



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2018 – 07:38 PM EDT

PDB ID : 6F7Q  
Title : Human Butyrylcholinesterase complexed with N-Propargylperidines  
Authors : Coquelle, N.; Knez, D.; Colletier, J.P.; Gobec, S.  
Deposited on : 2017-12-11  
Resolution : 2.60 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

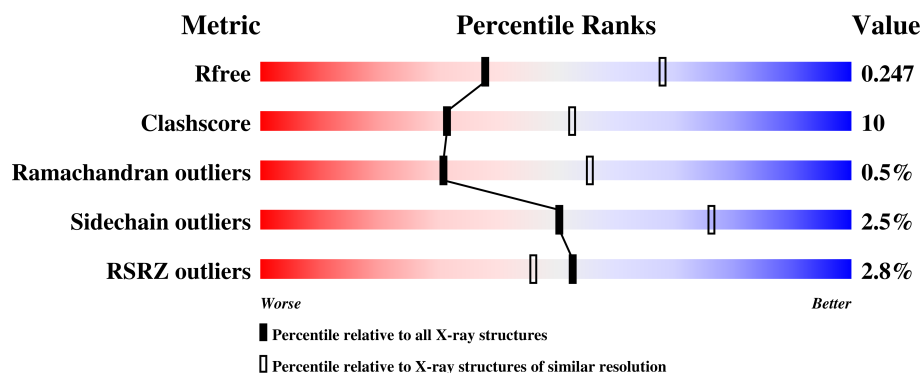
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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	529	<div> <div>3%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	B	529	<div> <div>2%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	614	-	-	-	X
5	NAG	A	618	-	-	-	X
5	NAG	B	605	-	-	X	-
5	NAG	B	614	-	-	-	X
6	FUL	A	613	-	-	-	X
6	FUL	B	613	-	-	-	X
7	SO4	A	620	-	-	X	-

## 2 Entry composition [i](#)

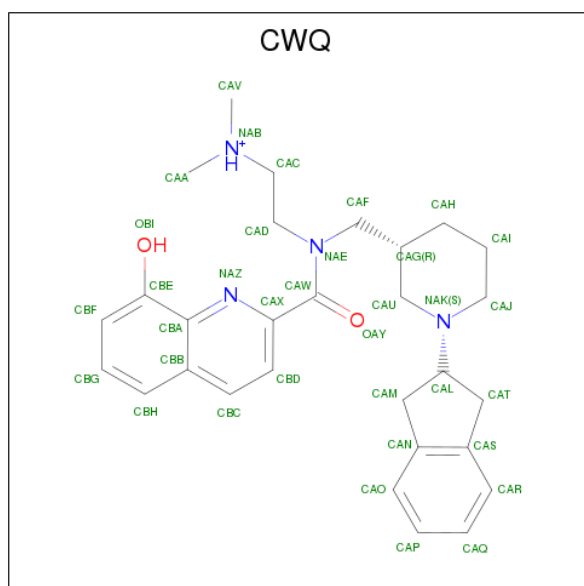
There are 10 unique types of molecules in this entry. The entry contains 8943 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	3	0
			4171	2690	696	770	15			
1	B	527	Total	C	N	O	S	0	2	0
			4189	2701	704	769	15			

- Molecule 2 is 2-[[[(3 {R})-1-(2,3-dihydro-1 {H}-inden-2-yl)piperidin-3-yl]methyl-(8-oxidany lquinolin-2-yl)carbonyl-amino]ethyl-dimethyl-azanium (three-letter code: CWQ) (formula: C<sub>29</sub>H<sub>37</sub>N<sub>4</sub>O<sub>2</sub>).



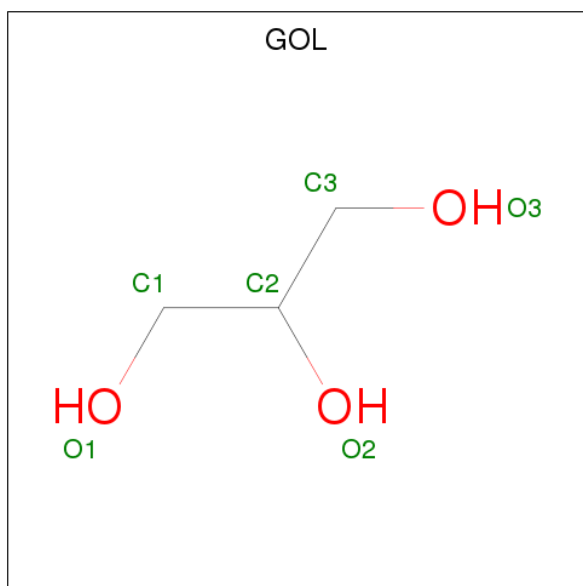
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	29	4	2		
2	A	1	Total	C	N	O	0	0
			35	29	4	2		
2	B	1	Total	C	N	O	0	0
			35	29	4	2		

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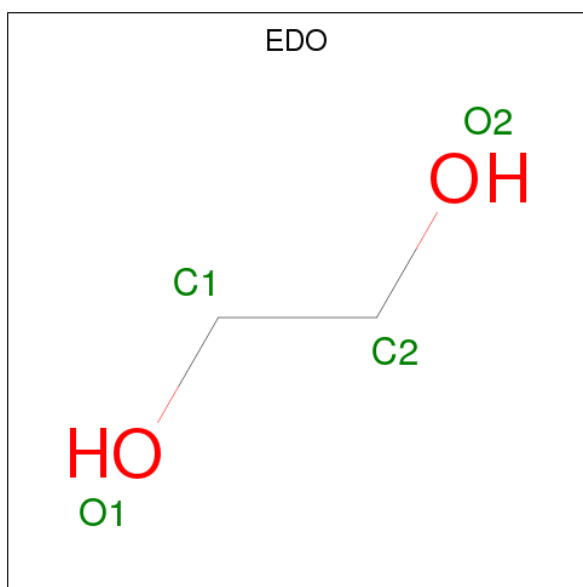
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			35	29	4	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



