



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2018 – 01:38 PM EST

PDB ID : 5FOQ
Title : Acetylcholinesterase in complex with C7653
Authors : Berg, L.; Mishra, B.K.; Andersson, D.C.; Ekstrom, F.; Linusson, A.
Deposited on : 2015-11-25
Resolution : 2.30 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

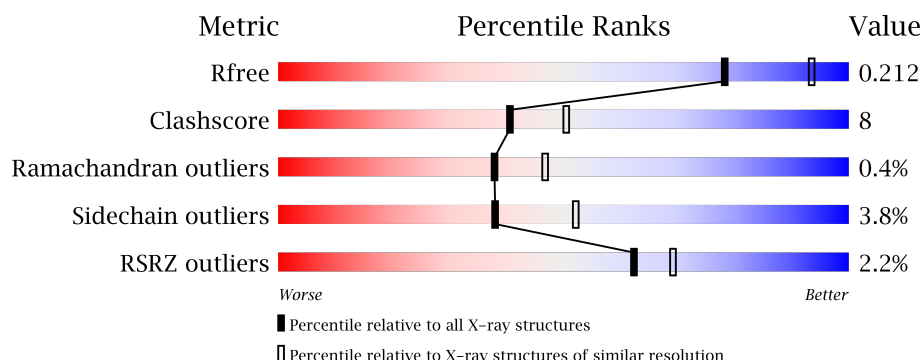
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	548	<div> <div>3%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	548	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	601	-	-	-	X
4	PG0	A	1544	-	-	-	X
4	PG0	A	1545	-	-	-	X
4	PG0	B	1546	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8853 atoms, of which 76 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 ACETYLCHOLINESTERASE.

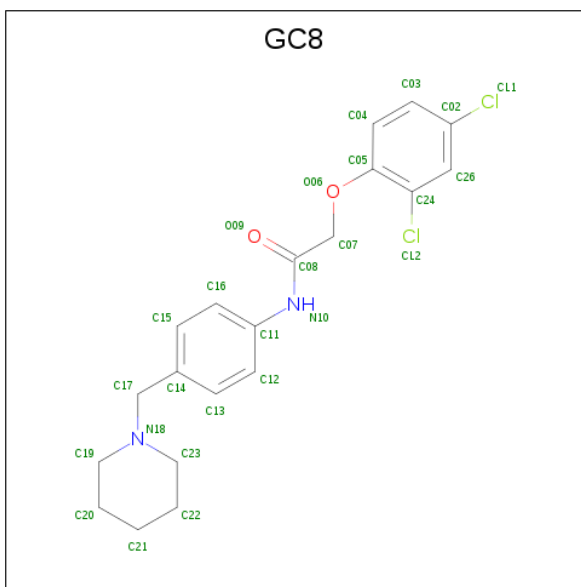
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	1	0
			4176	2680	722	759	15			
1	B	534	Total	C	N	O	S	0	2	1
			4160	2672	718	755	15			

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



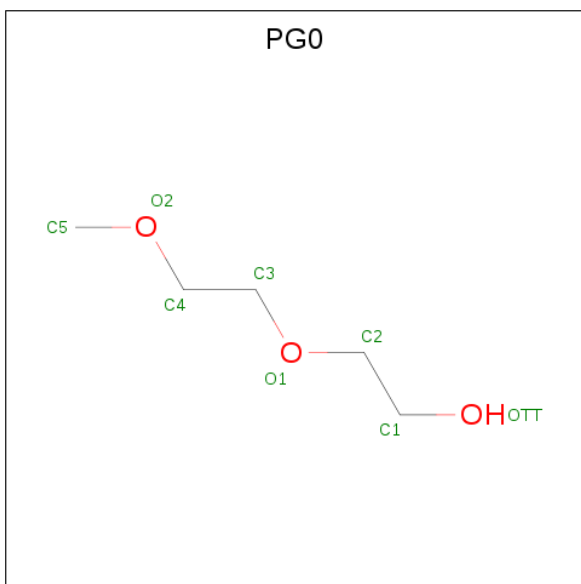
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-(2,4-dichlorophenoxy)-N-[4-(1-piperidinylmethyl)phenyl]acetamide (three-letter code: GC8) (formula: $C_{20}H_{22}Cl_2N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			26	20	2	2	2	
3	B	1	Total	C	Cl	N	O	0
			26	20	2	2	2	

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C₅H₁₂O₃).



