



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2018 – 04:55 PM EST

PDB ID : 5NN0
Title : Crystal structure of huBChE with N-((1-(2,3-dihydro-1H-inden-2-yl)piperidin-3-yl)methyl)-N-(2-(dimethylamino)ethyl)-2-naphthamide.
Authors : Coquelle, N.; Brus, B.; Colletier, J.P.
Deposited on : 2017-04-07
Resolution : 2.10 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : rb-20030736
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) : rb-20030736

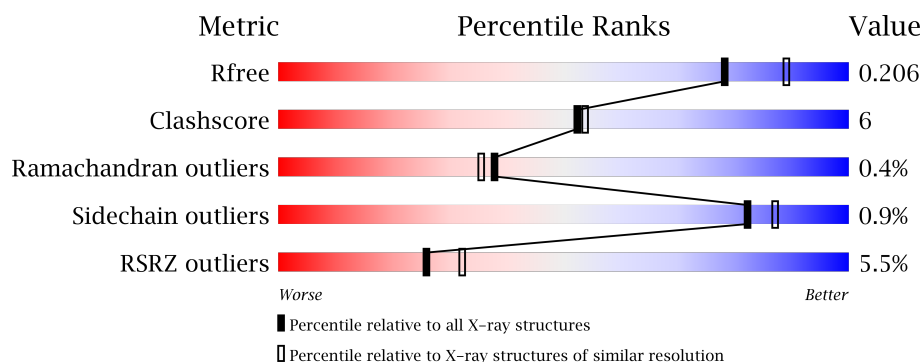
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 ≥ 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 style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> </div> <div> <div style="width: 5%;"></div> <div style="width: 86%;"></div> <div style="width: 13%;"></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
10	PEG	A	629	-	-	-	X
2	NAG	A	607	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	608	X	-	-	-
3	FUC	A	605	X	-	-	-
5	SO4	A	614	-	-	-	X
7	MES	A	624	-	-	-	X
7	MES	A	625	-	-	-	X
8	92H	A	626	-	-	-	X
9	1PG	A	628	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4858 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.

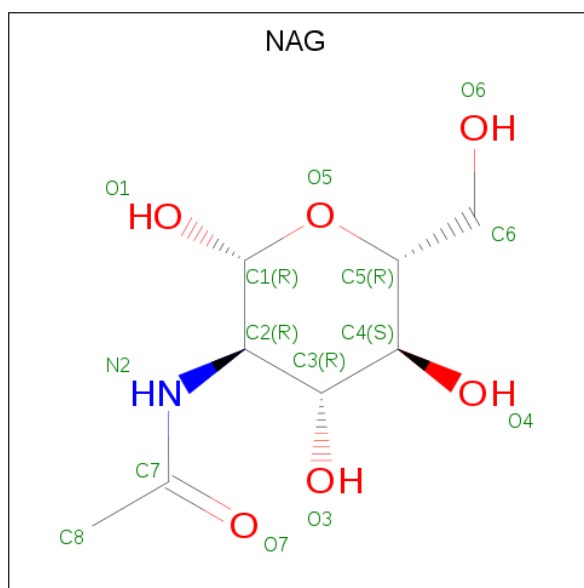
- Molecule 1 is a protein called Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4236	2743	701	777	15	0	14	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



