



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 10:53 am GMT

PDB ID : 5DYY  
Title : Crystal structure of human butyrylcholinesterase in complex with N-((1-benzylpiperidin-3-yl)methyl)naphthalene-2-sulfonamide  
Authors : Coquelle, N.; Brus, B.; Colletier, J.P.  
Deposited on : 2015-09-25  
Resolution : 2.65 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : recalc28906  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28906

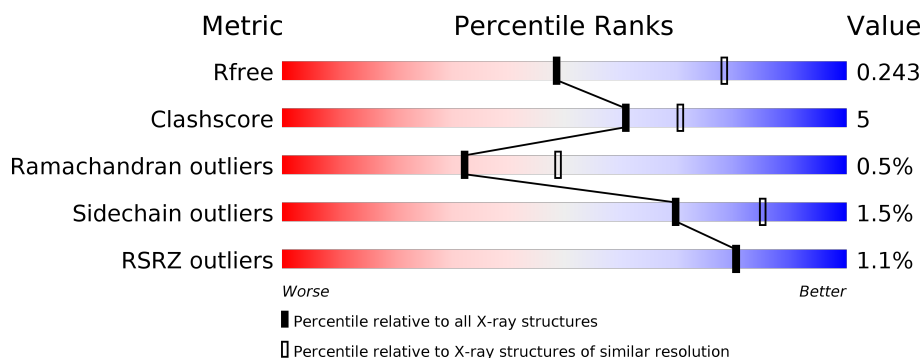
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	530	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; right: 0;">84%</div> <div style="position: absolute; top: 10px; right: 10px;">15%</div> <div style="position: absolute; top: 10px; right: 0;">•</div> </div> </div>
1	B	530	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; right: 0;">85%</div> <div style="position: absolute; top: 10px; right: 10px;">14%</div> <div style="position: absolute; top: 10px; right: 0;">•</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
2	GOL	A	601	-	-	-	X
2	GOL	A	602	-	-	-	X
2	GOL	A	603	-	-	-	X
2	GOL	B	601	-	-	-	X
2	GOL	B	602	-	-	-	X
5	CL	A	606	-	-	-	X
5	CL	B	606	-	-	-	X
6	NAG	A	611	X	-	-	-
6	NAG	A	612	X	-	-	-
6	NAG	A	614	X	-	-	-
6	NAG	A	617	X	-	-	-
6	NAG	B	607	X	-	-	-
6	NAG	B	608	X	-	-	-
6	NAG	B	609	X	-	-	-
6	NAG	B	616	X	-	-	X
8	FUL	A	613	X	-	-	X
8	FUL	A	619	-	-	-	X
8	FUL	B	612	-	-	-	X

## 2 Entry composition [i](#)

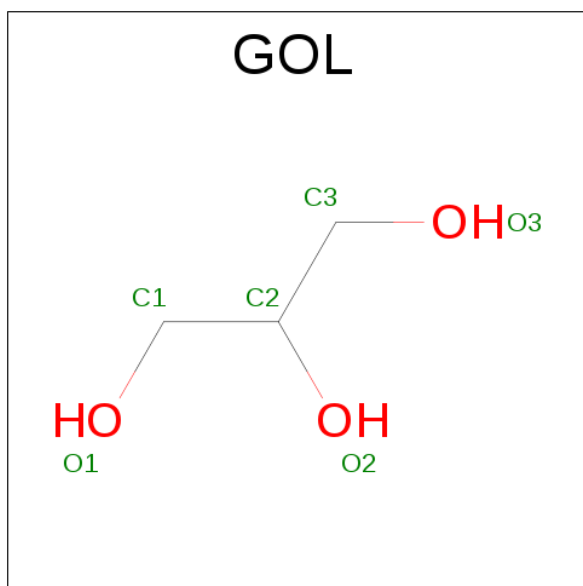
There are 9 unique types of molecules in this entry. The entry contains 9015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3	3	0
			4213	2718	710	770	15			
1	B	525	Total	C	N	O	S	4	0	0
			4163	2690	697	761	15			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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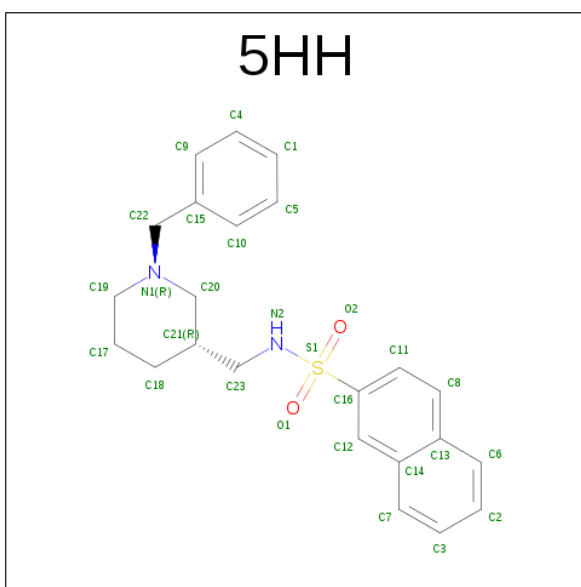
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is N-{[(3R)-1-benzylpiperidin-3-yl]methyl}naphthalene-2-sulfonamide (three-letter code: 5HH) (formula: C<sub>23</sub>H<sub>26</sub>N<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			28	23	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			28	23	2	2	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