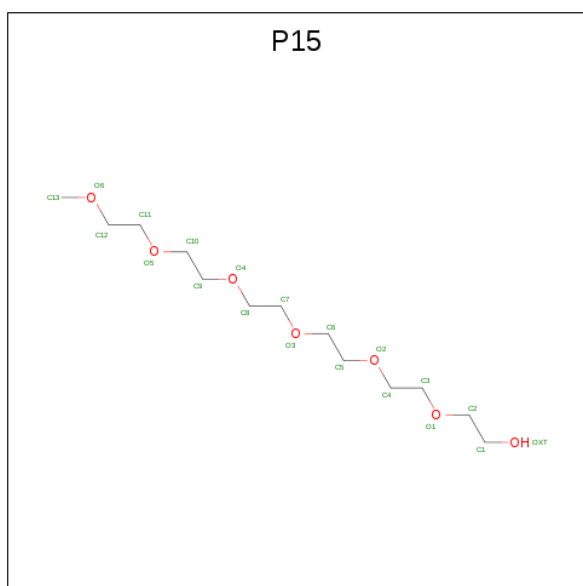
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			20	5	12	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			20	5	12	3		
4	B	1	Total	C	H	O	0	0
			20	5	12	3		
4	B	1	Total	C	H	O	0	0
			20	5	12	3		

- Molecule 5 is 2,5,8,11,14,17-HEXAOXANONADECAN-19-OL (three-letter code: P15) (formula: $C_{13}H_{28}O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			48	13	28	7		

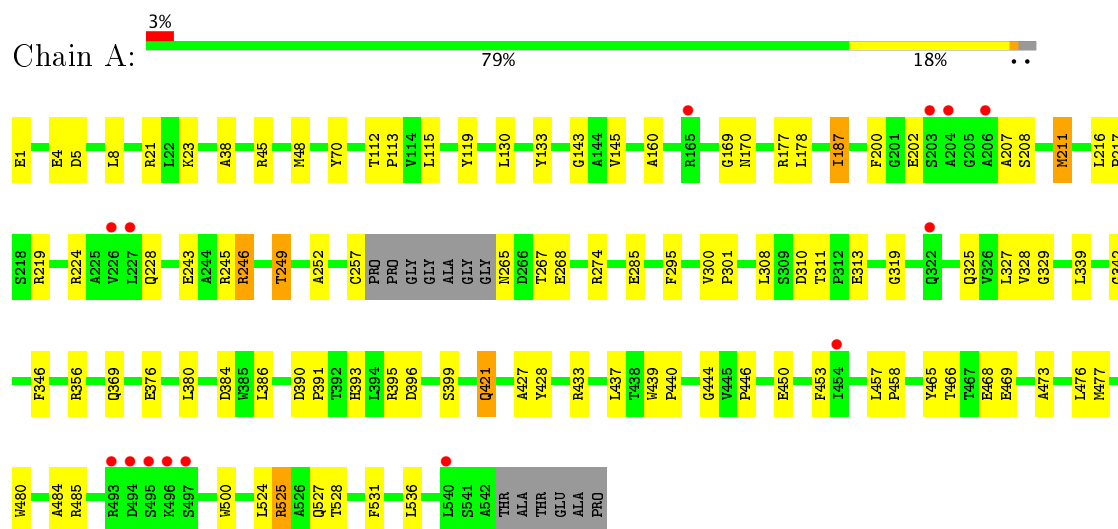
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	182	Total	O	0	0
			182	182		
6	B	113	Total	O	0	0
			113	113		

