



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2017 – 08:38 AM EDT

PDB ID : 5LKR
Title : Human Butyrylcholinesterase complexed with N-Propargylperidines
Authors : Coquelle, N.; Knez, D.; Colletier, J.P.; Gobec, S.
Deposited on : unknown
Resolution : 2.52 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-20029824
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-20029824

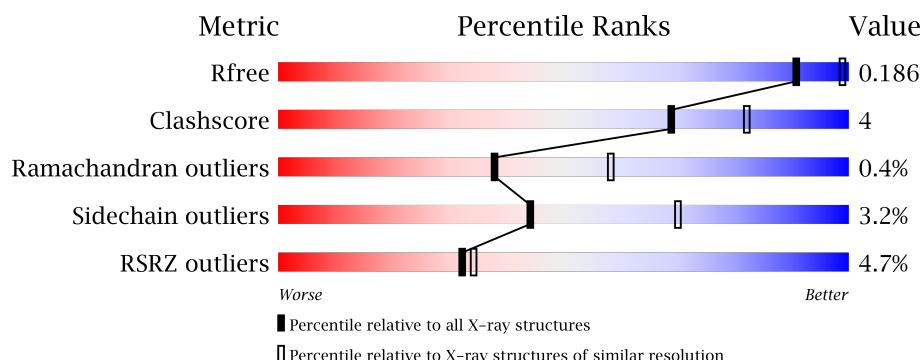
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	4636 (2.54-2.50)
Clashscore	112137	5382 (2.54-2.50)
Ramachandran outliers	110173	5282 (2.54-2.50)
Sidechain outliers	110143	5284 (2.54-2.50)
RSRZ outliers	101464	4669 (2.54-2.50)

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	574	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	B	574	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>9%</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
3	FUL	B	605	-	-	-	X
4	FUC	A	608	-	-	-	X
5	GOL	A	615	-	-	-	X
6	6YC	B	611	-	-	-	X
7	PEG	A	618	-	X	-	-

2 Entry composition [i](#)

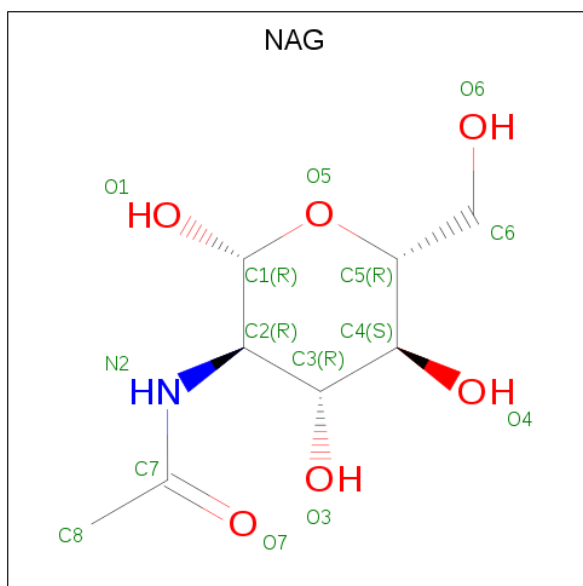
There are 8 unique types of molecules in this entry. The entry contains 8751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			4168	2694	695	763	16			
1	B	525	Total	C	N	O	S	0	0	1
			4130	2668	697	750	15			

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



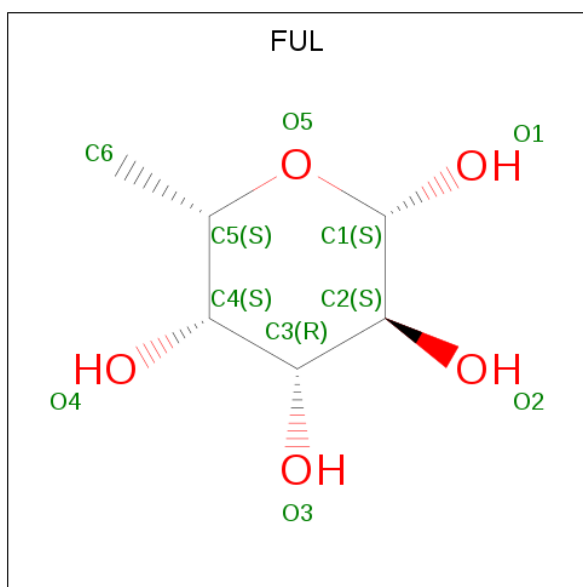
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

