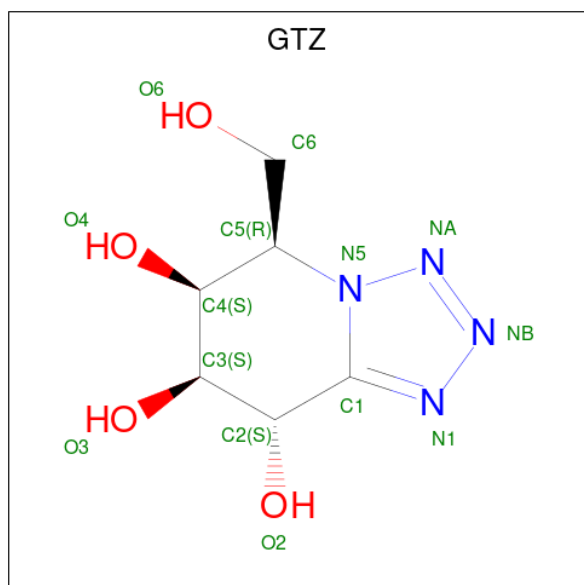
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	expression tag	UNP P00722
C	2	LYS	-	expression tag	UNP P00722
C	3	ASP	-	expression tag	UNP P00722
C	4	PRO	-	expression tag	UNP P00722
C	5	MET	-	expression tag	UNP P00722
C	6	ILE	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	460	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
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	SER	ASN	engineered mutation	UNP P00722

- Molecule 2 is (5R, 6S, 7S, 8S)-5-HYDROXYMETHYL-6,7,8-TRIHYDROXY-TETRAZOL O[1,5-A]PIPERIDINE (CCD ID: GTZ) (formula: C₆H₁₀N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	6	4	4		
2	B	1	Total	C	N	O	0	0
			14	6	4	4		
2	C	1	Total	C	N	O	0	0
			14	6	4	4		
2	D	1	Total	C	N	O	0	0
			14	6	4	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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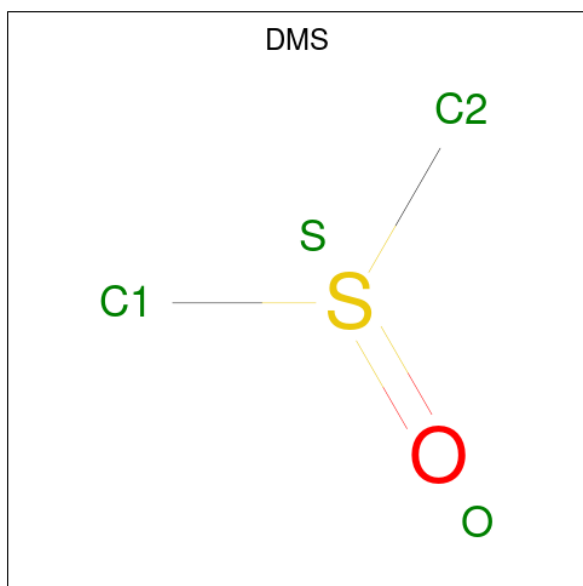
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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

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

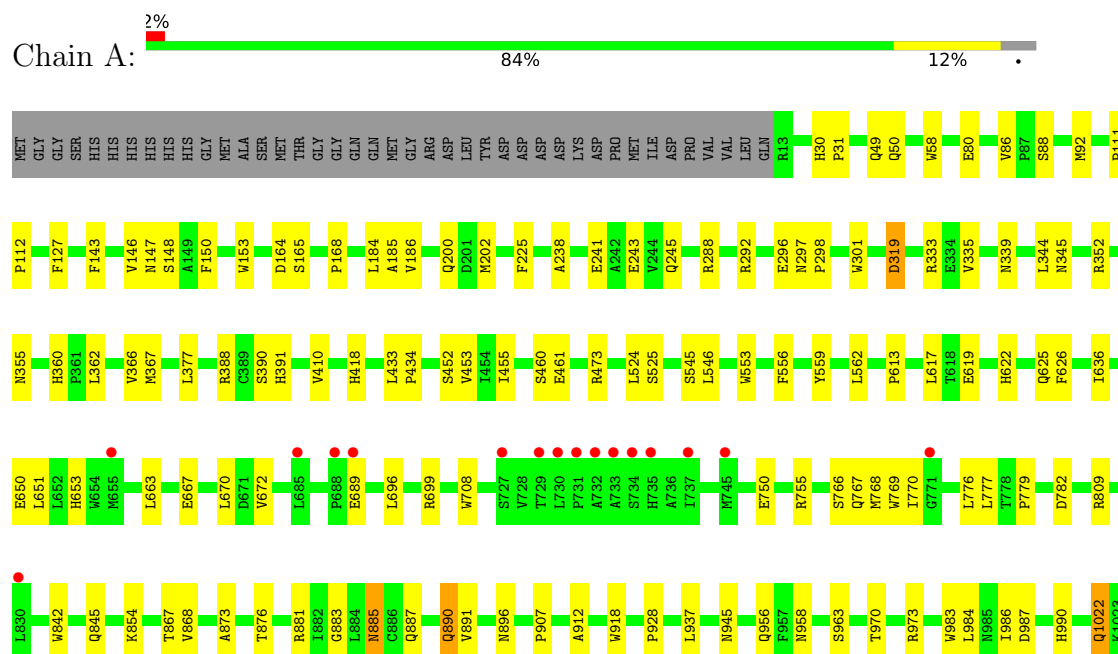
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	64	Total 64	O 64	0	0
6	B	93	Total 93	O 93	0	0
6	C	79	Total 79	O 79	0	0
6	D	123	Total 123	O 123	0	0

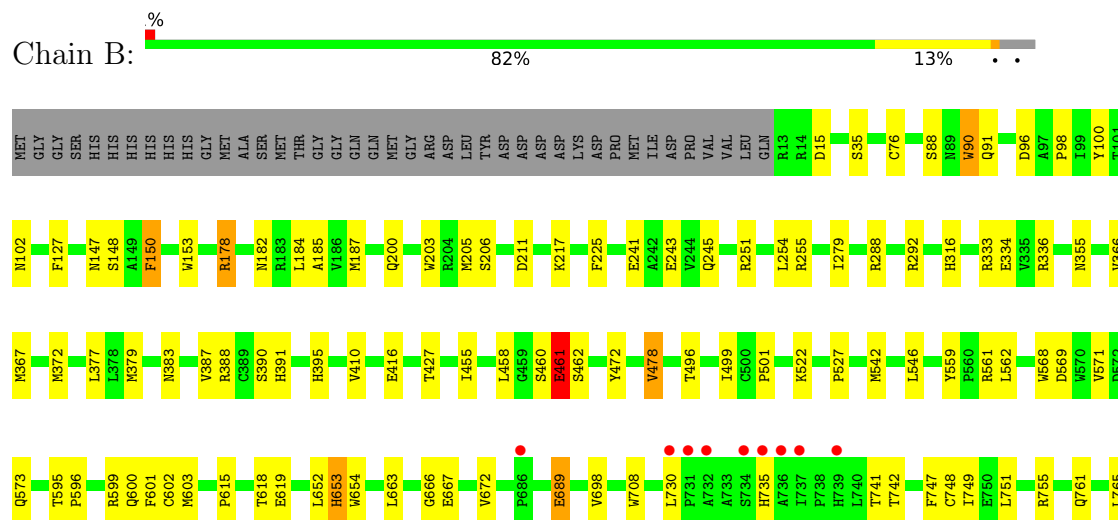
3 Residue-property plots [i](#)

