



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:32 PM GMT

PDB ID : 4TPK
Title : Human butyrylcholinesterase in complex with N-((1-(2,3-dihydro-1H-inden-2-yl)piperidin-3-yl)methyl)-N-(2-methoxyethyl)-2-naphthamide
Authors : Coquelle, N.; Brus, B.; Colletier, J.P.; Gobec, S.
Deposited on : 2014-06-07
Resolution : 2.70 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

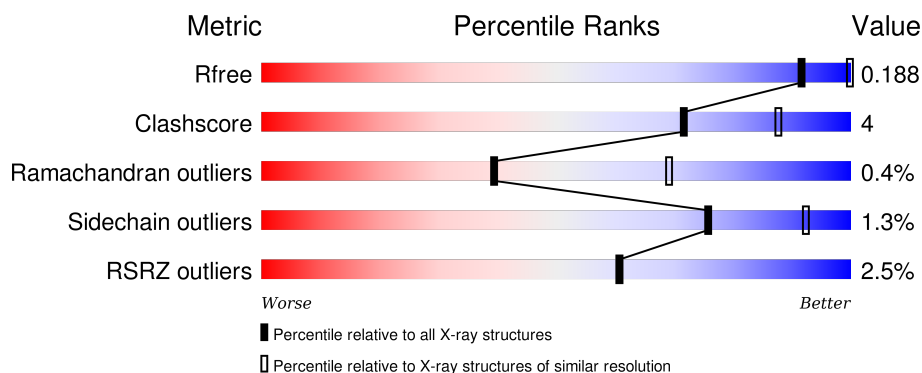
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


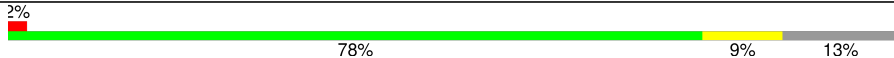
The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	602	
1	B	602	

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
3	FUL	B	606	-	-	-	X
8	GOL	A	616	-	-	-	X
8	GOL	B	612	-	-	-	X
8	GOL	B	613	-	-	-	X
8	GOL	B	614	-	-	-	X
8	GOL	B	615	-	-	-	X
9	EDO	B	616	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 8979 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	528	Total	C	N	O	S	0	3	1
			4208	2716	710	767	15			
1	B	525	Total	C	N	O	S	2	2	1
			4171	2694	702	760	15			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 3 is a polymer of unknown type called GLYCEROL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			24	14	1	9		
3	B	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

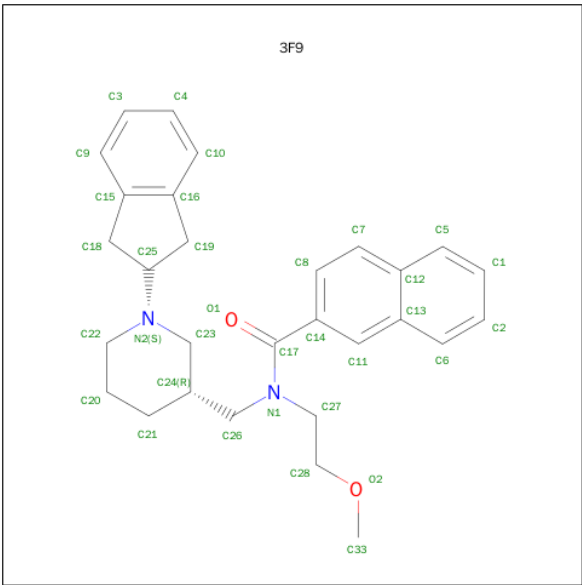
- Molecule 5 is a polymer of unknown type called GLYCEROL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

