



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:12 PM GMT

PDB ID : 3WF1  
Title : Crystal structure of human beta-galactosidase in complex with 6S-NBI-GJ  
Authors : Suzuki, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2013-07-16  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

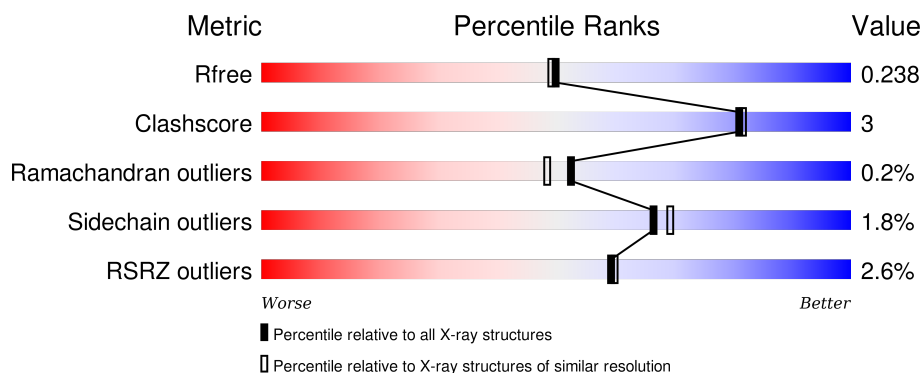
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




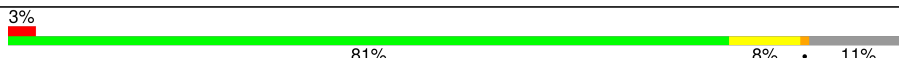
The reported resolution of this entry is 2.00 Å.

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	678	
1	C	678	
1	D	678	

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	A	702	-	-	-	X
2	NAG	A	703	-	-	-	X
2	NAG	B	703	-	-	-	X
4	6GJ	A	706	-	-	-	X
4	6GJ	B	710	-	-	X	X
4	6GJ	D	702	-	-	-	X
6	EDO	B	709	-	-	-	X
6	EDO	C	710	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21271 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	8	0
			4849	3144	805	882	18			
1	B	605	Total	C	N	O	S	0	4	0
			4831	3137	798	879	17			
1	C	603	Total	C	N	O	S	0	6	0
			4815	3126	792	880	17			
1	D	603	Total	C	N	O	S	0	5	0
			4808	3120	791	880	17			

There are 96 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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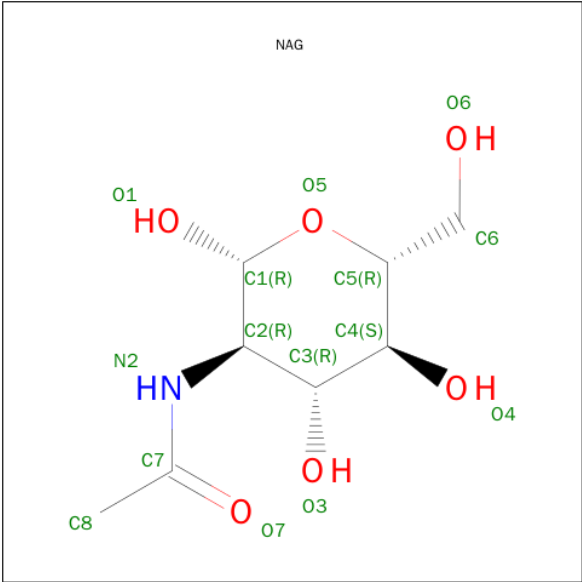
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	LYS	-	EXPRESSION TAG	UNP P16278
A	22	THR	-	EXPRESSION TAG	UNP P16278
A	23	SER	-	EXPRESSION TAG	UNP P16278
B	0	GLU	-	EXPRESSION TAG	UNP P16278
B	1	ALA	-	EXPRESSION TAG	UNP P16278
B	2	GLU	-	EXPRESSION TAG	UNP P16278
B	3	ALA	-	EXPRESSION TAG	UNP P16278
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
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
C	13	HIS	-	EXPRESSION TAG	UNP P16278
C	14	ASP	-	EXPRESSION TAG	UNP P16278

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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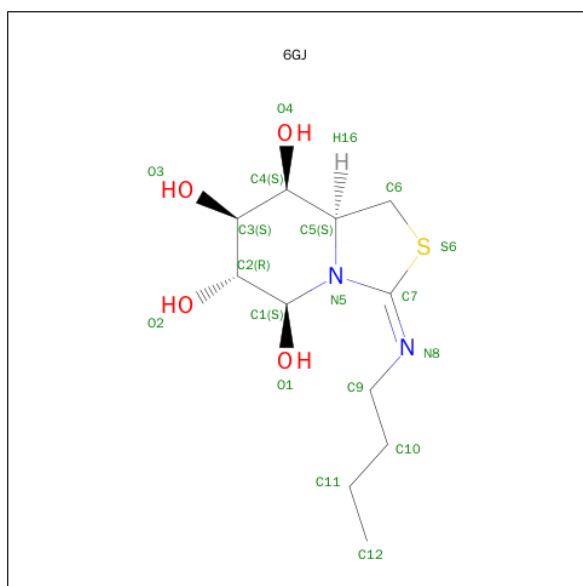
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is (3E,5S,6R,7S,8S,8AS)-3-(BUTYLIMINO)HEXAHYDRO[1,3]THIAZOLO[3,4-A]PYRIDINE-5,6,7,8-TETROL (three-letter code: 6GJ) (formula: C<sub>11</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			18	11	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			18	11	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			18	11	2	4	1		