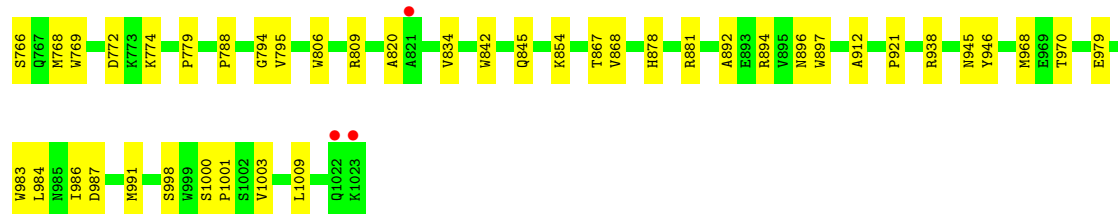
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-galactosidase



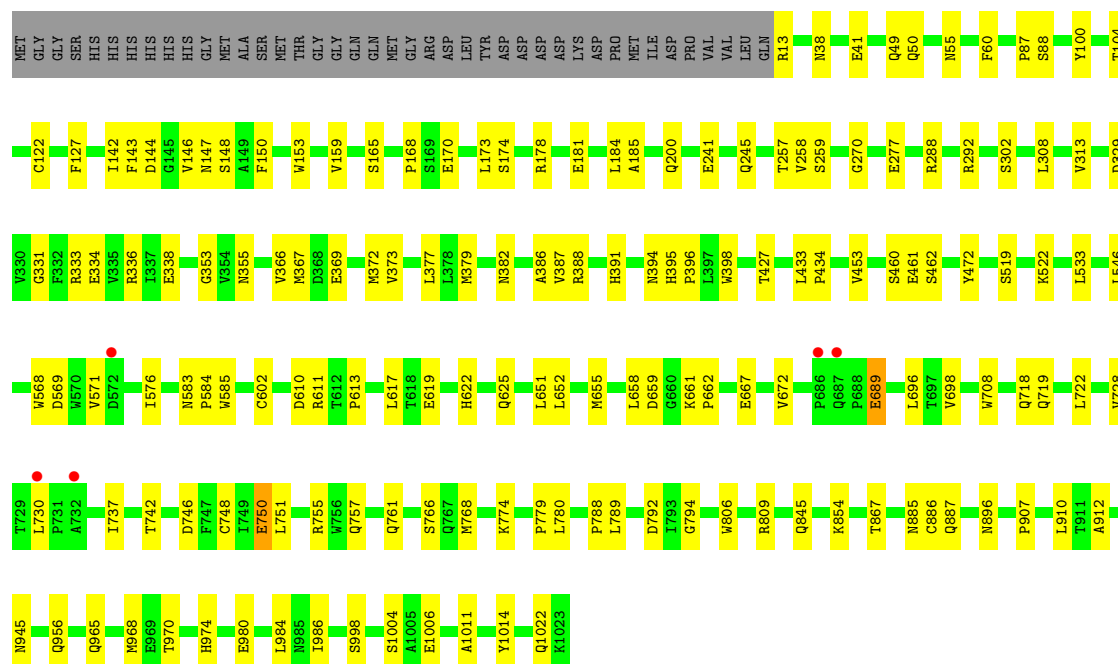
• Molecule 1: Beta-galactosidase





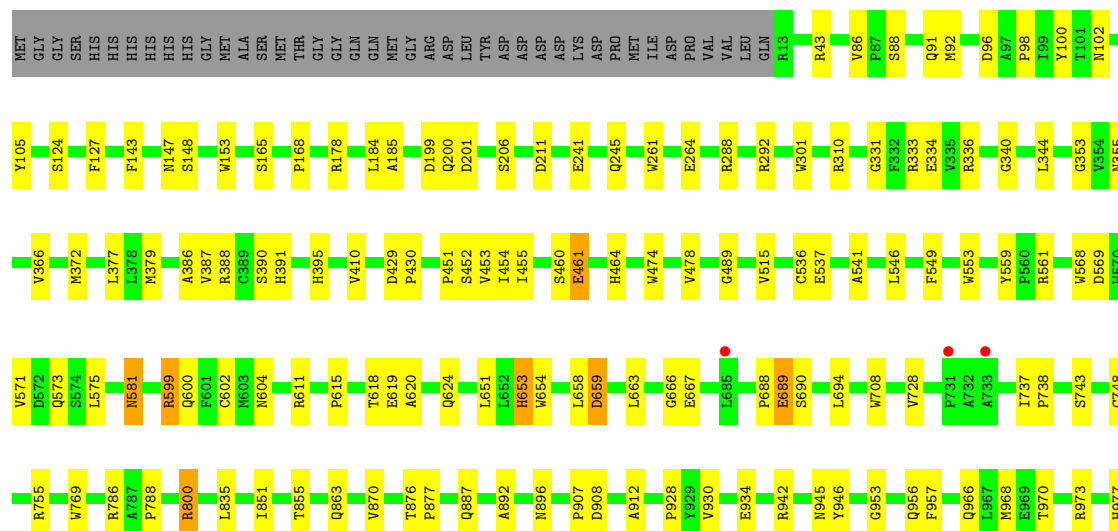
• Molecule 1: Beta-galactosidase

Chain C: 81% 15%



• Molecule 1: Beta-galactosidase

Chain D: 82% 14%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.46Å 152.37Å 135.11Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	44.78 – 2.87 44.78 – 2.87	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.78-2.87) 93.2 (44.78-2.87)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.188 , 0.250 0.188 , 0.247	Depositor DCC
R_{free} test set	4895 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33041	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, MG, GTZ, NA

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	0.51	0/8366	0.78	2/11412 (0.0%)
1	B	0.54	0/8366	0.79	5/11412 (0.0%)
1	C	0.52	0/8366	0.78	0/11412
1	D	0.53	0/8366	0.78	0/11412
All	All	0.53	0/33464	0.78	7/45648 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	VAL	N-CA-C	5.27	116.05	110.72
1	A	545	SER	N-CA-C	5.26	115.18	108.24
1	A	809	ARG	N-CA-C	-5.25	105.47	111.14
1	B	571	VAL	N-CA-C	5.19	115.75	108.17
1	B	150	PHE	N-CA-C	5.13	116.31	108.52
1	B	76	CYS	N-CA-C	5.12	117.03	108.99
1	B	496	THR	N-CA-C	5.03	117.26	108.76