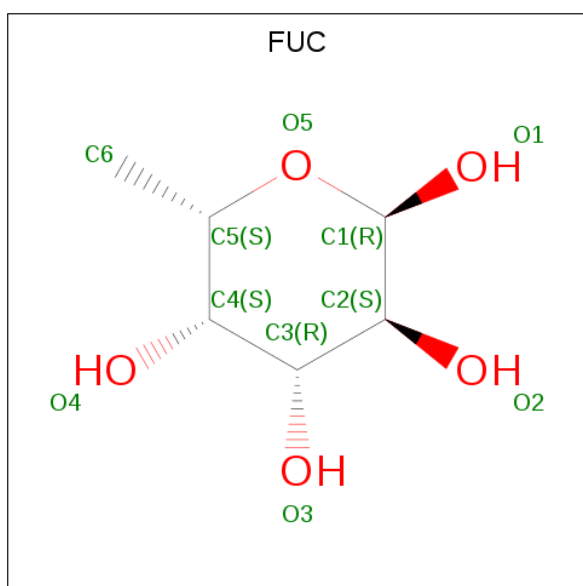
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

- Molecule 3 is BETA-L-FUCOSE (three-letter code: FUL) (formula: C₆H₁₂O₅).



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

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



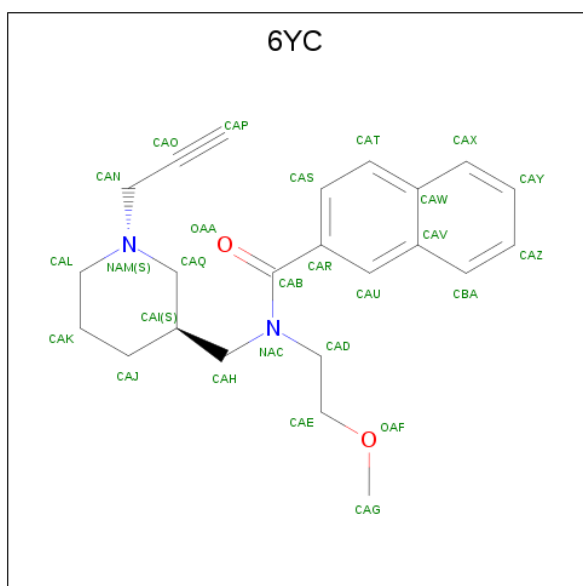
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



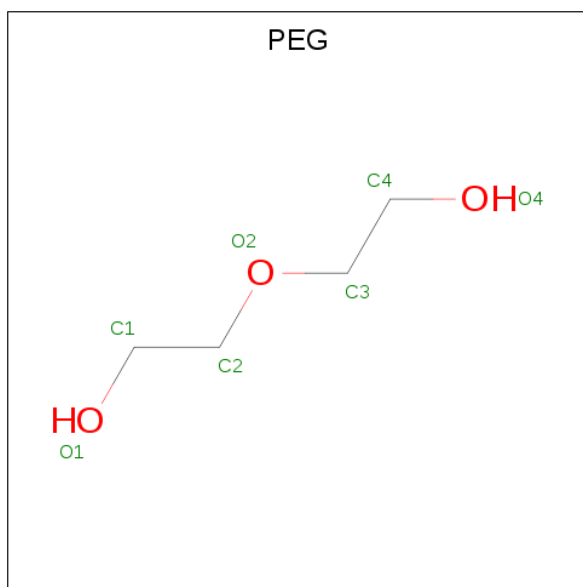
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is {N}-(2-methoxyethyl)- {N}-[[3 {S}]-1-prop-2-ynylpiperidin-3-yl]methyl]naphthalene-2-carboxamide (three-letter code: 6YC) (formula: C₂₃H₂₈N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	9	0
			27	23	2	2		
6	B	1	Total	C	N	O	0	0
			27	23	2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

