



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:25 AM UTC

PDB ID : 3THD / pdb\_00003thd  
Title : Crystal structure of human beta-galactosidase in complex with 1-deoxygalactonojirimycin  
Authors : Ohto, U.; Shimizu, T.  
Deposited on : 2011-08-18  
Resolution : 1.79 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

<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>.

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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)  
Xtrriage (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

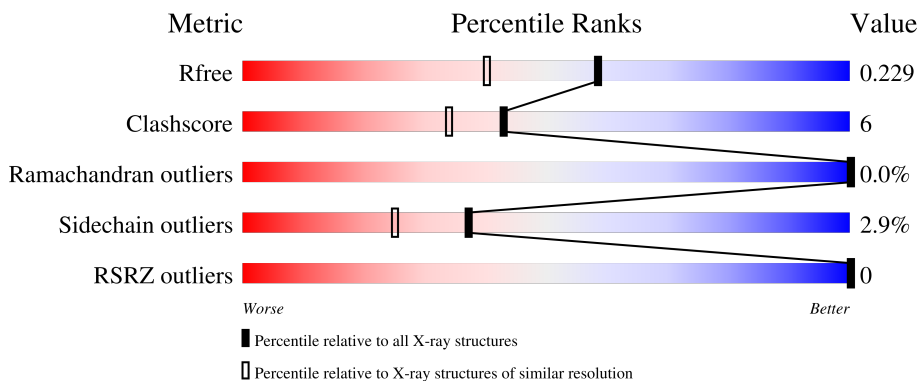
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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  $\geq 3$ , 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	654	
1	B	654	
1	C	654	
1	D	654	

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
6	EDO	D	1101	-	-	X	-

## 2 Entry composition [i](#)

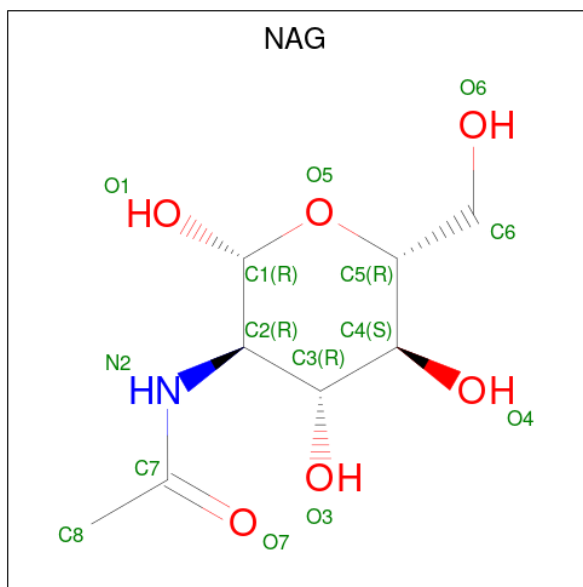
There are 7 unique types of molecules in this entry. The entry contains 21969 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	605	Total 4875	C 3161	N 803	O 893	S 18	0	8	0
1	B	605	Total 4850	C 3146	N 800	O 887	S 17	0	5	0
1	C	602	Total 4861	C 3153	N 798	O 893	S 17	0	9	0
1	D	602	Total 4855	C 3149	N 798	O 890	S 18	0	9	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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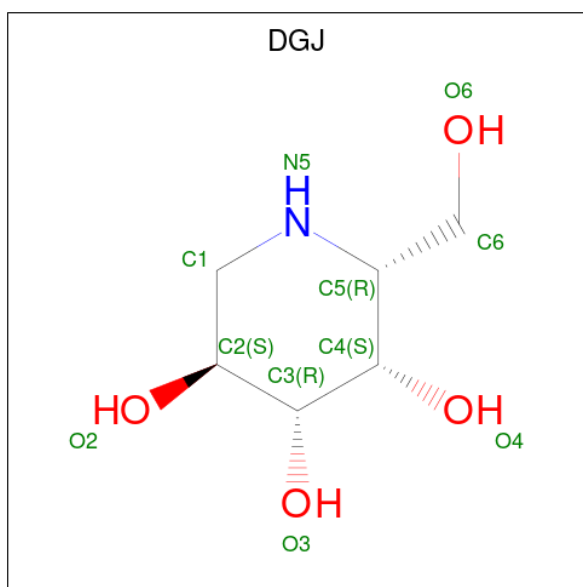
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
	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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

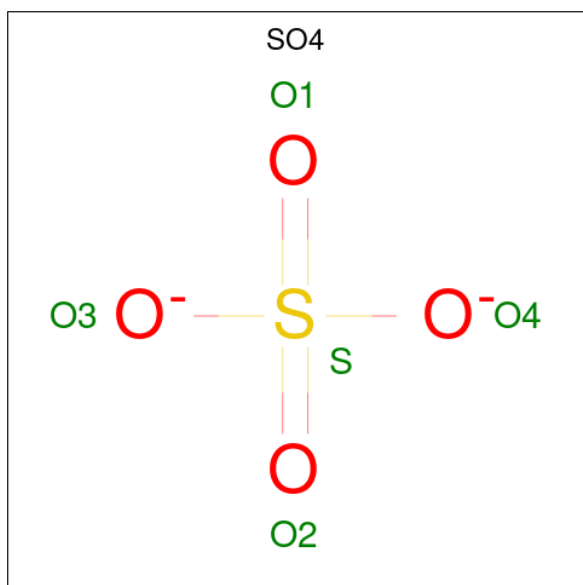
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is (2R,3S,4R,5S)-2-(hydroxymethyl)piperidine-3,4,5-triol (CCD ID: DGJ) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>).