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	78	0
1	B	8124	0	7715	79	0
1	C	8124	0	7715	86	0
1	D	8124	0	7715	84	0
2	A	14	0	9	0	0
2	B	14	0	9	0	0
2	C	14	0	9	0	0
2	D	14	0	9	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	24	0	36	1	0
5	B	32	0	48	1	0
5	C	32	0	48	2	0
5	D	28	0	42	5	0
6	A	64	0	0	1	0
6	B	93	0	0	1	0
6	C	79	0	0	2	0
6	D	123	0	0	0	0
All	All	33041	0	31070	322	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 (322) 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:88:SER:HA	1:A:366:VAL:HG21	1.49	0.95
1:D:800:ARG:HG3	1:D:800:ARG:O	1.71	0.91
1:D:653:HIS:CD2	1:D:667:GLU:HG3	2.07	0.90
1:C:750:GLU:HG2	1:C:755:ARG:HG2	1.57	0.84
1:B:200:GLN:HG2	1:B:391:HIS:HB2	1.61	0.81
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.97	0.80
1:A:768:MET:HE1	1:A:1022:GLN:OE1	1.83	0.78
1:C:38:ASN:HB3	1:C:41:GLU:HG3	1.63	0.78
1:A:890:GLN:HG3	1:A:891:VAL:N	2.00	0.75
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:HIS:NE2	1:D:667:GLU:HG3	2.03	0.72
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.71	0.72
1:C:367:MET:HB3	1:C:372:MET:HE3	1.72	0.71
1:D:689:GLU:H	1:D:689:GLU:CD	1.99	0.71
1:D:755:ARG:HB2	1:D:769:TRP:HB2	1.73	0.70
1:A:770:ILE:HD11	1:A:1022:GLN:HG2	1.72	0.70
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.74	0.70
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.74	0.70
1:C:88:SER:HA	1:C:366:VAL:HG21	1.74	0.69
1:B:91:GLN:HG3	1:B:96:ASP:OD1	1.95	0.67
1:B:410:VAL:HG22	1:B:455:ILE:HB	1.77	0.66
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.78	0.65
1:D:541:ALA:HB3	1:D:604:ASN:O	1.97	0.65
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.63	0.64
1:B:390:SER:HB2	1:B:391:HIS:CE1	2.33	0.64
1:B:806:TRP:HA	1:B:809:ARG:HD2	1.80	0.64
1:D:887:GLN:NE2	1:D:980:GLU:O	2.30	0.63
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.82	0.62
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.82	0.62
1:B:689:GLU:H	1:B:689:GLU:CD	2.08	0.62
1:A:524:LEU:HD11	1:A:562:LEU:HG	1.83	0.61
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.81	0.61
1:B:766:SER:HA	1:B:779:PRO:HB3	1.83	0.61
1:D:91:GLN:HB3	1:D:98:PRO:HD3	1.83	0.61
1:A:92:MET:HA	1:A:92:MET:HE2	1.83	0.61
1:A:963:SER:HB3	1:A:983:TRP:CE2	2.35	0.61
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.00	0.60
1:C:147:ASN:HA	1:C:165:SER:HB3	1.83	0.60
1:C:144:ASP:HA	1:C:168:PRO:HB3	1.84	0.60
1:B:788:PRO:HD2	1:B:968:MET:HG3	1.83	0.60
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.82	0.60
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.84	0.59
1:A:49:GLN:HB2	1:A:50:GLN:OE1	2.02	0.59
1:A:755:ARG:HB2	1:A:769:TRP:HB2	1.85	0.59
1:C:794:GLY:HA2	1:C:998:SER:O	2.02	0.59
1:A:885:ASN:OD1	1:A:885:ASN:C	2.45	0.58
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.84	0.58
1:D:88:SER:HA	1:D:366:VAL:HG21	1.84	0.58
1:B:854:LYS:HG2	1:B:868:VAL:HG22	1.86	0.58
1:A:766:SER:HA	1:A:779:PRO:HB3	1.86	0.57
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.05	0.57
1:C:806:TRP:HA	1:C:809:ARG:HD2	1.87	0.57
1:C:622:HIS:O	1:C:625:GLN:HG3	2.04	0.56
1:D:573:GLN:HB2	1:D:602:CYS:O	2.04	0.56
1:D:896:ASN:HB3	1:D:945:ASN:HB2	1.88	0.56
1:A:984:LEU:HD21	1:A:986:ILE:HD11	1.87	0.56
1:D:800:ARG:O	1:D:800:ARG:CG	2.49	0.56
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.70	0.55
1:B:599:ARG:HB2	1:B:600:GLN:OE1	2.07	0.55
1:A:147:ASN:HA	1:A:165:SER:HB3	1.88	0.55
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.87	0.55
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.88	0.55
1:A:854:LYS:HG2	1:A:868:VAL:HG22	1.88	0.54
1:D:331:GLY:O	5:D:8001:DMS:H13	2.07	0.54
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.42	0.54
1:D:200:GLN:HG2	1:D:391:HIS:HB2	1.89	0.54
1:A:896:ASN:HB3	1:A:945:ASN:HB2	1.90	0.54
1:A:319:ASP:OD1	1:A:319:ASP:N	2.39	0.54
1:C:696:LEU:HB2	1:C:722:LEU:HD11	1.89	0.54
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.43	0.54
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.89	0.54
1:A:767:GLN:HA	1:A:776:LEU:HD12	1.90	0.53
1:C:372:MET:CE	1:C:395:HIS:HB3	2.38	0.53
1:C:984:LEU:HD21	1:C:986:ILE:HD11	1.90	0.53
1:C:369:GLU:O	1:C:373:VAL:HG23	2.09	0.53
1:C:394:ASN:HD22	1:C:398:TRP:CD1	2.27	0.53
1:C:241:GLU:HG2	1:C:292:ARG:HG2	1.91	0.53
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.41	0.53
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.91	0.53
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.90	0.52
1:D:930:VAL:HA	1:D:973:ARG:HD3	1.90	0.52
1:C:522:LYS:HA	1:D:559:TYR:CE2	2.44	0.52
1:B:147:ASN:HB3	1:B:206:SER:HA	1.91	0.52
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.39	0.52
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.92	0.52
1:C:788:PRO:HD2	1:C:968:MET:HG3	1.91	0.52
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.91	0.52
1:A:352:ARG:HG2	1:A:553:TRP:CH2	2.44	0.52
1:C:372:MET:HE1	1:C:395:HIS:CB	2.39	0.52
1:B:88:SER:HA	1:B:366:VAL:HG21	1.92	0.52
1:B:854:LYS:HA	1:B:867:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:991:MET:HE3	1:B:1003:VAL:HG21	1.91	0.51
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.10	0.51
1:C:610:ASP:O	1:C:611:ARG:HB2	2.11	0.51
1:C:372:MET:HE1	1:C:395:HIS:CG	2.45	0.51
1:D:907:PRO:HG2	1:D:990:HIS:O	2.10	0.51
1:A:245:GLN:HG2	1:A:288:ARG:CG	2.41	0.51
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.92	0.51
1:C:382:ASN:ND2	1:C:617:LEU:HD21	2.25	0.51
