



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:17 PM GMT

PDB ID : 3THC  
Title : Crystal structure of human beta-galactosidase in complex with galactose  
Authors : Ohto, U.; Shimizu, T.  
Deposited on : 2011-08-18  
Resolution : 1.80 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

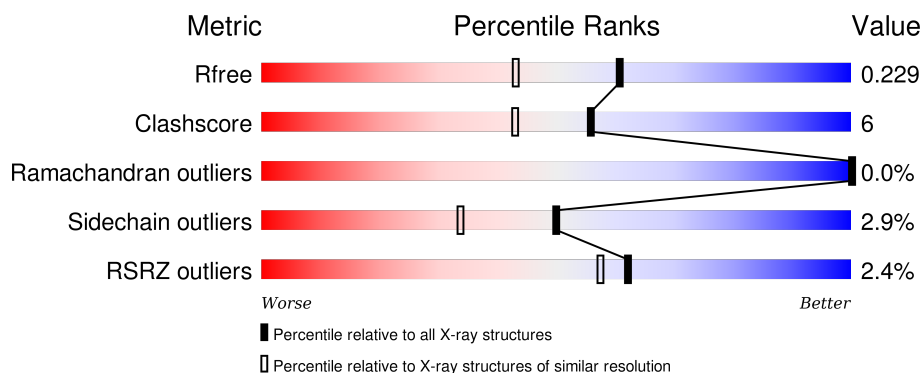
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 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	654	 2% 78% 12% • 7%
1	B	654	 2% 82% 10% 7%
1	C	654	 2% 79% 12% • 8%
1	D	654	 3% 82% 9% • 8%

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	702	-	-	-	X
2	NAG	C	704	-	-	-	X
2	NAG	D	702	-	-	-	X
2	NAG	D	703	-	-	-	X
2	NAG	D	704	-	-	-	X
5	SO4	A	1002	-	-	-	X
6	EDO	A	1101	-	-	-	X
6	EDO	C	1101	-	-	-	X
6	EDO	D	1101	-	-	X	-

## 2 Entry composition [i](#)

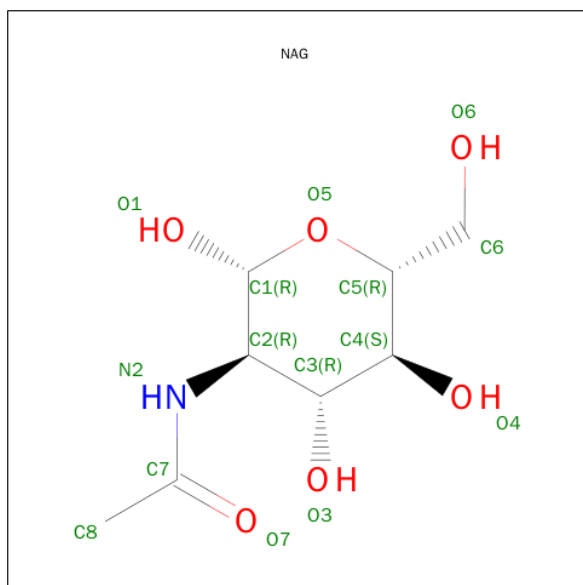
There are 7 unique types of molecules in this entry. The entry contains 22058 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	10	0
			4891	3170	805	898	18			
1	B	605	Total	C	N	O	S	0	5	0
			4850	3146	800	887	17			
1	C	602	Total	C	N	O	S	0	9	0
			4861	3153	798	893	17			
1	D	602	Total	C	N	O	S	0	10	0
			4866	3158	799	891	18			

- 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		

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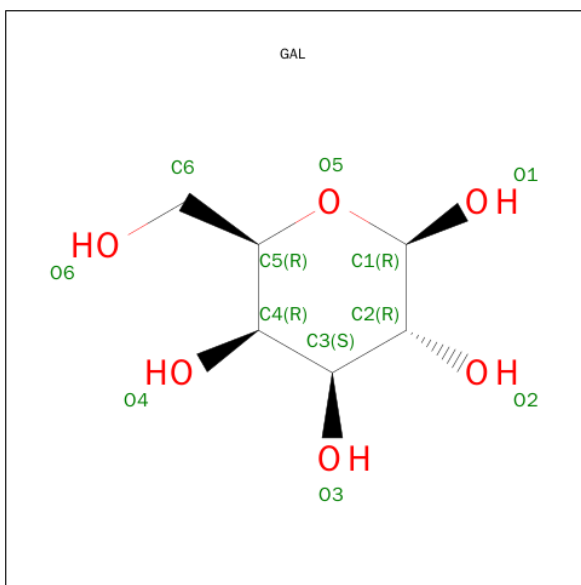
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			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 (three-letter code: CL) (formula: Cl).

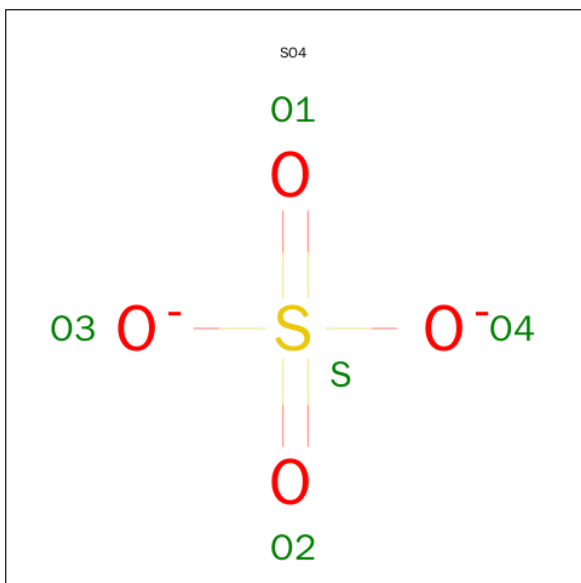
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