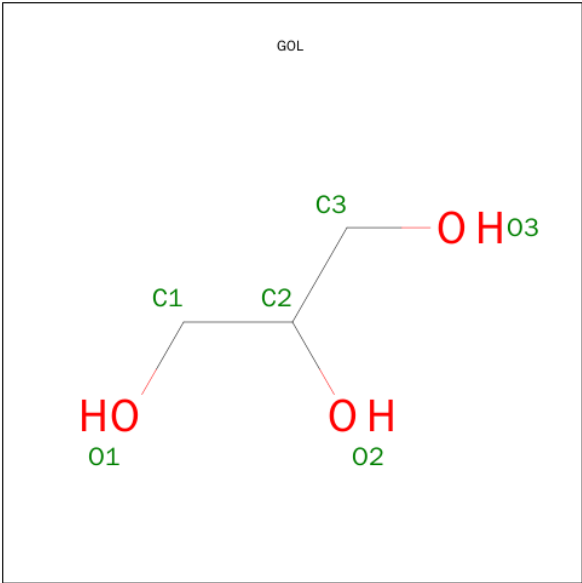
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 is N-{|(3R)-1-(2,3-dihydro-1H-inden-2-yl)piperidin-3-yl|methyl}-N-(2-methoxyethyl)naphthalene-2-carboxamide (three-letter code: 3F9) (formula: C₂₉H₃₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			33	29	2	2		
7	B	1	Total	C	N	O	0	0
			33	29	2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



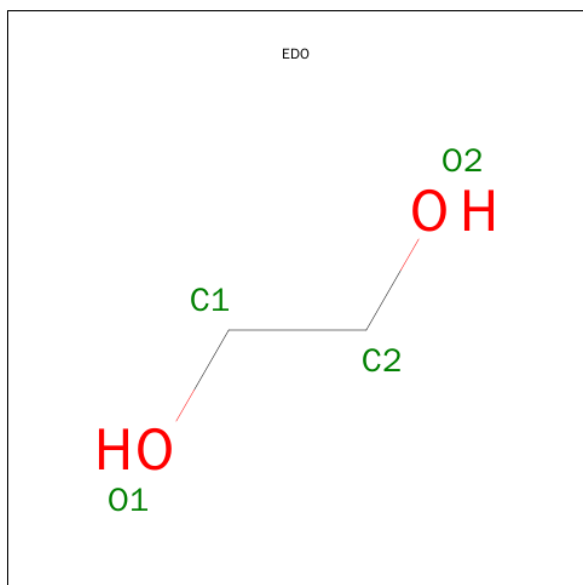
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

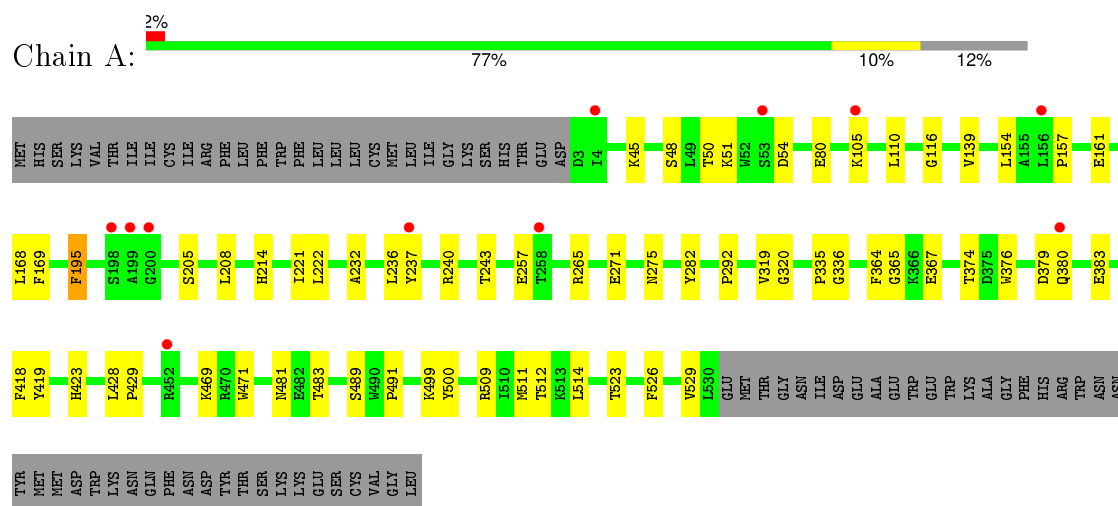
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	83	Total	O	0	0
			83	83		
10	B	89	Total	O	0	0
			89	89		

