



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:14 PM EDT

PDB ID : 3WF3 / pdb_00003wf3
Title : Crystal structure of human beta-galactosidase mutant I51T in complex with Galactose
Authors : Suzuki, H.; Ohto, U.; Shimizu, T.
Deposited on : 2013-07-16
Resolution : 2.15 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

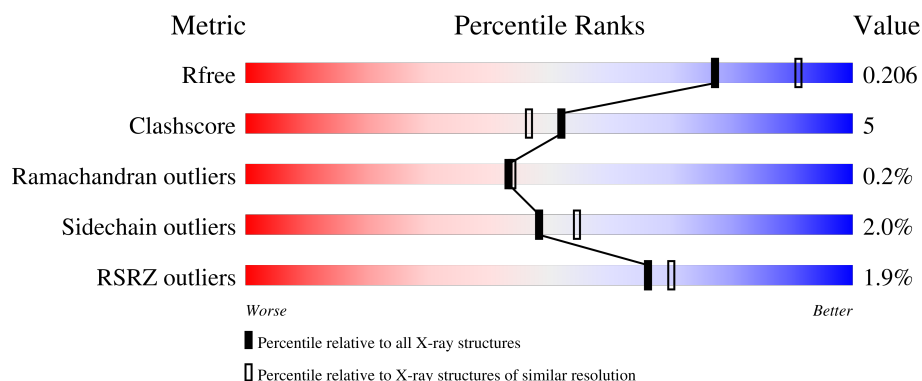
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	678	0% 78% 11% 11%
1	B	678	0% 79% 10% 11%
1	C	678	2% 77% 11% • 11%
1	D	678	3% 76% 12% • 11%

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
2	NAG	D	703	-	-	X	-
5	SO4	D	708	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21055 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	605	Total	C	N	O	S	0	6	0
			4841	3140	801	882	18			
1	B	605	Total	C	N	O	S	0	4	0
			4825	3131	796	881	17			
1	C	603	Total	C	N	O	S	0	6	0
			4808	3120	789	882	17			
1	D	603	Total	C	N	O	S	0	5	0
			4805	3115	790	883	17			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLU	-	expression tag	UNP P16278
A	1	ALA	-	expression tag	UNP P16278
A	2	GLU	-	expression tag	UNP P16278
A	3	ALA	-	expression tag	UNP P16278
A	4	TYR	-	expression tag	UNP P16278
A	5	VAL	-	expression tag	UNP P16278
A	6	GLU	-	expression tag	UNP P16278
A	7	PHE	-	expression tag	UNP P16278
A	8	HIS	-	expression tag	UNP P16278
A	9	HIS	-	expression tag	UNP P16278
A	10	HIS	-	expression tag	UNP P16278
A	11	HIS	-	expression tag	UNP P16278
A	12	HIS	-	expression tag	UNP P16278
A	13	HIS	-	expression tag	UNP P16278
A	14	ASP	-	expression tag	UNP P16278
A	15	TYR	-	expression tag	UNP P16278
A	16	LYS	-	expression tag	UNP P16278
A	17	ASP	-	expression tag	UNP P16278
A	18	ASP	-	expression tag	UNP P16278
A	19	ASP	-	expression tag	UNP P16278
A	20	ASP	-	expression tag	UNP P16278

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	LYS	-	expression tag	UNP P16278
A	22	THR	-	expression tag	UNP P16278
A	23	SER	-	expression tag	UNP P16278
A	51	THR	ILE	engineered mutation	UNP P16278
B	0	GLU	-	expression tag	UNP P16278
B	1	ALA	-	expression tag	UNP P16278
B	2	GLU	-	expression tag	UNP P16278
B	3	ALA	-	expression tag	UNP P16278
B	4	TYR	-	expression tag	UNP P16278
B	5	VAL	-	expression tag	UNP P16278
B	6	GLU	-	expression tag	UNP P16278
B	7	PHE	-	expression tag	UNP P16278
B	8	HIS	-	expression tag	UNP P16278
B	9	HIS	-	expression tag	UNP P16278
B	10	HIS	-	expression tag	UNP P16278
B	11	HIS	-	expression tag	UNP P16278
B	12	HIS	-	expression tag	UNP P16278
B	13	HIS	-	expression tag	UNP P16278
B	14	ASP	-	expression tag	UNP P16278
B	15	TYR	-	expression tag	UNP P16278
B	16	LYS	-	expression tag	UNP P16278
B	17	ASP	-	expression tag	UNP P16278
B	18	ASP	-	expression tag	UNP P16278
B	19	ASP	-	expression tag	UNP P16278
B	20	ASP	-	expression tag	UNP P16278
B	21	LYS	-	expression tag	UNP P16278
B	22	THR	-	expression tag	UNP P16278
B	23	SER	-	expression tag	UNP P16278
B	51	THR	ILE	engineered mutation	UNP P16278
C	0	GLU	-	expression tag	UNP P16278
C	1	ALA	-	expression tag	UNP P16278
C	2	GLU	-	expression tag	UNP P16278
C	3	ALA	-	expression tag	UNP P16278
C	4	TYR	-	expression tag	UNP P16278
C	5	VAL	-	expression tag	UNP P16278
C	6	GLU	-	expression tag	UNP P16278
C	7	PHE	-	expression tag	UNP P16278
C	8	HIS	-	expression tag	UNP P16278
C	9	HIS	-	expression tag	UNP P16278
C	10	HIS	-	expression tag	UNP P16278
C	11	HIS	-	expression tag	UNP P16278
C	12	HIS	-	expression tag	UNP P16278

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	HIS	-	expression tag	UNP P16278
C	14	ASP	-	expression tag	UNP P16278
C	15	TYR	-	expression tag	UNP P16278
C	16	LYS	-	expression tag	UNP P16278
C	17	ASP	-	expression tag	UNP P16278
C	18	ASP	-	expression tag	UNP P16278
C	19	ASP	-	expression tag	UNP P16278
C	20	ASP	-	expression tag	UNP P16278
C	21	LYS	-	expression tag	UNP P16278
C	22	THR	-	expression tag	UNP P16278
C	23	SER	-	expression tag	UNP P16278
C	51	THR	ILE	engineered mutation	UNP P16278
D	0	GLU	-	expression tag	UNP P16278
D	1	ALA	-	expression tag	UNP P16278
D	2	GLU	-	expression tag	UNP P16278
D	3	ALA	-	expression tag	UNP P16278
D	4	TYR	-	expression tag	UNP P16278
D	5	VAL	-	expression tag	UNP P16278
D	6	GLU	-	expression tag	UNP P16278
D	7	PHE	-	expression tag	UNP P16278
D	8	HIS	-	expression tag	UNP P16278
D	9	HIS	-	expression tag	UNP P16278
D	10	HIS	-	expression tag	UNP P16278
D	11	HIS	-	expression tag	UNP P16278
D	12	HIS	-	expression tag	UNP P16278
D	13	HIS	-	expression tag	UNP P16278
D	14	ASP	-	expression tag	UNP P16278
D	15	TYR	-	expression tag	UNP P16278
D	16	LYS	-	expression tag	UNP P16278
D	17	ASP	-	expression tag	UNP P16278
D	18	ASP	-	expression tag	UNP P16278
D	19	ASP	-	expression tag	UNP P16278
D	20	ASP	-	expression tag	UNP P16278
D	21	LYS	-	expression tag	UNP P16278
D	22	THR	-	expression tag	UNP P16278
D	23	SER	-	expression tag	UNP P16278
D	51	THR	ILE	engineered mutation	UNP P16278