1:A:782:ASP:HB2	1:A:842:TRP:CZ2	2.45	0.51
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.11	0.51
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.46	0.50
1:D:942:ARG:HA	1:D:953:GLY:O	2.11	0.50
1:B:573:GLN:HB2	1:B:602:CYS:O	2.10	0.50
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.93	0.50
1:D:654:TRP:HE1	1:D:666:GLY:HA3	1.76	0.50
1:C:766:SER:HA	1:C:779:PRO:HB3	1.92	0.50
1:A:143:PHE:O	1:A:168:PRO:HA	2.12	0.50
1:C:353:GLY:HA2	1:C:386:ALA:O	2.11	0.50
1:D:581:ASN:N	1:D:581:ASN:OD1	2.43	0.50
1:A:873:ALA:O	1:A:876:THR:HG22	2.12	0.50
1:C:49:GLN:HB2	1:C:50:GLN:OE1	2.12	0.50
1:C:896:ASN:HB3	1:C:945:ASN:HB2	1.94	0.50
1:D:454:ILE:HG13	1:D:455:ILE:HG13	1.94	0.49
1:B:203:TRP:CB	1:B:205:MET:HE3	2.42	0.49
1:C:60:PHE:HA	1:C:122:CYS:O	2.13	0.49
1:D:379:MET:HE1	1:D:387:VAL:HB	1.95	0.49
1:A:88:SER:HA	1:A:366:VAL:CG2	2.32	0.49
1:A:883:GLY:HA3	1:A:987:ASP:HA	1.93	0.49
1:D:147:ASN:HA	1:D:165:SER:HB3	1.95	0.49
1:D:331:GLY:O	5:D:8001:DMS:C1	2.60	0.49
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.77	0.49
1:C:331:GLY:O	5:C:8001:DMS:H13	2.12	0.49
1:B:600:GLN:HB2	1:B:603:MET:HE2	1.95	0.48
1:B:367:MET:HB3	1:B:372:MET:HE3	1.94	0.48
1:D:147:ASN:HA	1:D:148:SER:HA	1.62	0.48
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.48	0.48
1:D:536:CYS:O	1:D:537:GLU:HG3	2.13	0.48
1:A:525:SER:O	1:B:561:ARG:HD3	2.13	0.48
1:B:897:TRP:CZ2	1:B:938:ARG:HG2	2.49	0.48
1:D:908:ASP:HB3	1:D:1007:PHE:CD1	2.48	0.48
1:A:367:MET:HA	1:A:367:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.95	0.48
1:C:887:GLN:NE2	1:C:980:GLU:O	2.46	0.48
1:D:474:TRP:CZ2	1:D:478:VAL:HG21	2.48	0.48
1:B:794:GLY:HA2	1:B:998:SER:O	2.14	0.48
1:D:143:PHE:O	1:D:168:PRO:HA	2.13	0.48
1:B:427:THR:HG21	1:B:462:SER:HB3	1.95	0.48
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.95	0.48
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.48	0.47
1:A:241:GLU:HG2	1:A:292:ARG:HG2	1.95	0.47
1:C:854:LYS:HA	1:C:867:THR:O	2.13	0.47
1:D:658:LEU:O	1:D:659:ASP:C	2.57	0.47
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.49	0.47
1:B:878:HIS:HB3	1:B:1009:LEU:O	2.14	0.47
1:D:654:TRP:CE2	1:D:666:GLY:HA3	2.49	0.47
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.49	0.47
1:B:460:SER:O	1:B:461:GLU:C	2.58	0.47
1:B:894:ARG:NH1	1:B:921:PRO:HD3	2.30	0.47
1:B:383:ASN:OD1	5:B:8002:DMS:H23	2.14	0.47
1:C:746:ASP:OD2	1:C:757:GLN:NE2	2.48	0.47
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.45	0.47
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.50	0.47
1:D:615:PRO:O	1:D:618:THR:HG22	2.13	0.47
1:A:881:ARG:HE	1:A:987:ASP:CG	2.23	0.47
1:C:143:PHE:O	1:C:168:PRO:HA	2.14	0.47
1:C:146:VAL:HG11	1:C:150:PHE:CD2	2.50	0.47
1:C:571:VAL:HG21	1:C:611:ARG:NH1	2.30	0.47
1:B:595:THR:HA	1:B:596:PRO:C	2.39	0.46
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.98	0.46
1:C:789:LEU:HG	1:C:792:ASP:OD2	2.15	0.46
1:B:90:TRP:C	1:B:90:TRP:CD1	2.93	0.46
1:C:1022:GLN:HB2	6:C:4018:HOH:O	2.15	0.46
1:D:451:PRO:HA	5:D:8001:DMS:H23	1.97	0.46
1:D:651:LEU:O	1:D:651:LEU:HD12	2.14	0.46
1:C:55:ASN:ND2	1:C:87:PRO:HD3	2.29	0.46
1:B:241:GLU:HG2	1:B:292:ARG:HG2	1.96	0.46
1:A:30:HIS:ND1	1:A:31:PRO:O	2.32	0.46
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.98	0.46
1:D:43:ARG:HH12	1:D:264:GLU:HG2	1.81	0.46
1:A:937:LEU:HD11	1:A:956:GLN:HB2	1.98	0.46
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.51	0.46
1:D:261:TRP:HB2	1:D:310:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:PRO:HB2	1:A:973:ARG:NH1	2.29	0.46
1:B:91:GLN:HB3	1:B:98:PRO:HD3	1.97	0.46
1:B:881:ARG:HE	1:B:987:ASP:CG	2.23	0.46
1:C:730:LEU:HD12	1:C:730:LEU:H	1.81	0.46
1:D:241:GLU:HG2	1:D:292:ARG:HG2	1.97	0.46
1:D:991:MET:HE3	1:D:1003:VAL:HG21	1.98	0.46
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.51	0.46
1:A:50:GLN:N	1:A:50:GLN:CD	2.74	0.45
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.81	0.45
1:C:173:LEU:O	1:C:174:SER:C	2.59	0.45
1:C:689:GLU:CD	1:C:689:GLU:H	2.24	0.45
1:B:416:GLU:HG3	1:B:460:SER:O	2.16	0.45
1:D:957:PHE:HA	1:D:985:ASN:O	2.16	0.45
1:A:750:GLU:HG3	1:A:755:ARG:HG2	1.98	0.45
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.98	0.45
1:A:146:VAL:HG11	1:A:150:PHE:CD2	2.51	0.45
1:A:390:SER:HA	1:A:391:HIS:HA	1.75	0.45
1:D:301:TRP:CH2	1:D:452:SER:HA	2.52	0.45
1:A:651:LEU:HD13	1:A:667:GLU:HG2	1.99	0.45
1:B:979:GLU:OE1	1:B:983:TRP:NE1	2.44	0.45
1:C:379:MET:HE1	1:C:387:VAL:HB	1.99	0.45
1:B:147:ASN:O	1:B:206:SER:HB2	2.17	0.44
1:B:615:PRO:O	1:B:618:THR:HG22	2.17	0.44
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.16	0.44
1:A:301:TRP:CH2	1:A:452:SER:HA	2.53	0.44
1:B:742:THR:HG23	1:B:747:PHE:HE2	1.82	0.44
1:B:984:LEU:HD21	1:B:986:ILE:HD11	1.99	0.44
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.52	0.44
1:A:559:TYR:CE2	1:B:522:LYS:HA	2.53	0.44
1:B:379:MET:HE1	1:B:387:VAL:HB	1.99	0.44
1:D:390:SER:HA	1:D:391:HIS:HA	1.70	0.44
1:A:770:ILE:CD1	1:A:1022:GLN:HG2	2.46	0.44
1:C:718:GLN:HG3	1:C:719:GLN:N	2.32	0.44
1:C:1004:SER:OG	1:C:1006:GLU:OE2	2.34	0.44
1:D:928:PRO:HB2	1:D:973:ARG:HH11	1.83	0.44
1:A:148:SER:HA	1:A:165:SER:HB3	1.99	0.44
1:A:460:SER:O	1:A:461:GLU:C	2.61	0.44
1:D:464:HIS:HB2	1:D:489:GLY:HA3	1.99	0.44
1:A:335:VAL:HG22	1:A:344:LEU:HD12	2.00	0.44
1:A:650:GLU:HB3	1:A:670:LEU:HD12	2.00	0.44
1:B:559:TYR:HB2	1:B:562:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ALA:HB2	1:A:298:PRO:HG3	1.99	0.43