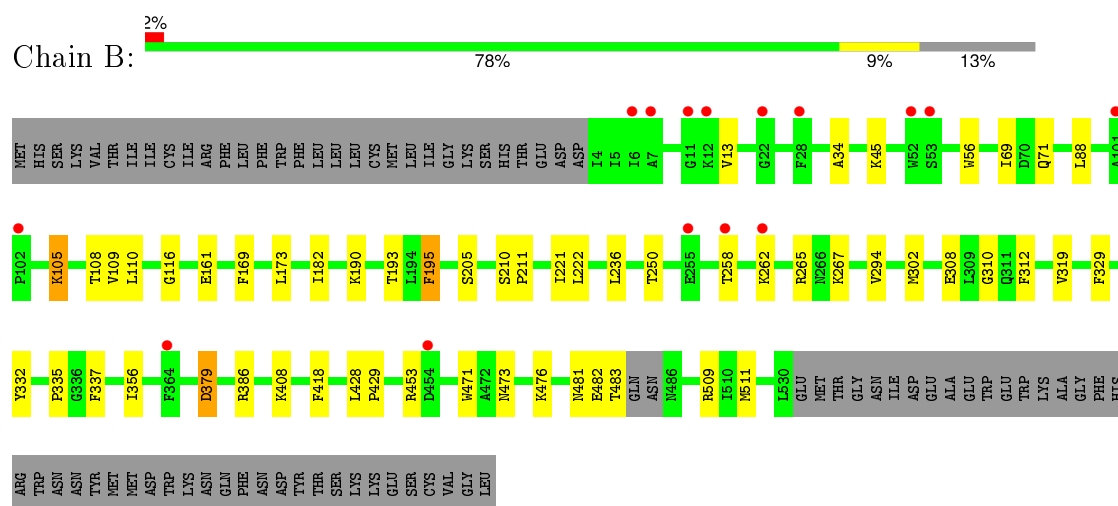
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, α , β , γ	76.60Å 80.20Å 231.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.70 46.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.20-2.70) 99.9 (46.20-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.184 , 0.239 0.193 , 0.188	Depositor DCC
R_{free} test set	2002 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.0	EDS
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 40039 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8979	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, 3F9, EDO, 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	0.36	0/4334	0.51	0/5887
1	B	0.36	0/4292	0.51	0/5829
All	All	0.36	0/8626	0.51	0/11716

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

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	4208	0	4096	40	1
1	B	4171	0	4046	30	1
2	A	14	0	13	0	0
2	B	84	0	78	0	0
3	A	24	0	22	0	0
3	B	24	0	22	0	0
4	A	84	0	75	1	0
4	B	28	0	25	2	0
5	A	24	0	22	0	0
6	A	38	0	34	2	0
7	A	33	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	33	0	34	4	0
8	A	6	0	8	1	0
8	B	24	0	32	2	0
9	A	8	0	12	0	0
9	B	4	0	6	0	0
10	A	83	0	0	2	0
10	B	89	0	0	1	0
All	All	8979	0	8559	74	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 4.