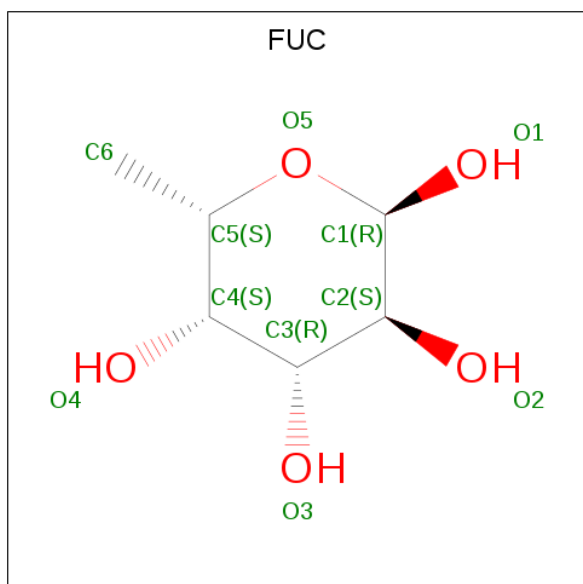
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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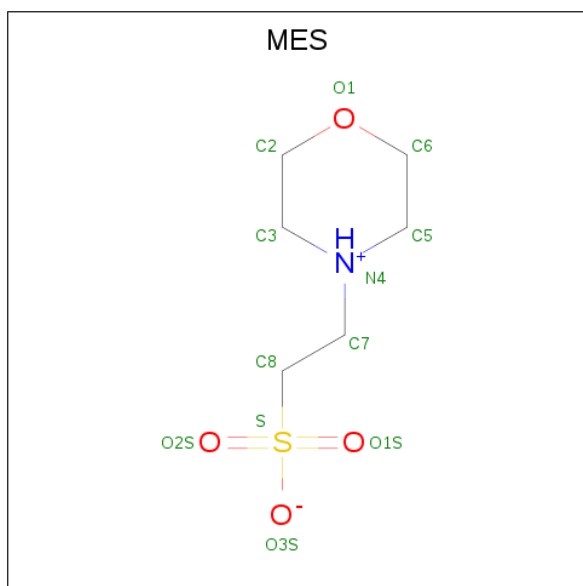
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Cl	0	0
			3	3		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0
			12	6	1	4	1	0
7	A	1	Total	C	N	O	S	0
			12	6	1	4	1	0

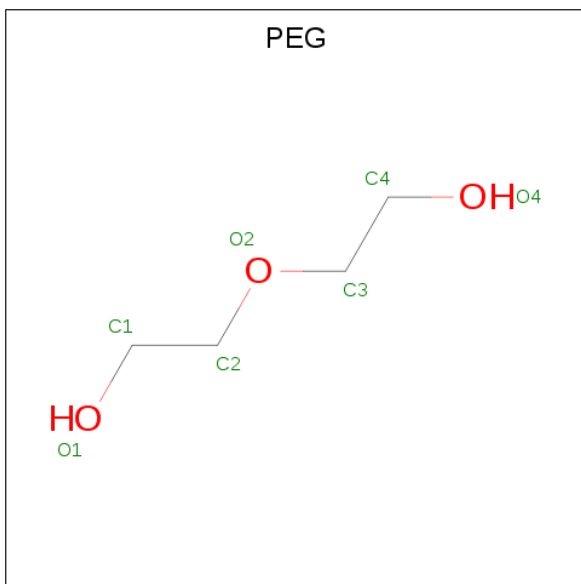
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 34	C 30	N 3	O 1	0	0
8	A	1	Total 34	C 30	N 3	O 1	0	0

- # 1PG

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			17	11	6		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

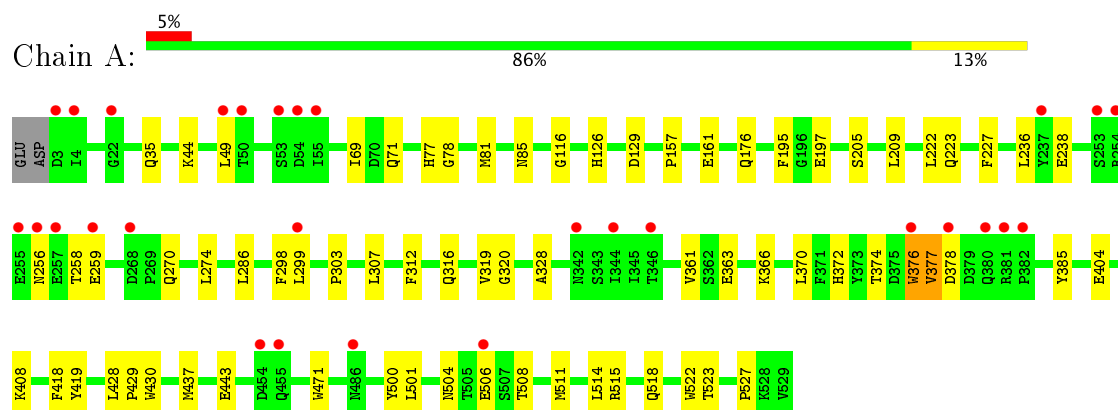
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	314	Total	O	0	0
			314	314		