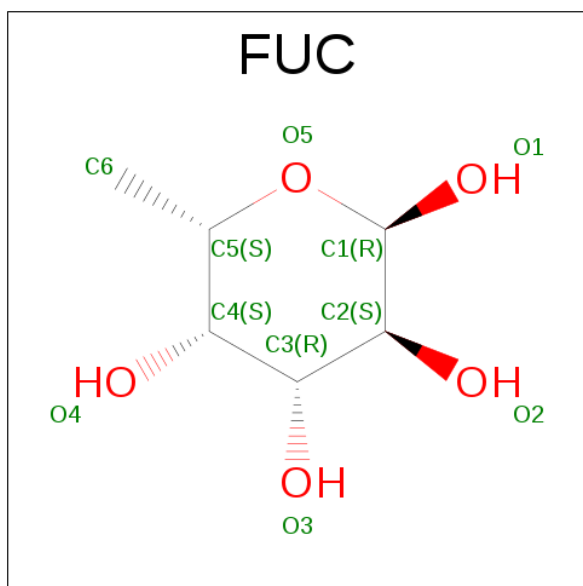
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1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

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

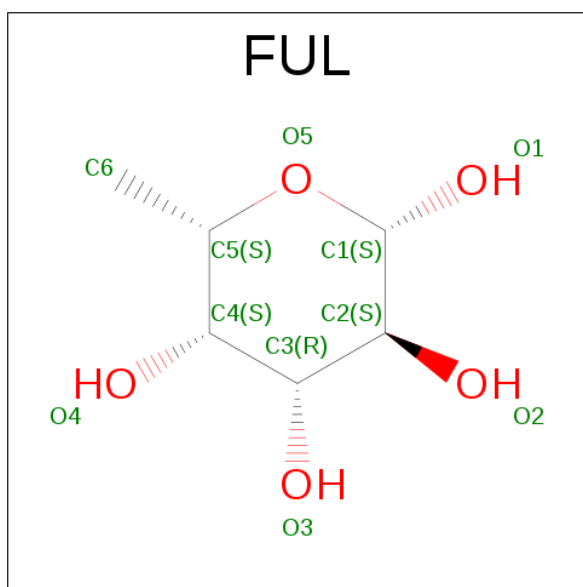
- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



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

- Molecule 8 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
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	B	1	Total	C	O	0	0
			10	6	4		

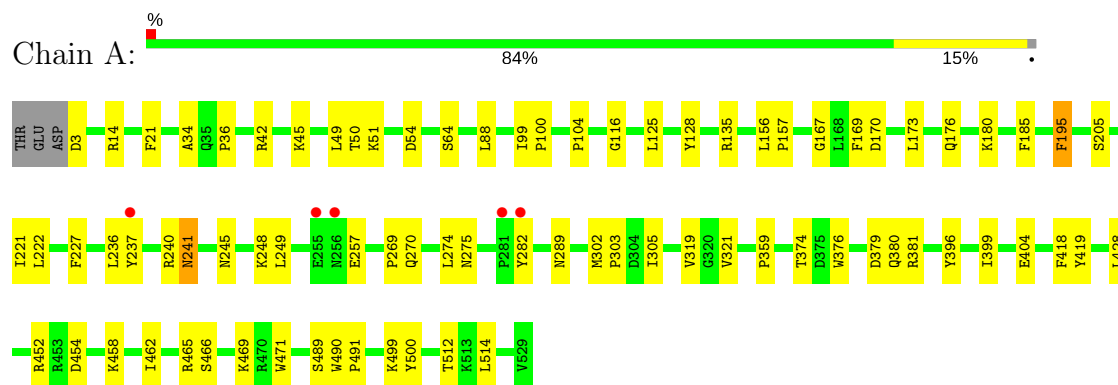
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	119	Total	O	0	0
			119	119		
9	B	114	Total	O	0	0
			114	114		