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



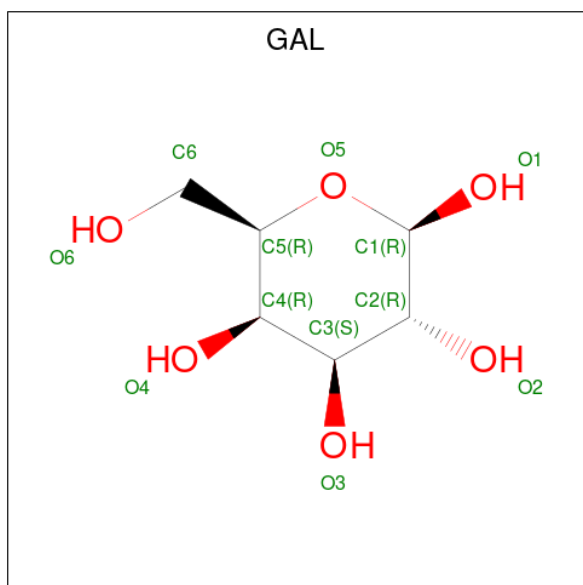
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

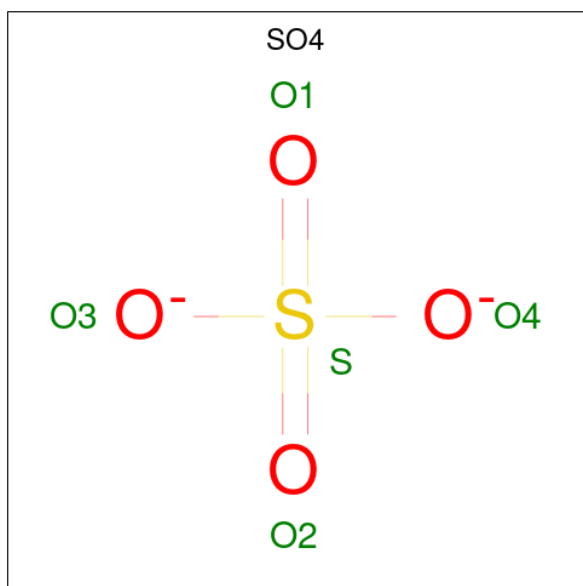
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

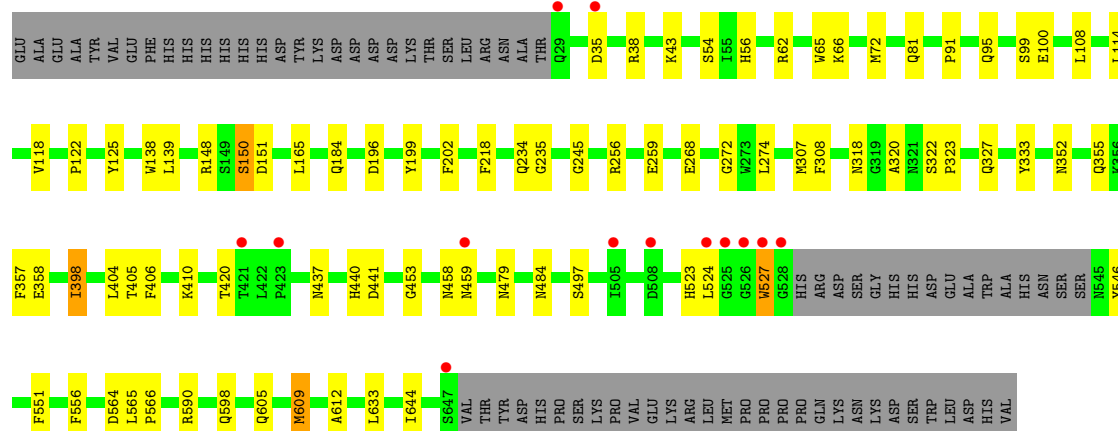
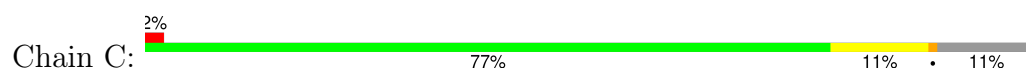
- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



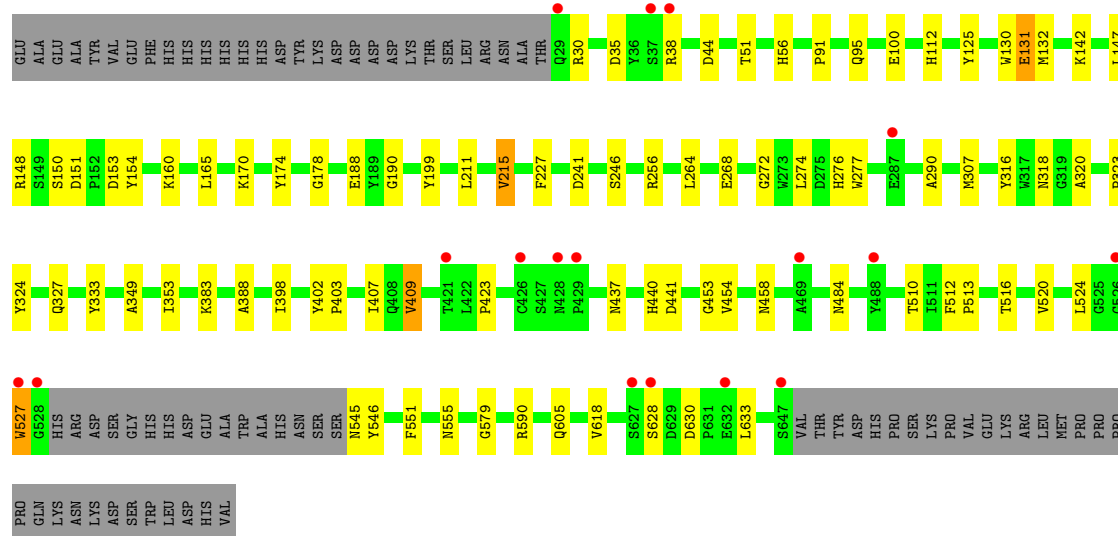
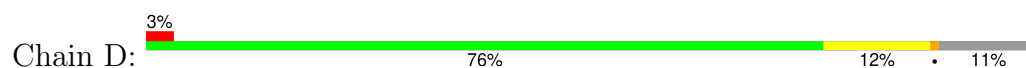
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	365	Total	O	0	0
			365	365		
7	B	369	Total	O	0	0
			369	369		
7	C	349	Total	O	0	0
			349	349		
7	D	345	Total	O	0	0
			345	345		