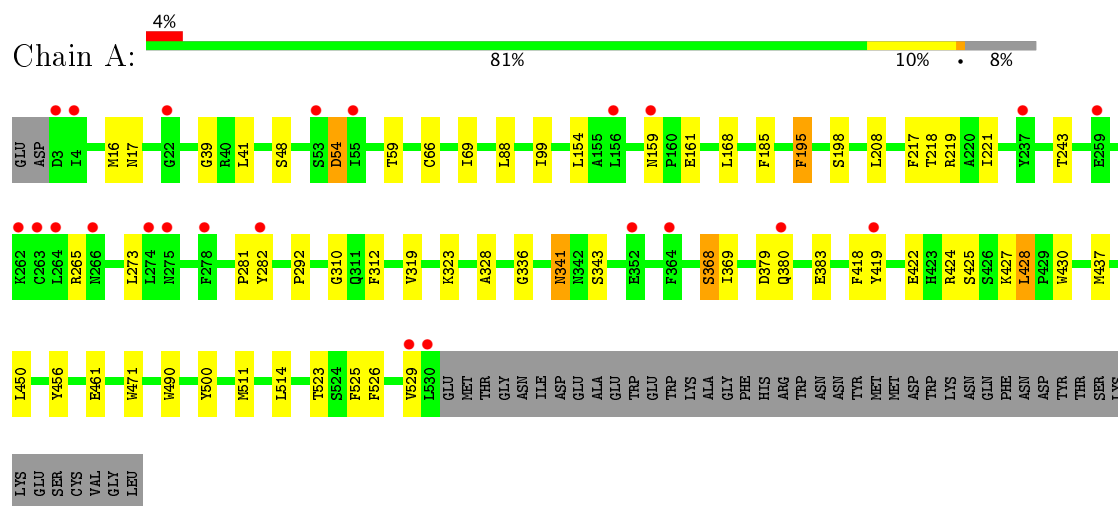
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	15	Total	O	0	0
			15	15		
8	B	21	Total	O	0	0
			21	21		

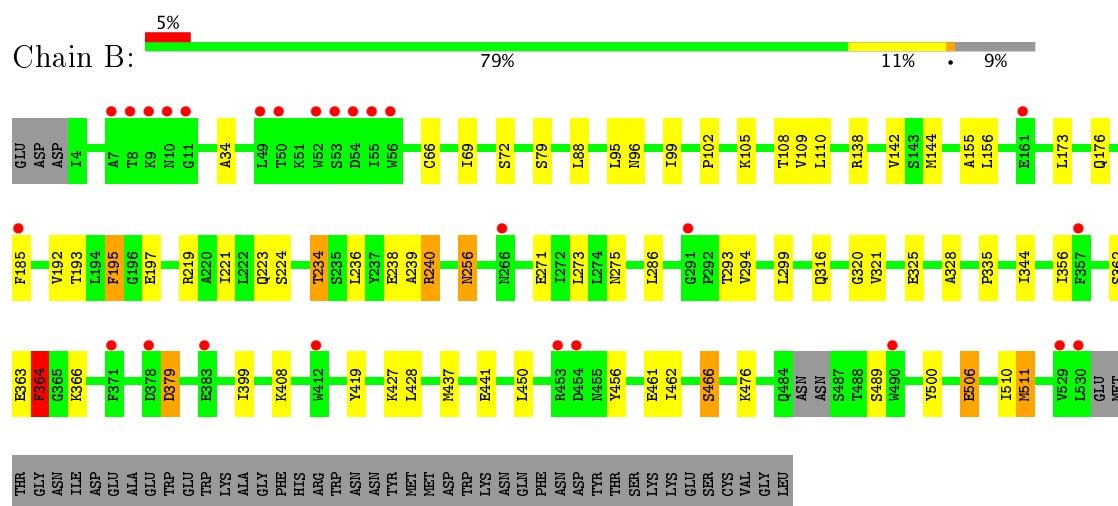
3 Residue-property plots [i](#)

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, α , β , γ	73.68 Å 79.46 Å 228.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.52 48.86 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.86-2.52) 94.7 (48.86-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.61 Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.185 , 0.238 0.187 , 0.186	Depositor DCC
R_{free} test set	1984 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8751	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: GOL, NAG, 6YC, FUC, FUL, PEG