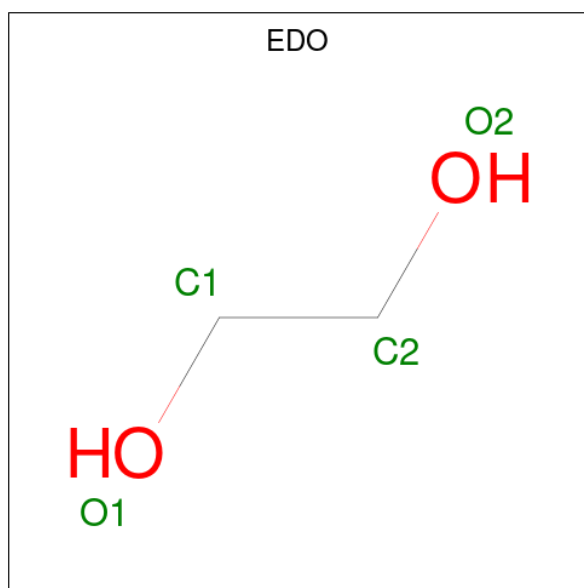
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	11	6	1	4	0	0
4	B	1	11	6	1	4	0	0
4	C	1	11	6	1	4	0	0
4	D	1	11	6	1	4	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: 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

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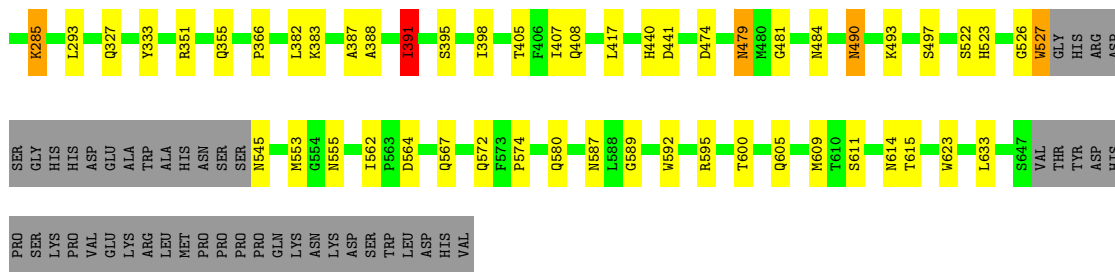
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0

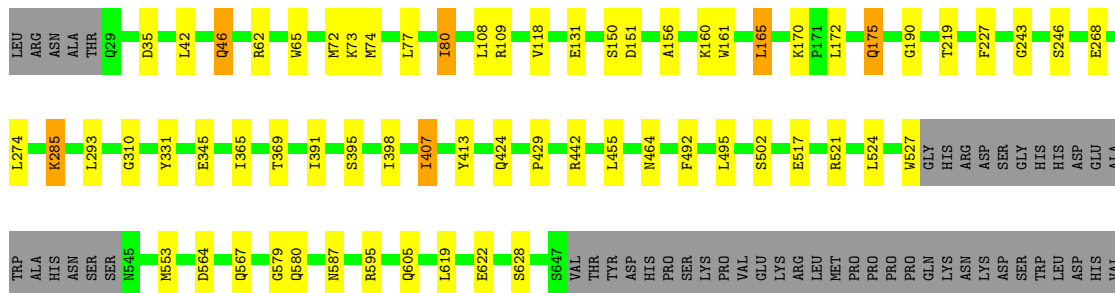
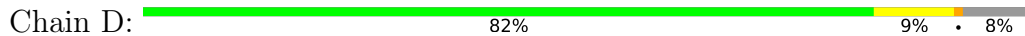
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	555	Total 555	O 555	0	0
7	B	603	Total 603	O 603	0	0
7	C	529	Total 529	O 529	0	0
7	D	497	Total 497	O 497	0	0





• Molecule 1: Beta-galactosidase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.79Å 116.00Å 140.33Å 90.00° 92.22° 90.00°	Depositor
Resolution (Å)	29.29 – 1.79 29.29 – 1.79	Depositor EDS
% Data completeness (in resolution range)	92.8 (29.29-1.79) 92.9 (29.29-1.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.198 , 0.228 0.200 , 0.229	Depositor DCC
$R_{free}$ test set	13274 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 30.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, 0.333 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: NAG, DGJ, CL, EDO, SO4

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	0.89	0/5026	0.94	8/6857 (0.1%)
1	B	0.89	1/5001 (0.0%)	0.89	2/6823 (0.0%)
1	C	0.86	1/5011 (0.0%)	0.87	1/6838 (0.0%)
1	D	0.85	0/5004	0.88	1/6828 (0.0%)
All	All	0.87	2/20042 (0.0%)	0.90	12/27346 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	562	ILE	N-CA	5.95	1.50	1.46
1	B	56	HIS	CG-CD2	5.40	1.41	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	VAL	CB-CA-C	-11.73	96.31	112.14
1	C	391	ILE	CB-CA-C	-7.08	102.75	112.24
1	B	492	PHE	N-CA-C	6.99	118.55	111.07
1	A	366	PRO	CA-C-N	-6.11	114.25	120.85
1	A	366	PRO	C-N-CA	-6.11	114.25	120.85
1	A	60	VAL	CA-C-N	-6.06	113.72	119.85
1	A	60	VAL	C-N-CA	-6.06	113.72	119.85
1	B	459	ASN	N-CA-C	5.99	117.89	111.36
1	A	215	VAL	CB-CA-C	-5.50	103.02	111.71
1	A	165	LEU	N-CA-C	5.46	117.03	111.14
1	A	492	PHE	N-CA-C	5.38	116.83	111.07
1	D	369	THR	N-CA-C	5.30	116.37	109.64

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	4875	0	4728	76	0
1	B	4850	0	4710	42	0
1	C	4861	0	4713	67	0
1	D	4855	0	4722	50	0
2	A	56	0	52	0	0
2	B	56	0	52	3	0
2	C	56	0	52	1	0
2	D	56	0	52	0	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	11	0	13	0	0
4	B	11	0	13	0	0
4	C	11	0	13	0	0
4	D	11	0	13	1	0
5	A	10	0	0	1	0
5	B	10	0	0	1	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	A	8	0	12	4	0
6	B	8	0	12	2	0
6	C	8	0	12	2	0
6	D	8	0	12	5	0
7	A	555	0	0	17	0
7	B	603	0	0	22	0
7	C	529	0	0	20	0
7	D	497	0	0	15	0
All	All	21969	0	19181	241	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 6.