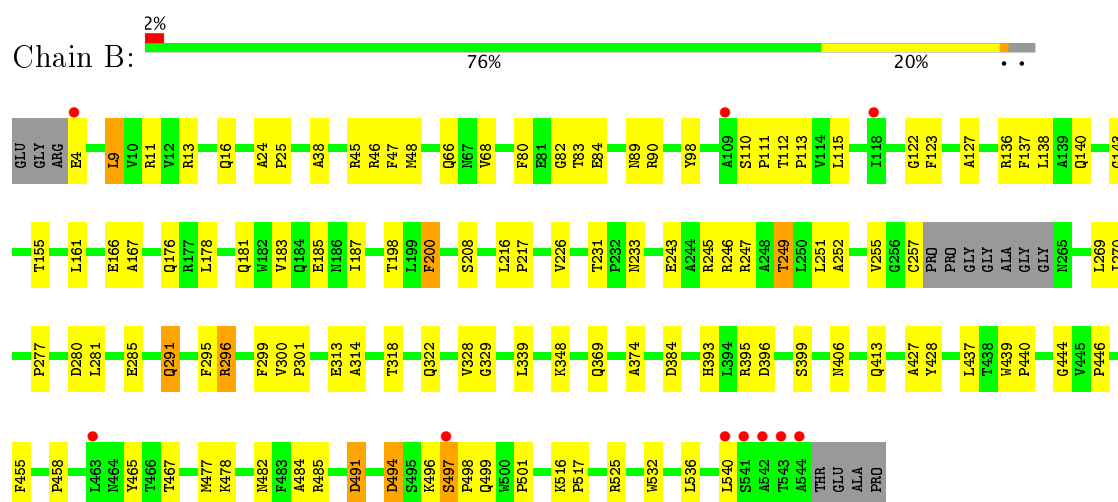
3 Residue-property plots

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: ACETYLCHOLINESTERASE



• Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.02Å 111.77Å 227.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.98 – 2.30 29.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.98-2.30) 82.7 (29.68-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.192 , 0.222 0.178 , 0.212	Depositor DCC
R_{free} test set	1466 reflections (1.97%)	DCC
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.800	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8853	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GC8, NAG, PG0, P15

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	0.42	1/4302 (0.0%)	0.54	0/5878
1	B	0.36	0/4287	0.53	0/5862
All	All	0.39	1/8589 (0.0%)	0.54	0/11740

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	TYR	CE1-CZ	5.78	1.46	1.38

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	4176	0	4061	65	0
1	B	4160	0	4035	71	0
2	A	28	0	26	0	0
2	B	14	0	13	1	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
4	A	16	24	24	2	0
4	B	16	24	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	20	28	28	2	0
6	A	182	0	0	4	0
6	B	113	0	0	4	0
All	All	8777	76	8211	137	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 8.