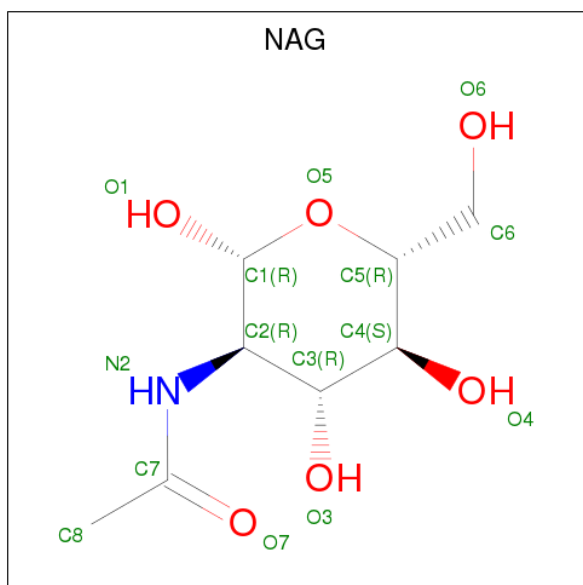
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



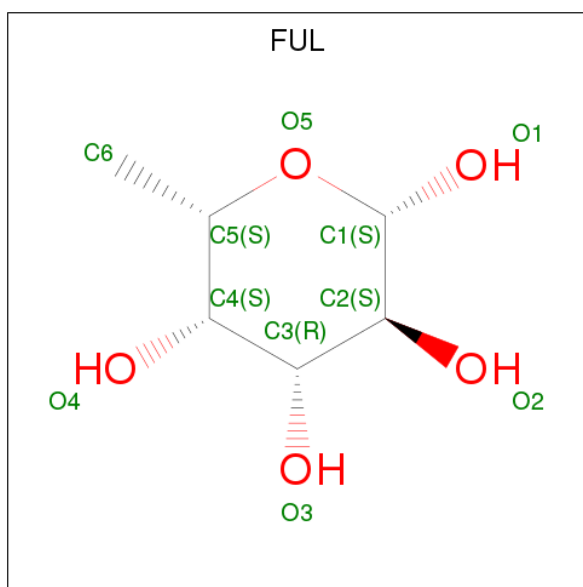
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



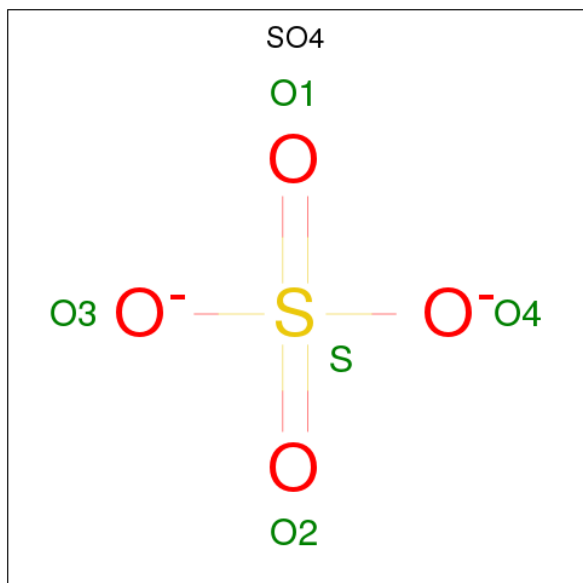
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1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

- Molecule 6 is BETA-L-FUCOSE (three-letter code: FUL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



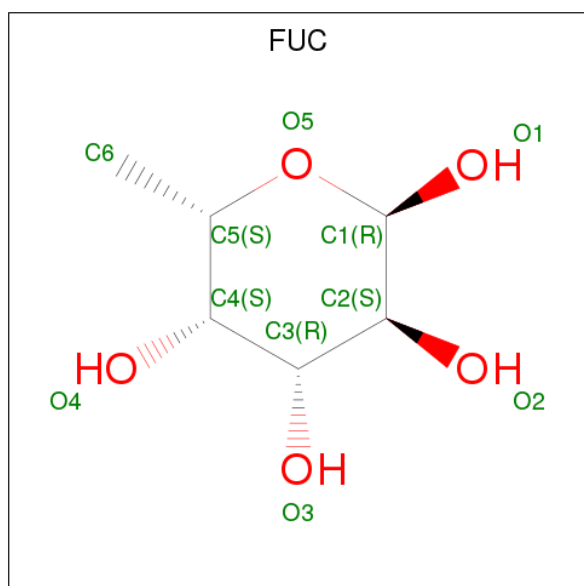


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cl 1 1	0	0

- Molecule 9 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 10 6 4	0	0

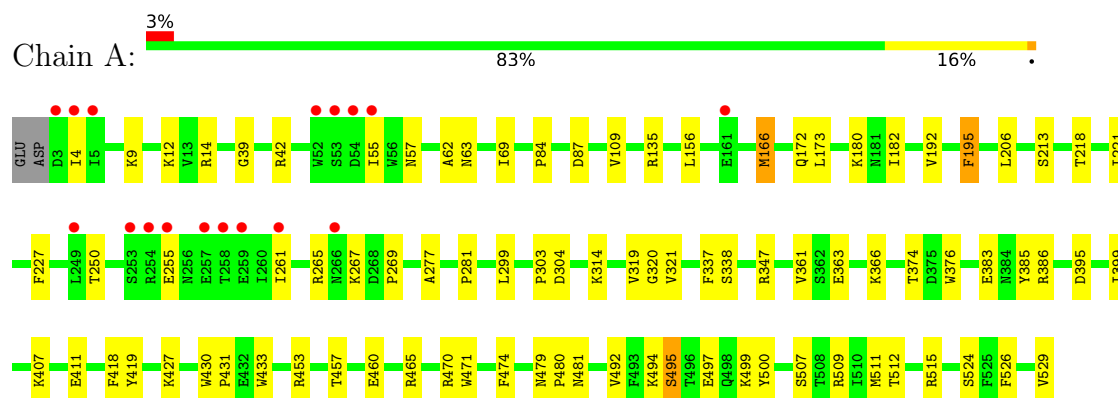
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	87	Total 87	O 87	0	0
10	B	36	Total 36	O 36	0	0