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	0.35	0/4298	0.52	0/5849
1	B	0.36	2/4247 (0.0%)	0.53	3/5773 (0.1%)
All	All	0.35	2/8545 (0.0%)	0.52	3/11622 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	PHE	CB-CG	-8.11	1.37	1.51
1	B	364	PHE	CD1-CE1	-6.00	1.27	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	PHE	N-CA-CB	-5.26	101.12	110.60
1	B	364	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	B	95	LEU	CA-CB-CG	5.02	126.86	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	4168	0	4015	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4130	0	3994	37	0
2	A	168	0	150	2	0
2	B	140	0	128	1	0
3	A	10	0	10	0	0
3	B	10	0	10	0	0
4	A	10	0	10	0	0
5	A	12	0	16	3	0
5	B	6	0	8	0	0
6	A	27	0	0	0	0
6	B	27	0	0	0	0
7	A	7	0	10	1	0
8	A	15	0	0	1	0
8	B	21	0	0	2	0
All	All	8751	0	8351	74	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 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:A:323:LYS:HD2	1:A:422:GLU:HG2	1.67	0.75
1:B:240:ARG:NH1	8:B:703:HOH:O	2.17	0.74
2:B:607:NAG:O4	8:B:701:HOH:O	2.09	0.70
1:B:271:GLU:O	1:B:275:ASN:ND2	2.26	0.67
1:B:69:ILE:HD11	1:B:88:LEU:HD11	1.75	0.67
1:A:424:ARG:NH2	1:A:430:TRP:O	2.27	0.66
1:B:99:ILE:HD11	1:B:185:PHE:HB3	1.78	0.66
1:B:335:PRO:HD3	1:B:356:ILE:HD12	1.78	0.65
1:A:198:SER:OG	8:A:701:HOH:O	2.14	0.65
1:A:523:THR:HG22	5:A:615:GOL:H32	1.82	0.61
5:A:617:GOL:O3	7:A:618:PEG:O4	2.19	0.58
1:B:102:PRO:O	1:B:138:ARG:NH2	2.26	0.58
1:B:108:THR:HG21	1:B:476:LYS:HA	1.86	0.58
1:B:256:ASN:OD1	1:B:256:ASN:N	2.38	0.56
1:B:234:THR:HG22	1:B:238:GLU:HB2	1.87	0.56
1:B:109:VAL:HB	1:B:192:VAL:HG22	1.88	0.56
1:B:363:GLU:HA	1:B:366:LYS:HE3	1.88	0.55
1:B:500:TYR:CZ	1:B:511:MET:HB2	2.42	0.55
1:B:110:LEU:HD23	1:B:193:THR:HB	1.90	0.54
1:B:195:PHE:CB	1:B:221:ILE:HB	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLY:H	2:A:610:NAG:H61	1.73	0.53
1:B:462:ILE:O	1:B:466:SER:OG	2.27	0.51
1:A:419:TYR:HB3	1:A:490:TRP:CZ2	2.47	0.50
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.46	0.50
1:A:99:ILE:HD11	1:A:185:PHE:HD2	1.77	0.50
1:B:34:ALA:HB2	1:B:173:LEU:HD23	1.93	0.50
1:B:239:ALA:HB2	1:B:293:THR:HG21	1.94	0.50
1:A:341:ASN:OD1	1:A:341:ASN:N	2.44	0.49
1:B:379:ASP:OD1	1:B:379:ASP:N	2.30	0.49
1:A:154:LEU:HD11	1:A:243:THR:HG23	1.95	0.49