All (241) 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:C:228:LEU:HD11	7:C:1610:HOH:O	1.48	1.14
1:A:409[A]:VAL:CG1	1:A:513:PRO:HG3	1.76	1.13
1:D:243:GLY:H	6:D:1101:EDO:H11	1.16	1.07
1:C:609:MET:SD	7:C:1351:HOH:O	2.16	1.02
1:B:252:PHE:HZ	7:B:1872:HOH:O	1.44	1.01
1:D:407:ILE:HD11	1:D:492:PHE:O	1.63	0.99
1:B:130:TRP:HB3	7:B:1575:HOH:O	1.63	0.97
1:B:243:GLY:H	6:B:1101:EDO:H22	1.29	0.93
1:A:500:THR:HG21	7:A:750:HOH:O	1.68	0.92
1:A:580:GLN:HE21	1:A:587:ASN:HD21	1.18	0.89
1:A:409[A]:VAL:HG12	1:A:513:PRO:HG3	1.53	0.88
1:D:407:ILE:H	1:D:407:ILE:CD1	1.87	0.88
1:A:437:ASN:HD21	1:A:458:ASN:H	1.16	0.88
1:A:409[A]:VAL:HG11	1:A:513:PRO:HG3	1.56	0.86
1:D:243:GLY:N	6:D:1101:EDO:H11	1.90	0.85
1:D:407:ILE:HD12	1:D:407:ILE:N	1.92	0.84
7:C:1347:HOH:O	1:D:46:GLN:HB2	1.76	0.84
1:B:95:GLN:HB2	7:B:1722:HOH:O	1.78	0.83
1:C:112:HIS:HD2	7:C:753:HOH:O	1.61	0.83
1:D:407:ILE:H	1:D:407:ILE:HD12	1.44	0.82
1:C:405:THR:H	1:C:408:GLN:HE21	1.26	0.81
1:A:500:THR:HG23	7:A:709:HOH:O	1.79	0.81
1:D:407:ILE:CD1	1:D:492:PHE:O	2.29	0.80
5:B:1002:SO4:O3	7:B:867:HOH:O	1.99	0.80
1:D:580:GLN:HE21	1:D:587:ASN:HD21	1.29	0.78
1:A:327:GLN:HE22	1:A:484:ASN:HD21	1.32	0.77
1:B:572[A]:GLN:OE1	7:B:1958:HOH:O	2.02	0.77
2:B:703:NAG:H81	7:D:1625:HOH:O	1.84	0.76
1:D:564:ASP:HB2	7:D:865:HOH:O	1.84	0.76
2:B:703:NAG:C8	7:D:1625:HOH:O	2.34	0.75
1:A:409[A]:VAL:HG12	1:A:409[A]:VAL:O	1.87	0.75
1:D:35:ASP:HB3	7:D:1448:HOH:O	1.85	0.75
1:C:580:GLN:HE21	1:C:587:ASN:HD21	1.35	0.74
1:D:246:SER:OG	6:D:1101:EDO:H12	1.88	0.73
1:A:398:ILE:HD13	7:A:2028:HOH:O	1.89	0.72
1:D:175:GLN:H	1:D:175:GLN:HE21	1.36	0.72
1:C:327:GLN:HE22	1:C:484:ASN:HD21	1.35	0.71
1:C:285:LYS:HE3	7:C:1152:HOH:O	1.89	0.71
1:A:255:GLN:HE22	1:A:265:ILE:H	1.37	0.71
1:D:243:GLY:H	6:D:1101:EDO:C1	1.98	0.69
1:D:391:ILE:HD13	1:D:524:LEU:O	1.92	0.69
1:C:623:TRP:HZ3	7:C:1999:HOH:O	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:HIS:CD2	1:C:527:TRP:CE2	2.82	0.68
1:A:382:LEU:HD23	1:A:524:LEU:HD12	1.76	0.67
1:B:160:LYS:NZ	7:B:2033:HOH:O	2.27	0.66
1:C:405:THR:H	1:C:408:GLN:NE2	1.92	0.66
1:B:623:TRP:HZ3	7:B:1629:HOH:O	1.79	0.66
1:C:234:GLN:NE2	7:C:1039:HOH:O	2.28	0.65
1:D:628:SER:HB3	7:D:1180:HOH:O	1.95	0.65
1:C:523:HIS:CE1	1:C:615:THR:HG21	2.32	0.65
1:C:564[A]:ASP:OD2	7:C:870:HOH:O	2.14	0.64
1:D:175:GLN:H	1:D:175:GLN:NE2	1.96	0.64
1:C:479:ASN:ND2	1:C:481:GLY:H	1.95	0.63
1:B:383:LYS:HG2	1:B:387:ALA:HB3	1.82	0.62
1:C:228:LEU:CD1	7:C:1610:HOH:O	2.23	0.62
1:C:523:HIS:HD2	1:C:527:TRP:CE2	2.17	0.61
1:A:479:ASN:ND2	1:A:481:GLY:H	1.99	0.61
1:B:529:HIS:HE1	7:B:1569:HOH:O	1.83	0.61
1:C:391:ILE:HG13	7:C:1528:HOH:O	2.00	0.61
1:A:160:LYS:HD3	7:A:888:HOH:O	2.01	0.61
1:A:318:ASN:HD21	1:A:590:ARG:HH21	1.49	0.61
1:A:490:ASN:ND2	7:A:1982:HOH:O	2.33	0.61
1:A:553:MET:HE2	1:A:617:THR:HG23	1.83	0.60
1:A:611:SER:CB	7:A:1885:HOH:O	2.49	0.60
1:B:91:PRO:O	7:B:1288:HOH:O	2.15	0.60
1:C:245:GLY:H	6:C:1101:EDO:H22	1.66	0.60
1:A:80:ILE:HD11	1:A:118:VAL:HG22	1.83	0.60
1:A:276:HIS:NE2	1:A:321:ASN:ND2	2.50	0.59
1:A:479:ASN:C	1:A:479:ASN:HD22	2.10	0.59
1:B:553:MET:HE3	7:B:1555:HOH:O	2.01	0.59
1:A:297:LEU:HD12	1:A:353:ILE:HD11	1.83	0.58
1:A:611:SER:HB2	7:A:1885:HOH:O	2.02	0.58
1:C:255:GLN:HE22	1:C:265:ILE:H	1.50	0.57
1:A:490:ASN:HD22	1:A:490:ASN:H	1.53	0.56
1:C:175[A]:GLN:NE2	7:C:1062:HOH:O	2.36	0.56
5:A:1002:SO4:O1	7:A:2000:HOH:O	2.17	0.56
1:C:526:GLY:C	1:C:527:TRP:HE3	2.14	0.56
1:A:112:HIS:HD2	7:A:1649:HOH:O	1.88	0.56
1:D:553:MET:CE	7:D:1133:HOH:O	2.53	0.56
1:A:409[A]:VAL:CG1	1:A:409[A]:VAL:O	2.54	0.55
1:A:587:ASN:HD22	1:A:589:GLY:H	1.53	0.55
1:A:105:GLU:HB3	1:A:109:ARG:HH12	1.71	0.55
1:A:630:ASP:HB3	1:A:633:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLY:H	6:A:1101:EDO:H11	1.73	0.54
1:D:442:ARG:NH1	1:D:622:GLU:OE2	2.29	0.54
1:D:587:ASN:C	1:D:587:ASN:HD22	2.15	0.54
1:A:293:LEU:HD13	1:A:353:ILE:CG1	2.37	0.54
1:B:31:MET:HE2	1:B:33:GLU:OE1	2.08	0.54
1:C:572[A]:GLN:HG2	1:C:574:PRO:HD3	1.90	0.54
1:D:395:SER:HB3	7:D:794:HOH:O	2.08	0.54
1:B:38:ARG:NH2	7:B:1798:HOH:O	2.41	0.54
1:C:523:HIS:HE1	1:C:615:THR:HG21	1.71	0.54
1:C:522:SER:HA	1:C:527:TRP:HB2	1.90	0.54
1:C:479:ASN:ND2	1:C:493:LYS:HE3	2.23	0.53
1:C:43:LYS:HE3	7:C:1303:HOH:O	2.07	0.53
1:B:623:TRP:CZ3	7:B:1629:HOH:O	2.53	0.53
1:A:398:ILE:HG21	1:A:409[B]:VAL:HG12	1.91	0.53
1:B:190:GLY:HA3	1:B:227:PHE:O	2.09	0.53
1:A:80:ILE:CD1	1:A:118:VAL:HG22	2.39	0.52
1:B:168:LYS:HE3	7:B:1973:HOH:O	2.08	0.52
6:B:1102:EDO:H22	7:B:1738:HOH:O	2.09	0.52
1:C:205:LYS:HG2	7:C:1434:HOH:O	2.10	0.52
1:C:395:SER:HB2	7:C:814:HOH:O	2.10	0.52
1:B:83:TYR:CE2	1:B:128:ALA:HB2	2.46	0.51
1:B:359:LYS:HE3	7:B:1851:HOH:O	2.11	0.51
1:C:592:TRP:CE2	1:C:595:ARG:HG3	2.45	0.51
1:C:479:ASN:C	1:C:479:ASN:HD22	2.18	0.51
1:D:72:MET:HB3	1:D:77:LEU:HD12	1.93	0.51
7:A:718:HOH:O	1:C:611:SER:HB3	2.11	0.51
1:A:479:ASN:ND2	1:A:479:ASN:C	2.69	0.51
1:A:245:GLY:H	6:A:1101:EDO:C1	2.24	0.50
1:B:598:GLN:HA	1:B:644:ILE:HA	1.93	0.50
1:D:131:GLU:HG2	1:D:413:TYR:CE2	2.46	0.50
1:D:219[A]:THR:HG23	7:D:741:HOH:O	2.10	0.50
1:B:112:HIS:CD2	7:B:1383:HOH:O	2.64	0.50
1:A:587:ASN:HD22	1:A:587:ASN:C	2.20	0.50
1:C:148:ARG:HB2	1:C:192:TYR:CE1	2.48	0.49
1:C:245:GLY:H	6:C:1101:EDO:C2	2.24	0.49
1:C:351:ARG:O	1:C:355:GLN:HG3	2.12	0.49
1:C:407[A]:ILE:HD12	7:C:813:HOH:O	2.12	0.49
1:C:223:ALA:HA	7:C:1610:HOH:O	2.13	0.49
1:A:437:ASN:ND2	1:A:458:ASN:H	1.99	0.48
1:A:211:LEU:HB3	1:A:215:VAL:HG21	1.95	0.48