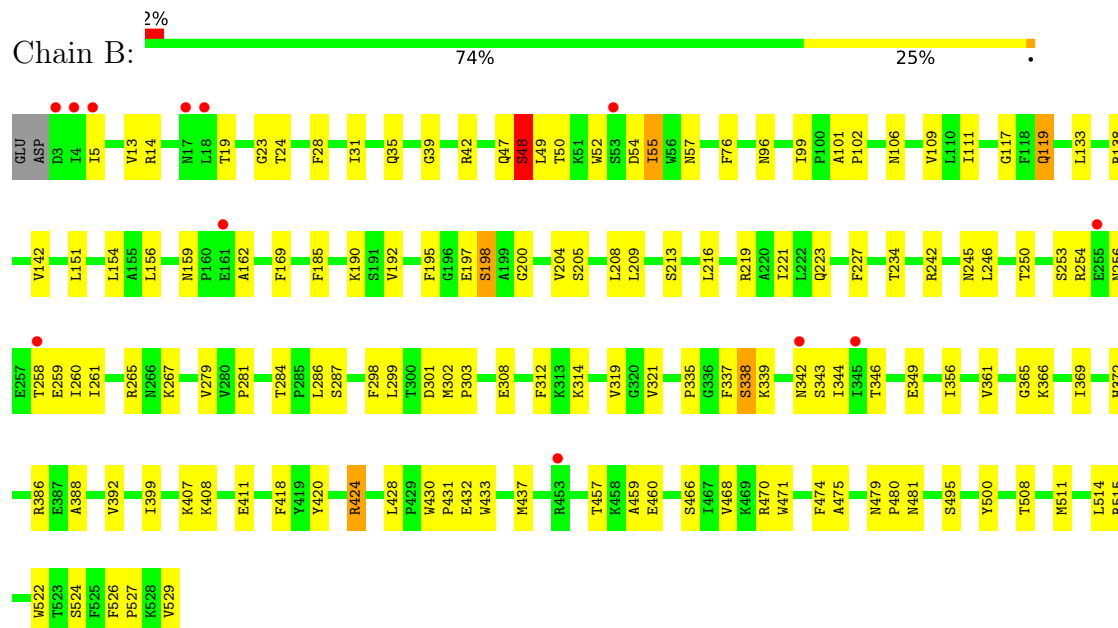
### 3 Residue-property plots

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

#### • Molecule 1: Cholinesterase



#### • Molecule 1: Cholinesterase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.14Å 152.14Å 141.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 2.60 49.11 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.11-2.60) 94.1 (49.11-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.192 , 0.248 0.192 , 0.247	Depositor DCC
$R_{free}$ test set	2435 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.3	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: GOL, NAG, CL, CWQ, EDO, FUC, FUL, 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	0.34	0/4297	0.52	0/5841
1	B	0.43	0/4311	0.58	0/5859
All	All	0.39	0/8608	0.55	0/11700

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4171	0	4034	61	0
1	B	4189	0	4060	103	0
2	A	70	0	0	0	0
2	B	70	0	0	1	0
3	A	18	0	24	4	0
4	A	12	0	18	2	0
4	B	4	0	6	2	0
5	A	98	0	86	1	0
5	B	112	0	99	20	0
6	A	30	0	30	1	0
6	B	10	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	15	0	0	3	0
7	B	10	0	0	1	0
8	B	1	0	0	0	0
9	B	10	0	10	0	0
10	A	87	0	0	4	0
10	B	36	0	0	1	0
All	All	8943	0	8377	166	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 10.