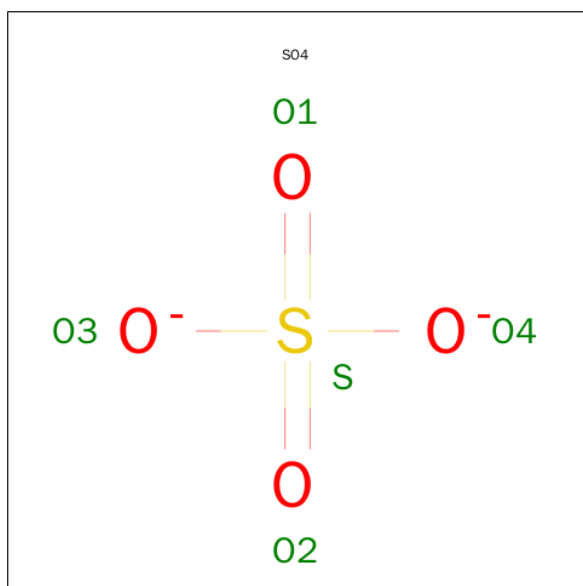
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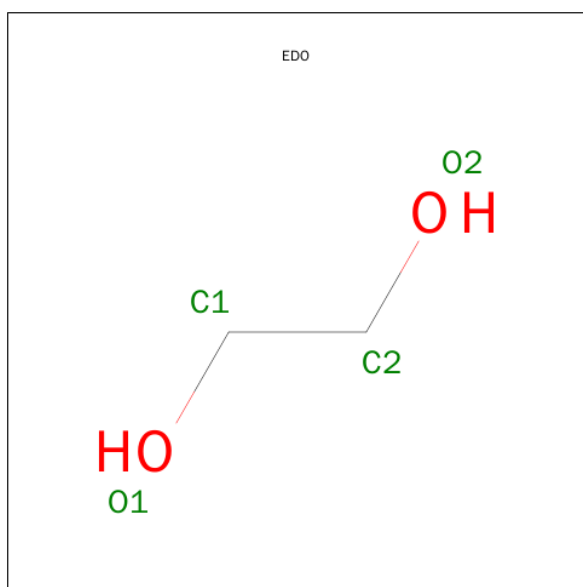
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			18	11	2	4	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	414	Total O 414 414	0	0
7	B	446	Total O 446 446	0	0
7	C	379	Total O 379 379	0	0
7	D	357	Total O 357 357	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.91Å 116.01Å 140.57Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	25.90 – 2.00 25.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (25.90-2.00) 97.5 (25.90-2.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.186 , 0.232 0.194 , 0.238	Depositor DCC
$R_{free}$ test set	10030 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.5	EDS
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 199401 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21271	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, NAG, 6GJ, CL

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	0.74	0/5041	0.81	4/6873 (0.1%)
1	B	0.75	0/5002	0.82	9/6822 (0.1%)
1	C	0.70	0/4995	0.79	2/6814 (0.0%)
1	D	0.69	0/4981	0.78	2/6796 (0.0%)
All	All	0.72	0/20019	0.80	17/27305 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ARG	NE-CZ-NH2	6.63	123.62	120.30
1	B	256	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	B	256	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	B	49	ARG	CG-CD-NE	-5.76	99.69	111.80
1	C	491	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	256	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	D	49	ARG	CG-CD-NE	-5.42	100.43	111.80
1	B	49	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	491	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	C	49	ARG	CG-CD-NE	-5.37	100.53	111.80
1	B	208	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	390	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	241	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	256	ARG	CG-CD-NE	-5.14	101.01	111.80
1	A	101	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	568	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	208	ARG	NE-CZ-NH2	-5.09	117.76	120.30

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	4849	0	4723	22	0
1	B	4831	0	4701	39	0
1	C	4815	0	4688	27	0
1	D	4808	0	4682	40	0
2	A	56	0	50	0	0
2	B	56	0	51	0	0
2	C	56	0	52	0	0
2	D	56	0	52	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	20	1	0
4	B	18	0	20	7	0
4	C	18	0	19	0	0
4	D	18	0	20	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	0	0
6	A	8	0	12	0	0
6	B	8	0	12	3	0
6	C	8	0	12	0	0
6	D	8	0	12	0	0
7	A	414	0	0	5	0
7	B	446	0	0	7	0
7	C	379	0	0	1	0
7	D	357	0	0	11	0
All	All	21271	0	19126	129	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 3.