1:D:109:ARG:NH2	7:D:1625:HOH:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:ASN:HD22	1:C:587:ASN:C	2.21	0.48
1:B:555:ASN:HA	1:B:614:ASN:O	2.15	0.47
1:C:190:GLY:HA3	1:C:227:PHE:O	2.14	0.47
1:A:580:GLN:HE21	1:A:587:ASN:ND2	1.98	0.47
1:A:57:TYR:CZ	1:A:104:VAL:HG13	2.49	0.47
1:C:479:ASN:ND2	1:C:479:ASN:C	2.70	0.47
1:A:321:ASN:ND2	1:A:327:GLN:HE21	2.12	0.47
1:A:318:ASN:HD21	1:A:590:ARG:NH2	2.12	0.47
1:A:382:LEU:HD23	1:A:524:LEU:CD1	2.43	0.47
1:C:175[A]:GLN:H	1:C:175[A]:GLN:CD	2.22	0.47
1:A:241:ASP:HB2	1:A:268:GLU:HB2	1.96	0.47
1:D:243:GLY:CA	6:D:1101:EDO:H11	2.42	0.47
1:D:310:GLY:HA3	1:D:331:TYR:O	2.15	0.47
1:C:440:HIS:HA	1:C:441:ASP:HA	1.73	0.47
1:D:35:ASP:HB2	1:D:42:LEU:HG	1.96	0.47
1:C:175[A]:GLN:NE2	1:C:175[A]:GLN:H	2.13	0.46
1:A:57:TYR:CE2	1:A:104:VAL:HG13	2.50	0.46
1:C:234:GLN:HG3	7:C:1463:HOH:O	2.15	0.46
1:A:287:GLU:HG3	7:A:1921:HOH:O	2.14	0.46
2:B:703:NAG:H83	7:D:1625:HOH:O	2.09	0.46
1:A:479:ASN:HD22	1:A:481:GLY:H	1.63	0.46
1:B:383:LYS:HD2	1:B:388:ALA:HB2	1.96	0.46
1:B:395:SER:HB2	7:B:748:HOH:O	2.15	0.46
1:C:72:MET:HB3	1:C:77:LEU:HD12	1.97	0.46
1:C:555:ASN:HA	1:C:614:ASN:O	2.16	0.46
1:A:160:LYS:CD	7:A:888:HOH:O	2.60	0.46
1:C:388:ALA:HB1	1:C:391:ILE:HD12	1.98	0.46
1:D:131:GLU:HG2	1:D:413:TYR:HE2	1.81	0.46
1:C:141:GLU:HB3	7:C:882:HOH:O	2.16	0.45
1:A:310:GLY:HA3	1:A:331:TYR:O	2.16	0.45
1:A:490:ASN:HD22	1:A:490:ASN:N	2.13	0.45
1:C:383:LYS:HG2	1:C:387:ALA:HB3	1.97	0.45
1:C:592:TRP:CZ2	1:C:595:ARG:HG3	2.50	0.45
1:B:322[A]:SER:HA	1:B:323:PRO:C	2.40	0.45
1:C:497:SER:HA	2:C:702:NAG:H81	1.99	0.45
1:C:221:ASP:O	1:C:240:VAL:HA	2.17	0.45
1:D:73:LYS:NZ	7:D:1529:HOH:O	2.50	0.45
1:C:405:THR:N	1:C:408:GLN:HE21	2.06	0.45
1:A:243:GLY:HA3	6:A:1101:EDO:H12	1.99	0.45
1:B:229:LYS:HE2	7:B:2022:HOH:O	2.17	0.45
1:C:417:LEU:HD11	1:C:474:ASP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:GLU:O	1:D:521:ARG:HG3	2.15	0.45
1:B:321:ASN:ND2	1:B:327:GLN:HE21	2.14	0.45
1:A:409[A]:VAL:HG12	1:A:513:PRO:CG	2.38	0.45
1:D:156:ALA:O	1:D:160:LYS:HG3	2.16	0.45
1:A:294:TYR:HA	1:A:353:ILE:HD13	1.99	0.45
1:D:564:ASP:O	1:D:567:GLN:HG3	2.17	0.45
1:B:241:ASP:HB2	1:B:268:GLU:HB2	1.99	0.44
1:B:355:GLN:HA	1:B:358:GLU:O	2.17	0.44
1:D:161:TRP:CZ2	1:D:165:LEU:HG	2.51	0.44
1:A:349:ALA:O	1:A:353:ILE:HG23	2.18	0.44
1:A:322[A]:SER:HA	1:A:323:PRO:C	2.42	0.44
1:D:80[A]:ILE:HD11	1:D:118:VAL:HG22	1.99	0.44
1:D:345:GLU:HG3	7:D:1370:HOH:O	2.18	0.44
1:A:598:GLN:HA	1:A:644:ILE:HA	2.00	0.44
1:C:382:LEU:HD22	1:C:553:MET:HE3	1.99	0.44
1:B:632:GLU:O	1:B:632:GLU:HG2	2.18	0.44
1:C:587:ASN:HD22	1:C:589:GLY:H	1.65	0.43
1:C:69:LEU:HD12	1:C:110:LEU:HD13	2.00	0.43
1:D:62:ARG:HA	1:D:65:TRP:CD2	2.53	0.43
1:A:587:ASN:ND2	1:A:589:GLY:H	2.16	0.43
1:B:440:HIS:HA	1:B:441:ASP:HA	1.81	0.43
1:D:407:ILE:H	1:D:407:ILE:HD13	1.78	0.43
1:A:83:TYR:CE2	1:A:128:ALA:HB2	2.53	0.43
1:A:440:HIS:HA	1:A:441:ASP:HA	1.73	0.43
1:A:360:VAL:HG13	1:A:361:PRO:HD2	2.00	0.43
1:C:490:ASN:N	1:C:490:ASN:HD22	2.15	0.43
1:A:406:PHE:HB3	1:A:411:GLN:O	2.18	0.43
1:C:272:GLY:HA3	1:C:333:TYR:O	2.18	0.43
1:A:433:SER:HB3	1:A:500:THR:HG22	1.99	0.42
1:A:500:THR:CG2	7:A:709:HOH:O	2.50	0.42
1:B:382:LEU:HD23	1:B:524:LEU:HD12	2.01	0.42
1:C:205:LYS:HE3	7:C:1434:HOH:O	2.18	0.42
1:D:108:LEU:HD12	1:D:172:LEU:HD13	2.01	0.42
1:D:268:GLU:OE1	4:D:900:DGJ:H1	2.20	0.42
1:D:429:PRO:HB3	1:D:464:ASN:HB3	2.02	0.42
1:A:479:ASN:ND2	1:A:493:LYS:HE3	2.34	0.42
1:C:490:ASN:HD22	1:C:490:ASN:H	1.66	0.42
1:B:529:HIS:CE1	7:B:1569:HOH:O	2.66	0.42
1:A:90:GLU:OE2	1:A:93:PRO:HA	2.20	0.42
1:B:154:TYR:HE2	1:B:199:TYR:CE1	2.38	0.42
1:B:631:PRO:HD3	7:B:1713:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HD23	1:C:366:PRO:HG3	2.02	0.42
1:A:35:ASP:HB2	1:A:42:LEU:HG	2.01	0.42
1:A:190:GLY:HA3	1:A:227:PHE:O	2.19	0.42
1:C:83:TYR:CD1	1:C:126:ILE:HB	2.55	0.42
1:D:407:ILE:HD11	1:D:492:PHE:C	2.43	0.42
1:B:112:HIS:HD2	7:B:1383:HOH:O	2.00	0.41
1:B:256:ARG:HA	1:B:256:ARG:HD3	1.83	0.41
1:C:522:SER:CA	1:C:527:TRP:HB2	2.50	0.41
1:A:318:ASN:ND2	1:A:590:ARG:HE	2.19	0.41
1:B:105:GLU:O	1:B:109:ARG:HG3	2.20	0.41
1:D:190:GLY:HA3	1:D:227:PHE:O	2.20	0.41
1:A:175:GLN:CG	7:A:858:HOH:O	2.69	0.41
1:A:52:SER:HA	1:A:79:ALA:O	2.21	0.41
1:A:523:HIS:HB2	1:A:527:TRP:CD2	2.55	0.41
1:B:35:ASP:HB2	1:B:42:LEU:HG	2.03	0.41
1:A:595:ARG:NE	7:A:2127:HOH:O	2.32	0.41
1:B:205:LYS:HG2	7:B:1375:HOH:O	2.19	0.41
1:B:306:TYR:HA	1:B:307:MET:HA	1.92	0.41
1:D:150:SER:O	1:D:151:ASP:C	2.63	0.41
1:D:219[A]:THR:CG2	7:D:685:HOH:O	2.68	0.41
1:D:285:LYS:HG3	7:D:776:HOH:O	2.21	0.41
1:A:413:TYR:CD1	6:A:1102:EDO:H22	2.56	0.41
1:A:523:HIS:CD2	1:A:553:MET:SD	3.14	0.41
1:B:174:TYR:HA	1:B:178:GLY:O	2.21	0.41
1:C:527:TRP:HE3	1:C:527:TRP:N	2.19	0.40
1:D:424:GLN:HE22	1:D:502:SER:HB2	1.85	0.40
1:A:91:PRO:O	7:A:955:HOH:O	2.22	0.40
1:A:429:PRO:HG2	7:A:2009:HOH:O	2.20	0.40
1:C:564[A]:ASP:O	1:C:567:GLN:HG3	2.20	0.40
1:B:581:VAL:HG13	1:B:588:LEU:HB2	2.03	0.40
1:D:74:MET:HB3	1:D:365:ILE:HG12	2.03	0.40
1:D:579:GLY:HA3	1:D:619:LEU:O	2.22	0.40
1:C:572[B]:GLN:HB3	1:C:600:THR:HG22	2.04	0.40
1:D:219[A]:THR:HG21	7:D:685:HOH:O	2.20	0.40
1:C:545:ASN:HB3	7:C:2153:HOH:O	2.20	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	609/654 (93%)	591 (97%)	17 (3%)	1 (0%)	43	31
1	B	606/654 (93%)	586 (97%)	20 (3%)	0	100	100
1	C	607/654 (93%)	589 (97%)	18 (3%)	0	100	100
1	D	607/654 (93%)	591 (97%)	16 (3%)	0	100	100
All	All	2429/2616 (93%)	2357 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	611	SER