1:A:328:ALA:HB2	1:A:437:MET:HE3	1.95	0.48
1:B:450:LEU:HA	1:B:461:GLU:HG3	1.93	0.48
1:B:195:PHE:HB2	1:B:221:ILE:HB	1.95	0.48
1:A:523:THR:HA	5:A:615:GOL:H12	1.96	0.48
1:A:526:PHE:O	1:A:529:VAL:HG12	2.13	0.47
1:B:328:ALA:HB2	1:B:437:MET:HE3	1.97	0.47
1:A:17:ASN:HD22	2:A:601:NAG:H83	1.79	0.47
1:B:236:LEU:HD11	1:B:294:VAL:O	2.14	0.47
1:A:368:SER:HG	1:A:525:PHE:HE2	1.60	0.47
1:A:218:THR:HG22	1:A:219:ARG:HG3	1.98	0.46
1:A:168:LEU:HD11	1:A:292:PRO:HB3	1.97	0.46
1:A:450:LEU:HA	1:A:461:GLU:HG3	1.98	0.46
1:B:224:SER:OG	1:B:325:GLU:OE2	2.25	0.46
1:B:320:GLY:HA3	1:B:419:TYR:CE2	2.51	0.46
1:A:39:GLY:O	1:A:265:ARG:HD3	2.15	0.46
1:B:219:ARG:HD3	1:B:316:GLN:OE1	2.16	0.46
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.82	0.45
1:B:321:VAL:HG21	1:B:399:ILE:HG12	1.98	0.45
1:A:16:MET:HB3	1:A:59:THR:HG22	1.99	0.45
1:A:424:ARG:HG3	1:A:428:LEU:HD23	1.99	0.45
1:B:155:ALA:HB3	1:B:239:ALA:HB1	1.99	0.45
1:A:369:ILE:HD11	1:A:526:PHE:CE1	2.52	0.44
1:A:69:ILE:HD11	1:A:88:LEU:HD11	1.99	0.44
1:B:362:SER:C	1:B:364:PHE:H	2.21	0.44
1:A:159:ASN:OD1	1:A:161:GLU:HB2	2.17	0.44
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.53	0.44
1:A:319:VAL:O	1:A:418:PHE:HA	2.18	0.43
1:A:500:TYR:CE1	1:A:514:LEU:HB2	2.53	0.43
1:B:362:SER:C	1:B:364:PHE:N	2.72	0.43
1:A:208:LEU:HD23	1:A:217:PHE:HZ	1.84	0.43
1:A:195:PHE:CB	1:A:221:ILE:HB	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:HB	1:B:293:THR:HG22	2.01	0.42
1:A:427:LYS:HD3	1:A:456:TYR:CZ	2.53	0.42
1:B:489:SER:O	1:B:510:ILE:HD11	2.19	0.42
1:A:66[B]:CYS:SG	1:A:273:LEU:HD11	2.60	0.42
1:B:66:CYS:HB3	1:B:273:LEU:HD11	2.02	0.41
1:B:96:ASN:O	1:B:142:VAL:HA	2.21	0.41
1:B:197:GLU:HA	1:B:223:GLN:O	2.20	0.41
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.85	0.41
1:B:427:LYS:HD3	1:B:456:TYR:CZ	2.56	0.40
1:A:379:ASP:O	1:A:380:GLN:HG2	2.21	0.40
1:A:341:ASN:HB2	1:A:343:SER:H	1.86	0.40
1:A:99:ILE:HD11	1:A:185:PHE:CD2	2.55	0.40
1:B:197:GLU:HG3	1:B:441:GLU:OE2	2.22	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	529/574 (92%)	503 (95%)	23 (4%)	3 (1%)	28	47
1	B	521/574 (91%)	488 (94%)	32 (6%)	1 (0%)	51	72
All	All	1050/1148 (92%)	991 (94%)	55 (5%)	4 (0%)	38	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	506	GLU
1	A	282	TYR
1	A	54	ASP
1	A	281	PRO