All (74) 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:250:THR:HB	1:B:267:LYS:HE2	1.65	0.79
1:B:13:VAL:HG12	1:B:56:TRP:HB3	1.75	0.69
1:A:80:GLU:OE1	10:A:714:HOH:O	2.15	0.65
1:B:161:GLU:OE1	1:B:265:ARG:NH2	2.32	0.63
1:B:71:GLN:H	8:B:614:GOL:H11	1.65	0.62
1:B:190:LYS:NZ	4:B:604:NAG:H5	2.15	0.61
1:A:335:PRO:HA	6:A:609:NAG:H61	1.81	0.61
1:B:34:ALA:HB2	1:B:173:LEU:HD23	1.83	0.60
1:A:240:ARG:NH1	1:A:257:GLU:OE2	2.34	0.60
1:A:509:ARG:HB2	1:A:511:MET:HE2	1.84	0.60
1:B:108:THR:HG21	1:B:476:LYS:HA	1.83	0.59
1:B:205:SER:HB3	1:B:222:LEU:HD21	1.85	0.59
1:B:236:LEU:HD21	1:B:294:VAL:HB	1.85	0.58
1:B:482:GLU:HG2	1:B:483:THR:H	1.68	0.58
1:B:109:VAL:HG21	1:B:182:ILE:HG12	1.86	0.57
1:A:526:PHE:O	1:A:529:VAL:HG12	2.03	0.57
1:B:379:ASP:OD1	1:B:379:ASP:N	2.27	0.56
1:A:428:LEU:HD12	1:A:429:PRO:HD2	1.88	0.55
1:A:154:LEU:HD11	1:A:243:THR:HG23	1.88	0.55
1:A:110:LEU:HD22	1:A:139:VAL:HG21	1.89	0.55
1:A:364[B]:PHE:C	1:A:364[B]:PHE:HD2	2.11	0.54
1:B:190:LYS:HZ3	4:B:604:NAG:H5	1.73	0.54
1:A:365:GLY:HA2	1:A:529:VAL:HG21	1.89	0.53
1:A:364[B]:PHE:C	1:A:364[B]:PHE:CD2	2.83	0.53
1:A:319:VAL:O	1:A:418:PHE:HA	2.09	0.53
1:B:473:ASN:ND2	1:B:481:ASN:O	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:THR:HG22	8:A:616:GOL:H32	1.92	0.52
1:A:423:HIS:ND1	10:A:754:HOH:O	2.34	0.52
1:A:168:LEU:HD11	1:A:292:PRO:HB3	1.92	0.51
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.93	0.51
7:B:611:3F9:C8	7:B:611:3F9:H27	2.41	0.51
1:A:208:LEU:O	1:A:214[A]:HIS:NE2	2.44	0.50
1:B:509:ARG:CZ	1:B:511:MET:HE1	2.42	0.49
1:A:374:THR:HG22	1:A:376:TRP:CZ2	2.48	0.49
1:B:337:PHE:CE2	1:B:386:ARG:HG3	2.48	0.49
1:B:319:VAL:O	1:B:418:PHE:HA	2.13	0.48
7:A:615:3F9:H27	7:A:615:3F9:C8	2.43	0.48
1:A:161:GLU:OE1	1:A:265:ARG:NH2	2.42	0.48
1:A:195:PHE:CB	1:A:221:ILE:HB	2.44	0.47
1:B:105:LYS:HD3	1:B:105:LYS:HA	1.65	0.47
1:A:499:LYS:HG2	1:A:512:THR:HG22	1.97	0.47
1:A:365:GLY:CA	1:A:529:VAL:HG21	2.45	0.47
1:A:45:LYS:HD2	1:A:169:PHE:CD2	2.50	0.47
1:B:335:PRO:HD3	1:B:356:ILE:HD12	1.96	0.47
1:B:258:THR:O	1:B:262:LYS:HD3	2.14	0.46
1:A:157:PRO:HB3	1:A:236:LEU:HD11	1.97	0.46
1:B:337:PHE:HE2	1:B:386:ARG:HG3	1.82	0.45
1:A:195:PHE:HB3	1:A:221:ILE:HB	1.98	0.45
1:B:310:GLY:HA2	1:B:312:PHE:CE2	2.51	0.45
1:B:332:TYR:CD1	7:B:611:3F9:H7	2.52	0.44
1:A:379:ASP:O	1:A:380:GLN:HG2	2.18	0.44
8:B:613:GOL:O3	10:B:783:HOH:O	2.21	0.44
1:B:329:PHE:CE2	7:B:611:3F9:H9	2.53	0.44
1:A:364[B]:PHE:O	1:A:367:GLU:N	2.51	0.44
1:A:481:ASN:OD1	1:A:481:ASN:N	2.51	0.43
1:A:50:THR:OG1	1:A:51:LYS:N	2.48	0.43
1:B:45:LYS:HD2	1:B:169:PHE:CD2	2.54	0.43
1:B:69:ILE:HD11	1:B:88:LEU:HD11	2.01	0.43
1:A:489:SER:O	1:A:491:PRO:HD3	2.19	0.43
1:B:110:LEU:HD23	1:B:193:THR:HB	2.00	0.42
7:B:611:3F9:H5	7:B:611:3F9:H27	2.00	0.42
1:A:428:LEU:HA	1:A:429:PRO:HD3	1.91	0.42
1:A:500:TYR:CE1	1:A:514:LEU:HB2	2.55	0.42
1:B:195:PHE:CB	1:B:221:ILE:HB	2.50	0.42
1:A:364[B]:PHE:HD2	1:A:364[B]:PHE:O	2.03	0.41
1:A:105:LYS:NZ	4:A:604:NAG:H81	2.36	0.41
1:A:336:GLY:H	6:A:609:NAG:H61	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:SER:HA	1:B:211:PRO:HD3	1.95	0.41
1:A:469:LYS:HB2	1:A:469:LYS:HE2	1.83	0.41
1:A:271:GLU:O	1:A:275:ASN:ND2	2.48	0.40
1:A:320:GLY:HA3	1:A:419:TYR:CD2	2.56	0.40
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.56	0.40
1:A:232:ALA:O	1:A:292:PRO:HG2	2.22	0.40
1:B:428:LEU:HD23	1:B:429:PRO:HD2	2.02	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_565]	2.19	0.01