All (129) 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:259:GLU:HB2	7:D:1103:HOH:O	1.64	0.96
1:D:555:ASN:HB2	2:D:704:NAG:O5	1.70	0.90
1:B:437:ASN:HD21	1:B:458:ASN:H	1.15	0.88
1:A:327:GLN:HE22	1:A:484:ASN:HD21	1.29	0.81
1:A:437:ASN:HD21	1:A:458:ASN:H	1.29	0.80
1:D:437:ASN:HD21	1:D:458:ASN:H	1.33	0.75
1:B:382:LEU:HD23	1:B:524:LEU:HD12	1.73	0.70
4:B:710:6GJ:H6	4:B:710:6GJ:O1	1.91	0.69
4:B:710:6GJ:C9	4:B:710:6GJ:O1	2.41	0.69
1:B:327:GLN:HE22	1:B:484:ASN:HD21	1.40	0.69
1:C:437:ASN:HD21	1:C:458:ASN:H	1.41	0.69
1:D:426:CYS:SG	7:D:1101:HOH:O	2.50	0.68
1:A:105:GLU:O	1:A:109[A]:ARG:HG3	1.93	0.68
1:C:615:THR:HG22	7:C:904:HOH:O	1.93	0.67
1:C:327:GLN:HE22	1:C:484:ASN:HD21	1.42	0.65
1:A:112:HIS:HD2	7:A:1048:HOH:O	1.79	0.64
1:B:109[A]:ARG:NH1	1:B:113:GLU:OE2	2.30	0.63
1:D:112:HIS:HD2	7:D:1104:HOH:O	1.80	0.63
1:B:273:TRP:CZ3	4:B:710:6GJ:S6	2.94	0.60
1:B:273:TRP:CH2	4:B:710:6GJ:S6	2.97	0.57
1:D:327:GLN:HE22	1:D:484:ASN:HD21	1.51	0.57
1:D:555:ASN:CB	2:D:704:NAG:O5	2.50	0.56
1:A:234[B]:GLN:HE21	1:A:235:GLY:N	2.04	0.55
1:D:255:GLN:HG2	7:D:1103:HOH:O	2.07	0.55
1:A:382:LEU:HD23	1:A:524:LEU:HD12	1.89	0.55
1:C:318:ASN:HD21	1:C:590:ARG:HH21	1.54	0.54
1:C:83:TYR:CE2	1:C:128:ALA:HB2	2.43	0.53
1:C:35:ASP:OD2	1:C:38:ARG:HB2	2.09	0.53
1:A:318:ASN:HD21	1:A:590:ARG:HH21	1.57	0.52
1:D:426:CYS:CB	7:D:1101:HOH:O	2.58	0.51
1:C:281:HIS:CE1	1:C:644:ILE:HD12	2.46	0.51
1:B:109[A]:ARG:NE	7:B:1086:HOH:O	2.44	0.50
1:C:523:HIS:CE1	1:C:527:TRP:CZ2	2.99	0.50
1:D:437:ASN:ND2	1:D:458:ASN:H	2.07	0.50
1:D:553:MET:CE	7:D:1116:HOH:O	2.60	0.50
1:B:106:TYR:HA	1:B:109[B]:ARG:HE	1.75	0.50
1:B:243:GLY:H	6:B:708:EDO:C2	2.25	0.50
1:A:327:GLN:HE22	1:A:484:ASN:ND2	2.05	0.50
1:A:598:GLN:NE2	7:A:1214:HOH:O	2.45	0.50
1:B:397:PRO:HD2	1:D:527:TRP:CD2	2.47	0.49
1:A:275:ASP:HB2	7:A:1179:HOH:O	2.12	0.49
1:B:629:ASP:O	1:B:631:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:GLN:HB2	1:D:218:PHE:CZ	2.48	0.49
1:D:30:ARG:HB3	1:D:174:TYR:CE2	2.48	0.49
1:D:112:HIS:CD2	7:D:1104:HOH:O	2.62	0.48
1:B:318:ASN:HD21	1:B:590:ARG:HE	1.60	0.48
1:D:320:ALA:H	1:D:484:ASN:HD22	1.60	0.48
1:A:644:ILE:HD12	7:A:1097:HOH:O	2.13	0.48
4:B:710:6GJ:H5	4:B:710:6GJ:C1	2.44	0.48
1:D:523:HIS:HA	7:D:1116:HOH:O	2.14	0.48
1:B:273:TRP:N	7:B:1155:HOH:O	2.46	0.48
1:B:553:MET:SD	1:B:617:THR:HG23	2.54	0.48
4:B:710:6GJ:C9	4:B:710:6GJ:C1	2.92	0.47
1:C:524:LEU:HD21	1:C:551:PHE:CD1	2.49	0.47
1:D:424:GLN:HE22	1:D:502:SER:HB2	1.78	0.47
1:A:310:GLY:HA3	1:A:331:TYR:O	2.15	0.47
1:D:527:TRP:HA	1:D:527:TRP:CE3	2.49	0.47
1:B:268:GLU:OE1	4:B:710:6GJ:H1	2.13	0.47
1:D:430:ALA:CB	7:D:1101:HOH:O	2.62	0.47
1:C:352[A]:ASN:OD1	1:C:355:GLN:NE2	2.47	0.47
1:B:318:ASN:ND2	1:B:590:ARG:HE	2.14	0.46
1:B:88:PHE:O	1:B:102:HIS:HD2	1.96	0.46
1:A:397:PRO:HD2	1:C:527:TRP:CG	2.50	0.46
1:D:551:PHE:HA	1:D:618:VAL:O	2.16	0.46
1:D:318:ASN:HD21	1:D:590:ARG:HH21	1.62	0.46
1:B:170:LYS:N	1:B:171:PRO:HD2	2.31	0.46
1:D:91:PRO:HD2	1:D:95:GLN:O	2.15	0.46
1:C:598:GLN:HA	1:C:644:ILE:HA	1.99	0.45
1:A:381:LYS:HB2	1:A:552:TYR:CE2	2.52	0.45
1:B:572[A]:GLN:HG3	1:B:637:THR:HB	1.97	0.45
1:B:243:GLY:H	6:B:708:EDO:H21	1.80	0.45