• 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	94.96Å 115.89Å 140.28Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	27.30 – 2.15 27.30 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.4 (27.30-2.15) 96.4 (27.30-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.196 , 0.242 0.205 , 0.206	Depositor DCC
R_{free} test set	7959 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21055	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: CL, NAG, EDO, SO4, GAL

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	0.99	2/5020 (0.0%)	1.01	6/6846 (0.1%)
1	B	1.02	0/4998	1.01	3/6818 (0.0%)
1	C	0.97	1/4990 (0.0%)	1.01	1/6808 (0.0%)
1	D	0.97	2/4979 (0.0%)	1.00	5/6795 (0.1%)
All	All	0.99	5/19987 (0.0%)	1.01	15/27267 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	PRO	N-CA	-6.90	1.42	1.47
1	D	316	TYR	N-CA	6.86	1.54	1.46
1	C	100	GLU	C-O	-5.54	1.19	1.24
1	D	51	THR	N-CA	-5.09	1.40	1.46
1	A	558	ILE	N-CA	-5.04	1.40	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	VAL	N-CA-C	-7.08	105.44	112.17
1	D	165	LEU	N-CA-C	6.70	118.28	110.97
1	A	409	VAL	CB-CA-C	5.98	119.44	111.85
1	B	335	ALA	CA-C-N	5.83	125.69	119.28
1	B	335	ALA	C-N-CA	5.83	125.69	119.28
1	D	407	ILE	CB-CA-C	-5.80	104.54	111.97
1	D	215	VAL	CB-CA-C	-5.79	101.88	111.32
1	C	165	LEU	N-CA-C	5.50	117.08	111.14
1	A	409	VAL	N-CA-CB	-5.31	105.22	112.28
1	B	492	PHE	N-CA-C	5.29	117.12	111.36
1	A	170	LYS	CA-C-N	-5.19	114.47	119.87
1	A	170	LYS	C-N-CA	-5.19	114.47	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	454	VAL	N-CA-C	5.14	115.68	108.17
1	A	383	LYS	CB-CA-C	-5.08	100.87	110.16
1	D	579	GLY	N-CA-C	5.07	117.94	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	4841	0	4714	48	0
1	B	4825	0	4686	40	0
1	C	4808	0	4667	51	0
1	D	4805	0	4669	61	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
2	C	56	0	52	2	0
2	D	56	0	52	7	0
3	A	12	0	12	0	0
3	B	12	0	12	1	0
3	C	12	0	12	1	0
3	D	12	0	12	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	2	0
6	A	8	0	12	0	0
6	B	8	0	12	0	0
6	C	8	0	12	1	0
6	D	8	0	12	1	0
7	A	365	0	0	8	0
7	B	369	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	349	0	0	5	0
7	D	345	0	0	8	0
All	All	21055	0	19040	198	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 (198) 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:555:ASN:HB2	2:D:703:NAG:O5	1.43	1.12
1:A:394:PRO:HB2	1:C:609[B]:MET:HE1	1.41	1.01
1:D:555:ASN:CB	2:D:703:NAG:O5	2.09	0.97
2:D:703:NAG:H3	7:D:1117:HOH:O	1.67	0.91
1:A:276:HIS:HE1	1:A:321:ASN:HD22	1.14	0.91
1:B:437:ASN:HD21	1:B:458:ASN:H	1.17	0.88
1:B:382:LEU:HD23	1:B:524:LEU:HD12	1.53	0.88
1:A:409:VAL:HG13	1:A:513:PRO:HG3	1.59	0.85
1:D:35:ASP:OD2	1:D:38:ARG:HG3	1.79	0.83
1:C:609[B]:MET:CE	1:C:612:ALA:HB3	2.09	0.81
1:D:327:GLN:HE22	1:D:484:ASN:HD21	1.30	0.78
1:D:35:ASP:OD2	1:D:38:ARG:CG	2.33	0.76
1:D:318:ASN:HD21	1:D:590:ARG:HH21	1.33	0.75
1:A:437:ASN:HD21	1:A:458:ASN:H	1.33	0.74
1:C:318:ASN:HD21	1:C:590:ARG:HH21	1.36	0.74
1:A:276:HIS:HE1	1:A:321:ASN:ND2	1.88	0.72
1:C:437:ASN:HD21	1:C:458:ASN:H	1.37	0.72
1:A:523:HIS:CD2	1:A:553:MET:SD	2.83	0.72
1:C:357:PHE:C	1:C:358:GLU:HG3	2.16	0.70
1:B:72:MET:HE2	1:B:80:ILE:HG22	1.74	0.69
1:A:327:GLN:HE22	1:A:484:ASN:HD21	1.37	0.69
1:D:324:TYR:N	5:D:708:SO4:O2	2.29	0.65
1:D:91:PRO:HD2	1:D:95:GLN:O	1.97	0.65
1:D:323:PRO:HA	5:D:708:SO4:O2	1.97	0.64
1:A:397:PRO:HD2	1:C:527:TRP:CE3	2.33	0.64
1:B:376:LYS:HD3	7:B:1136:HOH:O	1.97	0.64
1:C:327:GLN:HE22	1:C:484:ASN:HD21	1.46	0.62
1:D:211:LEU:HB3	1:D:215:VAL:HG21	1.81	0.61
1:C:43:LYS:HE3	7:C:1090:HOH:O	2.01	0.61
1:D:409:VAL:HG13	1:D:513:PRO:HG3	1.82	0.61
1:A:132:MET:HE3	1:A:147:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LYS:CE	7:C:1090:HOH:O	2.50	0.59
1:B:327:GLN:HE22	1:B:484:ASN:HD21	1.49	0.58