All (166) 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:57:ASN:HD21	5:B:605:NAG:C1	1.30	1.44
1:B:57:ASN:HD21	5:B:605:NAG:C2	1.45	1.29
1:B:57:ASN:CG	5:B:605:NAG:C1	2.35	0.94
1:B:346:THR:HG23	1:B:349:GLU:H	1.36	0.90
1:B:234:THR:HG22	7:B:615:SO4:O4	1.71	0.89
1:B:14:ARG:NH1	5:B:605:NAG:C1	2.37	0.86
1:B:457:THR:HG22	1:B:459:ALA:H	1.44	0.83
1:B:57:ASN:ND2	5:B:605:NAG:C2	2.30	0.78
1:B:14:ARG:HH11	5:B:605:NAG:C1	1.97	0.76
1:B:57:ASN:HD22	5:B:605:NAG:H83	1.51	0.74
1:B:57:ASN:OD1	5:B:605:NAG:C1	2.36	0.72
1:B:470:ARG:HH11	4:B:604:EDO:H21	1.54	0.71
1:A:499:LYS:HG2	1:A:512:THR:HG22	1.71	0.71
1:B:57:ASN:ND2	5:B:605:NAG:H83	2.09	0.68
1:B:250:THR:O	1:B:267:LYS:NZ	2.27	0.67
1:B:159:ASN:HD21	1:B:258:THR:HG22	1.60	0.67
1:A:63:ASN:N	7:A:620:SO4:O4	2.24	0.65
1:A:87:ASP:OD2	10:A:701:HOH:O	2.14	0.65
1:B:361:VAL:O	1:B:366:LYS:NZ	2.30	0.64
1:A:250:THR:O	1:A:267:LYS:NZ	2.23	0.64
1:B:308:GLU:OE2	1:B:408:LYS:HE2	1.96	0.64
1:B:319:VAL:O	1:B:418:PHE:HA	1.98	0.63
1:A:218:THR:HA	3:A:605:GOL:H31	1.80	0.62
1:A:509:ARG:NH2	10:A:706:HOH:O	2.32	0.62
1:B:57:ASN:ND2	5:B:605:NAG:N2	2.43	0.62
1:B:5:ILE:HD12	1:B:55:ILE:HD11	1.82	0.62
1:B:256:ASN:HB3	1:B:259:GLU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:N	1:A:383:GLU:OE1	2.27	0.60
1:A:277:ALA:N	10:A:704:HOH:O	2.30	0.60
1:B:479:ASN:OD1	1:B:481:ASN:ND2	2.35	0.59
1:B:213:SER:HA	1:B:216:LEU:HD12	1.84	0.59
1:B:109:VAL:HB	1:B:192:VAL:HG22	1.85	0.59
1:A:9:LYS:HD2	1:A:180:LYS:HB3	1.84	0.58
1:B:197:GLU:HB3	10:B:729:HOH:O	2.03	0.58
1:B:190:LYS:NZ	5:B:607:NAG:HN2	2.01	0.57
1:B:457:THR:HG22	1:B:459:ALA:N	2.18	0.57
1:B:76:PHE:CE2	1:B:339:LYS:HE2	2.40	0.57
1:B:515:ARG:HG2	1:B:515:ARG:HH21	1.69	0.57
1:B:522:TRP:O	1:B:527:PRO:HD3	2.06	0.56
1:B:111:ILE:HA	1:B:142:VAL:O	2.06	0.56
1:A:361:VAL:O	1:A:366:LYS:NZ	2.40	0.55
1:A:156:LEU:HD11	1:A:261:ILE:HD11	1.88	0.55
1:B:76:PHE:CZ	1:B:339:LYS:HE2	2.42	0.55
1:B:35[A]:GLN:HG3	1:B:48:SER:O	2.07	0.54
1:B:386:ARG:NH1	1:B:433:TRP:HB2	2.22	0.54
1:B:312:PHE:O	1:B:314:LYS:HE3	2.07	0.54
1:B:337:PHE:HA	1:B:343:SER:OG	2.08	0.54
1:A:319:VAL:O	1:A:418:PHE:HA	2.08	0.53
1:B:28:PHE:HB3	1:B:31:ILE:HD11	1.89	0.53
1:B:346:THR:HG22	1:B:349:GLU:OE1	2.08	0.53
1:B:254:ARG:HB2	1:B:260:ILE:HB	1.90	0.53
1:A:166:MET:HE2	1:A:166:MET:H	1.73	0.53
1:B:190:LYS:HZ3	5:B:607:NAG:HN2	1.55	0.53
1:A:135:ARG:HH12	3:A:603:GOL:H2	1.75	0.52
1:A:69:ILE:HD13	1:A:84:PRO:HD2	1.90	0.52
1:B:57:ASN:ND2	5:B:605:NAG:C7	2.72	0.52
1:A:62:ALA:HB1	7:A:620:SO4:O4	2.10	0.51
1:A:470:ARG:HH11	4:A:608:EDO:H22	1.76	0.51
1:B:386:ARG:HD3	1:B:433:TRP:CE3	2.47	0.50
1:B:156:LEU:HD12	1:B:261:ILE:HD11	1.93	0.50
1:B:474:PHE:HB2	1:B:480:PRO:HB3	1.92	0.50
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.46	0.50
1:B:197:GLU:OE1	1:B:198:SER:HB2	2.12	0.50
1:B:245:ASN:ND2	5:B:612:NAG:H62	2.27	0.50
1:A:135:ARG:NH1	3:A:603:GOL:H2	2.27	0.50
1:A:63:ASN:ND2	7:A:620:SO4:O1	2.45	0.49
1:B:227:PHE:CD1	1:B:303:PRO:HB2	2.47	0.49
1:B:500:TYR:CZ	1:B:511:MET:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:SER:HB3	5:B:608:NAG:H62	1.95	0.49
1:A:206:LEU:HD22	1:A:299:LEU:HD11	1.94	0.49
1:B:219:ARG:NH2	1:B:475:ALA:O	2.46	0.49
1:A:374:THR:HA	1:A:376:TRP:CZ3	2.47	0.49
1:B:200:GLY:O	1:B:204:VAL:HG23	2.13	0.49
1:B:76:PHE:CD2	1:B:339:LYS:HE2	2.48	0.48
1:A:314:LYS:NZ	10:A:710:HOH:O	2.40	0.48
1:B:42:ARG:HD2	1:B:151:LEU:HD22	1.93	0.48
1:B:39:GLY:O	1:B:265:ARG:HD3	2.13	0.47
1:B:365:GLY:O	1:B:369:ILE:HG13	2.13	0.47
1:A:218:THR:OG1	3:A:605:GOL:H2	2.13	0.47
1:A:494:LYS:HE2	1:A:497:GLU:HG3	1.95	0.47
1:B:99:ILE:HG21	1:B:185:PHE:HB3	1.96	0.47
1:A:109:VAL:HB	1:A:192:VAL:HG22	1.96	0.46
1:A:156:LEU:CD1	1:A:261:ILE:HD11	2.45	0.46
1:A:494:LYS:HB2	1:A:494:LYS:HE2	1.75	0.46
1:B:57:ASN:ND2	5:B:605:NAG:C8	2.76	0.46
1:A:453:ARG:H	1:A:453:ARG:HD2	1.81	0.46