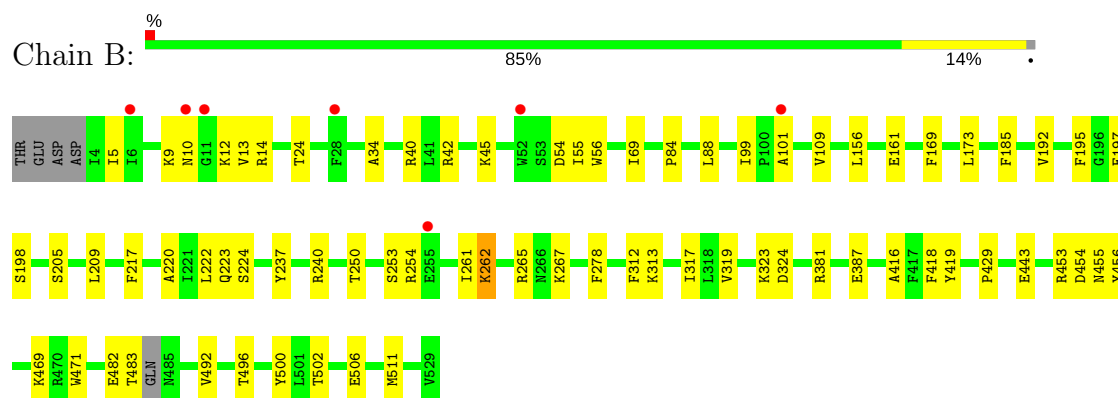
### 3 Residue-property plots [i](#)

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 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.97Å 80.19Å 232.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.21 – 2.65 46.21 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.21-2.65) 99.8 (46.21-2.65)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.187 , 0.244 0.185 , 0.243	Depositor DCC
$R_{free}$ test set	1255 reflections (2.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, CSO, NAG, CL, EDO, 5HH, FUC, FUL

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	0.45	1/4334 (0.0%)	0.60	1/5883 (0.0%)
1	B	0.47	0/4273	0.59	0/5801
All	All	0.46	1/8607 (0.0%)	0.60	1/11684 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	PRO	C-N	5.74	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	LEU	CA-CB-CG	5.12	127.06	115.30