### 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	526/563 (93%)	508 (97%)	18 (3%)	32	20
1	B	523/563 (93%)	511 (98%)	12 (2%)	44	33
1	C	525/563 (93%)	510 (97%)	15 (3%)	37	25
1	D	525/563 (93%)	509 (97%)	16 (3%)	36	24
All	All	2099/2252 (93%)	2038 (97%)	61 (3%)	37	25

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	104	VAL
1	A	110	LEU
1	A	119	ILE
1	A	160	LYS
1	A	175	GLN
1	A	215	VAL
1	A	274	LEU
1	A	293	LEU
1	A	353	ILE
1	A	398	ILE
1	A	460	VAL
1	A	479	ASN
1	A	490	ASN
1	A	500	THR
1	A	553	MET
1	A	605	GLN
1	A	633	LEU
1	B	110	LEU
1	B	170	LYS
1	B	274	LEU
1	B	293	LEU
1	B	345	GLU
1	B	398	ILE
1	B	521	ARG
1	B	553	MET
1	B	605	GLN
1	B	611	SER
1	B	632	GLU
1	B	633	LEU
1	C	33	GLU
1	C	110	LEU
1	C	170	LYS
1	C	175[A]	GLN
1	C	175[B]	GLN
1	C	274	LEU
1	C	285	LYS
1	C	293	LEU
1	C	391	ILE
1	C	398	ILE
1	C	479	ASN
1	C	490	ASN
1	C	527	TRP