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.96	0.46
1:B:35[B]:GLN:HG2	1:B:49:LEU:HD12	1.97	0.46
1:A:321:VAL:HG11	1:A:399:ILE:HA	1.97	0.46
1:A:411:GLU:HG3	1:A:495:SER:OG	2.16	0.46
1:B:52:TRP:HD1	1:B:54:ASP:H	1.63	0.46
1:B:301:ASP:OD1	1:B:302:MET:N	2.44	0.45
1:B:76:PHE:CE1	1:B:339:LYS:HE2	2.52	0.45
1:B:245:ASN:HD21	5:B:612:NAG:H62	1.81	0.45
1:A:12:LYS:HB2	1:A:55:ILE:HG12	1.97	0.45
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.52	0.45
1:B:342:ASN:OD1	1:B:344:ILE:HG12	2.16	0.45
1:B:284:THR:HG22	1:B:356:ILE:O	2.16	0.45
1:A:195:PHE:CB	1:A:221:ILE:HB	2.47	0.45
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.82	0.44
1:A:526:PHE:O	1:A:529:VAL:HG22	2.17	0.44
1:A:172:GLN:NE2	1:A:213:SER:OG	2.41	0.44
1:A:470:ARG:HE	4:A:608:EDO:H22	1.83	0.44
1:B:117:GLY:O	1:B:119:GLN:HG2	2.18	0.44
1:B:424:ARG:NH1	1:B:432:GLU:HA	2.33	0.44
5:B:612:NAG:H62	6:B:613:FUL:H2	1.76	0.44
1:A:4:ILE:H	1:A:4:ILE:HD12	1.83	0.44
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.52	0.44
1:B:500:TYR:CE1	1:B:514:LEU:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:CB	1:B:221:ILE:HB	2.47	0.44
1:B:49:LEU:HA	1:B:49:LEU:HD12	1.66	0.44
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.52	0.44
1:A:465:ARG:HD2	1:A:465:ARG:HA	1.87	0.44
1:B:205:SER:O	1:B:208:LEU:HB2	2.17	0.43
1:A:430:TRP:HB3	1:A:431:PRO:HD2	2.01	0.43
1:B:515:ARG:HH21	1:B:515:ARG:CG	2.31	0.43
1:B:335:PRO:HD3	1:B:356:ILE:CD1	2.48	0.43
1:A:182:ILE:HD12	1:A:182:ILE:HA	1.81	0.43
1:A:39:GLY:O	1:A:265:ARG:HD2	2.18	0.43
1:A:474:PHE:HB2	1:A:480:PRO:HB3	2.00	0.43
1:B:508:THR:HG21	4:B:604:EDO:H11	2.00	0.43
1:B:24:THR:O	1:B:101:ALA:HB3	2.19	0.43
1:B:13:VAL:HG12	1:B:28:PHE:HD2	1.83	0.43
1:B:14:ARG:HH12	5:B:605:NAG:C1	2.24	0.43
1:B:388:ALA:O	1:B:392:VAL:HG23	2.17	0.43
1:B:411:GLU:HG3	1:B:495:SER:OG	2.19	0.43
1:B:133:LEU:HD23	1:B:468:VAL:HG13	2.00	0.42
1:B:154:LEU:HD23	1:B:162:ALA:HB1	2.00	0.42
1:B:256:ASN:O	1:B:260:ILE:HG22	2.19	0.42
1:B:227:PHE:CE1	1:B:303:PRO:HB2	2.54	0.42
1:B:526:PHE:O	1:B:529:VAL:HB	2.19	0.42
1:A:195:PHE:HB3	1:A:221:ILE:HB	2.00	0.42
1:A:14:ARG:HD2	1:A:57:ASN:OD1	2.20	0.42
1:A:337:PHE:HE1	1:A:386:ARG:HG2	1.85	0.42
1:A:407:LYS:HB2	1:A:407:LYS:HE3	1.53	0.42
1:B:197:GLU:O	1:B:200:GLY:N	2.52	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.55	0.42
1:B:361:VAL:CG1	1:B:366:LYS:HG3	2.50	0.42
1:B:420:TYR:OH	1:B:515:ARG:NH1	2.52	0.41
1:B:195:PHE:HB2	1:B:221:ILE:HB	2.02	0.41
1:A:386:ARG:HD3	1:A:433:TRP:CE3	2.55	0.41
1:B:19:THR:HA	1:B:23:GLY:O	2.20	0.41
1:B:321:VAL:HG11	1:B:399:ILE:HA	2.02	0.41
1:B:407:LYS:HE3	1:B:407:LYS:HB2	1.43	0.41
1:B:457:THR:HB	1:B:460:GLU:HG3	2.01	0.41
1:A:173:LEU:HA	1:A:173:LEU:HD12	1.86	0.41
1:B:227:PHE:CD1	1:B:227:PHE:C	2.94	0.41
5:A:612:NAG:H62	6:A:613:FUL:H2	1.76	0.41
1:B:372:HIS:HB3	2:B:601:CWQ:CAQ	2.50	0.41
1:B:106:ASN:HB2	5:B:606:NAG:H83	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:THR:HG22	1:A:376:TRP:CH2	2.56	0.41
1:B:169:PHE:CZ	1:B:298:PHE:HB2	2.56	0.41
1:B:242:ARG:O	1:B:279:VAL:HG11	2.21	0.41
1:A:427:LYS:HB3	1:A:427:LYS:HE2	1.88	0.41
1:A:479:ASN:OD1	1:A:481:ASN:ND2	2.54	0.41
1:A:492:VAL:HG12	1:A:494:LYS:HG3	2.03	0.41
1:A:395:ASP:CG	1:A:515[A]:ARG:HE	2.25	0.40
1:B:197:GLU:HA	1:B:223:GLN:O	2.21	0.40
1:B:430:TRP:HB3	1:B:431:PRO:HD2	2.03	0.40
1:A:166:MET:CE	1:A:166:MET:H	2.34	0.40
1:B:102:PRO:O	1:B:138:ARG:NH2	2.54	0.40
1:B:299:LEU:HA	1:B:299:LEU:HD23	1.78	0.40
1:B:35[A]:GLN:HB2	1:B:47:GLN:HB2	2.02	0.40
1:A:457:THR:OG1	1:A:460:GLU:HG3	2.21	0.40
1:B:428:LEU:HD21	1:B:437:MET:SD	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	528/529 (100%)	500 (95%)	27 (5%)	1 (0%)	49	74
1	B	527/529 (100%)	489 (93%)	34 (6%)	4 (1%)	21	42
All	All	1055/1058 (100%)	989 (94%)	61 (6%)	5 (0%)	31	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	ILE
1	A	281	PRO
1	B	48	SER