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	444/494 (90%)	435 (98%)	9 (2%)	60	83
1	B	436/494 (88%)	417 (96%)	19 (4%)	33	55
All	All	880/988 (89%)	852 (97%)	28 (3%)	44	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	54	ASP
1	A	195	PHE
1	A	341	ASN
1	A	368	SER
1	A	383	GLU
1	A	425	SER
1	A	428	LEU
1	A	471	TRP
1	B	72	SER
1	B	79	SER
1	B	105	LYS
1	B	144	MET
1	B	156	LEU
1	B	176	GLN
1	B	195	PHE
1	B	234	THR
1	B	240	ARG
1	B	256	ASN
1	B	286	LEU
1	B	344	ILE
1	B	364	PHE
1	B	379	ASP
1	B	408	LYS
1	B	428	LEU
1	B	466	SER
1	B	506	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	511	MET

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

31 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	0.45	0	15,19,21	0.78	1 (6%)
2	NAG	A	602	2	14,14,15	0.30	0	15,19,21	0.55	0
2	NAG	A	603	1,2	14,14,15	0.19	0	15,19,21	0.54	0
3	FUL	A	604	-	9,10,11	1.69	2 (22%)	13,14,16	1.47	3 (23%)
2	NAG	A	605	1,2	14,14,15	0.40	0	15,19,21	0.91	1 (6%)
2	NAG	A	606	2	14,14,15	0.71	1 (7%)	15,19,21	0.56	0
2	NAG	A	607	1,4	14,14,15	0.38	0	15,19,21	0.51	0
4	FUC	A	608	2	9,10,11	1.02	0	13,14,16	1.31	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	609	1,2	14,14,15	0.47	0	15,19,21	1.11	2 (13%)
2	NAG	A	610	2	14,14,15	0.36	0	15,19,21	0.49	0
2	NAG	A	611	1,2	14,14,15	0.34	0	15,19,21	0.86	1 (6%)
2	NAG	A	612	2	14,14,15	0.58	1 (7%)	15,19,21	0.82	1 (6%)
2	NAG	A	613	1,2	14,14,15	0.57	0	15,19,21	0.73	0
2	NAG	A	614	2	14,14,15	0.32	0	15,19,21	0.61	0
5	GOL	A	615	-	5,5,5	0.36	0	5,5,5	0.27	0
6	6YC	A	616	-	29,29,29	1.52	2 (6%)	34,38,38	1.01	2 (5%)
5	GOL	A	617	-	5,5,5	0.80	0	5,5,5	0.88	0
7	PEG	A	618	-	6,6,6	2.36	5 (83%)	5,5,5	1.60	2 (40%)
2	NAG	B	601	1	14,14,15	0.74	1 (7%)	15,19,21	0.63	0
2	NAG	B	602	1,2	14,14,15	0.76	1 (7%)	15,19,21	0.89	1 (6%)
2	NAG	B	603	2	14,14,15	0.21	0	15,19,21	0.62	0
2	NAG	B	604	1,3	14,14,15	0.61	0	15,19,21	0.86	1 (6%)
3	FUL	B	605	2	9,10,11	1.97	2 (22%)	13,14,16	2.24	5 (38%)
2	NAG	B	606	-	14,14,15	0.67	1 (7%)	15,19,21	0.44	0
2	NAG	B	607	1	14,14,15	0.38	0	15,19,21	0.71	0
2	NAG	B	608	1	14,14,15	0.55	0	15,19,21	0.73	1 (6%)
2	NAG	B	609	1	14,14,15	1.06	1 (7%)	15,19,21	1.89	1 (6%)
5	GOL	B	610	-	5,5,5	0.35	0	5,5,5	0.26	0
6	6YC	B	611	-	29,29,29	1.52	2 (6%)	34,38,38	1.09	3 (8%)
2	NAG	B	612	-	14,14,15	0.77	1 (7%)	15,19,21	0.63	0
2	NAG	B	613	1	14,14,15	0.33	0	15,19,21	0.59	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
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	NAG	A	603	1,2	-	0/6/23/26	0/1/1/1
3	FUL	A	604	-	-	0/0/17/20	0/1/1/1
2	NAG	A	605	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	606	2	-	0/6/23/26	0/1/1/1
2	NAG	A	607	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	608	2	-	0/0/17/20	0/1/1/1
2	NAG	A	609	1,2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	610	2	-	0/6/23/26	0/1/1/1