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



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.97Å 154.97Å 126.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 2.10 47.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.83-2.10) 99.3 (47.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.169 , 0.206 0.168 , 0.206	Depositor DCC
R_{free} test set	2236 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4858	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 92H, GOL, NAG, CL, 1PG, FUC, MES, PEG, 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	0.38	0/4393	0.53	0/5970

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	4236	0	4141	55	0
2	A	112	0	99	0	0
3	A	30	0	30	0	0
4	A	12	0	16	4	0
5	A	35	0	0	1	0
6	A	3	0	0	0	0
7	A	24	0	24	7	0
8	A	68	0	0	1	0
9	A	17	0	24	8	0
10	A	7	0	10	2	0
11	A	314	0	0	5	0
All	All	4858	0	4344	56	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 (56) 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:A:77:HIS:HE2	9:A:628:1PG:H42	1.52	0.74
1:A:85:ASN:ND2	4:A:613:GOL:H11	2.05	0.72
1:A:372:HIS:NE2	5:A:620:SO4:O4	2.19	0.70
1:A:514:LEU:HD12	7:A:625:MES:H52	1.74	0.69
1:A:316:GLN:HE22	10:A:629:PEG:H22	1.59	0.66
1:A:504[B]:ASN:OD1	11:A:701:HOH:O	2.12	0.66
1:A:85:ASN:HD22	4:A:613:GOL:H11	1.62	0.63
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.35	0.62
1:A:157:PRO:HG2	1:A:236:LEU:HD12	1.83	0.60
1:A:377:VAL:HG23	1:A:378:ASP:H	1.67	0.60
1:A:515:ARG:NH2	7:A:625:MES:H71	2.18	0.59
1:A:81:MET:HE3	9:A:628:1PG:H21	1.85	0.57
1:A:69[B]:ILE:HG23	1:A:71[B]:GLN:HG2	1.87	0.57
1:A:116:GLY:HA2	8:A:627:92H:OAY	2.05	0.56
1:A:361:VAL:O	1:A:366:LYS:NZ	2.38	0.56
1:A:515:ARG:HD3	7:A:625:MES:H32	1.87	0.56
1:A:522:TRP:O	1:A:527:PRO:HD3	2.06	0.54
1:A:176[A]:GLN:NE2	11:A:714:HOH:O	2.40	0.54
1:A:508:THR:OG1	11:A:702:HOH:O	2.18	0.54
1:A:77:HIS:NE2	9:A:628:1PG:H42	2.20	0.53
1:A:319:VAL:O	1:A:418:PHE:HA	2.08	0.53
1:A:443:GLU:OE2	9:A:628:1PG:H13	2.10	0.52
1:A:316:GLN:NE2	10:A:629:PEG:H22	2.25	0.51
1:A:428:LEU:HD23	1:A:430:TRP:H	1.76	0.51
1:A:77:HIS:HE2	9:A:628:1PG:H32	1.76	0.50
1:A:126:HIS:HB2	4:A:613:GOL:H12	1.92	0.50
1:A:81:MET:HE3	9:A:628:1PG:H51	1.93	0.50
1:A:515:ARG:HH22	7:A:625:MES:H71	1.77	0.49
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.94	0.48
1:A:518:GLN:HG3	7:A:624:MES:H62	1.96	0.47
1:A:77:HIS:HE1	9:A:628:1PG:H72	1.78	0.47
1:A:81:MET:CE	9:A:628:1PG:H21	2.45	0.46
1:A:129:ASP:OD1	4:A:612:GOL:H31	2.14	0.46
1:A:270:GLN:O	1:A:274:LEU:HG	2.15	0.46
1:A:238:GLU:OE1	11:A:703:HOH:O	2.19	0.46
1:A:197:GLU:HA	1:A:223:GLN:O	2.16	0.46
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.51	0.46
1:A:328:ALA:HB2	1:A:437:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASN:OD1	1:A:259:GLU:HG2	2.17	0.45
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.82	0.45
1:A:363[A]:GLU:CD	1:A:363[A]:GLU:H	2.20	0.44
1:A:404[B]:GLU:OE2	1:A:408:LYS:HE2	2.16	0.44
1:A:370:LEU:O	1:A:374:THR:OG1	2.30	0.44
1:A:518:GLN:HA	7:A:624:MES:H62	2.01	0.43
1:A:35:GLN:HA	1:A:49:LEU:HD13	2.01	0.43
1:A:501:LEU:HD11	1:A:508:THR:CG2	2.48	0.43
1:A:370:LEU:HD12	1:A:374:THR:HG21	2.01	0.43
1:A:205:SER:HB3	1:A:222[A]:LEU:HD21	2.02	0.42
1:A:298:PHE:HD2	1:A:299[B]:LEU:HG	1.84	0.42
7:A:625:MES:H82	7:A:625:MES:H31	1.85	0.41
1:A:376:TRP:HH2	1:A:385:TYR:CE1	2.37	0.41
1:A:523:THR:HG22	11:A:974:HOH:O	2.20	0.41
1:A:78:GLY:HA2	1:A:429:PRO:HG2	2.01	0.41
1:A:44[B]:LYS:NZ	1:A:161:GLU:OE1	2.51	0.41
1:A:161:GLU:HG3	1:A:258:THR:HG23	2.03	0.40
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.56	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	539/529 (102%)	519 (96%)	18 (3%)	2 (0%)	38 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	VAL
1	A	506	GLU