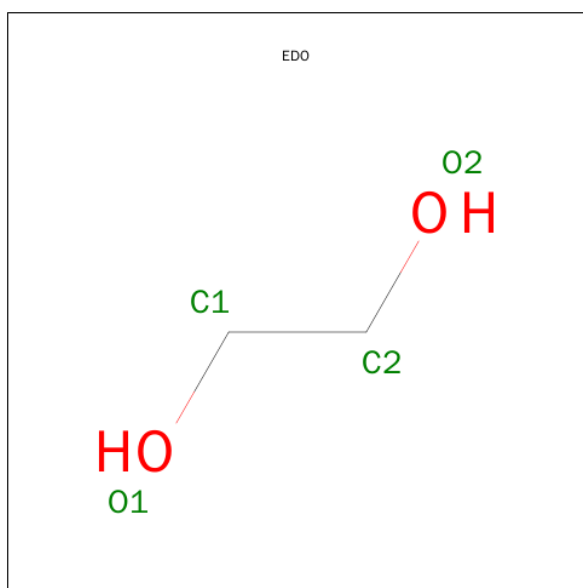
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	D	1	Total	C	O	0	0
			12	6	6		

- 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 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 (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

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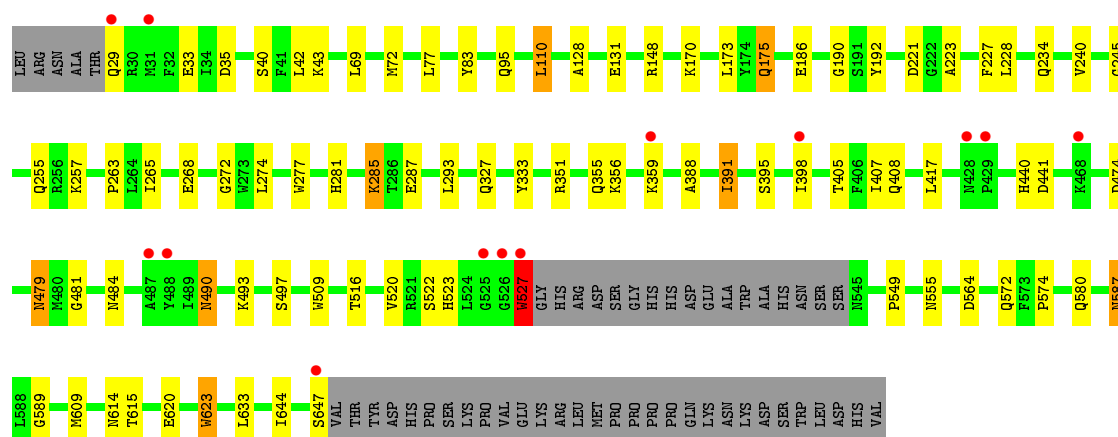
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0

- Molecule 7 is water.

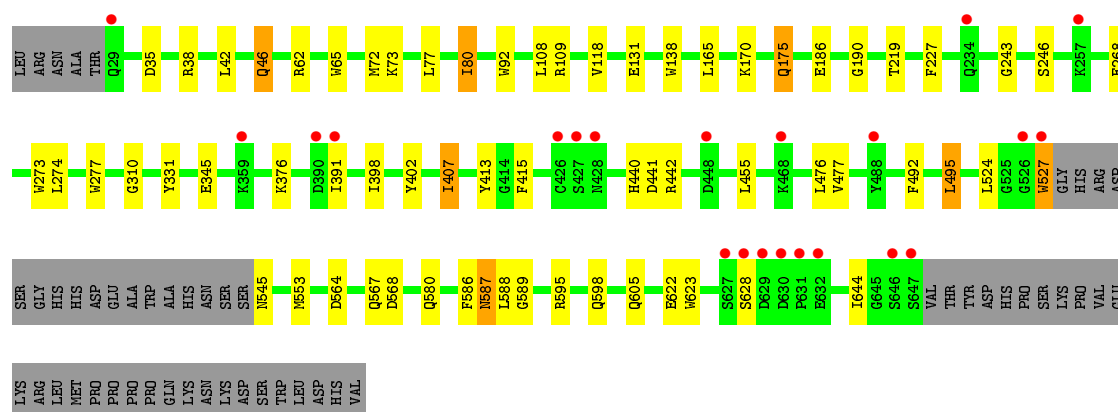
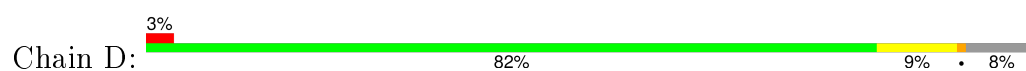
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	579	Total 579	O 579	0	0
7	B	617	Total 617	O 617	0	0
7	C	540	Total 540	O 540	0	0
7	D	506	Total 506	O 506	0	0







• Molecule 1: Beta-galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.80Å 116.10Å 140.33Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	28.88 – 1.80 28.88 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (28.88-1.80) 94.2 (28.88-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.190 , 0.228 0.192 , 0.229	Depositor DCC
$R_{free}$ test set	13357 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.2	EDS
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 264185 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, GAL, EDO, NAG, 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	0.69	4/5042 (0.1%)	0.72	1/6879 (0.0%)
1	B	0.70	2/5001 (0.0%)	0.70	0/6823
1	C	0.67	4/5011 (0.1%)	0.69	0/6838
1	D	0.67	6/5016 (0.1%)	0.68	1/6844 (0.0%)
All	All	0.68	16/20070 (0.1%)	0.70	2/27384 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	277	TRP	CD2-CE2	5.84	1.48	1.41
1	C	527	TRP	CD2-CE2	5.61	1.48	1.41
1	A	576	TRP	CD2-CE2	5.47	1.48	1.41
1	D	527	TRP	CD2-CE2	5.36	1.47	1.41
1	D	273	TRP	CD2-CE2	5.33	1.47	1.41
1	B	576	TRP	CD2-CE2	5.33	1.47	1.41
1	A	138	TRP	CD2-CE2	5.28	1.47	1.41
1	D	623	TRP	CD2-CE2	5.16	1.47	1.41
1	D	138	TRP	CD2-CE2	5.12	1.47	1.41
1	D	92	TRP	CD2-CE2	5.11	1.47	1.41
1	B	92	TRP	CD2-CE2	5.10	1.47	1.41
1	C	509	TRP	CD2-CE2	5.09	1.47	1.41
1	A	509	TRP	CD2-CE2	5.05	1.47	1.41
1	A	527	TRP	CD2-CE2	5.05	1.47	1.41
1	C	623	TRP	CD2-CE2	5.04	1.47	1.41
1	C	277	TRP	CD2-CE2	5.04	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	VAL	CB-CA-C	-6.58	98.89	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	568	ASP	CB-CG-OD1	5.01	122.81	118.30