1:C:583:ASN:HA	1:C:584:PRO:HD3	1.77	0.43
1:C:613:PRO:HB3	1:C:617:LEU:CD2	2.48	0.43
1:B:741:THR:HB	1:B:748:CYS:HB3	1.99	0.43
1:C:907:PRO:HA	1:C:910:LEU:HD23	2.00	0.43
1:A:653:HIS:HB3	1:A:699:ARG:HG3	2.00	0.43
1:B:896:ASN:HB3	1:B:945:ASN:HB2	2.01	0.43
1:C:245:GLN:HG2	1:C:288:ARG:HG2	2.00	0.43
1:C:568:TRP:HA	1:C:569:ASP:HA	1.76	0.43
1:C:651:LEU:HD13	1:C:667:GLU:HG2	2.00	0.43
1:B:769:TRP:HE1	1:B:774:LYS:HG2	1.83	0.43
1:C:142:ILE:HG12	1:C:170:GLU:CG	2.43	0.43
1:A:622:HIS:ND1	1:A:625:GLN:OE1	2.51	0.43
1:B:755:ARG:HB2	1:B:769:TRP:HB2	2.01	0.43
1:C:147:ASN:HA	1:C:148:SER:HA	1.63	0.43
1:A:339:ASN:O	1:B:527:PRO:HB3	2.18	0.43
1:A:410:VAL:HG22	1:A:455:ILE:HB	2.00	0.43
1:A:854:LYS:HA	1:A:867:THR:O	2.19	0.43
1:B:416:GLU:OE1	1:B:460:SER:HB3	2.19	0.43
1:C:200:GLN:CG	1:C:391:HIS:HB2	2.49	0.43
1:C:257:THR:HA	1:C:270:GLY:O	2.19	0.43
1:D:688:PRO:HG3	1:D:694:LEU:HD21	2.01	0.43
1:B:1000:SER:O	1:B:1001:PRO:C	2.62	0.43
1:D:553:TRP:CZ2	1:D:624:GLN:HG2	2.54	0.43
1:A:907:PRO:HG2	1:A:990:HIS:O	2.19	0.43
1:C:427:THR:HG21	1:C:462:SER:HB3	1.99	0.43
1:D:124:SER:HA	1:D:184:LEU:O	2.19	0.43
1:D:353:GLY:HA2	1:D:386:ALA:O	2.18	0.43
1:A:636:ILE:HD11	1:A:696:LEU:HD21	2.00	0.42
1:D:102:ASN:HA	1:D:201:ASP:OD1	2.19	0.42
1:D:966:GLN:OE1	1:D:977:HIS:HD2	2.02	0.42
1:A:559:TYR:HB2	1:A:562:LEU:HD12	2.00	0.42
1:C:302:SER:HB3	6:C:4026:HOH:O	2.18	0.42
1:B:653:HIS:CD2	1:B:667:GLU:HG3	2.55	0.42
1:C:308:LEU:HD22	1:C:329:ASP:HB3	2.01	0.42
1:D:571:VAL:HG21	1:D:611:ARG:NH1	2.34	0.42
1:A:296:GLU:O	1:A:297:ASN:C	2.63	0.42
1:C:395:HIS:HA	1:C:396:PRO:HD2	1.82	0.42
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.54	0.42
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.00	0.42
1:B:820:ALA:HB2	1:B:842:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:HG22	1:C:313:VAL:HG22	2.02	0.42
1:D:292:ARG:O	5:D:8003:DMS:H22	2.19	0.42
1:B:35:SER:HB2	1:B:217:LYS:HD2	2.02	0.42
1:D:92:MET:HE1	1:D:575:LEU:HD13	2.01	0.42
1:D:410:VAL:HG22	1:D:455:ILE:HB	2.02	0.42
1:C:533:LEU:C	1:C:533:LEU:HD23	2.44	0.42
1:C:576:ILE:HD13	1:C:576:ILE:HA	1.94	0.42
1:C:658:LEU:O	1:C:659:ASP:C	2.61	0.42
1:D:737:ILE:HA	1:D:738:PRO:HD3	1.90	0.42
1:A:200:GLN:HB2	1:A:202:MET:HE2	2.01	0.42
1:B:150:PHE:HA	1:B:187:MET:O	2.20	0.42
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.02	0.41
1:C:333:ARG:NH2	1:C:453:VAL:O	2.53	0.41
1:C:472:TYR:CD2	1:C:472:TYR:C	2.98	0.41
1:B:15:ASP:OD2	1:C:13:ARG:NH2	2.50	0.41
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.53	0.41
1:B:749:ILE:HG12	1:B:834:VAL:HG11	2.02	0.41
1:D:333:ARG:NH2	1:D:453:VAL:O	2.53	0.41
1:D:340:GLY:O	1:D:561:ARG:HG2	2.19	0.41
1:A:225:PHE:HA	1:A:243:GLU:O	2.20	0.41
1:A:333:ARG:NH2	1:A:453:VAL:O	2.53	0.41
1:B:225:PHE:HA	1:B:243:GLU:O	2.20	0.41
1:B:568:TRP:HA	1:B:569:ASP:HA	1.88	0.41
1:C:965:GLN:HA	1:C:968:MET:HE3	2.03	0.41
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.55	0.41
1:D:147:ASN:HB3	1:D:206:SER:HA	2.01	0.41
1:D:786:ARG:HD2	1:D:934:GLU:HG2	2.02	0.41
1:B:653:HIS:HD2	1:B:667:GLU:HG3	1.85	0.41
1:C:661:LYS:HA	1:C:662:PRO:HD3	1.95	0.41
1:A:111:PRO:HA	1:A:112:PRO:HA	1.88	0.41
1:B:333:ARG:NH2	6:B:4010:HOH:O	2.50	0.41
1:D:429:ASP:HA	1:D:430:PRO:HD2	1.93	0.41
1:A:58:TRP:CD1	1:A:86:VAL:HB	2.56	0.41
1:A:626:PHE:CE1	5:A:8001:DMS:H12	2.55	0.41
1:D:984:LEU:HD21	1:D:986:ILE:HD11	2.02	0.41
1:A:613:PRO:HB3	1:A:617:LEU:HD23	2.03	0.41
1:C:585:TRP:CE3	1:C:974:HIS:CE1	3.09	0.41
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.56	0.41
1:A:777:LEU:HD12	1:A:887:GLN:HG2	2.02	0.41
1:B:203:TRP:HB2	1:B:205:MET:HE3	2.03	0.41
1:C:622:HIS:NE2	5:C:8002:DMS:H13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:851:ILE:O	1:D:870:VAL:HA	2.21	0.41
1:A:344:LEU:O	1:A:345:ASN:C	2.64	0.41
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.93	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.41
1:B:251:ARG:HB2	1:B:254:LEU:HG	2.03	0.41
1:B:542:MET:HE3	1:B:601:PHE:HA	2.03	0.41
1:C:460:SER:O	1:C:461:GLU:C	2.63	0.41
1:D:460:SER:O	1:D:461:GLU:C	2.64	0.41
1:A:473:ARG:NH1	6:A:4040:HOH:O	2.53	0.41
1:B:458:LEU:HD11	1:B:472:TYR:HB2	2.03	0.41
1:A:418:HIS:ND1	1:A:461:GLU:OE1	2.54	0.40
1:A:553:TRP:CD2	1:A:556:PHE:HD1	2.38	0.40
1:D:333:ARG:HD3	5:D:8001:DMS:H12	2.02	0.40
1:A:200:GLN:HG2	1:A:391:HIS:HB2	2.03	0.40
1:B:178:ARG:HG3	1:B:182:ASN:OD1	2.21	0.40
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.56	0.40
1:D:835:LEU:HD11	1:D:855:THR:HB	2.03	0.40
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.21	0.40
1:C:50:GLN:CD	1:C:50:GLN:N	2.79	0.40
1:C:655:MET:HE2	1:C:655:MET:HB3	1.94	0.40
1:D:599:ARG:HH11	1:D:600:GLN:NE2	2.20	0.40
1:A:896:ASN:HA	1:A:918:TRP:O	2.22	0.40
1:B:730:LEU:HD12	1:B:730:LEU:H	1.85	0.40
1:C:768:MET:HE2	1:C:768:MET:HB3	1.98	0.40
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.57	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	1009/1052 (96%)	955 (95%)	53 (5%)	1 (0%)	48 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1009/1052 (96%)	949 (94%)	56 (6%)	4 (0%)	30	56
1	C	1009/1052 (96%)	951 (94%)	58 (6%)	0	100	100
1	D	1009/1052 (96%)	958 (95%)	47 (5%)	4 (0%)	30	56
All	All	4036/4208 (96%)	3813 (94%)	214 (5%)	9 (0%)	43	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	211	ASP
1	B	461	GLU
1	B	765	LEU
1	B	102	ASN
1	D	211	ASP
1	D	599	ARG
1	D	659	ASP
1	D	461	GLU
1	A	164	ASP