2:D:703:NAG:H62	7:D:989:HOH:O	2.03	0.58
1:B:95:GLN:HB2	7:B:1088:HOH:O	2.05	0.57
1:B:437:ASN:ND2	1:B:458:ASN:H	1.97	0.56
1:B:583:ILE:HD12	1:B:588:LEU:HD11	1.87	0.55
1:C:398:ILE:HD11	1:C:404:LEU:CD1	2.36	0.55
1:C:268:GLU:OE1	3:C:706:GAL:H1	2.07	0.55
1:D:44:ASP:OD2	1:D:174:TYR:OH	2.25	0.55
1:D:320:ALA:H	1:D:484:ASN:HD22	1.53	0.55
1:C:91:PRO:HD2	1:C:95:GLN:O	2.07	0.54
1:D:112:HIS:HD2	7:D:1113:HOH:O	1.89	0.54
1:D:290:ALA:HB1	1:D:353:ILE:HD11	1.90	0.54
1:D:112:HIS:CD2	7:D:1113:HOH:O	2.61	0.54
1:B:268:GLU:OE1	3:B:710:GAL:H1	2.08	0.53
1:C:35:ASP:OD2	1:C:38:ARG:HB2	2.09	0.53
1:A:150:SER:O	1:A:151:ASP:C	2.48	0.53
1:A:110:LEU:CD1	7:A:1138:HOH:O	2.57	0.53
1:C:524:LEU:HD11	1:C:551:PHE:CD2	2.44	0.52
1:B:572[A]:GLN:HG3	1:B:637:THR:HB	1.90	0.52
1:C:72:MET:HE3	1:C:308:PHE:HB3	1.90	0.52
1:A:437:ASN:ND2	1:A:458:ASN:H	2.05	0.52
1:D:318:ASN:HD21	1:D:590:ARG:NH2	2.06	0.52
1:A:155:LEU:HD22	1:A:202:PHE:CD2	2.45	0.52
1:A:196:ASP:O	1:A:199:TYR:HB3	2.10	0.51
1:B:359:LYS:HB2	7:B:1142:HOH:O	2.10	0.51
1:C:108:LEU:HD22	1:C:118:VAL:HG11	1.92	0.51
1:D:190:GLY:HA3	1:D:227:PHE:O	2.10	0.51
1:A:202:PHE:O	1:A:206:ARG:HG2	2.12	0.50
1:B:70:LEU:O	1:B:74:MET:HG2	2.12	0.50
1:B:241:ASP:HB2	1:B:268:GLU:HB2	1.93	0.50
1:A:239:THR:HG22	1:A:265:ILE:HD12	1.94	0.50
1:C:150[A]:SER:HB2	1:C:196:ASP:OD2	2.11	0.50
1:D:246:SER:OG	6:D:709:EDO:H11	2.12	0.50
1:A:175:GLN:NE2	7:A:957:HOH:O	2.45	0.50
1:B:175:GLN:HB3	7:B:801:HOH:O	2.12	0.49
1:B:598:GLN:HA	1:B:644:ILE:HA	1.94	0.49
1:A:110:LEU:HG	7:A:1138:HOH:O	2.13	0.49
1:B:31:MET:HE2	1:B:33:GLU:OE1	2.13	0.49
1:D:125:TYR:CE2	1:D:148:ARG:CZ	2.96	0.49
1:D:437:ASN:HD21	1:D:458:ASN:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:SER:HB2	7:C:1110:HOH:O	2.12	0.49
1:C:609[B]:MET:HE3	1:C:612:ALA:HB3	1.95	0.49
1:D:437:ASN:ND2	1:D:458:ASN:H	2.11	0.49
1:A:310:GLY:HA3	1:A:331:TYR:O	2.13	0.48
1:A:110:LEU:HD12	7:A:1138:HOH:O	2.12	0.48
1:A:150:SER:OG	1:A:196:ASP:OD2	2.31	0.48
1:D:30:ARG:HB3	1:D:174:TYR:CE2	2.48	0.48
1:B:35:ASP:HB2	1:B:42:LEU:HG	1.93	0.48
1:B:486:GLY:HA3	7:B:1084:HOH:O	2.14	0.48
1:A:276:HIS:CE1	1:A:321:ASN:HD22	2.07	0.48
1:A:397:PRO:HD2	1:C:527:TRP:CD2	2.48	0.48
1:A:360:VAL:HG12	7:A:912:HOH:O	2.14	0.48
1:A:564:ASP:O	1:A:567:GLN:HG3	2.14	0.48
1:B:397:PRO:HD2	1:D:527:TRP:CD1	2.49	0.48
1:B:409:VAL:HG13	1:B:513:PRO:HG3	1.95	0.47
1:D:56:HIS:CE1	1:D:307:MET:HE1	2.49	0.47
1:D:268:GLU:OE1	3:D:706:GAL:H1	2.14	0.47
1:B:389:LEU:HD21	1:B:417:LEU:HD23	1.95	0.47
1:C:54:SER:HA	1:C:81:GLN:O	2.14	0.47
1:A:318:ASN:HD21	1:A:590:ARG:HH21	1.62	0.47
1:D:590:ARG:HB3	7:D:1031:HOH:O	2.14	0.47
1:A:41:PHE:HB2	1:A:48:PHE:O	2.15	0.47
1:D:188:GLU:OE2	3:D:706:GAL:O1	2.32	0.47
1:C:598:GLN:HA	1:C:644:ILE:HA	1.97	0.47
1:B:346:LYS:O	1:B:350:LEU:HG	2.15	0.47
1:B:370:PRO:HD2	1:C:564[A]:ASP:CG	2.39	0.47
1:A:34:ILE:HG23	1:A:263:PRO:HD3	1.97	0.46
1:A:523:HIS:NE2	1:A:553:MET:SD	2.88	0.46
1:D:398:ILE:HD13	1:D:409:VAL:HG22	1.96	0.46
1:A:327:GLN:HE22	1:A:484:ASN:ND2	2.10	0.46
1:B:148:ARG:HB2	1:B:192:TYR:CE2	2.51	0.46
1:D:555:ASN:HB2	2:D:703:NAG:C5	2.42	0.46
1:D:555:ASN:HB2	2:D:703:NAG:H61	1.97	0.46
1:D:453:GLY:HA2	1:D:546:TYR:CE2	2.50	0.46
1:D:545:ASN:N	7:D:1057:HOH:O	2.48	0.46
1:C:453:GLY:HA2	1:C:546:TYR:CE1	2.51	0.46
1:A:190:GLY:HA3	1:A:227:PHE:O	2.15	0.46
2:D:703:NAG:C6	7:D:989:HOH:O	2.62	0.46
1:C:125:TYR:CD2	1:C:148:ARG:CZ	2.99	0.46
1:C:245:GLY:H	6:C:709:EDO:H22	1.81	0.46
1:D:130:TRP:O	1:D:131:GLU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:GLN:HB2	1:C:218:PHE:CZ	2.51	0.45
1:D:35:ASP:OD2	1:D:38:ARG:CB	2.63	0.45
1:D:516:THR:O	1:D:520:VAL:HG23	2.16	0.45
1:D:276:HIS:O	1:D:277:TRP:C	2.58	0.45
1:D:318:ASN:ND2	1:D:590:ARG:HH21	2.06	0.45
1:D:241:ASP:HB2	1:D:268:GLU:HB2	1.97	0.45