1:C:242:PHE:O	1:C:269:PHE:HA	2.16	0.45
1:D:440:HIS:HA	1:D:441:ASP:HA	1.79	0.45
1:D:62:ARG:HA	1:D:65:TRP:CD2	2.51	0.45
1:D:221:ASP:O	1:D:240:VAL:HA	2.17	0.44
1:B:327:GLN:HE22	1:B:484:ASN:ND2	2.13	0.44
1:C:91:PRO:HD2	1:C:95:GLN:O	2.17	0.44
1:C:507:THR:O	1:C:508:ASP:HB2	2.17	0.44
1:C:309:ILE:HB	1:C:337:LEU:HB2	1.99	0.44
1:B:318:ASN:HD21	1:B:590:ARG:HH21	1.66	0.44
1:C:221:ASP:O	1:C:240:VAL:HA	2.18	0.43
1:A:305:LEU:HD12	1:A:305:LEU:N	2.32	0.43
1:A:112:HIS:CD2	7:A:1048:HOH:O	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LYS:HB2	1:B:552:TYR:CE2	2.54	0.43
1:D:430:ALA:N	7:D:1101:HOH:O	2.51	0.43
1:B:310:GLY:HA3	1:B:331:TYR:O	2.19	0.43
1:D:253:LEU:HA	1:D:253:LEU:HD23	1.92	0.43
1:B:95:GLN:HG2	7:B:1181:HOH:O	2.19	0.43
1:A:598:GLN:HA	1:A:644:ILE:HA	2.01	0.43
1:B:321:ASN:ND2	1:B:327:GLN:HE21	2.17	0.42
1:B:440:HIS:HA	1:B:441:ASP:HA	1.78	0.42
1:A:273:TRP:CH2	4:A:706:6GJ:S6	3.12	0.42
1:B:299:ARG:HD3	7:B:1045:HOH:O	2.18	0.42
1:C:29:GLN:HE21	1:C:29:GLN:HA	1.84	0.42
1:D:424:GLN:HE22	1:D:502:SER:CB	2.33	0.42
1:B:383:LYS:NZ	1:D:100:GLU:OE2	2.51	0.42
1:B:190:GLY:HA3	1:B:227:PHE:O	2.19	0.42
1:D:62:ARG:HA	1:D:65:TRP:CG	2.54	0.42
1:C:76:GLY:HA3	1:C:360:VAL:HG22	2.01	0.42
2:D:701:NAG:O4	2:D:701:NAG:O6	2.32	0.42
1:A:399:LYS:HE2	1:C:528:GLY:O	2.20	0.42
1:A:52:SER:HA	1:A:79:ALA:O	2.20	0.41
1:D:321:ASN:ND2	1:D:327:GLN:HE21	2.18	0.41
1:D:318:ASN:HD21	1:D:590:ARG:HE	1.68	0.41
1:B:95:GLN:NE2	7:B:1083:HOH:O	2.54	0.41
1:B:555:ASN:HA	1:B:614:ASN:O	2.21	0.41
1:D:430:ALA:HB2	7:D:1101:HOH:O	2.19	0.41
1:D:592:TRP:CE2	1:D:595:ARG:HG3	2.55	0.41
1:C:49:ARG:HB2	1:C:302:SER:OG	2.21	0.41
1:B:205:LYS:HD2	7:B:1187:HOH:O	2.20	0.41
1:C:122:PRO:HD2	1:C:184:GLN:O	2.21	0.41
1:C:174:TYR:HA	1:C:178:GLY:O	2.21	0.41
1:B:579:GLY:HA3	1:B:619:LEU:O	2.21	0.41
1:B:125:TYR:CE2	1:B:148:ARG:CZ	3.04	0.41
1:B:598:GLN:HA	1:B:644:ILE:HA	2.03	0.41
1:D:64:TYR:O	1:D:68:ARG:HG2	2.20	0.41
1:D:72:MET:HB3	1:D:77:LEU:HD12	2.03	0.41
1:A:564:ASP:O	1:A:567:GLN:HG3	2.21	0.41
1:D:241:ASP:HB2	1:D:268:GLU:HB2	2.03	0.41
1:C:555:ASN:HA	1:C:614:ASN:O	2.21	0.41
1:B:275:ASP:HB2	7:B:1218:HOH:O	2.20	0.41
1:B:243:GLY:N	6:B:708:EDO:H22	2.35	0.40
1:A:415:PHE:CD1	1:A:415:PHE:N	2.89	0.40
1:D:399:LYS:HE3	1:D:510:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:TRP:CE2	1:C:595:ARG:HG3	2.56	0.40
1:B:174:TYR:HA	1:B:178:GLY:O	2.22	0.40
1:C:62:ARG:HA	1:C:65:TRP:CD2	2.57	0.40
1:C:150:SER:OG	1:C:196:ASP:OD2	2.39	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	609/678 (90%)	587 (96%)	20 (3%)	2 (0%)	46	41
1	B	605/678 (89%)	585 (97%)	19 (3%)	1 (0%)	52	48
1	C	605/678 (89%)	584 (96%)	20 (3%)	1 (0%)	52	48
1	D	604/678 (89%)	579 (96%)	25 (4%)	0	100	100
All	All	2423/2712 (89%)	2335 (96%)	84 (4%)	4 (0%)	52	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	611	SER
1	A	628	SER
1	C	503	SER
1	B	630	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	526/585 (90%)	520 (99%)	6 (1%)	80	83
1	B	522/585 (89%)	514 (98%)	8 (2%)	72	75
1	C	522/585 (89%)	507 (97%)	15 (3%)	50	49
1	D	521/585 (89%)	509 (98%)	12 (2%)	58	60
All	All	2091/2340 (89%)	2050 (98%)	41 (2%)	66	65