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Mol	Chain	Res	Type
1	B	281	PRO
1	B	253	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/454 (98%)	437 (98%)	9 (2%)	58	81
1	B	448/454 (99%)	435 (97%)	13 (3%)	45	72
All	All	894/908 (98%)	872 (98%)	22 (2%)	50	76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	MET
1	A	195	PHE
1	A	255	GLU
1	A	338	SER
1	A	363	GLU
1	A	471	TRP
1	A	495	SER
1	A	507	SER
1	A	524	SER
1	B	48	SER
1	B	50	THR
1	B	96	ASN
1	B	119	GLN
1	B	198	SER
1	B	246	LEU
1	B	286	LEU
1	B	287	SER
1	B	338	SER
1	B	424	ARG
1	B	466	SER
1	B	471	TRP

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Mol	Chain	Res	Type
1	B	524	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	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 37 ligands modelled in this entry, 1 is 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	CWQ	A	601	-	39,39,39	2.16	10 (25%)	49,55,55	1.46	7 (14%)
2	CWQ	A	602	-	39,39,39	1.97	7 (17%)	49,55,55	1.69	7 (14%)
3	GOL	A	603	-	5,5,5	0.38	0	5,5,5	0.31	0
3	GOL	A	604	-	5,5,5	0.39	0	5,5,5	0.67	0
3	GOL	A	605	-	5,5,5	0.22	0	5,5,5	0.34	0
4	EDO	A	606	-	3,3,3	0.64	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	607	-	3,3,3	0.42	0	2,2,2	0.72	0
4	EDO	A	608	-	3,3,3	0.58	0	2,2,2	0.30	0
5	NAG	A	609	1,6	14,14,15	0.24	0	17,19,21	0.52	0
6	FUL	A	610	5	9,10,11	1.68	2 (22%)	13,14,16	0.77	0
5	NAG	A	611	1	14,14,15	0.67	1 (7%)	17,19,21	0.59	0
5	NAG	A	612	1,5,6	14,14,15	0.42	0	17,19,21	1.43	1 (5%)
6	FUL	A	613	5	9,10,11	1.05	1 (11%)	13,14,16	1.51	3 (23%)
5	NAG	A	614	5	14,14,15	0.60	0	17,19,21	0.93	2 (11%)
5	NAG	A	615	1	14,14,15	0.50	0	17,19,21	0.57	0
5	NAG	A	616	1,5,6	14,14,15	0.58	0	17,19,21	1.36	2 (11%)
6	FUL	A	617	5	9,10,11	1.22	1 (11%)	13,14,16	1.94	6 (46%)
5	NAG	A	618	5	14,14,15	0.61	0	17,19,21	1.33	2 (11%)
7	SO4	A	619	-	4,4,4	0.39	0	6,6,6	0.19	0
7	SO4	A	620	-	4,4,4	0.20	0	6,6,6	0.49	0
7	SO4	A	621	-	4,4,4	0.26	0	6,6,6	0.38	0
2	CWQ	B	601	-	39,39,39	2.17	9 (23%)	49,55,55	1.26	4 (8%)
2	CWQ	B	602	-	39,39,39	2.21	10 (25%)	49,55,55	1.85	13 (26%)
4	EDO	B	604	-	3,3,3	0.58	0	2,2,2	0.19	0
5	NAG	B	605	1	14,14,15	0.38	0	17,19,21	1.19	2 (11%)
5	NAG	B	606	1,5	14,14,15	1.40	1 (7%)	17,19,21	1.47	2 (11%)
5	NAG	B	607	5	14,14,15	0.54	0	17,19,21	0.50	0
5	NAG	B	608	1,9,5	14,14,15	0.55	0	17,19,21	0.73	0
5	NAG	B	609	5	14,14,15	0.62	0	17,19,21	0.70	0
9	FUC	B	610	5	9,10,11	1.30	2 (22%)	13,14,16	1.23	1 (7%)
5	NAG	B	611	1	14,14,15	0.81	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	B	612	1,5,6	14,14,15	0.41	0	17,19,21	1.42	1 (5%)
6	FUL	B	613	5	9,10,11	1.04	1 (11%)	13,14,16	1.50	3 (23%)
5	NAG	B	614	5	14,14,15	0.61	0	17,19,21	0.93	2 (11%)
7	SO4	B	615	-	4,4,4	0.24	0	6,6,6	0.30	0
7	SO4	B	616	-	4,4,4	0.41	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CWQ	A	601	-	-	0/21/39/39	1/5/5/5
2	CWQ	A	602	-	-	0/21/39/39	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	603	-	-	0/4/4/4	0/0/0/0
3	GOL	A	604	-	-	0/4/4/4	0/0/0/0
3	GOL	A	605	-	-	0/4/4/4	0/0/0/0
4	EDO	A	606	-	-	0/1/1/1	0/0/0/0
4	EDO	A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	A	608	-	-	0/1/1/1	0/0/0/0
5	NAG	A	609	1,6	-	0/6/23/26	0/1/1/1
6	FUL	A	610	5	-	0/0/17/20	0/1/1/1
5	NAG	A	611	1	-	0/6/23/26	0/1/1/1
5	NAG	A	612	1,5,6	-	0/6/23/26	0/1/1/1
6	FUL	A	613	5	-	0/0/17/20	0/1/1/1
5	NAG	A	614	5	-	0/6/23/26	0/1/1/1
5	NAG	A	615	1	-	0/6/23/26	0/1/1/1
5	NAG	A	616	1,5,6	-	0/6/23/26	0/1/1/1
6	FUL	A	617	5	-	0/0/17/20	0/1/1/1
5	NAG	A	618	5	-	0/6/23/26	0/1/1/1
7	SO4	A	619	-	-	0/0/0/0	0/0/0/0
7	SO4	A	620	-	-	0/0/0/0	0/0/0/0
7	SO4	A	621	-	-	0/0/0/0	0/0/0/0
2	CWQ	B	601	-	-	0/21/39/39	0/5/5/5
2	CWQ	B	602	-	-	0/21/39/39	0/5/5/5
4	EDO	B	604	-	-	0/1/1/1	0/0/0/0
5	NAG	B	605	1	-	0/6/23/26	0/1/1/1
5	NAG	B	606	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	607	5	-	0/6/23/26	0/1/1/1
5	NAG	B	608	1,9,5	-	0/6/23/26	0/1/1/1
5	NAG	B	609	5	-	0/6/23/26	0/1/1/1
9	FUC	B	610	5	-	0/0/17/20	0/1/1/1
5	NAG	B	611	1	-	0/6/23/26	0/1/1/1
5	NAG	B	612	1,5,6	-	0/6/23/26	0/1/1/1
6	FUL	B	613	5	-	0/0/17/20	0/1/1/1
5	NAG	B	614	5	-	0/6/23/26	0/1/1/1
7	SO4	B	615	-	-	0/0/0/0	0/0/0/0
7	SO4	B	616	-	-	0/0/0/0	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	CWQ	CAM-CAN	-6.87	1.39	1.50
2	B	601	CWQ	CAT-CAS	-6.50	1.40	1.50
2	A	601	CWQ	CAM-CAN	-6.49	1.40	1.50