1:C:56:HIS:CE1	1:C:307:MET:HE1	2.50	0.45
1:B:310:GLY:HA3	1:B:331:TYR:O	2.17	0.45
1:C:122:PRO:HD2	1:C:184:GLN:O	2.17	0.45
1:D:132:MET:HE3	1:D:147:LEU:HD11	1.99	0.45
1:B:360:VAL:CG1	7:B:971:HOH:O	2.64	0.45
1:C:318:ASN:HD21	1:C:590:ARG:NH2	2.11	0.45
1:D:170:LYS:NZ	7:D:1029:HOH:O	2.48	0.45
1:A:388:ALA:O	1:A:391:ILE:HG22	2.17	0.44
1:A:175:GLN:HG2	7:A:811:HOH:O	2.17	0.44
1:B:76:GLY:HA3	1:B:360:VAL:HG22	2.00	0.44
1:A:401:LEU:HD12	1:A:507:THR:HB	2.00	0.44
1:C:609[B]:MET:HE2	1:C:612:ALA:HB3	1.93	0.44
1:A:382:LEU:HD23	1:A:524:LEU:HD12	2.00	0.44
1:C:479:ASN:OD1	1:C:479:ASN:C	2.57	0.44
1:D:551:PHE:HA	1:D:618:VAL:O	2.18	0.44
1:B:465:ILE:HD11	1:B:501:LEU:HD13	1.98	0.44
1:D:402:TYR:HB3	1:D:403:PRO:CD	2.48	0.44
1:D:174:TYR:HA	1:D:178:GLY:O	2.17	0.43
1:C:398:ILE:HD11	1:C:404:LEU:HD11	2.00	0.43
1:C:352[A]:ASN:OD1	1:C:355:GLN:NE2	2.51	0.43
1:A:289:VAL:HB	7:A:1135:HOH:O	2.17	0.43
1:D:35:ASP:OD2	1:D:38:ARG:HB2	2.17	0.43
1:D:383:LYS:HD3	1:D:388:ALA:HB2	2.00	0.43
1:C:523:HIS:CD2	1:C:527:TRP:CZ2	3.07	0.43
1:D:125:TYR:CD2	1:D:148:ARG:CZ	3.02	0.43
1:A:305:LEU:HD12	1:A:305:LEU:N	2.33	0.43
1:D:320:ALA:H	1:D:484:ASN:ND2	2.14	0.43
1:B:221:ASP:HB2	1:B:228:LEU:HD23	2.01	0.43
1:B:270:TYR:HA	1:B:306:TYR:O	2.19	0.43
1:B:553:MET:HE2	1:B:617:THR:HG23	2.01	0.43
1:C:62:ARG:HA	1:C:65:TRP:CD2	2.53	0.43
1:C:405:THR:O	1:C:406:PHE:C	2.62	0.43
1:C:565:LEU:HA	1:C:566:PRO:C	2.44	0.43
1:D:349:ALA:O	1:D:353:ILE:HD13	2.18	0.43
1:B:359:LYS:HA	7:B:1023:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:LYS:NZ	1:D:153:ASP:OD2	2.51	0.42
1:A:627:SER:O	1:A:628:SER:O	2.37	0.42
1:C:322:SER:HA	1:C:323:PRO:C	2.45	0.42
1:D:256:ARG:NE	1:D:264:LEU:HD21	2.35	0.42
1:A:381:LYS:HB2	1:A:552:TYR:CE2	2.55	0.42
1:B:383:LYS:HE3	1:D:100:GLU:OE1	2.19	0.42
1:D:241:ASP:CB	1:D:268:GLU:HB2	2.49	0.42
1:A:251:ALA:O	1:A:254:SER:OG	2.32	0.42
1:A:338:SER:O	1:A:339:GLU:C	2.62	0.42
1:D:150:SER:O	1:D:151:ASP:C	2.62	0.42
2:C:703:NAG:H61	7:C:1040:HOH:O	2.20	0.42
1:A:99:SER:HB3	1:A:100:GLU:OE1	2.20	0.42
1:B:382:LEU:CD2	1:B:524:LEU:HD12	2.38	0.42
1:C:234:GLN:OE1	1:C:235:GLY:N	2.52	0.42
1:A:360:VAL:HG13	1:A:361:PRO:HD2	2.01	0.41
1:B:420:THR:OG1	1:B:421:THR:N	2.53	0.41
1:C:66:LYS:HE3	1:C:114:LEU:HD21	2.01	0.41
1:C:62:ARG:HA	1:C:65:TRP:CG	2.54	0.41
1:A:437:ASN:O	1:A:437:ASN:CG	2.64	0.41
1:C:256:ARG:HA	1:C:259:GLU:O	2.20	0.41
1:A:130:TRP:O	1:A:131:GLU:C	2.62	0.41
1:B:318:ASN:HD21	1:B:590:ARG:HE	1.69	0.41
1:A:609[A]:MET:HG3	1:A:612:ALA:HB3	2.02	0.41
1:C:199:TYR:O	1:C:202:PHE:HB3	2.21	0.41
1:A:572:GLN:HG3	7:A:1088:HOH:O	2.21	0.41
1:B:91:PRO:HD2	1:B:95:GLN:O	2.21	0.41
1:B:241:ASP:CB	1:B:268:GLU:HB2	2.51	0.41
1:C:272:GLY:HA3	1:C:333:TYR:O	2.21	0.41
1:C:320:ALA:H	1:C:484:ASN:HD22	1.68	0.41
1:C:497:SER:HA	2:C:702:NAG:H81	2.02	0.41
1:D:440:HIS:HA	1:D:441:ASP:HA	1.84	0.41
1:D:628:SER:C	1:D:630:ASP:H	2.28	0.41
1:A:241:ASP:HA	1:A:266:ASN:OD1	2.20	0.41
1:D:35:ASP:OD2	1:D:38:ARG:CD	2.69	0.41
1:D:154:TYR:HE2	1:D:199:TYR:CE1	2.38	0.41
1:B:160:LYS:HE2	7:B:897:HOH:O	2.21	0.40
1:C:138:TRP:O	1:C:139:LEU:C	2.62	0.40
1:B:489:ILE:HD13	7:B:1060:HOH:O	2.20	0.40
1:D:510:THR:HG22	1:D:512:PHE:CE1	2.56	0.40
1:C:556:PHE:HA	7:C:1052:HOH:O	2.22	0.40
1:D:272:GLY:HA3	1:D:333:TYR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ASP:OD1	1:C:151:ASP:C	2.65	0.40
1:C:440:HIS:HA	1:C:441:ASP:HA	1.81	0.40
1:D:188:GLU:CD	3:D:706:GAL:O1	2.64	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	607/678 (90%)	576 (95%)	28 (5%)	3 (0%)	24	20
1	B	605/678 (89%)	579 (96%)	26 (4%)	0	100	100
1	C	605/678 (89%)	578 (96%)	27 (4%)	0	100	100
1	D	604/678 (89%)	576 (95%)	27 (4%)	1 (0%)	43	44
All	All	2421/2712 (89%)	2309 (95%)	108 (4%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	SER
1	A	611	SER
1	A	493	LYS
1	D	423	PRO