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%)	851 (98%)	13 (2%)	57	82
1	B	864/898 (96%)	846 (98%)	18 (2%)	47	75
1	C	864/898 (96%)	841 (97%)	23 (3%)	39	70
1	D	864/898 (96%)	847 (98%)	17 (2%)	48	76
All	All	3456/3592 (96%)	3385 (98%)	71 (2%)	47	75

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	186	VAL

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Mol	Chain	Res	Type
1	A	319	ASP
1	A	546	LEU
1	A	663	LEU
1	A	672	VAL
1	A	689	GLU
1	A	845	GLN
1	A	885	ASN
1	A	890	GLN
1	A	958	ASN
1	A	970	THR
1	A	1022	GLN
1	B	90	TRP
1	B	178	ARG
1	B	279	ILE
1	B	461	GLU
1	B	478	VAL
1	B	546	LEU
1	B	653	HIS
1	B	663	LEU
1	B	672	VAL
1	B	689	GLU
1	B	735	HIS
1	B	751	LEU
1	B	761	GLN
1	B	768	MET
1	B	772	ASP
1	B	795	VAL
1	B	845	GLN
1	B	970	THR
1	C	104	THR
1	C	159	VAL
1	C	178	ARG
1	C	181	GLU
1	C	259	SER
1	C	277	GLU
1	C	338	GLU
1	C	519	SER
1	C	546	LEU
1	C	672	VAL
1	C	689	GLU
1	C	728	VAL
1	C	737	ILE

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Mol	Chain	Res	Type
1	C	742	THR
1	C	748	CYS
1	C	750	GLU
1	C	751	LEU
1	C	761	GLN
1	C	774	LYS
1	C	845	GLN
1	C	885	ASN
1	C	956	GLN
1	C	970	THR
1	D	86	VAL
1	D	178	ARG
1	D	344	LEU
1	D	515	VAL
1	D	546	LEU
1	D	581	ASN
1	D	653	HIS
1	D	663	LEU
1	D	689	GLU
1	D	690	SER
1	D	728	VAL
1	D	743	SER
1	D	748	CYS
1	D	800	ARG
1	D	956	GLN
1	D	970	THR
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	216	HIS
1	A	221	GLN
1	A	445	GLN
1	A	702	GLN
1	A	757	GLN
1	A	887	GLN
1	A	903	GLN
1	A	974	HIS
1	A	977	HIS
1	B	135	GLN