2	B	602	CWQ	CAT-CAS	-6.06	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	CWQ	CAM-CAN	-5.96	1.41	1.50
2	B	601	CWQ	CAX-CAW	-5.82	1.40	1.50
2	A	602	CWQ	CAM-CAN	-5.71	1.41	1.50
2	B	602	CWQ	CAX-CAW	-5.69	1.40	1.50
2	A	601	CWQ	CAT-CAS	-5.65	1.41	1.50
2	A	601	CWQ	CAX-CAW	-5.64	1.40	1.50
2	A	602	CWQ	CAT-CAS	-5.61	1.41	1.50
2	A	602	CWQ	CAX-CAW	-5.01	1.41	1.50
5	B	606	NAG	O5-C1	-5.00	1.35	1.43
2	B	601	CWQ	CAR-CAS	-3.78	1.33	1.39
2	B	601	CWQ	CAM-CAL	-3.31	1.48	1.54
2	B	602	CWQ	CAO-CAN	-3.28	1.34	1.39
2	A	601	CWQ	CAM-CAL	-3.25	1.48	1.54
2	A	601	CWQ	CAT-CAL	-3.25	1.48	1.54
2	B	602	CWQ	CAT-CAL	-3.21	1.49	1.54
2	B	601	CWQ	CAO-CAN	-3.18	1.34	1.39
2	A	601	CWQ	CAR-CAS	-3.17	1.34	1.39
2	B	602	CWQ	CAR-CAS	-3.16	1.34	1.39
2	A	601	CWQ	CAO-CAN	-3.12	1.34	1.39
2	A	602	CWQ	CAR-CAS	-3.03	1.34	1.39
2	A	602	CWQ	CAM-CAL	-2.91	1.49	1.54
2	B	601	CWQ	CAT-CAL	-2.78	1.49	1.54
2	A	602	CWQ	CAO-CAN	-2.61	1.35	1.39
2	A	601	CWQ	CBE-CBA	-2.58	1.39	1.42
6	A	610	FUL	C2-C3	-2.44	1.48	1.52
2	B	601	CWQ	CAN-CAS	-2.44	1.35	1.39
2	B	602	CWQ	CAM-CAL	-2.32	1.50	1.54
2	B	602	CWQ	CBE-CBA	-2.29	1.39	1.42
2	A	601	CWQ	CAN-CAS	-2.28	1.35	1.39
2	A	602	CWQ	CBB-CBA	-2.21	1.39	1.42
2	A	601	CWQ	CBB-CBA	-2.12	1.39	1.42
2	B	601	CWQ	CBE-CBA	-2.04	1.39	1.42
2	B	602	CWQ	CAN-CAS	-2.04	1.35	1.39
2	B	602	CWQ	CBB-CBA	-2.01	1.39	1.42
5	A	611	NAG	C1-C2	2.11	1.55	1.52
9	B	610	FUC	C4-C3	2.17	1.57	1.52
6	A	617	FUL	C2-C3	2.57	1.56	1.52
6	B	613	FUL	C1-C2	2.61	1.58	1.52
6	A	613	FUL	C1-C2	2.61	1.58	1.52
9	B	610	FUC	C4-C5	2.78	1.58	1.52
5	B	611	NAG	O5-C1	2.91	1.48	1.43
6	A	610	FUL	O5-C1	4.06	1.50	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	CWQ	CAS-CAT-CAL	-4.78	98.25	103.38
2	A	602	CWQ	CBD-CAX-NAZ	-4.72	117.82	123.46
2	A	602	CWQ	CAN-CAM-CAL	-4.10	98.98	103.38
5	A	616	NAG	O4-C4-C3	-3.86	101.33	110.34
2	A	601	CWQ	CBD-CAX-NAZ	-3.77	118.95	123.46
2	B	602	CWQ	CBD-CAX-NAZ	-3.70	119.04	123.46
2	B	602	CWQ	CAS-CAT-CAL	-3.65	99.47	103.38
2	B	601	CWQ	CBD-CAX-NAZ	-3.36	119.45	123.46
2	A	602	CWQ	CAM-CAN-CAS	-3.19	108.33	110.56
5	A	618	NAG	O5-C1-C2	-3.14	107.18	111.52
2	B	602	CWQ	CAN-CAM-CAL	-3.12	100.03	103.38
2	B	602	CWQ	CAM-CAN-CAS	-3.03	108.44	110.56
2	A	601	CWQ	CAD-NAE-CAF	-2.70	113.13	116.30
2	A	601	CWQ	CAM-CAN-CAS	-2.65	108.71	110.56
5	B	605	NAG	O5-C1-C2	-2.51	108.06	111.52
2	A	602	CWQ	CAT-CAS-CAN	-2.49	108.82	110.56
2	B	602	CWQ	CAI-CAJ-NAK	-2.43	106.95	111.21
2	B	602	CWQ	CAU-NAK-CAL	-2.13	106.56	112.67
2	B	602	CWQ	CAT-CAS-CAN	-2.11	109.08	110.56
2	B	602	CWQ	CBG-CBF-CBE	-2.05	117.64	120.28
5	B	614	NAG	C1-O5-C5	2.00	114.94	112.19
5	A	614	NAG	C1-O5-C5	2.02	114.97	112.19
6	A	613	FUL	C1-C2-C3	2.04	112.24	109.66
6	B	613	FUL	C1-C2-C3	2.04	112.25	109.66
2	B	601	CWQ	CAX-NAZ-CBA	2.05	121.82	117.24
6	A	617	FUL	C2-C3-C4	2.11	114.54	110.87
5	A	618	NAG	C1-C2-N2	2.13	114.13	110.49
2	A	601	CWQ	CAH-CAI-CAJ	2.14	113.69	110.95
6	A	617	FUL	O5-C1-C2	2.22	114.24	110.78
2	B	601	CWQ	CBE-CBA-NAZ	2.23	119.64	117.32
5	B	614	NAG	C4-C3-C2	2.23	114.28	111.02
5	A	614	NAG	C4-C3-C2	2.24	114.29	111.02
2	B	602	CWQ	CAH-CAG-CAU	2.26	111.25	108.67
2	B	602	CWQ	CAX-NAZ-CBA	2.38	122.58	117.24
2	A	601	CWQ	CAX-NAZ-CBA	2.48	122.79	117.24
5	B	605	NAG	C1-O5-C5	2.50	115.63	112.19
6	A	617	FUL	C3-C4-C5	2.52	113.63	109.72
2	B	602	CWQ	CBD-CAX-CAW	2.55	123.79	119.17
2	B	601	CWQ	CAJ-NAK-CAU	2.56	110.61	108.17
2	A	602	CWQ	CAX-NAZ-CBA	2.70	123.28	117.24
2	A	601	CWQ	CBE-CBA-NAZ	2.74	120.18	117.32
6	A	617	FUL	C1-O5-C5	2.76	118.50	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	610	FUC	O5-C5-C4	2.85	114.24	109.62
2	B	602	CWQ	CAG-CAU-NAK	2.88	116.15	110.49
5	A	616	NAG	C4-C3-C2	2.91	115.28	111.02
5	B	611	NAG	C1-O5-C5	2.93	116.22	112.19
6	B	613	FUL	C1-O5-C5	3.09	119.23	112.39
6	A	613	FUL	C1-O5-C5	3.10	119.24	112.39
6	A	617	FUL	O5-C5-C4	3.11	114.67	109.62
6	B	613	FUL	O5-C1-C2	3.18	115.73	110.78
6	A	613	FUL	O5-C1-C2	3.20	115.77	110.78
6	A	617	FUL	C1-C2-C3	3.28	113.81	109.66
2	A	602	CWQ	CBE-CBA-NAZ	3.32	120.78	117.32
5	B	606	NAG	C4-C3-C2	3.73	116.48	111.02
5	B	606	NAG	C3-C4-C5	3.81	117.06	110.24
2	A	601	CWQ	CAJ-NAK-CAU	3.96	111.95	108.17
5	B	612	NAG	C1-O5-C5	5.25	119.42	112.19
5	A	612	NAG	C1-O5-C5	5.27	119.44	112.19
2	B	602	CWQ	CAJ-NAK-CAU	6.81	114.67	108.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CWQ	CAG-CAH-CAI-CAJ-CAU-NAK