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	4891	0	4739	76	0
1	B	4850	0	4710	44	0
1	C	4861	0	4713	66	0
1	D	4866	0	4730	50	0
2	A	56	0	52	0	0
2	B	56	0	52	2	0
2	C	56	0	52	1	0
2	D	56	0	52	1	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	12	0	12	1	0
4	B	12	0	12	1	0
4	C	12	0	12	1	0
4	D	12	0	12	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	3	0
6	B	8	0	12	2	0
6	C	8	0	12	1	0
6	D	8	0	12	4	0
7	A	579	0	0	24	0
7	B	617	0	0	20	0
7	C	540	0	0	21	0
7	D	506	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22058	0	19196	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:B:572[B]:GLN:HG3	7:B:1359:HOH:O	1.42	1.17
1:C:228:LEU:HD11	7:C:1632:HOH:O	1.50	1.11
1:A:409[A]:VAL:CG1	1:A:513:PRO:HG3	1.81	1.11
1:B:29:GLN:HG3	1:B:30:ARG:H	1.04	1.10
1:A:555:ASN:HB2	7:A:1310:HOH:O	1.57	1.03
1:C:609:MET:SD	7:C:1361:HOH:O	2.16	1.02
1:A:409[A]:VAL:HG12	1:A:513:PRO:HG3	1.41	1.02
1:A:234:GLN:HG3	7:A:2198:HOH:O	1.68	0.94
1:B:599:LEU:C	7:B:1359:HOH:O	2.08	0.92
1:B:29:GLN:HG3	1:B:30:ARG:N	1.85	0.91
1:A:500:THR:HG21	7:A:754:HOH:O	1.71	0.91
1:C:359:LYS:HG3	7:C:2132:HOH:O	1.70	0.90
1:D:407:ILE:H	1:D:407:ILE:HD12	1.38	0.88
1:A:437:ASN:HD21	1:A:458:ASN:H	1.20	0.88
1:D:407:ILE:HD11	1:D:492:PHE:O	1.74	0.87
1:A:580:GLN:HE21	1:A:587:ASN:HD21	1.22	0.85
1:B:29:GLN:CG	1:B:30:ARG:H	1.90	0.85
1:D:246:SER:OG	6:D:1101:EDO:H12	1.75	0.85
1:D:407:ILE:N	1:D:407:ILE:HD12	1.93	0.83
1:B:130:TRP:HB3	7:B:1594:HOH:O	1.76	0.83
1:A:500:THR:HG23	7:A:705:HOH:O	1.79	0.83
1:C:523:HIS:HD2	1:C:527:TRP:CE2	1.97	0.82
2:B:703:NAG:H83	7:D:1647:HOH:O	1.81	0.81
1:A:399:LYS:HE2	7:A:1509:HOH:O	1.81	0.80
1:D:407:ILE:CD1	1:D:407:ILE:H	1.95	0.79
1:B:555:ASN:HB2	7:B:1500:HOH:O	1.83	0.79
1:C:405:THR:H	1:C:408:GLN:HE21	1.29	0.77
1:A:318:ASN:HD21	1:A:590:ARG:HH21	1.33	0.76
1:A:258:CYS:SG	7:A:2312:HOH:O	2.42	0.76
7:C:1356:HOH:O	1:D:46:GLN:HB2	1.85	0.76
1:C:580:GLN:HE21	1:C:587:ASN:HD21	1.33	0.76
1:A:327:GLN:HE22	1:A:484:ASN:HD21	1.33	0.76
1:A:409[A]:VAL:HG11	1:A:513:PRO:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:GLN:HE22	1:C:484:ASN:HD21	1.34	0.75
1:D:243:GLY:H	6:D:1101:EDO:H11	1.52	0.75
1:B:243:GLY:H	6:B:1101:EDO:H22	1.50	0.75
1:A:490:ASN:ND2	7:A:2056:HOH:O	2.20	0.74
1:A:611:SER:HA	7:A:2125:HOH:O	1.85	0.74
1:B:599:LEU:O	7:B:1359:HOH:O	2.06	0.73
1:C:245:GLY:H	6:C:1101:EDO:H22	1.54	0.72
1:D:407:ILE:CD1	1:D:492:PHE:O	2.37	0.71
1:C:523:HIS:CD2	1:C:527:TRP:CE2	2.79	0.71
5:B:1002:SO4:O3	7:B:871:HOH:O	2.10	0.70
1:D:564:ASP:HB2	7:D:679:HOH:O	1.90	0.70
1:A:479:ASN:ND2	1:A:481:GLY:H	1.90	0.70
1:B:555:ASN:CB	7:B:1500:HOH:O	2.38	0.70
1:C:490:ASN:H	1:C:490:ASN:HD22	1.41	0.68
1:A:489:ILE:HG13	7:A:2074:HOH:O	1.91	0.68
1:A:398:ILE:HG21	1:A:409[B]:VAL:HG12	1.75	0.68
1:D:580:GLN:HE21	1:D:587:ASN:HD21	1.41	0.67
1:D:553:MET:CE	7:D:1138:HOH:O	2.43	0.67
1:A:160:LYS:HD3	7:A:1947:HOH:O	1.95	0.66
1:B:95:GLN:HB2	7:B:1749:HOH:O	1.94	0.66
1:A:409[A]:VAL:O	1:A:409[A]:VAL:HG12	1.95	0.65
1:C:479:ASN:ND2	1:C:481:GLY:H	1.93	0.65
5:A:1002:SO4:O1	7:A:2085:HOH:O	2.15	0.64
1:A:268:GLU:OE1	4:A:900:GAL:H1	1.97	0.64
1:A:245:GLY:HA3	7:A:1560:HOH:O	1.99	0.63
1:C:523:HIS:CE1	1:C:615:THR:HG21	2.33	0.63
1:D:175:GLN:CG	7:D:2050:HOH:O	2.47	0.63
1:C:479:ASN:ND2	1:C:493:LYS:HE3	2.15	0.62
1:B:168:LYS:HE3	7:B:2042:HOH:O	2.00	0.61
1:A:500:THR:CG2	7:A:705:HOH:O	2.43	0.61
2:B:703:NAG:C8	7:D:1647:HOH:O	2.42	0.61
1:C:523:HIS:HD2	1:C:527:TRP:CD2	2.18	0.61
1:C:255:GLN:HE22	1:C:265:ILE:H	1.47	0.61
1:C:268:GLU:OE1	4:C:900:GAL:H1	2.00	0.61
1:C:223:ALA:HA	7:C:1632:HOH:O	2.01	0.60
1:C:405:THR:H	1:C:408:GLN:NE2	1.99	0.59
1:C:490:ASN:ND2	7:C:1292:HOH:O	2.34	0.59
1:A:80:ILE:HD11	1:A:118:VAL:HG22	1.83	0.59
1:B:529:HIS:HE1	7:B:1587:HOH:O	1.85	0.59
1:B:160:LYS:NZ	7:B:2131:HOH:O	2.35	0.59
1:B:268:GLU:OE1	4:B:900:GAL:H1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:LYS:HE3	7:D:2064:HOH:O	2.02	0.58