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Mol	Chain	Res	Type
1	B	221	GLN
1	B	266	GLN
1	B	294	ASN
1	B	485	GLN
1	B	623	GLN
1	B	628	GLN
1	B	761	GLN
1	B	885	ASN
1	B	903	GLN
1	B	949	HIS
1	B	1022	GLN
1	C	221	GLN
1	C	363	HIS
1	C	445	GLN
1	C	624	GLN
1	C	739	HIS
1	C	757	GLN
1	C	804	ASN
1	C	845	GLN
1	C	903	GLN
1	C	945	ASN
1	C	950	GLN
1	D	49	GLN
1	D	50	GLN
1	D	163	GLN
1	D	221	GLN
1	D	485	GLN
1	D	757	GLN
1	D	845	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 47 ligands modelled in this entry, 14 are monoatomic - leaving 33 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
5	DMS	D	8006	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
5	DMS	D	8003	-	3,3,3	2.67	1 (33%)	3,3,3	0.77	0
5	DMS	C	8007	-	3,3,3	2.68	1 (33%)	3,3,3	0.46	0
5	DMS	B	8006	-	3,3,3	2.75	1 (33%)	3,3,3	0.72	0
5	DMS	B	8005	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
5	DMS	C	8008	-	3,3,3	2.69	1 (33%)	3,3,3	0.57	0
5	DMS	B	8008	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
5	DMS	D	8005	-	3,3,3	2.74	1 (33%)	3,3,3	0.73	0
2	GTZ	B	2001	4	13,15,15	2.55	4 (30%)	14,22,22	2.59	6 (42%)
5	DMS	C	8002	-	3,3,3	2.72	1 (33%)	3,3,3	0.66	0
5	DMS	C	8003	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
5	DMS	D	8001	-	3,3,3	2.72	1 (33%)	3,3,3	0.75	0
2	GTZ	D	2001	4	13,15,15	2.45	4 (30%)	14,22,22	2.64	5 (35%)
2	GTZ	A	2001	4	13,15,15	2.47	4 (30%)	14,22,22	2.49	5 (35%)
5	DMS	A	8002	-	3,3,3	2.75	1 (33%)	3,3,3	0.65	0
5	DMS	C	8001	-	3,3,3	2.72	1 (33%)	3,3,3	0.71	0
5	DMS	A	8003	-	3,3,3	2.69	1 (33%)	3,3,3	0.47	0
5	DMS	C	8004	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
5	DMS	D	8007	-	3,3,3	2.71	1 (33%)	3,3,3	0.61	0
5	DMS	A	8001	-	3,3,3	2.74	1 (33%)	3,3,3	0.63	0
5	DMS	B	8004	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
5	DMS	B	8003	-	3,3,3	2.79	1 (33%)	3,3,3	0.67	0
5	DMS	A	8006	-	3,3,3	2.71	1 (33%)	3,3,3	0.66	0
5	DMS	A	8005	-	3,3,3	2.69	1 (33%)	3,3,3	0.64	0
5	DMS	D	8004	-	3,3,3	2.76	1 (33%)	3,3,3	0.69	0
5	DMS	C	8006	-	3,3,3	2.72	1 (33%)	3,3,3	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8002	-	3,3,3	2.78	1 (33%)	3,3,3	0.60	0
5	DMS	D	8002	-	3,3,3	2.76	1 (33%)	3,3,3	0.69	0
5	DMS	C	8005	-	3,3,3	2.77	1 (33%)	3,3,3	0.82	0
5	DMS	A	8004	-	3,3,3	2.70	1 (33%)	3,3,3	0.35	0
5	DMS	B	8001	-	3,3,3	2.60	1 (33%)	3,3,3	0.60	0
2	GTZ	C	2001	4	13,15,15	2.45	4 (30%)	14,22,22	2.24	5 (35%)
5	DMS	B	8007	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	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
2	GTZ	D	2001	4	-	1/2/22/22	0/2/2/2
2	GTZ	C	2001	4	-	1/2/22/22	0/2/2/2
2	GTZ	A	2001	4	-	2/2/22/22	0/2/2/2
2	GTZ	B	2001	4	-	2/2/22/22	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	GTZ	NA-NB	5.17	1.41	1.30
2	A	2001	GTZ	NA-NB	5.03	1.41	1.30
2	D	2001	GTZ	NA-NB	5.02	1.41	1.30
2	B	2001	GTZ	NA-NB	4.99	1.41	1.30
5	B	8003	DMS	O-S	4.68	1.81	1.50
5	B	8002	DMS	O-S	4.67	1.81	1.50
5	D	8002	DMS	O-S	4.64	1.80	1.50
5	C	8005	DMS	O-S	4.63	1.80	1.50
5	D	8004	DMS	O-S	4.61	1.80	1.50
5	A	8001	DMS	O-S	4.60	1.80	1.50
5	A	8002	DMS	O-S	4.59	1.80	1.50
5	D	8005	DMS	O-S	4.59	1.80	1.50
5	B	8006	DMS	O-S	4.58	1.80	1.50
5	C	8002	DMS	O-S	4.58	1.80	1.50
5	D	8001	DMS	O-S	4.57	1.80	1.50
5	B	8007	DMS	O-S	4.56	1.80	1.50
5	C	8001	DMS	O-S	4.56	1.80	1.50
5	D	8007	DMS	O-S	4.55	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8004	DMS	O-S	4.55	1.80	1.50
5	C	8003	DMS	O-S	4.54	1.80	1.50
5	C	8006	DMS	O-S	4.54	1.80	1.50
5	C	8004	DMS	O-S	4.53	1.80	1.50
5	A	8006	DMS	O-S	4.52	1.80	1.50
5	B	8005	DMS	O-S	4.51	1.80	1.50
5	C	8007	DMS	O-S	4.51	1.80	1.50
2	B	2001	GTZ	N5-NA	4.51	1.41	1.35
5	A	8005	DMS	O-S	4.50	1.79	1.50
5	C	8008	DMS	O-S	4.49	1.79	1.50
5	A	8003	DMS	O-S	4.49	1.79	1.50
5	B	8004	DMS	O-S	4.47	1.79	1.50
5	D	8006	DMS	O-S	4.47	1.79	1.50
5	D	8003	DMS	O-S	4.47	1.79	1.50
5	B	8008	DMS	O-S	4.38	1.79	1.50
5	B	8001	DMS	O-S	4.35	1.78	1.50
2	D	2001	GTZ	N5-NA	4.30	1.41	1.35
2	B	2001	GTZ	C1-N1	4.28	1.36	1.32
2	A	2001	GTZ	N5-NA	4.20	1.41	1.35
2	A	2001	GTZ	C1-N1	4.13	1.36	1.32
2	C	2001	GTZ	N5-NA	4.07	1.40	1.35
2	C	2001	GTZ	C1-N1	4.01	1.36	1.32
2	D	2001	GTZ	C1-N1	3.97	1.36	1.32
2	B	2001	GTZ	N1-NB	3.68	1.41	1.36
2	D	2001	GTZ	N1-NB	3.65	1.41	1.36
2	A	2001	GTZ	N1-NB	3.61	1.41	1.36
2	C	2001	GTZ	N1-NB	3.58	1.41	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	GTZ	C1-N5-NA	5.15	111.89	108.47
2	C	2001	GTZ	C1-N5-NA	5.01	111.80	108.47
2	A	2001	GTZ	C1-N5-NA	4.91	111.73	108.47
2	D	2001	GTZ	C1-N5-NA	4.91	111.73	108.47
2	A	2001	GTZ	C1-N1-NB	4.77	109.04	105.81
2	D	2001	GTZ	C1-N1-NB	4.71	109.00	105.81
2	B	2001	GTZ	C1-N1-NB	4.65	108.96	105.81
2	D	2001	GTZ	C4-C3-C2	4.40	117.18	110.22
2	A	2001	GTZ	N1-NB-NA	-3.87	106.79	111.07
2	D	2001	GTZ	N1-NB-NA	-3.81	106.86	111.07
2	B	2001	GTZ	N1-NB-NA	-3.71	106.97	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	GTZ	C1-N1-NB	3.62	108.26	105.81
2	A	2001	GTZ	C4-C3-C2	3.47	115.70	110.22
2	B	2001	GTZ	C4-C3-C2	3.39	115.57	110.22
2	C	2001	GTZ	C4-C3-C2	3.32	115.47	110.22
2	C	2001	GTZ	N1-NB-NA	-3.19	107.54	111.07
2	B	2001	GTZ	O6-C6-C5	-2.95	105.04	111.55
2	D	2001	GTZ	C3-C4-C5	2.87	116.23	111.37
2	C	2001	GTZ	N5-NA-NB	-2.48	104.11	106.00
2	A	2001	GTZ	C3-C4-C5	2.10	114.91	111.37
2	B	2001	GTZ	N5-NA-NB	-2.03	104.45	106.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	GTZ	N5-C5-C6-O6
2	B	2001	GTZ	N5-C5-C6-O6
2	A	2001	GTZ	C4-C5-C6-O6
2	B	2001	GTZ	C4-C5-C6-O6
2	C	2001	GTZ	N5-C5-C6-O6
2	D	2001	GTZ	N5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8003	DMS	1	0
5	C	8002	DMS	1	0
5	D	8001	DMS	4	0
5	C	8001	DMS	1	0
5	A	8001	DMS	1	0
5	B	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 ⓘ