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	529/602 (88%)	507 (96%)	19 (4%)	3 (1%)	30	59
1	B	523/602 (87%)	499 (95%)	23 (4%)	1 (0%)	52	80
All	All	1052/1204 (87%)	1006 (96%)	42 (4%)	4 (0%)	39	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	282	TYR
1	A	116	GLY
1	B	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	452/521 (87%)	447 (99%)	5 (1%)	80	94
1	B	445/521 (85%)	438 (98%)	7 (2%)	70	91
All	All	897/1042 (86%)	885 (99%)	12 (1%)	76	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	195	PHE
1	A	383	GLU
1	A	471	TRP
1	A	483	THR
1	B	105	LYS
1	B	195	PHE
1	B	302	MET
1	B	308	GLU
1	B	379	ASP
1	B	408	LYS
1	B	471	TRP

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

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 ⓘ

17 carbohydrates 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$
3	NAG	A	602	1,3	14,14,15	0.24	0	15,19,21	0.31	0
3	FUL	A	603	3	10,10,11	1.42	2 (20%)	14,14,16	1.12	1 (7%)
4	NAG	A	604	1,4	14,14,15	0.21	0	15,19,21	0.41	0
4	NAG	A	605	4	14,14,15	0.20	0	15,19,21	0.33	0
5	NAG	A	606	1,5	14,14,15	0.29	0	15,19,21	0.30	0
5	FUC	A	607	5	10,10,11	1.48	2 (20%)	14,14,16	1.36	2 (14%)
6	NAG	A	608	-	14,14,15	0.27	0	15,19,21	0.61	0
6	NAG	A	609	-	14,14,15	0.60	0	15,19,21	0.46	0
6	FUC	A	610	-	10,10,11	1.55	2 (20%)	14,14,16	1.26	2 (14%)
4	NAG	A	611	1,4	14,14,15	0.21	0	15,19,21	0.47	0
4	NAG	A	612	4	14,14,15	0.63	0	15,19,21	0.61	1 (6%)
4	NAG	A	613	1,4	14,14,15	0.41	0	15,19,21	0.21	0
4	NAG	A	614	4	14,14,15	0.18	0	15,19,21	0.31	0
4	NAG	B	603	1,4	14,14,15	0.28	0	15,19,21	0.27	0
4	NAG	B	604	4	14,14,15	0.27	0	15,19,21	0.31	0
3	NAG	B	605	1,3	14,14,15	0.39	0	15,19,21	0.23	0
3	FUL	B	606	3	10,10,11	1.50	2 (20%)	14,14,16	1.69	3 (21%)