1:A:382:LEU:HD23	1:A:524:LEU:HD12	1.86	0.58
1:C:391:ILE:HG13	7:C:1544:HOH:O	2.02	0.58
1:C:234:GLN:NE2	7:C:1044:HOH:O	2.37	0.57
1:A:318:ASN:HD21	1:A:590:ARG:NH2	2.02	0.57
1:A:92:TRP:NE1	7:A:1876:HOH:O	2.30	0.57
1:C:522:SER:HA	1:C:527:TRP:HB2	1.87	0.57
1:C:623:TRP:HZ3	7:C:2084:HOH:O	1.87	0.57
1:B:383:LYS:HG2	1:B:387:ALA:HB3	1.85	0.57
1:D:442:ARG:NH1	1:D:622:GLU:OE2	2.26	0.56
1:D:268:GLU:OE1	4:D:900:GAL:H1	2.05	0.56
1:A:297:LEU:HD12	1:A:353:ILE:HD11	1.87	0.56
1:A:293:LEU:HG	1:A:353:ILE:HD11	1.87	0.56
1:C:490:ASN:N	1:C:490:ASN:HD22	2.01	0.55
1:A:490:ASN:H	1:A:490:ASN:HD22	1.54	0.55
1:A:261:LYS:HE3	7:A:2238:HOH:O	2.06	0.55
1:D:73:LYS:NZ	7:D:1545:HOH:O	2.39	0.55
1:D:175:GLN:HG2	7:D:2050:HOH:O	2.07	0.55
1:C:234:GLN:HG3	7:C:1477:HOH:O	2.06	0.55
1:A:580:GLN:HE21	1:A:587:ASN:ND2	2.01	0.55
1:D:243:GLY:N	6:D:1101:EDO:H11	2.20	0.54
1:C:43:LYS:HE3	7:C:1312:HOH:O	2.06	0.54
1:C:523:HIS:CD2	1:C:527:TRP:CZ2	2.95	0.54
1:A:91:PRO:O	7:A:959:HOH:O	2.19	0.54
1:D:243:GLY:H	6:D:1101:EDO:C1	2.21	0.53
1:B:91:PRO:O	7:B:1296:HOH:O	2.19	0.53
1:C:572[A]:GLN:HG2	1:C:574:PRO:HD3	1.91	0.53
1:C:175[A]:GLN:NE2	7:C:1067:HOH:O	2.37	0.52
1:A:479:ASN:HD22	1:A:481:GLY:H	1.58	0.52
1:A:318:ASN:ND2	1:A:590:ARG:HH21	2.04	0.52
1:A:89:HIS:CE1	1:A:104:VAL:HG22	2.45	0.51
1:C:72:MET:HB3	1:C:77:LEU:HD12	1.91	0.51
1:B:623:TRP:HZ3	7:B:1652:HOH:O	1.93	0.51
1:A:389:LEU:HD21	1:A:417:LEU:HD23	1.91	0.51
1:A:95:GLN:HB2	7:A:1892:HOH:O	2.09	0.51
1:B:40:SER:HA	1:B:263:PRO:HB3	1.91	0.51
1:D:131:GLU:HG2	1:D:413:TYR:CE2	2.45	0.51
1:D:175:GLN:NE2	1:D:175:GLN:H	2.09	0.51
1:C:407[A]:ILE:HD12	7:C:817:HOH:O	2.11	0.50
1:D:391:ILE:HD13	1:D:524:LEU:O	2.11	0.50
1:C:479:ASN:HD22	1:C:479:ASN:C	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:ASN:HB2	7:D:2022:HOH:O	2.12	0.50
1:D:586[B]:PHE:CE2	1:D:588:LEU:HD23	2.46	0.50
1:A:211:LEU:HB3	1:A:215:VAL:HG21	1.92	0.50
1:A:105:GLU:HB3	1:A:109:ARG:HH12	1.76	0.50
1:C:285:LYS:HE3	7:C:1157:HOH:O	2.12	0.49
1:D:310:GLY:HA3	1:D:331:TYR:O	2.12	0.49
1:A:245:GLY:H	6:A:1101:EDO:H11	1.77	0.49
1:A:479:ASN:C	1:A:479:ASN:HD22	2.15	0.49
1:C:388:ALA:HB1	1:C:391:ILE:HD12	1.95	0.49
1:C:287:GLU:HG3	7:C:764:HOH:O	2.13	0.49
1:B:83:TYR:CE2	1:B:128:ALA:HB2	2.48	0.49
1:B:190:GLY:HA3	1:B:227:PHE:O	2.13	0.48
1:A:112:HIS:HD2	7:A:1673:HOH:O	1.95	0.48
1:A:57:TYR:CZ	1:A:104:VAL:HG13	2.49	0.48
1:C:281:HIS:CE1	1:C:644:ILE:HD12	2.49	0.48
1:A:587:ASN:HD22	1:A:589:GLY:H	1.59	0.48
1:D:628:SER:HB3	7:D:1185:HOH:O	2.13	0.48
1:D:587:ASN:HD22	1:D:587:ASN:C	2.16	0.48
1:B:229:LYS:HE2	7:B:2114:HOH:O	2.14	0.48
1:B:108:LEU:HD22	1:B:118:VAL:HG11	1.96	0.48
6:A:1101:EDO:H12	7:A:1347:HOH:O	2.13	0.47
1:A:433:SER:HB3	1:A:500:THR:HG22	1.97	0.47
1:A:147:LEU:HD12	7:A:2074:HOH:O	2.14	0.47
1:C:173:LEU:HB3	1:C:175[A]:GLN:HE21	1.80	0.47
1:A:587:ASN:HD22	1:A:587:ASN:C	2.18	0.47
1:C:257:LYS:HD3	7:C:865:HOH:O	2.14	0.47
1:A:555:ASN:HA	1:A:614:ASN:O	2.15	0.46
1:C:479:ASN:ND2	1:C:479:ASN:C	2.68	0.46
1:D:131:GLU:HG2	1:D:413:TYR:HE2	1.81	0.46
1:D:477:VAL:HG21	1:D:495:LEU:HD13	1.96	0.46
1:D:440:HIS:HA	1:D:441:ASP:HA	1.77	0.46
1:A:80:ILE:CD1	1:A:118:VAL:HG22	2.46	0.46
1:A:245:GLY:H	6:A:1101:EDO:C1	2.28	0.46
1:C:391:ILE:HG13	1:C:391:ILE:H	1.61	0.46
1:B:598:GLN:HA	1:B:644:ILE:HA	1.98	0.46
1:A:437:ASN:ND2	1:A:458:ASN:H	2.01	0.45
1:A:294:TYR:HA	1:A:353:ILE:HD13	1.98	0.45
1:C:497:SER:HA	2:C:702:NAG:H81	1.98	0.45
1:D:38:ARG:HB2	7:D:1462:HOH:O	2.14	0.45
1:D:80[A]:ILE:HD11	1:D:118:VAL:HG22	1.98	0.45
1:C:190:GLY:HA3	1:C:227:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:ASN:C	1:C:587:ASN:HD22	2.20	0.45
1:A:175:GLN:NE2	7:A:788:HOH:O	2.47	0.45
1:C:356:LYS:HE2	7:C:2228:HOH:O	2.16	0.45
1:D:175:GLN:HG3	7:D:2050:HOH:O	2.15	0.45
1:A:409[A]:VAL:O	1:A:409[A]:VAL:CG1	2.64	0.45
1:C:351:ARG:O	1:C:355:GLN:HG3	2.17	0.45
1:C:647:SER:C	7:C:2107:HOH:O	2.55	0.45
1:B:204:GLN:HE22	1:B:235:GLY:HA3	1.82	0.45