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	16 (1%) 70 63	14, 41, 78, 121	0
1	B	1011/1052 (96%)	-0.27	12 (1%) 76 70	11, 34, 68, 116	0
1	C	1011/1052 (96%)	-0.24	5 (0%) 87 83	12, 35, 63, 99	0
1	D	1011/1052 (96%)	-0.33	4 (0%) 88 86	13, 33, 63, 101	0
All	All	4044/4208 (96%)	-0.22	37 (0%) 81 75	11, 35, 69, 121	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	735	HIS	3.3
1	C	686	PRO	3.1
1	D	685	LEU	2.9
1	B	686	PRO	2.8
1	A	731	PRO	2.6
1	C	732	ALA	2.6
1	B	731	PRO	2.6
1	A	685	LEU	2.6
1	D	733	ALA	2.6
1	B	1023	LYS	2.5
1	A	729	THR	2.5
1	B	736	ALA	2.5
1	A	730	LEU	2.4
1	B	739	HIS	2.4
1	B	730	LEU	2.4
1	B	1022	GLN	2.4
1	D	731	PRO	2.4
1	A	771	GLY	2.4
1	B	732	ALA	2.3
1	A	727	SER	2.3
1	A	737	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	734	SER	2.3
1	B	737	ILE	2.3
1	B	821	ALA	2.3
1	A	745	MET	2.2
1	C	687	GLN	2.2
1	A	735	HIS	2.2
1	A	689	GLU	2.2
1	A	830	LEU	2.1
1	A	655	MET	2.1
1	D	1023	LYS	2.1
1	A	733	ALA	2.1
1	B	734	SER	2.1
1	A	688	PRO	2.0
1	A	732	ALA	2.0
1	C	730	LEU	2.0
1	C	572	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	8008	4/4	0.76	0.25	74,76,77,78	0
5	DMS	A	8005	4/4	0.81	0.23	74,75,75,78	0
5	DMS	A	8006	4/4	0.81	0.24	69,70,71,73	0
2	GTZ	B	2001	14/14	0.81	0.18	53,71,77,79	0
2	GTZ	A	2001	14/14	0.83	0.16	56,76,80,81	0
5	DMS	D	8005	4/4	0.83	0.18	61,65,65,68	0
5	DMS	A	8002	4/4	0.85	0.21	70,72,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GTZ	D	2001	14/14	0.86	0.18	63,80,90,90	0
5	DMS	C	8006	4/4	0.88	0.21	74,75,76,78	0
5	DMS	B	8007	4/4	0.88	0.20	68,72,72,74	0
5	DMS	C	8008	4/4	0.89	0.19	62,62,63,63	0
5	DMS	B	8005	4/4	0.89	0.19	64,66,66,70	0
2	GTZ	C	2001	14/14	0.90	0.12	51,61,64,65	0
5	DMS	C	8005	4/4	0.91	0.17	55,55,56,58	0
5	DMS	B	8003	4/4	0.91	0.16	59,60,60,62	0
4	NA	C	3101	1/1	0.91	0.07	49,49,49,49	0
5	DMS	D	8004	4/4	0.91	0.18	62,65,66,67	0
5	DMS	C	8003	4/4	0.91	0.17	59,59,60,61	0
5	DMS	C	8004	4/4	0.93	0.13	48,49,51,51	0
5	DMS	B	8006	4/4	0.93	0.12	52,52,54,54	0
5	DMS	B	8004	4/4	0.93	0.12	44,45,45,46	0
5	DMS	D	8006	4/4	0.93	0.16	58,60,60,61	0
4	NA	A	3101	1/1	0.94	0.09	46,46,46,46	0
5	DMS	C	8007	4/4	0.94	0.11	65,66,66,67	0
5	DMS	B	8002	4/4	0.95	0.11	51,52,52,53	0
5	DMS	A	8004	4/4	0.95	0.12	57,59,60,60	0
5	DMS	C	8002	4/4	0.95	0.15	63,63,64,64	0
5	DMS	A	8001	4/4	0.95	0.12	52,53,53,55	0
5	DMS	A	8003	4/4	0.95	0.10	50,52,53,53	0
5	DMS	B	8001	4/4	0.95	0.14	44,45,46,47	0
5	DMS	D	8001	4/4	0.96	0.11	45,45,46,47	0
5	DMS	D	8003	4/4	0.96	0.10	38,39,41,42	0
3	MG	B	3002	1/1	0.96	0.03	36,36,36,36	0
4	NA	B	3102	1/1	0.96	0.05	19,19,19,19	0
3	MG	D	3001	1/1	0.96	0.04	37,37,37,37	0
5	DMS	D	8007	4/4	0.96	0.13	47,48,51,52	0
4	NA	C	3102	1/1	0.97	0.05	29,29,29,29	0
3	MG	C	3002	1/1	0.97	0.03	31,31,31,31	0
4	NA	A	2102	1/1	0.97	0.05	25,25,25,25	0
5	DMS	C	8001	4/4	0.97	0.09	44,45,45,51	0
5	DMS	D	8002	4/4	0.97	0.12	44,46,47,47	0
4	NA	D	3102	1/1	0.98	0.03	21,21,21,21	0
3	MG	A	3001	1/1	0.98	0.06	44,44,44,44	0
4	NA	D	3101	1/1	0.98	0.05	46,46,46,46	0
3	MG	C	3001	1/1	0.99	0.04	35,35,35,35	0
4	NA	B	3101	1/1	0.99	0.04	44,44,44,44	0
3	MG	B	3001	1/1	0.99	0.05	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.