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Mol	Chain	Res	Type
1	C	605	GLN
1	C	633	LEU
1	D	46	GLN
1	D	80[A]	ILE
1	D	80[B]	ILE
1	D	165	LEU
1	D	170	LYS
1	D	175	GLN
1	D	274	LEU
1	D	285	LYS
1	D	293	LEU
1	D	398	ILE
1	D	407	ILE
1	D	455	LEU
1	D	495	LEU
1	D	527	TRP
1	D	595	ARG
1	D	605	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	112	HIS
1	A	204	GLN
1	A	255	GLN
1	A	318	ASN
1	A	321	ASN
1	A	437	ASN
1	A	459	ASN
1	A	479	ASN
1	A	484	ASN
1	A	490	ASN
1	A	523	HIS
1	A	587	ASN
1	B	112	HIS
1	B	321	ASN
1	B	355	GLN
1	B	424	GLN
1	B	529	HIS
1	C	102	HIS
1	C	112	HIS

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Mol	Chain	Res	Type
1	C	204	GLN
1	C	234	GLN
1	C	255	GLN
1	C	279	GLN
1	C	408	GLN
1	C	479	ASN
1	C	484	ASN
1	C	490	ASN
1	C	523	HIS
1	C	587	ASN
1	D	175	GLN
1	D	424	GLN
1	D	587	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	$\# Z  > 2$
6	EDO	A	1102	-	3,3,3	0.46	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	D	703	1	14,14,15	0.68	0	17,19,21	1.29	2 (11%)
5	SO4	C	1001	-	4,4,4	0.50	0	6,6,6	0.15	0
4	DGJ	D	900	-	11,11,11	1.20	1 (9%)	13,15,15	3.10	6 (46%)
2	NAG	B	702	1	14,14,15	0.71	0	17,19,21	1.18	0
5	SO4	B	1001	-	4,4,4	0.42	0	6,6,6	0.15	0
2	NAG	C	702	1	14,14,15	0.61	0	17,19,21	1.35	2 (11%)
2	NAG	C	704	1	14,14,15	0.45	0	17,19,21	0.96	0
5	SO4	C	1002	-	4,4,4	0.46	0	6,6,6	0.18	0
5	SO4	A	1001	-	4,4,4	0.46	0	6,6,6	0.24	0
5	SO4	A	1002	-	4,4,4	0.60	0	6,6,6	0.26	0
6	EDO	D	1101	-	3,3,3	0.34	0	2,2,2	0.83	0
6	EDO	A	1101	-	3,3,3	0.32	0	2,2,2	1.35	0
2	NAG	C	703	1	14,14,15	0.42	0	17,19,21	1.48	3 (17%)
2	NAG	A	703	1	14,14,15	0.64	0	17,19,21	2.17	4 (23%)
5	SO4	D	1001	-	4,4,4	0.46	0	6,6,6	0.17	0
6	EDO	D	1102	-	3,3,3	0.67	0	2,2,2	0.30	0
5	SO4	D	1002	-	4,4,4	0.45	0	6,6,6	0.24	0
2	NAG	A	704	1	14,14,15	0.53	0	17,19,21	1.16	1 (5%)
2	NAG	B	703	1	14,14,15	0.74	0	17,19,21	2.44	9 (52%)
2	NAG	D	701	1	14,14,15	0.47	0	17,19,21	1.23	2 (11%)
5	SO4	B	1002	-	4,4,4	0.60	0	6,6,6	0.55	0
2	NAG	A	701	1	14,14,15	0.71	0	17,19,21	2.10	6 (35%)
4	DGJ	A	900	-	11,11,11	1.28	2 (18%)	13,15,15	2.81	6 (46%)
6	EDO	C	1102	-	3,3,3	0.95	0	2,2,2	0.19	0
6	EDO	B	1101	-	3,3,3	0.61	0	2,2,2	0.78	0
2	NAG	D	702	1	14,14,15	0.75	0	17,19,21	1.26	2 (11%)
6	EDO	C	1101	-	3,3,3	0.25	0	2,2,2	0.99	0
4	DGJ	C	900	-	11,11,11	1.67	3 (27%)	13,15,15	2.01	7 (53%)
4	DGJ	B	900	-	11,11,11	1.78	3 (27%)	13,15,15	2.64	5 (38%)
2	NAG	B	701	1	14,14,15	0.74	0	17,19,21	1.97	6 (35%)
2	NAG	C	701	1	14,14,15	0.60	0	17,19,21	1.27	2 (11%)
6	EDO	B	1102	-	3,3,3	0.64	0	2,2,2	1.20	0
2	NAG	B	704	1	14,14,15	0.50	0	17,19,21	1.17	2 (11%)
2	NAG	A	702	1	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	D	704	1	14,14,15	0.46	0	17,19,21	1.38	2 (11%)