15 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	GOL	2	0
3	A	605	GOL	2	0
4	A	608	EDO	2	0
5	A	612	NAG	1	0
6	A	613	FUL	1	0
7	A	620	SO4	3	0
2	B	601	CWQ	1	0
4	B	604	EDO	2	0
5	B	605	NAG	13	0
5	B	606	NAG	1	0
5	B	607	NAG	2	0
5	B	608	NAG	1	0
5	B	612	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	613	FUL	1	0
7	B	615	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	527/529 (99%)	-0.17	17 (3%)	47 40	38, 57, 90, 113	6 (1%)
1	B	527/529 (99%)	-0.17	12 (2%)	60 54	45, 69, 96, 129	7 (1%)
All	All	1054/1058 (99%)	-0.17	29 (2%)	53 46	38, 63, 94, 129	13 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ILE	3.8
1	B	3	ASP	3.8
1	A	254	ARG	3.5
1	B	53	SER	3.5
1	A	54	ASP	3.4
1	A	5	ILE	3.4
1	A	253	SER	3.2
1	A	55	ILE	3.1
1	A	53	SER	3.1
1	A	257	GLU	3.1
1	A	3	ASP	2.9
1	B	258	THR	2.9
1	A	255	GLU	2.9
1	A	258	THR	2.5
1	B	345	ILE	2.4
1	B	342	ASN	2.4
1	A	249	LEU	2.4
1	B	453	ARG	2.3
1	B	255	GLU	2.3
1	B	4	ILE	2.3
1	A	266	ASN	2.3
1	A	52	TRP	2.2
1	A	261	ILE	2.2
1	A	259	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	5	ILE	2.1
1	B	18	LEU	2.1
1	B	17	ASN	2.1
1	A	161	GLU	2.0
1	B	161	GLU	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. 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
5	NAG	A	618	14/15	0.59	0.50	111,127,135,139	0
5	NAG	A	614	14/15	0.59	0.53	121,134,138,142	0
3	GOL	A	604	6/6	0.62	0.30	67,78,84,85	0
3	GOL	A	603	6/6	0.66	0.33	79,84,89,95	0
5	NAG	B	605	14/15	0.69	0.27	106,116,122,124	0
6	FUL	A	613	10/11	0.69	0.49	92,114,121,129	0
7	SO4	A	620	5/5	0.70	0.39	85,87,102,106	5
6	FUL	B	613	10/11	0.72	0.45	98,111,116,122	0
5	NAG	B	614	14/15	0.72	0.50	116,127,131,134	0
6	FUL	A	617	10/11	0.73	0.26	105,113,115,115	0
5	NAG	B	607	14/15	0.78	0.22	97,120,133,135	0
7	SO4	A	621	5/5	0.81	0.29	74,80,89,106	5
5	NAG	B	609	14/15	0.81	0.30	95,105,117,125	0
5	NAG	B	612	14/15	0.83	0.31	109,123,128,133	0
7	SO4	B	615	5/5	0.83	0.20	92,94,102,119	5
3	GOL	A	605	6/6	0.84	0.25	61,63,71,75	0
5	NAG	A	612	14/15	0.85	0.29	107,120,130,135	0
5	NAG	B	606	14/15	0.87	0.11	81,95,106,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	FUC	B	610	10/11	0.88	0.32	102,111,125,125	0
5	NAG	A	616	14/15	0.89	0.23	86,99,111,122	0
5	NAG	B	611	14/15	0.89	0.14	71,84,100,100	0
4	EDO	A	607	4/4	0.90	0.17	66,67,68,72	0
5	NAG	A	615	14/15	0.90	0.16	62,86,97,99	0
5	NAG	A	611	14/15	0.91	0.16	58,70,79,83	0
6	FUL	A	610	10/11	0.91	0.29	80,90,93,99	0
8	CL	B	603	1/1	0.92	0.17	78,78,78,78	0
5	NAG	A	609	14/15	0.93	0.28	90,96,101,106	0
4	EDO	A	606	4/4	0.94	0.21	53,74,75,76	0
2	CWQ	A	602	35/35	0.94	0.24	38,54,63,69	0
2	CWQ	B	602	35/35	0.94	0.20	54,69,89,94	0
5	NAG	B	608	14/15	0.94	0.20	84,91,103,109	0
7	SO4	B	616	5/5	0.95	0.15	62,79,89,100	5
7	SO4	A	619	5/5	0.95	0.19	62,73,84,93	5
2	CWQ	A	601	35/35	0.96	0.14	49,61,73,76	0
4	EDO	A	608	4/4	0.96	0.13	57,61,68,68	0
2	CWQ	B	601	35/35	0.97	0.12	50,57,66,72	0
4	EDO	B	604	4/4	0.98	0.11	57,64,68,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.