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	4213	0	4104	45	1
1	B	4163	0	4038	45	1
2	A	18	0	24	0	0
2	B	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	6	0	0
3	B	8	0	12	0	0
4	A	28	0	0	0	0
4	B	28	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	140	0	124	1	0
6	B	126	0	115	1	0
7	A	10	0	10	0	0
8	A	20	0	20	2	0
8	B	10	0	10	1	0
9	A	119	0	0	4	0
9	B	114	0	0	4	0
All	All	9015	0	8479	90	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (90) 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:217:PHE:O	1:B:313:LYS:NZ	2.03	0.92
1:B:99:ILE:HD11	1:B:185:PHE:HB3	1.65	0.78
1:A:100:PRO:HG2	1:A:104:PRO:HG3	1.67	0.74
1:B:250:THR:HB	1:B:267:LYS:HE2	1.72	0.71
1:B:161:GLU:OE1	1:B:265:ARG:NH1	2.22	0.71
1:A:156:LEU:HD13	1:A:257:GLU:HB3	1.73	0.71
1:B:482:GLU:HG2	1:B:483:THR:H	1.55	0.71
1:B:69:ILE:CD1	1:B:84:PRO:HD2	2.22	0.70
1:B:381:ARG:NH2	1:B:387:GLU:OE1	2.27	0.68
1:A:3:ASP:N	9:A:702:HOH:O	2.26	0.68
1:B:99:ILE:CD1	1:B:185:PHE:HB3	2.28	0.63
1:A:396:TYR:OH	9:A:701:HOH:O	2.15	0.63
1:B:34:ALA:HB2	1:B:173:LEU:HD23	1.80	0.61
1:B:253:SER:O	1:B:254:ARG:HD3	2.01	0.61
1:B:42:ARG:O	1:B:265:ARG:NH2	2.35	0.60
1:B:220:ALA:HB3	1:B:317:ILE:HG22	1.84	0.59
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.87	0.57
1:B:319:VAL:O	1:B:418:PHE:HA	2.05	0.57
1:A:245:ASN:HB3	8:A:613:FUL:H5	1.88	0.56
1:A:3:ASP:OD2	1:A:14:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:HD12	1:B:84:PRO:HD2	1.87	0.56
1:A:42:ARG:NH2	1:A:269:PRO:HD3	2.20	0.55
1:A:157:PRO:HD2	1:A:240:ARG:CZ	2.37	0.55
1:B:109:VAL:HB	1:B:192:VAL:HG22	1.89	0.55
1:B:69:ILE:CD1	1:B:84:PRO:CD	2.85	0.55
1:A:248:LYS:HD3	8:A:613:FUL:H61	1.89	0.54
1:B:262:LYS:C	1:B:262:LYS:HD2	2.28	0.53
1:B:12:LYS:HB2	1:B:55:ILE:HG12	1.90	0.53
1:B:323:LYS:HE2	1:B:324:ASP:OD2	2.08	0.53
1:B:454:ASP:O	1:B:456:TYR:N	2.38	0.53
1:B:492:VAL:HG13	9:B:709:HOH:O	2.08	0.52
1:A:21:PHE:O	1:A:135:ARG:NH2	2.37	0.52
1:A:404:GLU:HG2	9:A:815:HOH:O	2.08	0.52
1:B:278:PHE:O	8:B:612:FUL:O4	2.27	0.52
1:A:319:VAL:O	1:A:418:PHE:HA	2.10	0.52
1:A:45:LYS:HD2	1:A:169:PHE:CD2	2.45	0.52
1:B:13:VAL:HG12	1:B:56:TRP:HB3	1.92	0.51
1:A:419:TYR:HB3	1:A:490:TRP:CZ2	2.46	0.51
1:B:5:ILE:HD13	1:B:55:ILE:HD13	1.93	0.51
1:A:282:TYR:CE2	1:A:359:PRO:HB2	2.45	0.51
1:A:195:PHE:HB3	1:A:221:ILE:HB	1.94	0.49