1:A:35:ASP:HB2	1:A:42:LEU:HG	1.98	0.45
1:D:345:GLU:HG3	7:D:1382:HOH:O	2.17	0.45
1:C:35:ASP:HB2	1:C:42:LEU:HG	1.99	0.44
1:C:95:GLN:HG2	7:C:2206:HOH:O	2.18	0.44
1:B:382:LEU:HD22	1:B:553:MET:HE2	1.99	0.44
1:B:321:ASN:ND2	1:B:327:GLN:HE21	2.16	0.44
1:C:564[A]:ASP:OD2	7:C:874:HOH:O	2.21	0.44
1:C:175[A]:GLN:H	1:C:175[A]:GLN:NE2	2.16	0.44
1:A:598:GLN:HA	1:A:644:ILE:HA	2.00	0.44
1:C:417:LEU:HD11	1:C:474:ASP:HB3	1.98	0.44
1:C:69:LEU:HD12	1:C:110:LEU:HD13	2.00	0.44
1:B:316:TYR:HB2	6:B:1102:EDO:H11	2.00	0.44
1:B:440:HIS:HA	1:B:441:ASP:HA	1.80	0.43
1:D:62:ARG:HA	1:D:65:TRP:CD2	2.53	0.43
1:C:587:ASN:HD22	1:C:589:GLY:H	1.67	0.43
1:A:479:ASN:ND2	1:A:479:ASN:C	2.71	0.43
1:A:564:ASP:O	1:A:567:GLN:HG3	2.18	0.43
1:D:219[A]:THR:HG21	7:D:687:HOH:O	2.18	0.43
1:C:148:ARG:HB2	1:C:192:TYR:CE1	2.54	0.43
1:A:83:TYR:CE2	1:A:128:ALA:HB2	2.53	0.43
1:A:398:ILE:HD13	7:A:2123:HOH:O	2.18	0.43
1:C:522:SER:CA	1:C:527:TRP:HB2	2.48	0.43
1:B:241:ASP:HB2	1:B:268:GLU:HB2	2.00	0.43
1:B:276:HIS:NE2	1:B:321:ASN:ND2	2.62	0.43
1:D:190:GLY:HA3	1:D:227:PHE:O	2.19	0.43
1:B:555:ASN:HA	1:B:614:ASN:O	2.19	0.43
1:B:581:VAL:HG13	1:B:588:LEU:HB2	2.00	0.43
1:C:440:HIS:HA	1:C:441:ASP:HA	1.71	0.42
1:B:488:TYR:HD1	7:B:1651:HOH:O	2.01	0.42
1:D:72:MET:HB3	1:D:77:LEU:HD12	2.01	0.42
1:A:346:LYS:O	1:A:350:LEU:HG	2.19	0.42
1:D:402:TYR:CZ	2:D:702:NAG:H5	2.54	0.42
1:D:586[B]:PHE:HE2	1:D:588:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219[A]:THR:HG23	7:D:741:HOH:O	2.18	0.42
1:C:516:THR:O	1:C:520:VAL:HG23	2.20	0.42
1:A:69:LEU:HD12	1:A:110:LEU:HD13	2.01	0.42
1:A:440:HIS:HA	1:A:441:ASP:HA	1.73	0.42
1:D:587:ASN:HD22	1:D:589:GLY:H	1.68	0.42
1:B:97:GLN:OE1	7:B:1763:HOH:O	2.22	0.42
1:C:272:GLY:HA3	1:C:333:TYR:O	2.19	0.42
1:D:219[A]:THR:CG2	7:D:687:HOH:O	2.68	0.42
1:B:582:TRP:HA	1:B:586[B]:PHE:O	2.20	0.42
1:C:83:TYR:CE2	1:C:128:ALA:HB2	2.55	0.42
1:C:228:LEU:CD1	7:C:1632:HOH:O	2.33	0.41
1:A:490:ASN:N	1:A:490:ASN:HD22	2.18	0.41
1:D:553:MET:HE3	7:D:1138:HOH:O	2.16	0.41
1:B:529:HIS:CE1	7:B:1587:HOH:O	2.68	0.41
1:C:221:ASP:O	1:C:240:VAL:HA	2.19	0.41
1:B:553:MET:HE3	7:B:1572:HOH:O	2.19	0.41
1:A:174:TYR:HA	1:A:178:GLY:O	2.20	0.41
1:A:553:MET:HE2	1:A:617:THR:HG23	2.02	0.41
1:C:549:PRO:HA	1:C:620:GLU:O	2.20	0.41
1:B:457:ARG:O	1:B:458:ASN:HB2	2.21	0.41
1:A:406:PHE:HB3	1:A:411:GLN:O	2.20	0.41
1:A:310:GLY:HA3	1:A:331:TYR:O	2.20	0.41
1:A:160:LYS:HE2	7:A:2119:HOH:O	2.19	0.41
1:B:310:GLY:HA3	1:B:331:TYR:O	2.21	0.41
1:A:57:TYR:CE2	1:A:104:VAL:HG13	2.55	0.41
1:A:190:GLY:HA3	1:A:227:PHE:O	2.21	0.41
1:D:109:ARG:NH2	7:D:1647:HOH:O	2.54	0.41
1:B:555:ASN:HB3	7:B:1500:HOH:O	2.15	0.41
1:D:108:LEU:HD22	1:D:118:VAL:HG11	2.03	0.41
1:A:502:SER:O	1:A:503:SER:HB2	2.21	0.41
1:A:401:LEU:HD12	1:A:507:THR:HB	2.03	0.41
1:B:272:GLY:HA3	1:B:333:TYR:O	2.20	0.41
1:B:447:VAL:HG23	1:B:452:GLN:HG3	2.03	0.41
1:B:205:LYS:HG2	7:B:1388:HOH:O	2.21	0.41
1:D:415:PHE:HB3	1:D:476:LEU:HD11	2.03	0.41
1:A:360:VAL:HG13	1:A:361:PRO:HD2	2.03	0.41
1:A:611:SER:CB	7:A:1931:HOH:O	2.69	0.40
1:C:40:SER:HA	1:C:263:PRO:HB3	2.03	0.40
1:D:564:ASP:O	1:D:567:GLN:HG3	2.21	0.40
1:C:479:ASN:HD22	1:C:481:GLY:H	1.65	0.40
1:D:35:ASP:HB2	1:D:42:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:ASN:HA	1:C:614:ASN:O	2.22	0.40
1:C:572[B]:GLN:HG3	1:C:574:PRO:HD3	2.03	0.40
1:D:598:GLN:HA	1:D:644:ILE:HA	2.04	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	611/654 (93%)	593 (97%)	17 (3%)	1 (0%)	52	35
1	B	606/654 (93%)	587 (97%)	19 (3%)	0	100	100
1	C	607/654 (93%)	587 (97%)	20 (3%)	0	100	100
1	D	608/654 (93%)	591 (97%)	17 (3%)	0	100	100
All	All	2432/2616 (93%)	2358 (97%)	73 (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	528/563 (94%)	511 (97%)	17 (3%)	46	29
1	B	523/563 (93%)	512 (98%)	11 (2%)	61	47
1	C	525/563 (93%)	505 (96%)	20 (4%)	40	22
1	D	526/563 (93%)	510 (97%)	16 (3%)	48	31
All	All	2102/2252 (93%)	2038 (97%)	64 (3%)	50	31