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38[A]	ARG
1	A	38[B]	ARG
1	A	186	GLU
1	A	360	VAL
1	A	553	MET
1	A	605	GLN
1	B	40	SER
1	B	47	PRO
1	B	49	ARG
1	B	131	GLU
1	B	234	GLN
1	B	274	LEU
1	B	605	GLN
1	B	628	SER
1	C	29	GLN
1	C	35	ASP
1	C	40	SER
1	C	49	ARG
1	C	150	SER
1	C	186	GLU
1	C	274	LEU
1	C	359	LYS
1	C	420	THR
1	C	459[A]	ASN
1	C	459[B]	ASN
1	C	466	THR
1	C	572[A]	GLN
1	C	572[B]	GLN
1	C	646	SER
1	D	29	GLN

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Mol	Chain	Res	Type
1	D	38	ARG
1	D	49	ARG
1	D	160	LYS
1	D	186	GLU
1	D	274	LEU
1	D	359	LYS
1	D	424	GLN
1	D	527	TRP
1	D	605	GLN
1	D	628	SER
1	D	647	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	318	ASN
1	A	321	ASN
1	A	355	GLN
1	A	437	ASN
1	A	484	ASN
1	A	523	HIS
1	B	102	HIS
1	B	318	ASN
1	B	321	ASN
1	B	355	GLN
1	B	437	ASN
1	B	484	ASN
1	B	529	HIS
1	C	29	GLN
1	C	279	GLN
1	C	318	ASN
1	C	321	ASN
1	C	355	GLN
1	C	437	ASN
1	C	484	ASN
1	C	523	HIS
1	D	102	HIS
1	D	204	GLN
1	D	279	GLN
1	D	318	ASN
1	D	321	ASN

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Mol	Chain	Res	Type
1	D	355	GLN
1	D	424	GLN
1	D	437	ASN
1	D	484	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	NAG	A	701	1	14,14,15	0.45	0	15,19,21	1.21	2 (13%)
2	NAG	A	702	1	14,14,15	1.05	1 (7%)	15,19,21	3.07	5 (33%)
2	NAG	A	703	1	14,14,15	1.09	1 (7%)	15,19,21	2.61	7 (46%)
2	NAG	A	704	1	14,14,15	0.54	0	15,19,21	0.86	0
4	6GJ	A	706	-	17,19,19	1.48	4 (23%)	16,27,27	4.45	9 (56%)
5	SO4	A	707	-	4,4,4	0.53	0	6,6,6	0.21	0
5	SO4	A	708	-	4,4,4	0.53	0	6,6,6	0.44	0
6	EDO	A	709	-	3,3,3	0.26	0	2,2,2	1.39	0
6	EDO	A	710	-	3,3,3	0.49	0	2,2,2	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	701	1	14,14,15	0.58	0	15,19,21	1.68	2 (13%)
2	NAG	B	702	1	14,14,15	1.02	0	15,19,21	2.24	5 (33%)
2	NAG	B	703	1	14,14,15	0.67	0	15,19,21	2.06	6 (40%)
2	NAG	B	704	1	14,14,15	0.55	0	15,19,21	0.80	0
5	SO4	B	706	-	4,4,4	0.41	0	6,6,6	0.36	0
5	SO4	B	707	-	4,4,4	0.42	0	6,6,6	0.53	0
6	EDO	B	708	-	3,3,3	0.50	0	2,2,2	0.26	0
6	EDO	B	709	-	3,3,3	0.53	0	2,2,2	0.60	0
4	6GJ	B	710	-	17,19,19	1.53	3 (17%)	16,27,27	2.94	6 (37%)
2	NAG	C	701	1	14,14,15	0.29	0	15,19,21	0.53	0
2	NAG	C	702	1	14,14,15	0.50	0	15,19,21	1.57	1 (6%)
2	NAG	C	703	1	14,14,15	0.48	0	15,19,21	1.13	2 (13%)
2	NAG	C	704	1	14,14,15	0.67	0	15,19,21	1.01	1 (6%)
4	6GJ	C	705	-	17,19,19	1.72	3 (17%)	16,27,27	4.34	8 (50%)
5	SO4	C	706	-	4,4,4	0.47	0	6,6,6	0.26	0
5	SO4	C	707	-	4,4,4	0.54	0	6,6,6	0.41	0
6	EDO	C	709	-	3,3,3	0.44	0	2,2,2	0.86	0
6	EDO	C	710	-	3,3,3	0.49	0	2,2,2	1.24	0
2	NAG	D	701	1	14,14,15	0.91	1 (7%)	15,19,21	1.34	1 (6%)
4	6GJ	D	702	-	17,19,19	1.62	4 (23%)	16,27,27	4.20	5 (31%)
2	NAG	D	703	1	14,14,15	0.47	0	15,19,21	1.22	2 (13%)
2	NAG	D	704	1	14,14,15	0.57	0	15,19,21	1.65	2 (13%)
2	NAG	D	705	1	14,14,15	0.72	0	15,19,21	1.30	3 (20%)
6	EDO	D	707	-	3,3,3	0.51	0	2,2,2	0.75	0
6	EDO	D	708	-	3,3,3	0.14	0	2,2,2	1.25	0
5	SO4	D	709	-	4,4,4	0.42	0	6,6,6	0.41	0
5	SO4	D	710	-	4,4,4	0.57	0	6,6,6	0.96	1 (16%)