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
3	NAG	A	602	1,3	-	0/6/23/26	0/1/1/1
3	FUL	A	603	3	-	0/0/17/20	0/1/1/1
4	NAG	A	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	605	4	-	0/6/23/26	0/1/1/1
5	NAG	A	606	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	607	5	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	608	-	-	0/6/23/26	0/1/1/1
6	NAG	A	609	-	-	0/6/23/26	0/1/1/1
6	FUC	A	610	-	-	0/0/17/20	0/1/1/1
4	NAG	A	611	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	612	4	-	0/6/23/26	0/1/1/1
4	NAG	A	613	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	614	4	-	0/6/23/26	0/1/1/1
4	NAG	B	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	604	4	-	0/6/23/26	0/1/1/1
3	NAG	B	605	1,3	-	0/6/23/26	0/1/1/1
3	FUL	B	606	3	-	0/0/17/20	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	606	FUL	C2-C3	-2.71	1.48	1.52
5	A	607	FUC	C2-C3	-2.64	1.48	1.52
6	A	610	FUC	C2-C3	-2.63	1.48	1.52
3	A	603	FUL	C2-C3	-2.50	1.49	1.52
3	A	603	FUL	O5-C1	3.14	1.49	1.43
5	A	607	FUC	O5-C1	3.34	1.49	1.43
3	B	606	FUL	O5-C1	3.34	1.49	1.43
6	A	610	FUC	O5-C1	3.61	1.49	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	606	FUL	C3-C4-C5	2.09	113.25	109.72
6	A	610	FUC	O5-C5-C6	2.14	109.67	106.13
3	A	603	FUL	O5-C5-C4	2.17	113.28	109.53
4	A	612	NAG	C1-O5-C5	2.18	115.01	112.25
3	B	606	FUL	O5-C5-C4	2.21	113.35	109.53
5	A	607	FUC	O5-C5-C4	2.24	113.41	109.53
5	A	607	FUC	C1-C2-C3	2.45	112.44	109.54
6	A	610	FUC	C1-C2-C3	2.52	112.52	109.54
3	B	606	FUL	C1-C2-C3	3.87	114.12	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	NAG	1	0
6	A	609	NAG	2	0
4	B	604	NAG	2	0