1:A:321:VAL:HG21	1:A:399:ILE:HG12	1.94	0.49
1:B:429:PRO:HD3	2:B:602:GOL:H32	1.94	0.49
1:B:443:GLU:HG2	9:B:740:HOH:O	2.13	0.49
1:A:302:MET:HB2	1:A:305:ILE:HD12	1.95	0.48
1:B:198:SER:HA	1:B:224:SER:O	2.14	0.48
1:B:69:ILE:HD13	1:B:84:PRO:CD	2.44	0.47
1:A:469:LYS:HB2	1:A:469:LYS:HE2	1.67	0.47
1:A:374:THR:HG22	1:A:376:TRP:CZ2	2.50	0.47
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.79	0.47
1:B:381:ARG:HH22	1:B:387:GLU:CD	2.18	0.46
1:A:458:LYS:O	1:A:462:ILE:HD12	2.16	0.46
1:B:500:TYR:CZ	1:B:511:MET:HB2	2.51	0.45
1:A:241:ASN:ND2	6:A:612:NAG:C7	2.79	0.45
1:B:9:LYS:C	1:B:10:ASN:HD22	2.20	0.45
1:A:50:THR:OG1	1:A:51:LYS:N	2.49	0.45
1:A:465[A]:ARG:HH22	1:A:469:LYS:NZ	2.14	0.45
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.51	0.44
1:A:176:GLN:OE1	1:A:180:LYS:HE3	2.18	0.44
1:B:205:SER:HB3	1:B:222:LEU:HD21	1.99	0.44
1:B:262:LYS:HE3	9:B:701:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLY:O	1:A:170:ASP:HB2	2.18	0.44
1:A:99:ILE:HD11	1:A:185:PHE:HD2	1.83	0.44
1:A:452:ARG:C	1:A:454:ASP:H	2.22	0.43
1:A:64:SER:HB2	1:A:88:LEU:HD23	1.99	0.43
1:A:282:TYR:HE2	1:A:359:PRO:HB2	1.84	0.43
1:B:156:LEU:HD12	1:B:261:ILE:HD11	2.00	0.43
1:A:34:ALA:HB2	1:A:173:LEU:HD23	2.00	0.43
1:B:209:LEU:HD23	1:B:312:PHE:HB3	2.01	0.43
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.85	0.42
1:B:223:GLN:HG2	1:B:419:TYR:OH	2.19	0.42
1:A:500:TYR:CE1	1:A:514:LEU:HB2	2.55	0.42
1:B:469:LYS:HB2	1:B:469:LYS:HE2	1.79	0.42
1:A:380:GLN:HA	1:A:381:ARG:C	2.39	0.42
1:A:249:LEU:HB3	1:A:275:ASN:OD1	2.20	0.42
1:B:45:LYS:HD2	1:B:169:PHE:CD2	2.55	0.42
1:B:161:GLU:HB3	1:B:265:ARG:HH12	1.84	0.42
1:B:84:PRO:HG2	1:B:88:LEU:HD21	2.00	0.42
1:A:270:GLN:O	1:A:274:LEU:HB2	2.20	0.41
1:A:125:LEU:HD12	1:A:128:TYR:CE2	2.55	0.41
1:B:24:THR:O	1:B:101:ALA:HB3	2.20	0.41
1:B:5:ILE:HD11	1:B:14:ARG:HH21	1.86	0.41
1:A:99:ILE:HD11	1:A:185:PHE:CD2	2.56	0.41
1:A:489:SER:O	1:A:491:PRO:HD3	2.21	0.41
1:A:499:LYS:HG2	1:A:512:THR:HG22	2.03	0.41
1:A:34:ALA:C	1:A:49:LEU:HD13	2.42	0.40
1:B:237:TYR:HE2	6:B:610:NAG:H82	1.86	0.40
1:A:289:ASN:ND2	9:A:717:HOH:O	2.54	0.40
1:B:197:GLU:HA	1:B:223:GLN:O	2.21	0.40
1:B:416:ALA:N	9:B:709:HOH:O	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:OH	1:B:453:ARG:O[1_545]	2.00	0.20