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
6	EDO	A	1102	-	-	0/1/1/1	-
2	NAG	D	703	1	-	2/6/23/26	0/1/1/1
4	DGJ	D	900	-	-	0/2/19/19	0/1/1/1
2	NAG	B	702	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	704	1	-	0/6/23/26	0/1/1/1
6	EDO	D	1101	-	-	1/1/1/1	-
6	EDO	A	1101	-	-	0/1/1/1	-
2	NAG	C	703	1	-	2/6/23/26	0/1/1/1
2	NAG	A	703	1	-	1/6/23/26	0/1/1/1
6	EDO	D	1102	-	-	0/1/1/1	-
2	NAG	A	704	1	-	0/6/23/26	0/1/1/1
2	NAG	B	703	1	-	0/6/23/26	0/1/1/1
2	NAG	D	701	1	-	2/6/23/26	0/1/1/1
2	NAG	A	701	1	-	2/6/23/26	0/1/1/1
4	DGJ	A	900	-	-	0/2/19/19	0/1/1/1
6	EDO	C	1102	-	-	0/1/1/1	-
6	EDO	B	1101	-	-	1/1/1/1	-
2	NAG	D	702	1	-	0/6/23/26	0/1/1/1
6	EDO	C	1101	-	-	0/1/1/1	-
4	DGJ	C	900	-	-	0/2/19/19	0/1/1/1
4	DGJ	B	900	-	-	0/2/19/19	0/1/1/1
2	NAG	B	701	1	-	0/6/23/26	0/1/1/1
2	NAG	C	701	1	-	1/6/23/26	0/1/1/1
6	EDO	B	1102	-	-	1/1/1/1	-
2	NAG	B	704	1	-	0/6/23/26	0/1/1/1
2	NAG	A	702	1	-	1/6/23/26	0/1/1/1
2	NAG	D	704	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	DGJ	C1-C2	3.73	1.55	1.52
4	C	900	DGJ	C1-C2	3.22	1.55	1.52
4	C	900	DGJ	C4-C3	-2.97	1.44	1.52
4	C	900	DGJ	C5-N5	2.92	1.51	1.47
4	D	900	DGJ	C1-C2	2.65	1.54	1.52
4	B	900	DGJ	C5-N5	2.55	1.51	1.47
4	B	900	DGJ	C4-C3	-2.19	1.46	1.52
4	A	900	DGJ	C2-C3	2.13	1.55	1.52
4	A	900	DGJ	C1-C2	2.03	1.54	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	DGJ	C4-C5-N5	-5.99	97.04	109.12
4	D	900	DGJ	C4-C5-N5	-5.94	97.16	109.12
2	B	703	NAG	C1-O5-C5	5.82	119.99	112.19
2	A	703	NAG	C1-O5-C5	5.20	119.15	112.19
4	D	900	DGJ	C2-C3-C4	-5.18	101.75	110.86
4	A	900	DGJ	O4-C4-C3	5.13	122.47	110.38
2	A	701	NAG	C1-C2-N2	-5.11	102.38	110.43
2	A	703	NAG	C2-N2-C7	-4.71	116.58	122.90
4	D	900	DGJ	C3-C4-C5	4.63	117.80	111.02
4	B	900	DGJ	C4-C5-N5	-4.46	100.13	109.12
4	B	900	DGJ	C1-C2-C3	4.45	115.69	110.25
4	B	900	DGJ	O4-C4-C3	4.13	120.11	110.38
2	B	703	NAG	C4-C3-C2	-4.11	105.00	111.02
4	A	900	DGJ	C2-C3-C4	-4.09	103.66	110.86
2	C	702	NAG	C1-O5-C5	4.04	117.60	112.19
2	B	701	NAG	O4-C4-C3	-3.85	101.31	110.38
2	D	702	NAG	C4-C3-C2	3.81	116.60	111.02
4	B	900	DGJ	C2-C3-C4	-3.72	104.31	110.86
4	D	900	DGJ	O4-C4-C5	3.67	117.02	109.40
4	D	900	DGJ	O4-C4-C3	3.61	118.90	110.38
2	B	703	NAG	C2-N2-C7	-3.60	118.08	122.90
4	C	900	DGJ	C2-C3-C4	-3.56	104.61	110.86
2	D	704	NAG	O7-C7-C8	-3.36	116.08	122.05
2	A	703	NAG	O5-C1-C2	-3.27	106.23	111.29
2	C	703	NAG	C2-N2-C7	3.26	127.28	122.90
2	A	701	NAG	O4-C4-C5	-3.23	101.38	109.32
2	B	701	NAG	C4-C3-C2	-3.16	106.39	111.02
2	C	703	NAG	O5-C5-C6	3.04	113.57	107.66
2	A	701	NAG	O5-C1-C2	-2.97	106.70	111.29
4	C	900	DGJ	O4-C4-C3	2.91	117.25	110.38
2	D	702	NAG	C1-O5-C5	2.82	115.97	112.19
4	D	900	DGJ	C6-C5-C4	2.82	122.17	112.03
2	D	703	NAG	C2-N2-C7	2.76	126.60	122.90
4	C	900	DGJ	C4-C5-N5	-2.66	103.76	109.12
4	A	900	DGJ	C1-C2-C3	2.65	113.48	110.25
2	B	701	NAG	O5-C1-C2	-2.60	107.27	111.29
2	A	704	NAG	C1-O5-C5	2.57	115.63	112.19
2	C	701	NAG	C1-O5-C5	2.52	115.57	112.19
4	C	900	DGJ	C6-C5-C4	2.49	120.98	112.03
2	B	703	NAG	C6-C5-C4	-2.45	107.01	113.02
2	B	703	NAG	O5-C5-C4	2.44	116.77	110.83
2	B	704	NAG	C3-C4-C5	2.40	114.59	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	703	NAG	C6-C5-C4	-2.40	107.12	113.02
2	C	701	NAG	C4-C3-C2	2.38	114.50	111.02
2	B	704	NAG	C1-O5-C5	2.36	115.34	112.19
2	B	703	NAG	C8-C7-N2	-2.36	112.21	116.12
2	C	702	NAG	C3-C4-C5	-2.32	106.02	110.23
4	B	900	DGJ	O4-C4-C5	2.32	114.22	109.40
2	D	701	NAG	C2-N2-C7	2.28	125.95	122.90
2	A	702	NAG	C1-O5-C5	2.24	115.19	112.19
2	B	701	NAG	C2-N2-C7	2.21	125.86	122.90
4	C	900	DGJ	O2-C2-C3	-2.21	105.58	110.15
2	B	701	NAG	O5-C5-C6	-2.20	103.38	107.66
2	B	703	NAG	O7-C7-N2	2.17	125.82	121.98
2	A	701	NAG	O4-C4-C3	-2.14	105.32	110.38
4	A	900	DGJ	C1-N5-C5	2.14	114.40	109.71
2	D	703	NAG	O5-C5-C6	2.14	111.82	107.66
4	C	900	DGJ	O4-C4-C5	2.13	113.82	109.40
2	A	701	NAG	O5-C5-C6	-2.12	103.53	107.66
2	B	701	NAG	C6-C5-C4	2.12	118.22	113.02
2	B	703	NAG	O5-C1-C2	-2.11	108.02	111.29
4	A	900	DGJ	O4-C4-C5	2.10	113.77	109.40
2	D	701	NAG	C1-O5-C5	2.08	114.98	112.19
2	A	703	NAG	O3-C3-C2	2.07	113.70	109.40
2	D	704	NAG	C8-C7-N2	2.04	119.50	116.12
2	B	703	NAG	O3-C3-C2	2.04	113.64	109.40
4	C	900	DGJ	C1-N5-C5	2.03	114.18	109.71
2	A	701	NAG	C8-C7-N2	-2.02	112.77	116.12