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	457/454 (101%)	453 (99%)	4 (1%)	82	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	PHE
1	A	286	LEU
1	A	376	TRP
1	A	471	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	601	1,3,2	14,14,15	0.60	0	15,19,21	0.50	0
2	NAG	A	602	2	14,14,15	0.34	0	15,19,21	0.36	0
3	FUC	A	603	2	9,10,11	1.62	2 (22%)	13,14,16	1.43	2 (15%)
2	NAG	A	604	1,3	14,14,15	0.34	0	15,19,21	0.44	0
3	FUC	A	605	2	9,10,11	1.89	2 (22%)	13,14,16	1.18	2 (15%)
2	NAG	A	606	1	14,14,15	0.30	0	15,19,21	0.91	1 (6%)
2	NAG	A	607	1	14,14,15	0.31	0	15,19,21	0.47	0
2	NAG	A	608	1	14,14,15	0.42	0	15,19,21	0.54	0
2	NAG	A	609	1,3,2	14,14,15	0.34	0	15,19,21	0.64	0
2	NAG	A	610	2	14,14,15	0.29	0	15,19,21	0.54	0
3	FUC	A	611	2	9,10,11	1.84	2 (22%)	13,14,16	1.24	2 (15%)
4	GOL	A	612	-	5,5,5	0.50	0	5,5,5	0.46	0
4	GOL	A	613	-	5,5,5	0.35	0	5,5,5	0.63	0
5	SO4	A	614	-	4,4,4	0.16	0	6,6,6	0.16	0
5	SO4	A	615	-	4,4,4	0.17	0	6,6,6	0.11	0
5	SO4	A	616	-	4,4,4	0.22	0	6,6,6	0.16	0
5	SO4	A	617	8	4,4,4	0.18	0	6,6,6	0.23	0
5	SO4	A	618	8	4,4,4	0.39	0	6,6,6	0.27	0
5	SO4	A	619	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	620	-	4,4,4	0.13	0	6,6,6	0.18	0
7	MES	A	624	-	12,12,12	2.21	1 (8%)	14,16,16	2.09	4 (28%)
7	MES	A	625	-	12,12,12	2.01	1 (8%)	14,16,16	2.35	6 (42%)
8	92H	A	626	5	38,38,38	2.10	7 (18%)	47,53,53	1.43	6 (12%)
8	92H	A	627	-	38,38,38	2.05	7 (18%)	47,53,53	1.20	3 (6%)
9	1PG	A	628	-	16,16,16	0.54	0	15,15,15	0.36	0
10	PEG	A	629	-	6,6,6	0.50	0	5,5,5	0.20	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	NAG	A	601	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
3	FUC	A	603	2	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	604	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	605	2	1/1/4/5	0/0/17/20	0/1/1/1
2	NAG	A	606	1	-	0/6/23/26	0/1/1/1
2	NAG	A	607	1	-	0/6/23/26	0/1/1/1
2	NAG	A	608	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	609	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	610	2	-	0/6/23/26	0/1/1/1
3	FUC	A	611	2	-	0/0/17/20	0/1/1/1
4	GOL	A	612	-	-	0/4/4/4	0/0/0/0
4	GOL	A	613	-	-	0/4/4/4	0/0/0/0
5	SO4	A	614	-	-	0/0/0/0	0/0/0/0
5	SO4	A	615	-	-	0/0/0/0	0/0/0/0
5	SO4	A	616	-	-	0/0/0/0	0/0/0/0
5	SO4	A	617	8	-	0/0/0/0	0/0/0/0
5	SO4	A	618	8	-	0/0/0/0	0/0/0/0