5.6 Ligand geometry

17 ligands 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$
2	NAG	A	601	1	14,14,15	0.37	0	15,19,21	0.23	0
7	3F9	A	615	-	37,37,37	2.04	7 (18%)	47,51,51	1.00	2 (4%)
8	GOL	A	616	-	5,5,5	0.24	0	5,5,5	0.35	0
9	EDO	A	617	-	3,3,3	0.54	0	2,2,2	0.30	0
9	EDO	A	618	-	3,3,3	0.52	0	2,2,2	0.36	0
2	NAG	B	601	1	14,14,15	0.38	0	15,19,21	0.67	1 (6%)
2	NAG	B	602	1	14,14,15	0.36	0	15,19,21	0.19	0
2	NAG	B	607	-	14,14,15	0.32	0	15,19,21	0.29	0
2	NAG	B	608	1	14,14,15	0.23	0	15,19,21	0.49	0
2	NAG	B	609	1	14,14,15	0.22	0	15,19,21	0.42	0
2	NAG	B	610	-	14,14,15	0.28	0	15,19,21	0.46	0
7	3F9	B	611	-	37,37,37	2.13	8 (21%)	47,51,51	1.23	5 (10%)
8	GOL	B	612	-	5,5,5	0.33	0	5,5,5	0.27	0
8	GOL	B	613	-	5,5,5	0.30	0	5,5,5	0.33	0
8	GOL	B	614	-	5,5,5	0.31	0	5,5,5	0.21	0
8	GOL	B	615	-	5,5,5	0.33	0	5,5,5	0.44	0
9	EDO	B	616	-	3,3,3	0.64	0	2,2,2	0.14	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	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	3F9	A	615	-	-	0/20/38/38	0/5/5/5
8	GOL	A	616	-	-	0/4/4/4	0/0/0/0
9	EDO	A	617	-	-	0/1/1/1	0/0/0/0
9	EDO	A	618	-	-	0/1/1/1	0/0/0/0
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	-	0/6/23/26	0/1/1/1
2	NAG	B	607	-	-	0/6/23/26	0/1/1/1
2	NAG	B	608	1	-	0/6/23/26	0/1/1/1
2	NAG	B	609	1	-	0/6/23/26	0/1/1/1
2	NAG	B	610	-	-	0/6/23/26	0/1/1/1
7	3F9	B	611	-	-	0/20/38/38	0/5/5/5
8	GOL	B	612	-	-	0/4/4/4	0/0/0/0
8	GOL	B	613	-	-	0/4/4/4	0/0/0/0
8	GOL	B	614	-	-	0/4/4/4	0/0/0/0
8	GOL	B	615	-	-	0/4/4/4	0/0/0/0
9	EDO	B	616	-	-	0/1/1/1	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	611	3F9	C18-C15	-6.73	1.39	1.50
7	A	615	3F9	C18-C15	-6.04	1.40	1.50
7	A	615	3F9	C19-C16	-5.88	1.40	1.50
7	B	611	3F9	C19-C16	-5.68	1.41	1.50
7	A	615	3F9	C14-C17	-5.57	1.41	1.50
7	B	611	3F9	C14-C17	-5.30	1.41	1.50
7	A	615	3F9	C9-C15	-3.36	1.33	1.39
7	B	611	3F9	C9-C15	-3.35	1.33	1.39
7	A	615	3F9	C10-C16	-3.25	1.34	1.39
7	B	611	3F9	C10-C16	-3.15	1.34	1.39
7	B	611	3F9	C18-C25	-2.85	1.48	1.54
7	A	615	3F9	C18-C25	-2.42	1.49	1.54
7	B	611	3F9	C19-C25	-2.34	1.49	1.54
7	B	611	3F9	C15-C16	-2.06	1.35	1.39
7	A	615	3F9	C15-C16	-2.03	1.35	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	611	3F9	C16-C19-C25	-3.80	99.24	103.09
7	B	611	3F9	C22-N2-C25	-2.88	106.74	112.37
7	B	611	3F9	C15-C18-C25	-2.77	100.28	103.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	611	3F9	C18-C15-C16	-2.50	108.82	110.59
7	B	611	3F9	C19-C16-C15	-2.45	108.85	110.59
7	A	615	3F9	C19-C16-C15	-2.26	108.99	110.59
7	A	615	3F9	C18-C15-C16	-2.12	109.08	110.59
2	B	601	NAG	C1-O5-C5	2.40	115.29	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	615	3F9	1	0
8	A	616	GOL	1	0
7	B	611	3F9	4	0
8	B	613	GOL	1	0
8	B	614	GOL	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, 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	528/602 (87%)	-0.14	11 (2%) 67 68	32, 53, 80, 108	0
1	B	525/602 (87%)	-0.06	15 (2%) 55 55	35, 56, 86, 113	2 (0%)
All	All	1053/1204 (87%)	-0.10	26 (2%) 61 61	32, 54, 84, 113	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	TYR	4.7
1	B	12	LYS	4.1
1	B	53	SER	3.8
1	B	22	GLY	3.4
1	A	199	ALA	3.2
1	B	6	ILE	3.1
1	B	262	LYS	3.0
1	A	4	ILE	2.9
1	B	258	THR	2.9
1	B	52	TRP	2.8
1	B	101	ALA	2.7
1	A	258	THR	2.6
1	B	454	ASP	2.6
1	B	28	PHE	2.5
1	B	255	GLU	2.4
1	B	102	PRO	2.4
1	B	364[A]	PHE	2.3
1	A	198	SER	2.3
1	B	11	GLY	2.2
1	A	380	GLN	2.2
1	B	7	ALA	2.2
1	A	200	GLY	2.2
1	A	53	SER	2.1
1	A	452	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	105	LYS	2.0
1	A	156	LEU	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](#)