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	524/585 (90%)	512 (98%)	12 (2%)	44	49
1	B	522/585 (89%)	510 (98%)	12 (2%)	44	49
1	C	522/585 (89%)	510 (98%)	12 (2%)	44	49
1	D	521/585 (89%)	513 (98%)	8 (2%)	57	64
All	All	2089/2340 (89%)	2045 (98%)	44 (2%)	48	52

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	100	GLU
1	A	150	SER
1	A	257	LYS
1	A	274	LEU
1	A	309	ILE
1	A	409	VAL
1	A	425	ASP
1	A	503	SER
1	A	605	GLN
1	A	632[A]	GLU
1	A	632[B]	GLU
1	B	234	GLN
1	B	256	ARG
1	B	274	LEU
1	B	358	GLU
1	B	360	VAL
1	B	421	THR
1	B	424	GLN
1	B	553	MET
1	B	611	SER
1	B	627	SER
1	B	628	SER
1	B	633	LEU
1	C	150[A]	SER
1	C	150[B]	SER
1	C	274	LEU
1	C	398	ILE
1	C	410	LYS
1	C	420	THR
1	C	459	ASN

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Mol	Chain	Res	Type
1	C	527	TRP
1	C	605	GLN
1	C	609[A]	MET
1	C	609[B]	MET
1	C	633	LEU
1	D	131	GLU
1	D	160	LYS
1	D	274	LEU
1	D	409	VAL
1	D	524	LEU
1	D	527	TRP
1	D	605	GLN
1	D	633	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	97	GLN
1	A	102	HIS
1	A	175	GLN
1	A	204	GLN
1	A	276	HIS
1	A	279	GLN
1	A	318	ASN
1	A	321	ASN
1	A	355	GLN
1	A	424	GLN
1	A	437	ASN
1	A	484	ASN
1	A	523	HIS
1	A	605	GLN
1	B	97	GLN
1	B	204	GLN
1	B	318	ASN
1	B	321	ASN
1	B	355	GLN
1	B	412	HIS
1	B	424	GLN
1	B	437	ASN
1	B	484	ASN
1	C	46	GLN