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	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	702	1	-	0/6/23/26	0/1/1/1
2	NAG	A	703	1	-	0/6/23/26	0/1/1/1
2	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	6GJ	A	706	-	-	1/4/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	707	-	-	0/0/0/0	0/0/0/0
5	SO4	A	708	-	-	0/0/0/0	0/0/0/0
6	EDO	A	709	-	-	0/1/1/1	0/0/0/0
6	EDO	A	710	-	-	0/1/1/1	0/0/0/0
2	NAG	B	701	1	-	0/6/23/26	0/1/1/1
2	NAG	B	702	1	-	0/6/23/26	0/1/1/1
2	NAG	B	703	1	-	0/6/23/26	0/1/1/1
2	NAG	B	704	1	-	0/6/23/26	0/1/1/1
5	SO4	B	706	-	-	0/0/0/0	0/0/0/0
5	SO4	B	707	-	-	0/0/0/0	0/0/0/0
6	EDO	B	708	-	-	0/1/1/1	0/0/0/0
6	EDO	B	709	-	-	0/1/1/1	0/0/0/0
4	6GJ	B	710	-	-	1/4/38/38	0/2/2/2
2	NAG	C	701	1	-	0/6/23/26	0/1/1/1
2	NAG	C	702	1	-	0/6/23/26	0/1/1/1
2	NAG	C	703	1	-	0/6/23/26	0/1/1/1
2	NAG	C	704	1	-	0/6/23/26	0/1/1/1
4	6GJ	C	705	-	-	1/4/38/38	0/2/2/2
5	SO4	C	706	-	-	0/0/0/0	0/0/0/0
5	SO4	C	707	-	-	0/0/0/0	0/0/0/0
6	EDO	C	709	-	-	0/1/1/1	0/0/0/0
6	EDO	C	710	-	-	0/1/1/1	0/0/0/0
2	NAG	D	701	1	-	0/6/23/26	0/1/1/1
4	6GJ	D	702	-	-	1/4/38/38	0/2/2/2
2	NAG	D	703	1	-	0/6/23/26	0/1/1/1
2	NAG	D	704	1	-	0/6/23/26	0/1/1/1
2	NAG	D	705	1	-	0/6/23/26	0/1/1/1
6	EDO	D	707	-	-	0/1/1/1	0/0/0/0
6	EDO	D	708	-	-	0/1/1/1	0/0/0/0
5	SO4	D	709	-	-	0/0/0/0	0/0/0/0
5	SO4	D	710	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	6GJ	C7-S6	-4.26	1.67	1.75
4	C	705	6GJ	C7-S6	-4.00	1.68	1.75
4	B	710	6GJ	C6-S6	-3.85	1.74	1.81
4	C	705	6GJ	C6-S6	-3.42	1.74	1.81
4	A	706	6GJ	C7-S6	-3.22	1.69	1.75
4	D	702	6GJ	C6-S6	-3.02	1.75	1.81
2	A	702	NAG	O3-C3	-2.62	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	710	6GJ	C7-S6	-2.37	1.71	1.75
4	A	706	6GJ	C6-S6	-2.17	1.77	1.81
4	A	706	6GJ	C7-N8	2.01	1.30	1.26
4	D	702	6GJ	C7-N8	2.30	1.31	1.26
2	D	701	NAG	C1-C2	2.40	1.55	1.52
2	A	703	NAG	C2-N2	2.46	1.50	1.46
4	A	706	6GJ	O1-C1	2.48	1.44	1.41
4	D	702	6GJ	O1-C1	2.77	1.44	1.41
4	B	710	6GJ	C7-N8	2.93	1.32	1.26
4	C	705	6GJ	O1-C1	2.94	1.44	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	6GJ	C5-C6-S6	-6.28	98.59	105.67
4	B	710	6GJ	O1-C1-C2	-5.27	94.76	109.36
2	A	702	NAG	C6-C5-C4	-5.12	100.38	113.02
4	A	706	6GJ	C5-C6-S6	-4.65	100.42	105.67
4	C	705	6GJ	O1-C1-C2	-4.24	97.62	109.36
2	B	702	NAG	O6-C6-C5	-4.22	97.37	111.33
4	B	710	6GJ	C3-C4-C5	-3.99	106.01	111.39
4	C	705	6GJ	C5-C6-S6	-3.97	101.19	105.67
2	A	703	NAG	O3-C3-C4	-3.86	101.64	110.34
2	A	703	NAG	O7-C7-C8	-3.75	115.18	122.06
4	A	706	6GJ	C3-C4-C5	-3.66	106.45	111.39
4	D	702	6GJ	O1-C1-C2	-3.62	99.33	109.36