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
3	FUL	B	606	10/11	0.88	0.48	7.40	91,106,115,119	0
4	NAG	A	612	14/15	0.83	0.23	1.65	61,76,87,93	0
5	FUC	A	607	10/11	0.94	0.30	1.37	102,110,117,117	0
6	NAG	A	608	14/15	0.91	0.22	1.33	83,91,100,105	0
4	NAG	A	611	14/15	0.93	0.13	-0.54	61,71,80,82	0
6	NAG	A	609	14/15	0.86	0.32	-	86,107,109,109	0
6	FUC	A	610	10/11	0.85	0.43	-	95,106,111,113	0
4	NAG	A	605	14/15	0.85	0.31	-	97,106,112,112	0
3	FUL	A	603	10/11	0.86	0.26	-	98,103,113,115	0
4	NAG	A	604	14/15	0.95	0.20	-	68,79,86,98	0
4	NAG	A	613	14/15	0.80	0.28	-	104,116,123,129	0
4	NAG	A	614	14/15	0.71	0.48	-	133,134,141,142	0
3	NAG	A	602	14/15	0.83	0.32	-	92,99,109,109	0
4	NAG	B	604	14/15	0.83	0.41	-	100,114,119,119	0
4	NAG	B	603	14/15	0.90	0.32	-	95,105,112,116	0
5	NAG	A	606	14/15	0.85	0.27	-	102,114,122,123	0
3	NAG	B	605	14/15	0.90	0.26	-	86,98,105,108	0

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(\AA^2)	Q<0.9
8	GOL	B	612	6/6	0.87	0.39	7.64	56,60,67,79	0
8	GOL	B	614	6/6	0.84	0.41	7.49	57,62,74,79	0
8	GOL	B	613	6/6	0.82	0.28	5.28	59,74,75,89	0
8	GOL	B	615	6/6	0.84	0.25	4.23	53,69,78,80	0
8	GOL	A	616	6/6	0.92	0.17	2.61	54,60,65,95	0
9	EDO	B	616	4/4	0.86	0.20	2.05	55,67,70,74	0
7	3F9	A	615	33/33	0.94	0.28	1.53	38,51,63,66	33
7	3F9	B	611	33/33	0.94	0.21	0.62	36,47,60,65	0
2	NAG	B	609	14/15	0.89	0.21	0.58	70,76,82,93	0
9	EDO	A	618	4/4	0.90	0.19	0.46	65,66,66,73	0
2	NAG	B	610	14/15	0.86	0.15	0.43	85,96,104,105	0
9	EDO	A	617	4/4	0.87	0.15	-0.55	73,77,80,82	0
2	NAG	A	601	14/15	0.82	0.31	-	81,99,102,107	0
2	NAG	B	608	14/15	0.88	0.25	-	89,98,104,104	0
2	NAG	B	607	14/15	0.76	0.55	-	108,123,128,131	0
2	NAG	B	602	14/15	0.68	0.24	-	95,110,119,119	0
2	NAG	B	601	14/15	0.78	0.41	-	105,119,125,127	0

6.5 Other polymers

There are no such residues in this entry.