5	SO4	A	619	-	-	0/0/0/0	0/0/0/0
5	SO4	A	620	-	-	0/0/0/0	0/0/0/0
7	MES	A	624	-	-	0/6/14/14	0/1/1/1
7	MES	A	625	-	-	0/6/14/14	0/1/1/1
8	92H	A	626	5	-	0/21/39/39	1/5/5/5
8	92H	A	627	-	-	0/21/39/39	0/5/5/5
9	1PG	A	628	-	-	0/14/14/14	0/0/0/0
10	PEG	A	629	-	-	0/4/4/4	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	624	MES	C8-S	-7.35	1.66	1.77
8	A	626	92H	CAT-CAS	-7.14	1.38	1.50
8	A	626	92H	CAX-CAW	-6.75	1.39	1.50
7	A	625	MES	C8-S	-6.64	1.67	1.77
8	A	627	92H	CAM-CAN	-6.13	1.40	1.50
8	A	627	92H	CAT-CAS	-5.97	1.40	1.50
8	A	627	92H	CAX-CAW	-5.61	1.41	1.50
8	A	626	92H	CAM-CAN	-4.34	1.43	1.50
8	A	627	92H	CAO-CAN	-3.47	1.33	1.39
8	A	627	92H	CAR-CAS	-3.30	1.34	1.39
8	A	626	92H	CAO-CAN	-3.26	1.34	1.39
8	A	626	92H	CAR-CAS	-3.20	1.34	1.39
3	A	611	FUC	C2-C3	-2.76	1.48	1.52
3	A	605	FUC	C2-C3	-2.65	1.49	1.52
8	A	626	92H	CAT-CAL	-2.52	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	626	92H	CAN-CAS	-2.19	1.35	1.39
3	A	603	FUC	C2-C3	-2.17	1.49	1.52
8	A	627	92H	CAM-CAL	-2.10	1.50	1.54
8	A	627	92H	CAN-CAS	-2.08	1.35	1.39
3	A	603	FUC	O5-C1	3.94	1.50	1.43
3	A	611	FUC	O5-C1	4.39	1.50	1.43
3	A	605	FUC	O5-C1	4.60	1.51	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	626	92H	CAN-CAM-CAL	-5.28	97.72	103.38
8	A	626	92H	CAH-CAI-CAJ	-3.96	105.74	110.96
3	A	605	FUC	C6-C5-C4	-2.67	108.31	113.07
8	A	626	92H	CAZ-CAX-CAW	-2.58	115.66	120.43
8	A	626	92H	CAT-CAS-CAN	-2.13	109.09	110.58
3	A	611	FUC	C6-C5-C4	-2.12	109.30	113.07
8	A	626	92H	CAP-CAQ-CAR	-2.12	117.30	120.21
8	A	626	92H	CAJ-NAK-CAU	2.02	110.16	108.18
3	A	611	FUC	O5-C5-C4	2.12	113.12	109.62
3	A	603	FUC	C2-C3-C4	2.25	114.80	110.88
7	A	625	MES	C7-N4-C5	2.27	117.07	111.26
7	A	624	MES	O1S-S-C8	2.28	108.75	106.79
3	A	605	FUC	O5-C5-C4	2.34	113.49	109.62
7	A	625	MES	C7-N4-C3	2.62	117.97	111.26
2	A	606	NAG	C1-O5-C5	2.70	115.89	112.17
7	A	624	MES	O2S-S-C8	2.79	109.19	106.79
7	A	625	MES	O1S-S-C8	2.80	109.19	106.79
7	A	624	MES	O3S-S-C8	2.81	109.51	106.06
8	A	627	92H	CAG-CAU-NAK	2.82	115.67	110.46
8	A	627	92H	CAX-CAW-NAE	3.04	122.71	118.77
7	A	625	MES	O3S-S-C8	3.25	110.06	106.06
3	A	603	FUC	C1-C2-C3	3.64	114.27	109.65
7	A	625	MES	C5-N4-C3	3.76	117.39	108.87
8	A	627	92H	CAJ-NAK-CAU	4.53	112.63	108.18
7	A	625	MES	O2S-S-C8	4.64	110.78	106.79
7	A	624	MES	C5-N4-C3	5.82	122.06	108.87