## 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	527/530 (99%)	502 (95%)	23 (4%)	2 (0%)	38	54
1	B	520/530 (98%)	495 (95%)	22 (4%)	3 (1%)	28	43
All	All	1047/1060 (99%)	997 (95%)	45 (4%)	5 (0%)	32	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	ASN
1	A	54	ASP
1	B	54	ASP
1	B	506	GLU
1	A	116	GLY

### 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	452/454 (100%)	446 (99%)	6 (1%)	73	88
1	B	443/454 (98%)	436 (98%)	7 (2%)	68	84
All	All	895/908 (99%)	882 (98%)	13 (2%)	70	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	PHE

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	379	ASP
1	A	428	LEU
1	A	466	SER
1	A	471	TRP
1	B	40	ARG
1	B	195	PHE
1	B	240	ARG
1	B	262	LYS
1	B	471	TRP
1	B	496	THR
1	B	502	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	ASN
1	B	479	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	CSO	A	66	1	4,6,7	1.15	1 (25%)	1,6,8	1.38	0
1	CSO	B	66	1	4,6,7	0.87	0	1,6,8	1.74	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
1	CSO	A	66	1	-	0/1/5/7	0/0/0/0
1	CSO	B	66	1	-	0/1/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CSO	CA-C	2.09	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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	GOL	A	601	-	5,5,5	0.30	0	5,5,5	0.54	0
2	GOL	A	602	-	5,5,5	0.55	0	5,5,5	0.30	0
2	GOL	A	603	-	5,5,5	0.43	0	5,5,5	0.29	0
3	EDO	A	604	-	3,3,3	0.58	0	2,2,2	0.11	0
4	5HH	A	605	-	31,31,31	2.71	4 (12%)	42,43,43	2.67	12 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	607	1	14,14,15	0.77	1 (7%)	15,19,21	0.72	0
6	NAG	A	608	1,7	14,14,15	0.60	1 (7%)	15,19,21	0.54	0
7	FUC	A	609	6	9,10,11	1.84	4 (44%)	13,14,16	1.06	2 (15%)
6	NAG	A	610	1,6	14,14,15	0.23	0	15,19,21	0.70	0
6	NAG	A	611	6	14,14,15	0.58	0	15,19,21	0.49	0
6	NAG	A	612	1,8	14,14,15	0.21	0	15,19,21	1.02	1 (6%)
8	FUL	A	613	6	9,10,11	1.73	2 (22%)	13,14,16	1.67	3 (23%)
6	NAG	A	614	1	14,14,15	0.88	1 (7%)	15,19,21	1.40	1 (6%)
6	NAG	A	615	1,6	14,14,15	0.27	0	15,19,21	0.57	0
6	NAG	A	616	6	14,14,15	1.01	1 (7%)	15,19,21	0.87	1 (6%)
6	NAG	A	617	1,8,6	14,14,15	1.21	2 (14%)	15,19,21	1.05	1 (6%)
6	NAG	A	618	6	14,14,15	0.26	0	15,19,21	0.44	0
8	FUL	A	619	6	9,10,11	1.77	3 (33%)	13,14,16	1.13	1 (7%)
2	GOL	B	601	-	5,5,5	0.34	0	5,5,5	0.33	0
2	GOL	B	602	-	5,5,5	0.26	0	5,5,5	0.81	0
3	EDO	B	603	-	3,3,3	0.61	0	2,2,2	0.04	0
3	EDO	B	604	-	3,3,3	0.67	0	2,2,2	0.35	0
4	5HH	B	605	-	31,31,31	2.49	4 (12%)	42,43,43	3.10	12 (28%)
6	NAG	B	607	1	14,14,15	1.26	2 (14%)	15,19,21	1.66	3 (20%)
6	NAG	B	608	1	14,14,15	0.70	1 (7%)	15,19,21	0.76	0
6	NAG	B	609	1	14,14,15	0.37	0	15,19,21	1.31	3 (20%)
6	NAG	B	610	1,8,6	14,14,15	0.16	0	15,19,21	0.60	0
6	NAG	B	611	6	14,14,15	0.18	0	15,19,21	0.56	0
8	FUL	B	612	6	9,10,11	1.80	3 (33%)	13,14,16	1.97	3 (23%)
6	NAG	B	613	1	14,14,15	0.36	0	15,19,21	0.81	1 (6%)
6	NAG	B	614	1	14,14,15	0.29	0	15,19,21	0.59	0
6	NAG	B	615	1	14,14,15	0.56	0	15,19,21	0.71	1 (6%)
6	NAG	B	616	1	14,14,15	0.59	0	15,19,21	1.07	1 (6%)