2	B	703	NAG	C4-C3-C2	-3.43	105.89	111.23
2	B	702	NAG	C6-C5-C4	-3.40	104.63	113.02
2	A	702	NAG	O6-C6-C5	-3.27	100.52	111.33
4	B	710	6GJ	C6-C5-C4	-3.27	112.30	115.73
4	D	702	6GJ	C6-C5-C4	-3.22	112.35	115.73
4	B	710	6GJ	C5-C6-S6	-3.06	102.21	105.67
4	C	705	6GJ	C6-C5-C4	-3.03	112.55	115.73
2	D	705	NAG	O7-C7-C8	-2.97	116.61	122.06
4	A	706	6GJ	O1-C1-C2	-2.92	101.26	109.36
2	B	702	NAG	O3-C3-C4	-2.92	103.76	110.34
4	A	706	6GJ	C6-C5-C4	-2.86	112.73	115.73
2	B	702	NAG	C4-C3-C2	-2.84	106.82	111.23
2	B	701	NAG	O6-C6-C5	-2.80	102.08	111.33
2	B	703	NAG	O3-C3-C4	-2.68	104.31	110.34
2	B	703	NAG	C6-C5-C4	-2.63	106.53	113.02
4	C	705	6GJ	C10-C9-N8	-2.50	106.65	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAG	O6-C6-C5	-2.47	103.16	111.33
2	A	703	NAG	C4-C3-C2	-2.42	107.47	111.23
2	D	703	NAG	C2-N2-C7	-2.33	120.04	123.04
2	A	702	NAG	O4-C4-C5	-2.32	103.09	109.24
2	A	702	NAG	O3-C3-C4	-2.28	105.20	110.34
2	C	704	NAG	O4-C4-C3	-2.26	105.26	110.34
2	D	705	NAG	C3-C2-N2	-2.19	105.32	110.56
2	A	701	NAG	O3-C3-C2	-2.17	104.81	109.11
5	D	710	SO4	O2-S-O1	-2.16	102.67	109.50
2	D	704	NAG	O7-C7-C8	-2.02	118.35	122.06
2	C	703	NAG	O3-C3-C2	-2.01	105.13	109.11
4	D	702	6GJ	C10-C9-N8	-2.01	107.46	110.73
2	B	703	NAG	O7-C7-N2	2.08	126.11	121.86
2	D	705	NAG	C8-C7-N2	2.13	120.18	116.11
2	D	703	NAG	O5-C5-C6	2.35	112.43	107.35
2	A	703	NAG	C1-O5-C5	2.42	115.32	112.25
2	D	701	NAG	O5-C5-C6	2.44	112.63	107.35
4	A	706	6GJ	O4-C4-C3	2.48	115.92	110.34
4	C	705	6GJ	O2-C2-C1	2.68	114.30	109.07
2	B	703	NAG	C3-C2-N2	2.77	117.21	110.56
2	C	703	NAG	C1-O5-C5	2.80	115.81	112.25
4	A	706	6GJ	O2-C2-C3	3.06	117.23	110.34
2	A	703	NAG	C8-C7-N2	3.09	122.01	116.11
4	A	706	6GJ	O2-C2-C1	3.40	115.72	109.07
2	B	703	NAG	C1-O5-C5	3.68	116.92	112.25
2	A	703	NAG	O3-C3-C2	3.86	116.75	109.11
2	B	701	NAG	C1-O5-C5	4.14	117.50	112.25
4	C	705	6GJ	O2-C2-C3	4.36	120.15	110.34
2	C	702	NAG	C1-O5-C5	4.64	118.14	112.25
2	B	702	NAG	C1-O5-C5	4.76	118.30	112.25
2	D	704	NAG	C1-O5-C5	5.15	118.79	112.25
4	B	710	6GJ	C10-C9-N8	5.25	119.31	110.73
2	A	703	NAG	C3-C2-N2	5.49	123.71	110.56
4	B	710	6GJ	C9-N8-C7	6.30	128.31	117.86
4	C	705	6GJ	C3-C2-C1	7.13	120.45	109.13
4	A	706	6GJ	C3-C2-C1	7.31	120.74	109.13
2	A	702	NAG	C1-O5-C5	9.51	124.32	112.25
4	C	705	6GJ	C9-N8-C7	12.96	139.37	117.86
4	A	706	6GJ	C9-N8-C7	13.36	140.03	117.86
4	D	702	6GJ	C9-N8-C7	14.27	141.54	117.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	710	6GJ	S6-C7-N8-C9
4	D	702	6GJ	S6-C7-N8-C9
4	A	706	6GJ	S6-C7-N8-C9
4	C	705	6GJ	S6-C7-N8-C9