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Mol	Chain	Res	Type
1	C	176	ASN
1	C	318	ASN
1	C	321	ASN
1	C	355	GLN
1	C	437	ASN
1	C	484	ASN
1	D	102	HIS
1	D	318	ASN
1	D	321	ASN
1	D	355	GLN
1	D	437	ASN
1	D	484	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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	SO4	D	708	-	4,4,4	0.46	0	6,6,6	0.69	0
2	NAG	B	701	1	14,14,15	1.04	0	17,19,21	1.84	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	710	-	3,3,3	0.51	0	2,2,2	0.65	0
2	NAG	A	703	1	14,14,15	0.74	0	17,19,21	2.64	6 (35%)
2	NAG	D	703	1	14,14,15	0.30	0	17,19,21	0.56	0
5	SO4	C	708	-	4,4,4	0.53	0	6,6,6	0.43	0
6	EDO	A	709	-	3,3,3	0.42	0	2,2,2	0.45	0
6	EDO	D	710	-	3,3,3	0.56	0	2,2,2	0.60	0
6	EDO	C	710	-	3,3,3	0.46	0	2,2,2	0.14	0
2	NAG	D	702	1	14,14,15	0.64	0	17,19,21	3.30	6 (35%)
2	NAG	A	701	1	14,14,15	0.82	0	17,19,21	1.11	1 (5%)
6	EDO	B	708	-	3,3,3	0.52	0	2,2,2	0.12	0
2	NAG	B	703	1	14,14,15	0.65	0	17,19,21	1.68	2 (11%)
6	EDO	D	709	-	3,3,3	0.20	0	2,2,2	0.57	0
2	NAG	C	703	1	14,14,15	0.66	0	17,19,21	1.68	4 (23%)
5	SO4	A	707	-	4,4,4	0.51	0	6,6,6	0.42	0
2	NAG	A	702	1	14,14,15	0.68	0	17,19,21	2.87	7 (41%)
2	NAG	B	704	1	14,14,15	0.56	0	17,19,21	0.76	0
5	SO4	D	707	-	4,4,4	0.48	0	6,6,6	0.34	0
3	GAL	B	710	-	12,12,12	0.88	0	17,17,17	1.23	1 (5%)
5	SO4	C	707	-	4,4,4	0.60	0	6,6,6	0.39	0
2	NAG	A	704	1	14,14,15	0.54	0	17,19,21	1.48	3 (17%)
2	NAG	C	701	1	14,14,15	0.61	0	17,19,21	1.43	2 (11%)
5	SO4	B	706	-	4,4,4	0.50	0	6,6,6	0.23	0
5	SO4	B	707	-	4,4,4	0.44	0	6,6,6	0.72	0
2	NAG	C	702	1	14,14,15	0.63	0	17,19,21	1.29	1 (5%)
3	GAL	C	706	-	12,12,12	0.83	0	17,17,17	1.02	1 (5%)
3	GAL	D	706	-	12,12,12	0.69	0	17,17,17	0.97	0
5	SO4	A	708	-	4,4,4	0.53	0	6,6,6	0.66	0
3	GAL	A	705	-	12,12,12	0.74	0	17,17,17	1.12	2 (11%)
2	NAG	B	702	1	14,14,15	0.86	0	17,19,21	2.72	6 (35%)
2	NAG	D	704	1	14,14,15	0.61	0	17,19,21	1.25	2 (11%)
6	EDO	B	709	-	3,3,3	0.38	0	2,2,2	0.57	0
2	NAG	C	704	1	14,14,15	0.66	0	17,19,21	1.33	1 (5%)
2	NAG	D	701	1	14,14,15	0.88	1 (7%)	17,19,21	1.30	2 (11%)
6	EDO	C	709	-	3,3,3	0.21	0	2,2,2	0.81	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	NAG	B	701	1	-	2/6/23/26	0/1/1/1
6	EDO	A	710	-	-	1/1/1/1	-
2	NAG	A	703	1	-	0/6/23/26	0/1/1/1
2	NAG	D	703	1	-	2/6/23/26	0/1/1/1
6	EDO	A	709	-	-	0/1/1/1	-
6	EDO	D	710	-	-	1/1/1/1	-
6	EDO	C	710	-	-	1/1/1/1	-
2	NAG	D	702	1	-	0/6/23/26	0/1/1/1
2	NAG	A	701	1	-	1/6/23/26	0/1/1/1
6	EDO	B	708	-	-	1/1/1/1	-
2	NAG	B	703	1	-	0/6/23/26	0/1/1/1
6	EDO	D	709	-	-	1/1/1/1	-
2	NAG	C	703	1	-	0/6/23/26	0/1/1/1
2	NAG	A	702	1	-	2/6/23/26	0/1/1/1
2	NAG	B	704	1	-	0/6/23/26	0/1/1/1
3	GAL	B	710	-	-	1/2/22/22	0/1/1/1
2	NAG	A	704	1	-	0/6/23/26	0/1/1/1
2	NAG	C	701	1	-	3/6/23/26	0/1/1/1
2	NAG	C	702	1	-	0/6/23/26	0/1/1/1
3	GAL	C	706	-	-	1/2/22/22	0/1/1/1
3	GAL	D	706	-	-	1/2/22/22	0/1/1/1
3	GAL	A	705	-	-	1/2/22/22	0/1/1/1
2	NAG	B	702	1	-	2/6/23/26	0/1/1/1
2	NAG	D	704	1	-	0/6/23/26	0/1/1/1
6	EDO	B	709	-	-	0/1/1/1	-
2	NAG	C	704	1	-	0/6/23/26	0/1/1/1
2	NAG	D	701	1	-	2/6/23/26	0/1/1/1
6	EDO	C	709	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	NAG	C1-C2	2.68	1.56	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	NAG	C1-O5-C5	10.50	126.26	112.19
2	A	702	NAG	C1-O5-C5	8.29	123.30	112.19
2	B	702	NAG	C1-O5-C5	7.07	121.67	112.19
2	A	703	NAG	C1-O5-C5	6.86	121.38	112.19
2	B	703	NAG	C1-O5-C5	4.98	118.86	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	NAG	C1-C2-N2	-4.70	103.02	110.43
2	D	702	NAG	C4-C3-C2	4.60	117.76	111.02
2	B	701	NAG	C1-O5-C5	4.59	118.34	112.19
2	A	702	NAG	C6-C5-C4	-4.51	101.94	113.02
2	C	701	NAG	C1-O5-C5	3.91	117.42	112.19
2	C	702	NAG	C1-O5-C5	3.87	117.37	112.19
2	B	702	NAG	C6-C5-C4	-3.83	103.61	113.02
2	A	703	NAG	C4-C3-C2	-3.57	105.78	111.02
2	D	702	NAG	C3-C4-C5	3.57	116.71	110.23
2	A	704	NAG	C1-C2-N2	-3.50	104.92	110.43
2	C	703	NAG	O5-C1-C2	-3.41	106.02	111.29
2	A	703	NAG	O7-C7-C8	-3.40	116.00	122.05
2	B	702	NAG	O5-C5-C4	3.40	119.09	110.83
2	A	703	NAG	O5-C1-C2	-3.38	106.07	111.29
2	A	701	NAG	C1-C2-N2	-3.37	105.12	110.43
2	A	703	NAG	C8-C7-N2	3.35	121.68	116.12
2	A	702	NAG	C1-C2-N2	-3.33	105.18	110.43
2	C	704	NAG	O4-C4-C3	-3.33	102.54	110.38
2	D	702	NAG	O5-C5-C4	3.21	118.63	110.83
2	B	702	NAG	O5-C1-C2	3.16	116.19	111.29
2	D	702	NAG	C6-C5-C4	-3.13	105.32	113.02
2	A	703	NAG	O3-C3-C2	3.12	115.88	109.40
2	A	702	NAG	O4-C4-C5	-3.06	101.79	109.32
2	C	701	NAG	O5-C1-C2	3.04	116.00	111.29
2	C	703	NAG	C1-O5-C5	2.96	116.15	112.19
2	B	701	NAG	C1-C2-N2	-2.95	105.78	110.43
2	B	703	NAG	C1-C2-N2	-2.79	106.04	110.43
2	D	702	NAG	O3-C3-C4	-2.71	103.98	110.38
2	A	702	NAG	O5-C5-C4	2.70	117.39	110.83
2	B	702	NAG	O6-C6-C5	-2.62	102.40	111.33
2	D	704	NAG	C1-O5-C5	2.48	115.51	112.19
2	D	701	NAG	O5-C1-C2	2.44	115.06	111.29
2	A	702	NAG	O5-C5-C6	2.43	112.39	107.66
2	B	701	NAG	O6-C6-C5	-2.38	103.22	111.33
3	A	705	GAL	C4-C3-C2	-2.37	106.66	110.83
3	B	710	GAL	O1-C1-O5	-2.29	103.62	110.41
3	C	706	GAL	C1-C2-C3	-2.27	105.72	110.36
2	A	704	NAG	O5-C5-C6	2.26	112.06	107.66
2	A	704	NAG	C1-O5-C5	2.20	115.14	112.19
2	D	701	NAG	O5-C5-C4	-2.16	105.57	110.83
2	C	703	NAG	O3-C3-C2	-2.13	104.97	109.40
2	C	703	NAG	C8-C7-N2	2.11	119.61	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	NAG	O5-C1-C2	-2.09	108.06	111.29
3	A	705	GAL	O5-C5-C4	-2.03	106.04	109.70
2	D	704	NAG	O3-C3-C2	-2.02	105.20	109.40
2	A	702	NAG	O6-C6-C5	-2.02	104.45	111.33