2	NAG	A	611	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	612	2	-	0/6/23/26	0/1/1/1
2	NAG	A	613	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	614	2	-	0/6/23/26	0/1/1/1
5	GOL	A	615	-	-	0/4/4/4	0/0/0/0
6	6YC	A	616	-	-	0/18/29/29	0/3/3/3
5	GOL	A	617	-	-	0/4/4/4	0/0/0/0
7	PEG	A	618	-	-	0/4/4/4	0/0/0/0
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	603	2	-	0/6/23/26	0/1/1/1
2	NAG	B	604	1,3	-	0/6/23/26	0/1/1/1
3	FUL	B	605	2	-	0/0/17/20	0/1/1/1
2	NAG	B	606	-	-	0/6/23/26	0/1/1/1
2	NAG	B	607	1	-	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
5	GOL	B	610	-	-	0/4/4/4	0/0/0/0
6	6YC	B	611	-	-	0/18/29/29	0/3/3/3
2	NAG	B	612	-	-	0/6/23/26	0/1/1/1
2	NAG	B	613	1	-	0/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	611	6YC	CAR-CAB	-6.46	1.39	1.50
6	A	616	6YC	CAR-CAB	-6.44	1.39	1.50
3	B	605	FUL	C2-C3	-2.78	1.48	1.52
3	A	604	FUL	C2-C3	-2.74	1.48	1.52
2	B	602	NAG	O5-C1	-2.51	1.39	1.43
6	A	616	6YC	CAO-CAP	-2.44	1.12	1.18
2	B	606	NAG	O5-C1	-2.39	1.39	1.43
6	B	611	6YC	CAO-CAP	-2.07	1.13	1.18
2	B	612	NAG	O5-C1	-2.03	1.40	1.43
2	A	612	NAG	C1-C2	2.00	1.55	1.52
7	A	618	PEG	C2-C1	2.02	1.59	1.49
2	A	606	NAG	C1-C2	2.07	1.55	1.52
7	A	618	PEG	O2-C2	2.13	1.51	1.42
7	A	618	PEG	C3-C4	2.13	1.60	1.49
2	B	601	NAG	O5-C1	2.22	1.47	1.43
7	A	618	PEG	O4-C4	2.75	1.56	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	618	PEG	O2-C3	3.20	1.55	1.42
2	B	609	NAG	O5-C1	3.62	1.49	1.43
3	A	604	FUL	O5-C1	3.88	1.50	1.43
3	B	605	FUL	O5-C1	4.84	1.51	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	605	FUL	C6-C5-C4	-3.23	107.32	113.07
2	A	605	NAG	O4-C4-C3	-2.52	104.87	110.36
6	B	611	6YC	CAR-CAB-NAC	-2.39	115.67	118.77
3	A	604	FUL	C6-C5-C4	-2.27	109.02	113.07
2	A	609	NAG	C4-C3-C2	-2.17	107.84	111.02
6	B	611	6YC	CAN-NAM-CAL	-2.17	109.00	111.70
7	A	618	PEG	O1-C1-C2	-2.14	99.62	111.89
2	B	602	NAG	O4-C4-C5	-2.11	103.96	109.28
6	B	611	6YC	CAJ-CAK-CAL	-2.09	108.21	110.96
6	A	616	6YC	CAR-CAB-NAC	-2.08	116.07	118.77
6	A	616	6YC	CAN-NAM-CAL	-2.04	109.17	111.70
2	A	611	NAG	C1-O5-C5	2.26	115.28	112.17
2	B	608	NAG	C1-O5-C5	2.27	115.30	112.17
2	B	604	NAG	C3-C4-C5	2.31	114.30	110.22
2	A	609	NAG	C1-O5-C5	2.33	115.38	112.17
2	A	601	NAG	C1-O5-C5	2.40	115.48	112.17
4	A	608	FUC	O5-C5-C4	2.49	113.72	109.62
2	A	612	NAG	C1-O5-C5	2.62	115.78	112.17
4	A	608	FUC	O2-C2-C1	2.66	114.58	109.18
7	A	618	PEG	C3-O2-C2	2.68	124.90	113.30
3	B	605	FUL	C1-O5-C5	2.86	118.72	112.39
3	B	605	FUL	O5-C1-C2	2.86	115.28	110.79
3	B	605	FUL	O5-C5-C4	3.16	114.84	109.62
3	A	604	FUL	O5-C5-C4	3.21	114.91	109.62
3	A	604	FUL	C3-C4-C5	3.21	114.72	109.68
3	B	605	FUL	C1-C2-C3	4.31	115.11	109.65
2	B	609	NAG	C1-O5-C5	7.03	121.85	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	1	0
2	A	610	NAG	1	0