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	GOL	A	601	-	-	0/4/4/4	0/0/0/0
2	GOL	A	602	-	-	0/4/4/4	0/0/0/0
2	GOL	A	603	-	-	0/4/4/4	0/0/0/0
3	EDO	A	604	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5HH	A	605	-	-	0/16/26/26	0/4/4/4
6	NAG	A	607	1	-	0/6/23/26	0/1/1/1
6	NAG	A	608	1,7	-	0/6/23/26	0/1/1/1
7	FUC	A	609	6	-	0/0/17/20	0/1/1/1
6	NAG	A	610	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	611	6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	612	1,8	1/1/5/7	0/6/23/26	0/1/1/1
8	FUL	A	613	6	1/1/4/5	0/0/17/20	0/1/1/1
6	NAG	A	614	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	615	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	616	6	-	0/6/23/26	0/1/1/1
6	NAG	A	617	1,8,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	618	6	-	0/6/23/26	0/1/1/1
8	FUL	A	619	6	-	0/0/17/20	0/1/1/1
2	GOL	B	601	-	-	0/4/4/4	0/0/0/0
2	GOL	B	602	-	-	0/4/4/4	0/0/0/0
3	EDO	B	603	-	-	0/1/1/1	0/0/0/0
3	EDO	B	604	-	-	0/1/1/1	0/0/0/0
4	5HH	B	605	-	-	0/16/26/26	0/4/4/4
6	NAG	B	607	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	608	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	609	1	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	610	1,8,6	-	0/6/23/26	0/1/1/1
6	NAG	B	611	6	-	0/6/23/26	0/1/1/1
8	FUL	B	612	6	-	0/0/17/20	0/1/1/1
6	NAG	B	613	1	-	0/6/23/26	0/1/1/1
6	NAG	B	614	1	-	0/6/23/26	0/1/1/1
6	NAG	B	615	1	-	0/6/23/26	0/1/1/1
6	NAG	B	616	1	1/1/5/7	0/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	5HH	C22-C15	-6.16	1.40	1.51
4	B	605	5HH	C22-C15	-5.14	1.41	1.51
4	A	605	5HH	S1-N2	-4.24	1.56	1.61
8	A	619	FUL	O5-C1	-3.29	1.38	1.43
8	B	612	FUL	O5-C1	-3.28	1.38	1.43
8	A	613	FUL	O5-C1	-3.25	1.38	1.43
7	A	609	FUC	O5-C1	-2.98	1.38	1.43
8	B	612	FUL	O2-C2	-2.23	1.38	1.43
7	A	609	FUC	O2-C2	-2.18	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	612	FUL	O4-C4	-2.17	1.38	1.43
7	A	609	FUC	O3-C3	-2.09	1.38	1.43
8	A	613	FUL	O2-C2	-2.08	1.38	1.43
7	A	609	FUC	C2-C3	-2.06	1.49	1.52
8	A	619	FUL	O2-C2	-2.05	1.38	1.43
8	A	619	FUL	O3-C3	-2.03	1.38	1.43
6	A	607	NAG	C1-C2	2.04	1.55	1.52
6	A	608	NAG	C1-C2	2.06	1.55	1.52
6	B	608	NAG	C1-C2	2.25	1.55	1.52
4	B	605	5HH	C12-C16	2.34	1.40	1.36
6	B	607	NAG	C1-C2	2.41	1.55	1.52
6	A	617	NAG	O5-C1	2.98	1.48	1.43
6	A	614	NAG	O5-C1	3.18	1.48	1.43
6	A	617	NAG	C1-C2	3.22	1.56	1.52
6	A	616	NAG	O5-C1	3.38	1.49	1.43
6	B	607	NAG	O5-C1	3.93	1.50	1.43
4	B	605	5HH	O2-S1	7.47	1.51	1.43
4	A	605	5HH	O1-S1	8.01	1.52	1.43
4	B	605	5HH	O1-S1	8.72	1.52	1.43
4	A	605	5HH	O2-S1	9.20	1.53	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	5HH	O1-S1-O2	-11.37	105.00	119.55
4	B	605	5HH	C21-C23-N2	-7.45	100.96	111.81
4	B	605	5HH	O1-S1-O2	-7.01	110.58	119.55
4	B	605	5HH	C17-C18-C21	-5.17	102.69	112.19
4	B	605	5HH	C11-C16-S1	-4.63	114.66	119.77
4	B	605	5HH	C18-C17-C19	-4.48	105.06	110.96
4	A	605	5HH	C23-N2-S1	-4.46	111.47	119.91
4	A	605	5HH	C17-C18-C21	-4.35	104.20	112.19
8	A	613	FUL	O5-C1-C2	-4.03	104.48	110.79
4	A	605	5HH	C21-C23-N2	-3.78	106.31	111.81
4	A	605	5HH	C11-C16-S1	-2.74	116.74	119.77
4	B	605	5HH	C8-C13-C6	-2.31	117.70	123.18
7	A	609	FUC	C1-C2-C3	-2.21	106.86	109.65
8	B	612	FUL	C6-C5-C4	-2.14	109.26	113.07
7	A	609	FUC	C2-C3-C4	-2.01	107.37	110.88
4	B	605	5HH	C16-C12-C14	-2.01	117.64	120.22
6	B	615	NAG	C1-O5-C5	2.01	114.93	112.17
6	B	609	NAG	C1-O5-C5	2.05	114.99	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	619	FUL	O5-C5-C4	2.08	113.06	109.62
8	B	612	FUL	C2-C3-C4	2.32	114.93	110.88
4	A	605	5HH	O2-S1-C16	2.32	110.83	107.95
4	A	605	5HH	O1-S1-N2	2.32	110.79	107.03
8	A	613	FUL	O5-C5-C4	2.45	113.66	109.62
6	A	612	NAG	C1-O5-C5	2.47	115.57	112.17
8	A	613	FUL	C3-C4-C5	2.48	113.58	109.68
4	A	605	5HH	C17-C19-N1	2.49	115.55	111.40
6	B	613	NAG	C1-O5-C5	2.51	115.63	112.17
6	B	609	NAG	C1-C2-N2	2.53	114.81	110.49
6	A	616	NAG	C1-O5-C5	2.76	115.97	112.17
6	B	607	NAG	C1-C2-N2	3.13	115.83	110.49
4	A	605	5HH	C19-N1-C20	3.15	114.70	109.74
4	B	605	5HH	C22-N1-C19	3.17	117.80	111.08
6	B	609	NAG	C2-N2-C7	3.31	127.78	122.94
6	B	607	NAG	C1-O5-C5	3.49	116.98	112.17
4	A	605	5HH	C16-S1-N2	3.61	112.27	107.53
6	B	616	NAG	C1-O5-C5	3.65	117.20	112.17
6	A	617	NAG	C1-O5-C5	3.75	117.33	112.17
4	A	605	5HH	C12-C16-S1	3.77	123.13	120.10
6	B	607	NAG	C2-N2-C7	4.04	128.84	122.94
4	B	605	5HH	C18-C21-C20	4.09	113.35	108.67
6	A	614	NAG	C1-O5-C5	4.77	118.75	112.17
4	A	605	5HH	C22-N1-C19	4.93	121.51	111.08
4	B	605	5HH	C12-C16-S1	5.20	124.28	120.10
8	B	612	FUL	C1-C2-C3	5.27	116.34	109.65
4	B	605	5HH	C22-N1-C20	5.69	119.56	111.14
4	B	605	5HH	C16-S1-N2	10.33	121.09	107.53