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	80	ILE
1	A	104	VAL
1	A	110	LEU
1	A	131	GLU
1	A	175	GLN
1	A	186	GLU
1	A	274	LEU
1	A	345	GLU
1	A	353	ILE
1	A	398	ILE
1	A	479	ASN
1	A	490	ASN
1	A	500	THR
1	A	587	ASN
1	A	605	GLN
1	A	633	LEU
1	B	110	LEU
1	B	131	GLU
1	B	170	LYS
1	B	186	GLU
1	B	234	GLN
1	B	274	LEU
1	B	293	LEU
1	B	358	GLU
1	B	398	ILE
1	B	553	MET
1	B	605	GLN
1	C	29	GLN
1	C	33	GLU
1	C	110	LEU
1	C	131[A]	GLU
1	C	131[B]	GLU

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Mol	Chain	Res	Type
1	C	170	LYS
1	C	175[A]	GLN
1	C	175[B]	GLN
1	C	186	GLU
1	C	274	LEU
1	C	285	LYS
1	C	293	LEU
1	C	391	ILE
1	C	395	SER
1	C	398	ILE
1	C	479	ASN
1	C	490	ASN
1	C	527	TRP
1	C	587	ASN
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	186	GLU
1	D	274	LEU
1	D	398	ILE
1	D	407	ILE
1	D	455	LEU
1	D	495	LEU
1	D	527	TRP
1	D	587	ASN
1	D	595	ARG
1	D	605	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	112	HIS
1	A	175	GLN
1	A	318	ASN
1	A	321	ASN
1	A	355	GLN
1	A	437	ASN