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706	6GJ	1	0
6	B	708	EDO	3	0
4	B	710	6GJ	7	0
2	D	701	NAG	1	0
2	D	704	NAG	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	605/678 (89%)	-0.07	12 (1%) 68 69	17, 25, 41, 91	0
1	B	605/678 (89%)	-0.17	14 (2%) 64 64	17, 24, 41, 87	0
1	C	603/678 (88%)	-0.03	14 (2%) 64 64	17, 27, 50, 77	0
1	D	603/678 (88%)	0.04	23 (3%) 44 45	18, 28, 52, 87	0
All	All	2416/2712 (89%)	-0.06	63 (2%) 59 60	17, 26, 46, 91	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	647	SER	8.0
1	D	528	GLY	7.1
1	D	527	TRP	6.5
1	C	527	TRP	5.7
1	D	29	GLN	5.7
1	C	525	GLY	5.6
1	A	645	GLY	5.3
1	D	629	ASP	5.2
1	D	526	GLY	5.2
1	D	647	SER	5.0
1	A	628	SER	4.9
1	A	29	GLN	4.5
1	C	647	SER	4.2
1	A	629	ASP	4.2
1	A	646	SER	4.2
1	B	29	GLN	4.1
1	A	647	SER	4.0
1	D	646	SER	3.9
1	C	29	GLN	3.9
1	B	611	SER	3.9
1	B	31	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	629	ASP	3.5
1	B	628	SER	3.4
1	B	646	SER	3.4
1	D	545	ASN	3.3
1	B	627	SER	3.3
1	D	627	SER	3.3
1	D	427	SER	3.3
1	D	628	SER	3.2
1	A	644	ILE	3.2
1	D	359	LYS	3.2
1	A	359	LYS	3.0
1	C	359	LYS	2.9
1	D	631	PRO	2.9
1	D	488	TYR	2.9
1	C	31	MET	2.8
1	B	644	ILE	2.8
1	B	488	TYR	2.8
1	B	645	GLY	2.7
1	D	428	ASN	2.6
1	D	390	ASP	2.6
1	D	426	CYS	2.5
1	C	476	LEU	2.5
1	D	632	GLU	2.4
1	A	627	SER	2.4
1	C	488	TYR	2.4
1	D	425	ASP	2.3
1	D	623	TRP	2.3
1	D	459	ASN	2.3
1	C	502	SER	2.2
1	C	646	SER	2.2
1	A	109[A]	ARG	2.2
1	C	426	CYS	2.2
1	B	283	THR	2.1
1	D	234	GLN	2.1
1	C	427	SER	2.1
1	A	31	MET	2.1
1	A	273	TRP	2.1
1	B	359	LYS	2.1
1	C	229	LYS	2.1
1	B	282	SER	2.1
1	D	38	ARG	2.0
1	C	505	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	C	710	4/4	0.81	0.20	5.14	31,31,35,42	0
6	EDO	B	709	4/4	0.92	0.15	4.35	28,29,31,33	0
2	NAG	A	703	14/15	0.78	0.18	4.22	36,41,51,52	0
2	NAG	B	703	14/15	0.77	0.20	4.19	36,43,57,61	0
2	NAG	A	702	14/15	0.90	0.15	3.63	24,30,35,35	0
4	6GJ	B	710	18/18	0.88	0.16	2.43	19,26,59,61	0
4	6GJ	D	702	18/18	0.84	0.17	2.27	24,31,56,57	0
4	6GJ	A	706	18/18	0.84	0.19	2.11	20,31,63,64	0
4	6GJ	C	705	18/18	0.86	0.16	1.64	23,31,54,54	0
2	NAG	C	703	14/15	0.86	0.20	1.59	35,46,49,50	0
5	SO4	C	707	5/5	0.95	0.20	1.58	44,52,54,56	0
2	NAG	C	702	14/15	0.82	0.23	1.12	40,47,54,58	0
5	SO4	B	707	5/5	0.97	0.13	1.00	31,39,44,44	0
6	EDO	B	708	4/4	0.85	0.15	1.00	37,43,43,45	0
6	EDO	A	709	4/4	0.92	0.14	0.80	44,48,49,54	0
2	NAG	D	703	14/15	0.84	0.19	0.60	41,44,51,53	0
2	NAG	B	702	14/15	0.93	0.10	0.58	25,28,32,35	0
6	EDO	D	708	4/4	0.92	0.13	0.49	38,40,43,45	0
5	SO4	D	710	5/5	0.98	0.17	0.47	52,53,54,54	0
5	SO4	A	708	5/5	0.97	0.13	0.37	38,47,49,52	0
2	NAG	B	701	14/15	0.91	0.10	-0.01	21,28,36,36	0
2	NAG	D	705	14/15	0.94	0.10	-0.07	27,31,34,36	0
2	NAG	C	704	14/15	0.93	0.10	-0.12	25,31,33,36	0
2	NAG	A	701	14/15	0.94	0.09	-0.94	23,27,32,41	0
3	CL	D	706	1/1	0.99	0.10	-1.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	C	708	1/1	0.99	0.08	-2.00	22,22,22,22	0
3	CL	B	705	1/1	0.99	0.05	-3.59	20,20,20,20	0
3	CL	A	705	1/1	1.00	0.04	-3.72	21,21,21,21	0
5	SO4	B	706	5/5	0.96	0.24	-	64,67,70,71	0
6	EDO	A	710	4/4	0.87	0.19	-	29,31,32,40	0
6	EDO	C	709	4/4	0.91	0.23	-	29,35,36,39	0
5	SO4	A	707	5/5	0.87	0.29	-	60,60,63,63	0
2	NAG	A	704	14/15	0.85	0.33	-	49,55,63,67	0
2	NAG	D	701	14/15	0.64	0.36	-	69,76,92,92	0
2	NAG	B	704	14/15	0.86	0.26	-	46,49,52,58	0
5	SO4	D	709	5/5	0.84	0.28	-	67,70,74,74	0
6	EDO	D	707	4/4	0.88	0.17	-	28,33,36,37	0
2	NAG	D	704	14/15	0.56	0.39	-	75,85,89,91	0
2	NAG	C	701	14/15	0.73	0.39	-	79,88,98,103	0
5	SO4	C	706	5/5	0.95	0.23	-	61,62,64,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.