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	613	FUL	C1
6	B	616	NAG	C1
6	A	614	NAG	C1
6	A	611	NAG	C1
6	B	609	NAG	C1
6	B	607	NAG	C1
6	A	612	NAG	C1
6	B	608	NAG	C1
6	A	617	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	612	NAG	1	0
8	A	613	FUL	2	0
2	B	602	GOL	1	0
6	B	610	NAG	1	0
8	B	612	FUL	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	526/530 (99%)	-0.23	5 (0%) 82 82	27, 45, 71, 115	1 (0%)
1	B	524/530 (98%)	-0.25	7 (1%) 77 77	27, 44, 78, 128	4 (0%)
All	All	1050/1060 (99%)	-0.24	12 (1%) 80 80	27, 44, 73, 128	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	3.1
1	A	237	TYR	2.9
1	B	52	TRP	2.8
1	B	101	ALA	2.6
1	A	255	GLU	2.6
1	B	6	ILE	2.4
1	B	10	ASN	2.2
1	B	28	PHE	2.2
1	B	11	GLY	2.1
1	B	255	GLU	2.1
1	A	256	ASN	2.1
1	A	281	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	B	66	7/8	0.98	0.14	-	33,35,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSO	A	66	7/8	0.97	0.10	-	41,42,53,59	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	FUL	A	619	10/11	0.83	0.29	8.94	94,100,109,109	0
5	CL	B	606	1/1	0.96	0.45	6.52	50,50,50,50	0
2	GOL	A	602	6/6	0.87	0.31	5.89	43,52,55,55	0
2	GOL	A	603	6/6	0.86	0.28	5.80	59,63,67,72	0
5	CL	A	606	1/1	0.97	0.47	5.78	48,48,48,48	0
2	GOL	B	602	6/6	0.75	0.26	4.99	45,50,55,60	0
8	FUL	A	613	10/11	0.90	0.46	4.64	90,97,100,109	0
2	GOL	A	601	6/6	0.95	0.28	4.60	58,62,66,69	0
8	FUL	B	612	10/11	0.92	0.40	4.38	76,85,88,93	0
6	NAG	B	616	14/15	0.77	0.23	3.88	88,101,106,107	0
2	GOL	B	601	6/6	0.94	0.27	2.74	49,54,60,65	0
6	NAG	B	614	14/15	0.90	0.20	0.51	58,63,70,75	0
4	5HH	A	605	28/28	0.95	0.18	0.44	39,49,56,57	0
3	EDO	B	604	4/4	0.94	0.17	0.26	49,50,51,52	0
4	5HH	B	605	28/28	0.95	0.17	0.22	31,41,53,60	0
3	EDO	A	604	4/4	0.91	0.14	0.05	61,64,70,71	0
3	EDO	B	603	4/4	0.90	0.14	-0.00	47,50,55,55	0
6	NAG	A	615	14/15	0.94	0.14	-0.46	53,63,67,68	0
6	NAG	B	613	14/15	0.76	0.23	-	91,99,102,104	0
6	NAG	B	611	14/15	0.82	0.44	-	96,102,110,111	0
7	FUC	A	609	10/11	0.87	0.35	-	91,105,108,109	0
6	NAG	A	614	14/15	0.86	0.20	-	66,69,76,78	0
6	NAG	A	618	14/15	0.69	0.50	-	118,123,130,130	0
6	NAG	A	610	14/15	0.94	0.15	-	62,68,81,84	0
6	NAG	A	611	14/15	0.88	0.33	-	88,97,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	B	609	14/15	0.79	0.34	-	86,91,96,102	0
6	NAG	B	607	14/15	0.67	0.38	-	91,108,111,115	0
6	NAG	A	616	14/15	0.78	0.20	-	57,71,79,81	0
6	NAG	A	612	14/15	0.85	0.26	-	92,109,111,111	0
6	NAG	B	608	14/15	0.66	0.29	-	87,110,115,117	0
6	NAG	A	617	14/15	0.73	0.22	-	89,109,115,117	0
6	NAG	B	615	14/15	0.66	0.34	-	88,106,109,112	0
6	NAG	A	608	14/15	0.84	0.28	-	78,93,101,103	0
6	NAG	A	607	14/15	0.82	0.34	-	75,85,93,94	0
6	NAG	B	610	14/15	0.91	0.28	-	80,86,96,101	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.