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Mol	Chain	Res	Type
1	A	479	ASN
1	A	484	ASN
1	A	490	ASN
1	A	572	GLN
1	A	587	ASN
1	A	605	GLN
1	B	204	GLN
1	B	279	GLN
1	B	321	ASN
1	B	355	GLN
1	B	459	ASN
1	B	529	HIS
1	C	81	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	234	GLN
1	D	424	GLN
1	D	523	HIS
1	D	572	GLN
1	D	587	ASN
1	D	605	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no 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	$\# Z  > 2$
5	SO4	A	1001	-	4,4,4	0.44	0	6,6,6	0.18	0
5	SO4	A	1002	-	4,4,4	0.62	0	6,6,6	0.35	0
6	EDO	A	1101	-	3,3,3	0.32	0	2,2,2	1.00	0
6	EDO	A	1102	-	3,3,3	0.58	0	2,2,2	0.64	0
2	NAG	A	701	1	14,14,15	0.55	0	15,19,21	1.23	2 (13%)
2	NAG	A	702	1	14,14,15	0.51	0	15,19,21	1.02	2 (13%)
2	NAG	A	703	1	14,14,15	0.60	0	15,19,21	2.08	3 (20%)
2	NAG	A	704	1	14,14,15	0.52	0	15,19,21	1.09	2 (13%)
4	GAL	A	900	-	12,12,12	0.78	0	17,17,17	1.05	1 (5%)
5	SO4	B	1001	-	4,4,4	0.42	0	6,6,6	0.10	0
5	SO4	B	1002	-	4,4,4	0.54	0	6,6,6	0.72	0
6	EDO	B	1101	-	3,3,3	0.68	0	2,2,2	0.65	0
6	EDO	B	1102	-	3,3,3	0.67	0	2,2,2	1.33	0
2	NAG	B	701	1	14,14,15	0.67	0	15,19,21	1.16	1 (6%)
2	NAG	B	702	1	14,14,15	0.42	0	15,19,21	0.98	1 (6%)
2	NAG	B	703	1	14,14,15	0.69	0	15,19,21	2.37	7 (46%)
2	NAG	B	704	1	14,14,15	0.58	0	15,19,21	1.05	0
4	GAL	B	900	-	12,12,12	0.62	0	17,17,17	1.13	2 (11%)
5	SO4	C	1001	-	4,4,4	0.46	0	6,6,6	0.12	0
5	SO4	C	1002	-	4,4,4	0.59	0	6,6,6	0.18	0
6	EDO	C	1101	-	3,3,3	0.12	0	2,2,2	0.83	0
6	EDO	C	1102	-	3,3,3	0.87	0	2,2,2	0.22	0
2	NAG	C	701	1	14,14,15	0.69	1 (7%)	15,19,21	1.63	4 (26%)
2	NAG	C	702	1	14,14,15	0.60	0	15,19,21	1.59	1 (6%)
2	NAG	C	703	1	14,14,15	0.39	0	15,19,21	1.40	2 (13%)
2	NAG	C	704	1	14,14,15	0.43	0	15,19,21	1.06	1 (6%)
4	GAL	C	900	-	12,12,12	0.67	0	17,17,17	0.87	1 (5%)
5	SO4	D	1001	-	4,4,4	0.47	0	6,6,6	0.10	0
5	SO4	D	1002	-	4,4,4	0.47	0	6,6,6	0.21	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	D	1101	-	3,3,3	0.17	0	2,2,2	0.80	0
6	EDO	D	1102	-	3,3,3	0.64	0	2,2,2	0.44	0
2	NAG	D	701	1	14,14,15	0.41	0	15,19,21	1.52	2 (13%)
2	NAG	D	702	1	14,14,15	0.66	0	15,19,21	1.12	2 (13%)
2	NAG	D	703	1	14,14,15	0.59	0	15,19,21	0.99	1 (6%)
2	NAG	D	704	1	14,14,15	0.29	0	15,19,21	1.02	0
4	GAL	D	900	-	12,12,12	0.74	0	17,17,17	1.15	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
5	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
6	EDO	A	1101	-	-	0/1/1/1	0/0/0/0
6	EDO	A	1102	-	-	0/1/1/1	0/0/0/0
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	GAL	A	900	-	-	0/2/22/22	0/1/1/1
5	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
6	EDO	B	1101	-	-	0/1/1/1	0/0/0/0
6	EDO	B	1102	-	-	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
4	GAL	B	900	-	-	0/2/22/22	0/1/1/1
5	SO4	C	1001	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
6	EDO	C	1101	-	-	0/1/1/1	0/0/0/0
6	EDO	C	1102	-	-	0/1/1/1	0/0/0/0
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	GAL	C	900	-	-	0/2/22/22	0/1/1/1
5	SO4	D	1001	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	D	1002	-	-	0/0/0/0	0/0/0/0
6	EDO	D	1101	-	-	0/1/1/1	0/0/0/0
6	EDO	D	1102	-	-	0/1/1/1	0/0/0/0
2	NAG	D	701	1	-	0/6/23/26	0/1/1/1
2	NAG	D	702	1	-	0/6/23/26	0/1/1/1
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
4	GAL	D	900	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	NAG	C1-C2	2.11	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	NAG	C2-N2-C7	-4.26	117.57	123.04
2	B	703	NAG	C4-C3-C2	-3.97	105.05	111.23
4	B	900	GAL	O1-C1-O5	-2.69	102.89	110.25
2	A	701	NAG	O4-C4-C3	-2.59	104.51	110.34
4	A	900	GAL	O1-C1-O5	-2.53	103.34	110.25
2	C	701	NAG	C3-C4-C5	-2.49	105.86	110.20
4	B	900	GAL	O5-C5-C4	-2.46	105.07	109.68
2	B	703	NAG	C6-C5-C4	-2.36	107.19	113.02
2	A	704	NAG	O4-C4-C3	-2.34	105.06	110.34
4	D	900	GAL	O1-C1-O5	-2.34	103.85	110.25
2	B	701	NAG	O4-C4-C3	-2.28	105.20	110.34
2	A	701	NAG	O6-C6-C5	-2.28	103.81	111.33
2	B	703	NAG	C8-C7-N2	-2.27	111.77	116.11
4	C	900	GAL	O1-C1-O5	-2.23	104.16	110.25
2	B	703	NAG	C2-N2-C7	-2.20	120.21	123.04
2	C	704	NAG	C3-C2-N2	-2.19	105.31	110.56
2	A	702	NAG	C3-C4-C5	-2.05	106.62	110.20
2	D	702	NAG	C4-C3-C2	2.00	114.34	111.23
2	A	703	NAG	O3-C3-C2	2.00	113.08	109.11
2	B	702	NAG	C1-O5-C5	2.03	114.83	112.25
2	C	701	NAG	O3-C3-C2	2.07	113.22	109.11
4	D	900	GAL	O4-C4-C5	2.22	115.12	109.24
2	D	703	NAG	C2-N2-C7	2.31	126.01	123.04
2	A	704	NAG	C1-O5-C5	2.50	115.42	112.25