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	703	NAG	O5-C5-C6-O6
2	C	703	NAG	O5-C5-C6-O6
2	D	703	NAG	C4-C5-C6-O6
6	B	1102	EDO	O1-C1-C2-O2
2	C	703	NAG	C4-C5-C6-O6
6	D	1101	EDO	O1-C1-C2-O2
2	A	701	NAG	C4-C5-C6-O6
2	A	701	NAG	O5-C5-C6-O6
6	B	1101	EDO	O1-C1-C2-O2
2	D	701	NAG	C4-C5-C6-O6
2	D	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	702	NAG	C1-C2-N2-C7
2	A	703	NAG	C1-C2-N2-C7
2	C	701	NAG	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1102	EDO	1	0
4	D	900	DGJ	1	0
2	C	702	NAG	1	0
5	A	1002	SO4	1	0
6	D	1101	EDO	5	0
6	A	1101	EDO	3	0
2	B	703	NAG	3	0
5	B	1002	SO4	1	0
6	B	1101	EDO	1	0
6	C	1101	EDO	2	0
6	B	1102	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	605/654 (92%)	-1.43	0 100 100	5, 16, 31, 69	8 (1%)
1	B	605/654 (92%)	-1.46	0 100 100	4, 15, 29, 62	5 (0%)
1	C	602/654 (92%)	-1.38	0 100 100	6, 18, 39, 61	9 (1%)
1	D	602/654 (92%)	-1.37	0 100 100	5, 19, 43, 73	9 (1%)
All	All	2414/2616 (92%)	-1.41	0 100 100	4, 17, 38, 73	31 (1%)

There are no RSRZ outliers to report.

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	C	701	14/15	0.96	0.06	51,58,62,64	0
2	NAG	D	703	14/15	0.96	0.07	55,62,64,66	0
2	NAG	C	703	14/15	0.98	0.04	23,25,29,32	0
2	NAG	D	701	14/15	0.98	0.04	52,59,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	704	14/15	0.98	0.04	31,37,42,44	0
5	SO4	A	1001	5/5	0.98	0.05	55,57,57,61	0
5	SO4	D	1001	5/5	0.98	0.04	62,63,64,65	0
6	EDO	A	1101	4/4	0.98	0.05	16,16,21,24	0
6	EDO	C	1101	4/4	0.98	0.04	16,20,23,26	0
6	EDO	D	1101	4/4	0.98	0.04	12,15,16,20	0
2	NAG	C	704	14/15	0.99	0.02	10,11,15,16	0
2	NAG	A	701	14/15	0.99	0.03	6,9,15,17	0
2	NAG	D	702	14/15	0.99	0.03	24,26,29,32	0
2	NAG	B	701	14/15	0.99	0.03	5,8,16,17	0
2	NAG	D	704	14/15	0.99	0.03	11,15,17,19	0
4	DGJ	B	900	11/11	0.99	0.02	2,2,4,4	0
2	NAG	B	703	14/15	0.99	0.03	20,24,34,34	0
5	SO4	A	1002	5/5	0.99	0.05	30,35,37,40	0
5	SO4	B	1001	5/5	0.99	0.03	55,55,56,57	0
5	SO4	C	1001	5/5	0.99	0.03	52,52,53,56	0
5	SO4	C	1002	5/5	0.99	0.06	28,32,35,36	0
2	NAG	B	704	14/15	0.99	0.03	28,34,40,43	0
2	NAG	A	702	14/15	0.99	0.02	11,15,19,19	0
6	EDO	A	1102	4/4	0.99	0.03	7,10,11,15	0
6	EDO	B	1101	4/4	0.99	0.05	17,17,22,27	0
6	EDO	B	1102	4/4	0.99	0.03	9,16,16,21	0
2	NAG	C	702	14/15	0.99	0.03	25,29,31,33	0
2	NAG	A	703	14/15	0.99	0.03	19,23,32,36	0
6	EDO	D	1102	4/4	0.99	0.03	10,13,13,18	0
4	DGJ	A	900	11/11	1.00	0.02	2,3,4,5	0
2	NAG	B	702	14/15	1.00	0.02	11,13,16,16	0
5	SO4	D	1002	5/5	1.00	0.05	30,32,34,37	0
4	DGJ	C	900	11/11	1.00	0.02	4,5,5,7	0
4	DGJ	D	900	11/11	1.00	0.02	2,5,6,6	0
3	CL	A	801	1/1	1.00	0.03	7,7,7,7	0
3	CL	B	801	1/1	1.00	0.02	5,5,5,5	0
3	CL	C	801	1/1	1.00	0.02	6,6,6,6	0
6	EDO	C	1102	4/4	1.00	0.02	9,12,17,21	0
5	SO4	B	1002	5/5	1.00	0.04	32,32,37,41	0
3	CL	D	801	1/1	1.00	0.02	6,6,6,6	0

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

There are no such residues in this entry.