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	608	NAG	C1

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Mol	Chain	Res	Type	Atom
3	A	605	FUC	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	626	92H	CAG-CAH-CAI-CAJ-CAU-NAK

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	612	GOL	1	0
4	A	613	GOL	3	0
5	A	620	SO4	1	0
7	A	624	MES	2	0
7	A	625	MES	5	0
8	A	627	92H	1	0
9	A	628	1PG	8	0
10	A	629	PEG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	527/529 (99%)	0.10	29 (5%)	26 32	24, 37, 63, 90	6 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	6.1
1	A	53	SER	6.0
1	A	255	GLU	4.5
1	A	380	GLN	4.5
1	A	378	ASP	4.0
1	A	259	GLU	3.8
1	A	4	ILE	3.2
1	A	454	ASP	3.2
1	A	455	GLN	3.2
1	A	376	TRP	3.2
1	A	253	SER	3.1
1	A	54	ASP	3.1
1	A	256	ASN	3.1
1	A	344	ILE	2.9
1	A	254	ARG	2.7
1	A	381	ARG	2.5
1	A	50	THR	2.4
1	A	382	PRO	2.4
1	A	49	LEU	2.3
1	A	299[A]	LEU	2.3
1	A	22	GLY	2.3
1	A	268	ASP	2.3
1	A	486	ASN	2.3
1	A	506	GLU	2.3
1	A	342	ASN	2.2
1	A	257[A]	GLU	2.2
1	A	346	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	237	TYR	2.0
1	A	55	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
7	MES	A	625	12/12	0.81	0.21	10.50	45,58,61,68	12
10	PEG	A	629	7/7	0.82	0.21	6.95	45,52,62,63	7
2	NAG	A	607	14/15	0.78	0.23	6.16	43,74,88,90	0
5	SO4	A	614	5/5	0.87	0.20	4.98	30,49,51,60	5
9	1PG	A	628	17/17	0.81	0.17	4.75	41,55,67,71	0
8	92H	A	626	34/34	0.67	0.28	4.14	37,51,67,71	34
7	MES	A	624	12/12	0.72	0.22	2.74	38,51,84,97	12
3	FUC	A	611	10/11	0.91	0.26	1.65	60,65,72,81	0
5	SO4	A	616	5/5	0.93	0.18	1.55	36,42,54,57	5
4	GOL	A	612	6/6	0.92	0.11	1.51	41,45,46,50	0
8	92H	A	627	34/34	0.92	0.16	0.43	28,34,46,47	0
2	NAG	A	601	14/15	0.96	0.20	0.40	43,55,66,71	0
5	SO4	A	619	5/5	0.96	0.11	-0.13	54,56,59,67	5
6	CL	A	621	1/1	0.96	0.07	-	70,70,70,70	0
3	FUC	A	603	10/11	0.81	0.34	-	58,65,74,77	0
2	NAG	A	610	14/15	0.75	0.38	-	72,85,93,94	0
2	NAG	A	609	14/15	0.91	0.27	-	68,74,78,79	0
5	SO4	A	617	5/5	0.81	0.35	-	80,85,93,100	0
3	FUC	A	605	10/11	0.76	0.24	-	50,57,65,72	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CL	A	622	1/1	0.86	0.04	-	79,79,79,79	0
5	SO4	A	620	5/5	0.81	0.40	-	81,84,89,118	5
6	CL	A	623	1/1	0.85	0.06	-	85,85,85,85	0
2	NAG	A	602	14/15	0.91	0.31	-	70,75,90,91	0
2	NAG	A	604	14/15	0.90	0.19	-	63,67,73,74	0
2	NAG	A	606	14/15	0.74	0.35	-	87,93,99,103	0
2	NAG	A	608	14/15	0.86	0.37	-	81,85,90,91	0
5	SO4	A	615	5/5	0.98	0.11	-	27,42,43,44	5
5	SO4	A	618	5/5	0.82	0.23	-	66,66,75,79	0
4	GOL	A	613	6/6	0.62	0.24	-	49,64,65,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.