5	A	615	GOL	2	0
5	A	617	GOL	1	0
7	A	618	PEG	1	0
2	B	607	NAG	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	528/574 (91%)	0.51	23 (4%)	35 38	45, 74, 101, 118	1 (0%)
1	B	525/574 (91%)	0.57	26 (4%)	30 31	47, 73, 104, 129	0
All	All	1053/1148 (91%)	0.54	49 (4%)	32 34	45, 73, 102, 129	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	530	LEU	17.3
1	B	52	TRP	6.8
1	A	530	LEU	6.7
1	B	53	SER	6.1
1	A	53	SER	6.0
1	B	49	LEU	4.3
1	B	54	ASP	4.2
1	B	11	GLY	4.0
1	A	4	ILE	4.0
1	A	529	VAL	3.9
1	A	156	LEU	3.3
1	B	55	ILE	3.1
1	A	3	ASP	3.1
1	B	10	ASN	3.0
1	B	8	THR	3.0
1	A	22	GLY	3.0
1	B	529	VAL	2.9
1	B	454	ASP	2.9
1	A	352	GLU	2.9
1	B	185	PHE	2.8
1	A	278	PHE	2.8
1	B	266	ASN	2.8
1	B	50	THR	2.8
1	A	264	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	CYS	2.5
1	B	161	GLU	2.5
1	B	371	PHE	2.5
1	A	262	LYS	2.4
1	B	9	LYS	2.3
1	A	419	TYR	2.3
1	A	259	GLU	2.3
1	A	364[A]	PHE	2.2
1	A	159	ASN	2.2
1	A	380	GLN	2.2
1	A	55	ILE	2.2
1	B	291	GLY	2.2
1	B	378	ASP	2.2
1	A	266	ASN	2.2
1	A	274	LEU	2.2
1	B	412	TRP	2.2
1	B	56	TRP	2.2
1	B	453	ARG	2.2
1	B	490	TRP	2.1
1	B	7	ALA	2.1
1	A	237	TYR	2.1
1	B	357	PHE	2.1
1	B	383	GLU	2.1
1	A	282	TYR	2.1
1	A	275	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	GOL	A	615	6/6	0.78	0.32	6.17	74,83,96,96	0
3	FUL	B	605	10/11	0.93	0.32	5.63	91,101,107,124	0
6	6YC	B	611	27/27	0.88	0.29	3.57	58,79,105,110	27
6	6YC	A	616	27/27	0.90	0.23	1.72	67,96,117,128	9
4	FUC	A	608	10/11	0.91	0.44	1.53	105,111,118,121	0
2	NAG	A	612	14/15	0.82	0.21	1.47	75,94,100,101	14
2	NAG	A	611	14/15	0.89	0.21	1.34	70,81,93,95	14
5	GOL	B	610	6/6	0.92	0.20	1.10	77,78,93,94	0
2	NAG	B	609	14/15	0.82	0.20	0.39	106,119,133,134	0
2	NAG	A	609	14/15	0.89	0.15	-0.62	95,105,125,132	0
2	NAG	B	608	14/15	0.94	0.12	-1.71	81,91,101,105	0
7	PEG	A	618	7/7	0.84	0.14	-	93,96,100,103	0
2	NAG	A	607	14/15	0.81	0.29	-	120,131,139,139	0
2	NAG	B	612	14/15	0.87	0.15	-	85,105,120,127	0
2	NAG	A	614	14/15	0.73	0.33	-	145,151,158,159	0
2	NAG	B	613	14/15	0.78	0.27	-	109,129,137,137	0
2	NAG	B	602	14/15	0.91	0.23	-	100,113,129,133	0
2	NAG	A	613	14/15	0.78	0.14	-	98,127,141,146	0
2	NAG	B	606	14/15	0.81	0.42	-	93,112,118,119	0
3	FUL	A	604	10/11	0.73	0.48	-	109,116,125,133	0
2	NAG	A	610	14/15	0.90	0.33	-	113,122,131,132	0
2	NAG	A	605	14/15	0.88	0.27	-	74,93,117,125	0
2	NAG	A	603	14/15	0.83	0.19	-	87,111,121,132	0
2	NAG	B	603	14/15	0.85	0.47	-	107,135,138,142	0
2	NAG	B	604	14/15	0.90	0.17	-	83,99,109,116	0
5	GOL	A	617	6/6	0.72	0.18	-	89,97,103,109	0
2	NAG	A	602	14/15	0.87	0.27	-	90,124,132,135	0
2	NAG	A	606	14/15	0.82	0.40	-	114,133,142,145	0
2	NAG	B	601	14/15	0.81	0.20	-	104,127,134,137	0
2	NAG	A	601	14/15	0.92	0.25	-	86,91,107,108	0
2	NAG	B	607	14/15	0.91	0.12	-	95,106,113,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.