2	B	703	NAG	O7-C7-N2	2.51	126.98	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	NAG	C1-O5-C5	2.55	115.49	112.25
2	D	701	NAG	C2-N2-C7	2.62	126.40	123.04
2	B	703	NAG	C3-C2-N2	2.68	116.98	110.56
2	A	702	NAG	C1-O5-C5	2.69	115.66	112.25
2	C	701	NAG	C2-N2-C7	3.02	126.92	123.04
2	C	703	NAG	C2-N2-C7	3.19	127.13	123.04
2	C	701	NAG	C1-O5-C5	3.27	116.40	112.25
2	D	701	NAG	C1-O5-C5	3.70	116.94	112.25
2	C	703	NAG	C1-O5-C5	3.83	117.11	112.25
2	C	702	NAG	C1-O5-C5	5.08	118.69	112.25
2	A	703	NAG	C1-O5-C5	5.09	118.70	112.25
2	B	703	NAG	C1-O5-C5	5.52	119.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	SO4	1	0
6	A	1101	EDO	3	0
4	A	900	GAL	1	0
5	B	1002	SO4	1	0
6	B	1101	EDO	1	0
6	B	1102	EDO	1	0
2	B	703	NAG	2	0
4	B	900	GAL	1	0
6	C	1101	EDO	1	0
2	C	702	NAG	1	0
4	C	900	GAL	1	0
6	D	1101	EDO	4	0
2	D	702	NAG	1	0
4	D	900	GAL	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	605/654 (92%)	-0.12	13 (2%) 67 62	7, 16, 31, 69	0
1	B	605/654 (92%)	-0.18	10 (1%) 73 69	6, 14, 29, 58	0
1	C	602/654 (92%)	-0.06	13 (2%) 65 60	7, 17, 38, 55	0
1	D	602/654 (92%)	0.01	22 (3%) 45 39	8, 18, 40, 69	0
All	All	2414/2616 (92%)	-0.09	58 (2%) 62 57	6, 16, 36, 69	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	ASP	6.2
1	A	646	SER	5.9
1	C	527	TRP	5.5
1	B	646	SER	5.5
1	B	628	SER	5.1
1	B	629	ASP	5.1
1	D	29	GLN	4.9
1	D	527	TRP	4.8
1	D	628	SER	4.7
1	B	29	GLN	4.6
1	A	29	GLN	4.5
1	D	629	ASP	4.5
1	D	488	TYR	4.2
1	B	647	SER	4.2
1	A	647	SER	4.0
1	C	488	TYR	3.7
1	C	525	GLY	3.6
1	B	488	TYR	3.5
1	A	628	SER	3.5
1	A	627	SER	3.4
1	B	627	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	359	LYS	3.2
1	C	647	SER	3.1
1	A	488	TYR	3.1
1	D	631	PRO	3.0
1	C	487	ALA	3.0
1	D	627	SER	3.0
1	C	526	GLY	2.9
1	D	427	SER	2.9
1	D	359	LYS	2.9
1	D	428	ASN	2.8
1	C	398	ILE	2.8
1	D	647	SER	2.7
1	D	526	GLY	2.6
1	A	427	SER	2.6
1	D	646	SER	2.6
1	D	234	GLN	2.6
1	C	428	ASN	2.5
1	D	468	LYS	2.5
1	C	359	LYS	2.4
1	B	631	PRO	2.4
1	A	31	MET	2.4
1	C	29	GLN	2.4
1	C	429	PRO	2.4
1	D	391	ILE	2.3
1	D	390	ASP	2.3
1	D	630	ASP	2.2
1	C	31	MET	2.2
1	D	632	GLU	2.2
1	D	257	LYS	2.2
1	C	468	LYS	2.1
1	B	611	SER	2.1
1	A	545	ASN	2.1
1	A	611	SER	2.1
1	A	92	TRP	2.1
1	B	359	LYS	2.1
1	D	426	CYS	2.0
1	D	448	ASP	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 carbohydrates 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. 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	1101	4/4	0.78	0.20	11.05	22,26,29,33	0
2	NAG	D	703	14/15	0.64	0.41	8.90	45,49,51,52	0
2	NAG	D	704	14/15	0.96	0.12	7.83	11,14,18,18	0
6	EDO	A	1101	4/4	0.74	0.21	6.34	23,25,29,31	0
2	NAG	A	702	14/15	0.94	0.14	4.27	14,16,19,22	0
2	NAG	C	704	14/15	0.96	0.12	3.41	11,12,14,16	0
2	NAG	D	702	14/15	0.86	0.20	2.92	23,25,29,30	0
2	NAG	A	703	14/15	0.89	0.17	2.84	21,24,30,33	0
5	SO4	A	1002	5/5	0.94	0.22	2.37	32,35,39,40	0
2	NAG	B	702	14/15	0.95	0.10	2.24	11,13,16,17	0
2	NAG	B	703	14/15	0.84	0.16	1.84	22,25,30,32	0
6	EDO	C	1102	4/4	0.95	0.10	1.67	11,13,17,20	0
6	EDO	D	1101	4/4	0.88	0.12	1.64	16,19,20,23	0
6	EDO	B	1101	4/4	0.85	0.15	1.61	22,22,24,26	0
2	NAG	C	702	14/15	0.83	0.23	1.50	23,26,28,33	0
5	SO4	C	1002	5/5	0.94	0.21	1.46	28,30,31,31	0
2	NAG	C	703	14/15	0.90	0.21	1.26	23,26,30,30	0
5	SO4	B	1002	5/5	0.96	0.18	1.25	31,31,35,36	0
5	SO4	D	1002	5/5	0.97	0.17	0.52	31,32,33,34	0
2	NAG	A	701	14/15	0.95	0.09	-0.12	8,10,16,17	0
2	NAG	B	701	14/15	0.95	0.09	-0.44	8,10,17,18	0
4	GAL	A	900	12/12	0.96	0.07	-0.53	6,7,9,12	0
4	GAL	B	900	12/12	0.96	0.08	-0.55	4,7,10,13	0
4	GAL	D	900	12/12	0.96	0.08	-0.94	7,8,9,16	0
4	GAL	C	900	12/12	0.97	0.07	-1.09	6,7,10,16	0
3	CL	B	801	1/1	1.00	0.04	-2.63	7,7,7,7	0
3	CL	A	801	1/1	1.00	0.03	-3.04	8,8,8,8	0
3	CL	D	801	1/1	1.00	0.02	-4.18	7,7,7,7	0
3	CL	C	801	1/1	1.00	0.03	-5.40	6,6,6,6	0
5	SO4	D	1001	5/5	0.86	0.28	-	63,63,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	1102	4/4	0.97	0.07	-	9,11,12,15	0
2	NAG	A	704	14/15	0.81	0.34	-	29,33,39,41	0
5	SO4	C	1001	5/5	0.92	0.26	-	57,57,59,60	0
2	NAG	C	701	14/15	0.61	0.46	-	44,48,51,51	0
5	SO4	B	1001	5/5	0.96	0.26	-	54,55,56,56	0
6	EDO	B	1102	4/4	0.88	0.17	-	12,18,18,23	0
2	NAG	D	701	14/15	0.66	0.42	-	43,47,50,54	0
5	SO4	A	1001	5/5	0.91	0.26	-	54,55,57,58	0
2	NAG	B	704	14/15	0.84	0.33	-	29,34,39,41	0
6	EDO	D	1102	4/4	0.97	0.10	-	11,14,15,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.