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	NAG	C4-C5-C6-O6
2	B	702	NAG	O5-C5-C6-O6
2	B	702	NAG	C4-C5-C6-O6
2	D	701	NAG	O5-C5-C6-O6
2	D	703	NAG	O5-C5-C6-O6
2	D	703	NAG	C4-C5-C6-O6
2	C	701	NAG	C4-C5-C6-O6
2	A	702	NAG	C4-C5-C6-O6
2	B	701	NAG	C4-C5-C6-O6
2	B	701	NAG	O5-C5-C6-O6
6	A	710	EDO	O1-C1-C2-O2
2	C	701	NAG	O5-C5-C6-O6
3	C	706	GAL	O5-C5-C6-O6
3	B	710	GAL	O5-C5-C6-O6
3	D	706	GAL	O5-C5-C6-O6
6	B	708	EDO	O1-C1-C2-O2
6	D	709	EDO	O1-C1-C2-O2
3	A	705	GAL	O5-C5-C6-O6
2	A	702	NAG	O5-C5-C6-O6
6	D	710	EDO	O1-C1-C2-O2
6	C	709	EDO	O1-C1-C2-O2
2	C	701	NAG	C1-C2-N2-C7
6	C	710	EDO	O1-C1-C2-O2
2	A	701	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	708	SO4	2	0
2	D	703	NAG	7	0
6	D	709	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	703	NAG	1	0
3	B	710	GAL	1	0
2	C	702	NAG	1	0
3	C	706	GAL	1	0
3	D	706	GAL	3	0
6	C	709	EDO	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	605/678 (89%)	0.11	9 (1%) 72 76	13, 26, 41, 85	6 (0%)
1	B	605/678 (89%)	0.03	7 (1%) 76 79	12, 25, 40, 83	4 (0%)
1	C	603/678 (88%)	0.16	13 (2%) 62 66	15, 26, 49, 81	6 (0%)
1	D	603/678 (88%)	0.21	17 (2%) 55 59	16, 28, 50, 83	5 (0%)
All	All	2416/2712 (89%)	0.13	46 (1%) 66 70	12, 26, 46, 85	21 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	527	TRP	7.3
1	C	527	TRP	6.5
1	D	526	GLY	5.7
1	C	528	GLY	5.2
1	B	646	SER	4.5
1	C	525	GLY	4.4
1	C	526	GLY	4.3
1	B	647	SER	4.3
1	D	469	ALA	3.9
1	A	629	ASP	3.8
1	A	647	SER	3.7
1	A	646	SER	3.4
1	B	627	SER	3.1
1	D	37	SER	3.0
1	D	528	GLY	2.9
1	D	421	THR	2.8
1	B	489	ILE	2.8
1	D	38	ARG	2.8
1	C	524	LEU	2.8
1	A	628	SER	2.7
1	D	628	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	29	GLN	2.7
1	B	628	SER	2.7
1	D	287	GLU	2.6
1	A	109	ARG	2.6
1	D	632	GLU	2.6
1	C	35	ASP	2.6
1	A	545	ASN	2.5
1	C	508	ASP	2.4
1	D	429	PRO	2.4
1	C	505	ILE	2.4
1	D	647	SER	2.3
1	D	488	TYR	2.3
1	C	421	THR	2.2
1	B	359	LYS	2.2
1	C	423	PRO	2.2
1	C	29	GLN	2.2
1	C	647	SER	2.2
1	D	428	ASN	2.2
1	D	627	SER	2.1
1	A	421	THR	2.1
1	A	257	LYS	2.1
1	D	426	CYS	2.1
1	C	459	ASN	2.1
1	A	627	SER	2.0
1	B	29	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	NAG	D	703	14/15	0.48	0.19	72,93,100,101	0
2	NAG	A	704	14/15	0.71	0.15	54,60,64,65	0
2	NAG	D	701	14/15	0.72	0.15	81,88,93,93	0
2	NAG	C	701	14/15	0.72	0.14	79,88,98,103	0
5	SO4	C	707	5/5	0.74	0.17	55,55,59,63	0
2	NAG	B	703	14/15	0.77	0.17	45,53,61,68	0
2	NAG	A	703	14/15	0.78	0.14	40,45,50,61	0
6	EDO	A	709	4/4	0.78	0.23	45,49,52,53	0
5	SO4	A	707	5/5	0.80	0.10	69,72,73,78	0
6	EDO	C	709	4/4	0.80	0.14	41,44,46,54	0
6	EDO	B	708	4/4	0.82	0.16	45,47,47,49	0
2	NAG	D	702	14/15	0.84	0.11	35,46,49,51	0
5	SO4	D	707	5/5	0.85	0.10	64,69,73,80	0
2	NAG	C	702	14/15	0.85	0.11	43,51,56,56	0
6	EDO	D	709	4/4	0.85	0.12	35,38,39,45	0
2	NAG	C	703	14/15	0.86	0.12	36,41,44,44	0
2	NAG	A	702	14/15	0.87	0.10	28,33,36,42	0
2	NAG	B	701	14/15	0.87	0.11	28,31,34,43	0
6	EDO	D	710	4/4	0.88	0.13	28,30,33,33	0
2	NAG	B	704	14/15	0.89	0.10	46,51,59,63	0
6	EDO	A	710	4/4	0.89	0.13	25,29,30,35	0
5	SO4	B	706	5/5	0.89	0.16	56,63,64,67	0
5	SO4	A	708	5/5	0.91	0.12	45,48,54,56	0
2	NAG	B	702	14/15	0.91	0.08	25,30,34,35	0
5	SO4	D	708	5/5	0.91	0.11	49,50,52,56	0
5	SO4	B	707	5/5	0.92	0.12	47,47,54,55	0
6	EDO	C	710	4/4	0.92	0.08	36,41,41,45	0
2	NAG	C	704	14/15	0.93	0.08	24,26,29,35	0
2	NAG	A	701	14/15	0.93	0.07	24,30,33,41	0
5	SO4	C	708	5/5	0.93	0.12	40,43,47,48	0
2	NAG	D	704	14/15	0.93	0.07	27,30,32,36	0
3	GAL	B	710	12/12	0.94	0.08	19,21,23,30	0
6	EDO	B	709	4/4	0.94	0.09	33,33,33,37	0
3	GAL	C	706	12/12	0.95	0.07	18,22,25,32	0
3	GAL	A	705	12/12	0.96	0.07	16,20,24,29	0
3	GAL	D	706	12/12	0.96	0.06	21,25,27,31	0
4	CL	A	706	1/1	0.99	0.06	21,21,21,21	0
4	CL	B	705	1/1	0.99	0.07	20,20,20,20	0
4	CL	C	705	1/1	0.99	0.05	21,21,21,21	0
4	CL	D	705	1/1	0.99	0.04	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.