All (137) 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:374:ALA:HB2	1:B:540:LEU:HD21	1.47	0.96
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.60	0.84
1:B:13:ARG:HE	1:B:185:GLU:HB3	1.45	0.80
1:A:245:ARG:O	1:A:249:THR:HG23	1.84	0.77
1:A:211:MET:HE2	1:A:308:LEU:HD21	1.68	0.75
1:A:145:VAL:HG11	1:A:187:ILE:HD11	1.72	0.71
1:B:45:ARG:NH2	1:B:48:MET:SD	2.63	0.71
1:A:265:ASN:HD21	1:A:267:THR:HB	1.53	0.71
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.73	0.69
1:B:115:LEU:HD21	1:B:484:ALA:HB2	1.78	0.66
1:B:245:ARG:O	1:B:249:THR:HG23	1.96	0.66
1:B:374:ALA:CB	1:B:540:LEU:HD21	2.25	0.65
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.79	0.65
1:A:145:VAL:HG11	1:A:187:ILE:CD1	2.27	0.64
1:A:393:HIS:HB2	6:A:2147:HOH:O	1.96	0.64
1:B:233:ASN:HD22	1:B:413:GLN:HE21	1.45	0.64
1:B:161:LEU:HD12	1:B:270:ILE:CD1	2.28	0.64
1:B:369:GLN:HB2	6:B:2067:HOH:O	1.98	0.63
1:A:265:ASN:HD22	1:A:268:GLU:H	1.48	0.61
1:B:497:SER:HB2	1:B:498:PRO:C	2.22	0.60
1:B:348:LYS:O	1:B:440:PRO:HG3	1.99	0.60
1:A:531:PHE:HB2	5:B:1547:P15:H81	1.83	0.60
1:A:216:LEU:HB3	1:A:217:PRO:HD3	1.83	0.60
1:A:369:GLN:HB2	6:A:2122:HOH:O	2.03	0.59
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.84	0.59
1:A:376:GLU:O	1:A:380:LEU:HD23	2.03	0.58
1:A:207:ALA:O	1:A:211:MET:HG2	2.02	0.58
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.38	0.58
1:B:516:LYS:NZ	6:B:2104:HOH:O	2.37	0.58
1:B:112:THR:HG21	1:B:143:GLY:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PHE:CB	1:B:226:VAL:HB	2.34	0.56
1:A:328:VAL:O	1:A:427:ALA:HA	2.05	0.56
1:B:384:ASP:HB2	1:B:393[B]:HIS:CE1	2.41	0.56
1:A:211:MET:CE	1:A:308:LEU:HD11	2.37	0.55
1:B:115:LEU:HD23	1:B:198:THR:HB	1.88	0.54
1:B:167:ALA:HB2	1:B:270:ILE:HD12	1.89	0.54
1:B:328:VAL:O	1:B:427:ALA:HA	2.07	0.54
1:B:532:TRP:CE3	1:B:536:LEU:HD12	2.43	0.53
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.42	0.53
1:B:24:ALA:HB1	1:B:25:PRO:HD2	1.90	0.52
1:B:110:SER:HB2	1:B:111:PRO:HD2	1.91	0.52
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.45	0.52
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.92	0.51
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.93	0.51
1:A:145:VAL:CG1	1:A:187:ILE:HD11	2.40	0.51
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.10	0.51
1:A:211:MET:HE2	1:A:308:LEU:HD11	1.93	0.51
1:A:450:GLU:OE1	1:A:450:GLU:N	2.40	0.51
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.46	0.51
1:B:167:ALA:CB	1:B:270:ILE:HD12	2.41	0.50
1:A:313:GLU:HB2	6:A:2092:HOH:O	2.11	0.50
1:B:231:THR:HB	1:B:233:ASN:OD1	2.12	0.49
1:B:252:ALA:HB1	1:B:257:CYS:HB2	1.94	0.49
1:B:313:GLU:HG3	6:B:2081:HOH:O	2.12	0.49
1:A:439:TRP:HB3	1:A:440:PRO:HD2	1.93	0.49
1:B:80:PHE:O	1:B:84:GLU:HG2	2.12	0.49
1:A:525:ARG:HD3	4:A:1545:PG0:H51	1.93	0.49
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.95	0.49
1:B:291:GLN:NE2	1:B:369:GLN:HE21	2.10	0.49
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.49	0.48
1:A:112:THR:HG21	1:A:143:GLY:O	2.12	0.48
1:A:384:ASP:HB2	1:A:393:HIS:CE1	2.49	0.48
1:A:252:ALA:HB1	1:A:257:CYS:HB2	1.96	0.48
1:B:300:VAL:HB	1:B:301:PRO:HD2	1.96	0.48
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.48	0.48
1:B:251:LEU:O	1:B:255:VAL:HG22	2.13	0.48
1:B:269:LEU:HD23	1:B:269:LEU:C	2.33	0.48
1:B:138:LEU:HD23	1:B:477:MET:HE3	1.96	0.47
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.50	0.47
1:B:46:ARG:HD3	1:B:47:PHE:CZ	2.49	0.47
1:A:433:ARG:CZ	1:A:437:LEU:HD23	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ALA:O	1:B:318:THR:HG23	2.16	0.46
1:A:527:GLN:HG3	5:B:1547:P15:H61	1.98	0.46
1:A:457:LEU:N	1:A:458:PRO:CD	2.79	0.46
1:A:310:ASP:OD1	1:A:311:THR:N	2.40	0.46
1:A:528:THR:O	1:A:531:PHE:HB3	2.16	0.46
1:B:66:GLN:HG3	1:B:98:TYR:CD2	2.51	0.46
1:B:497:SER:HB2	1:B:498:PRO:O	2.16	0.45
1:A:224:ARG:HG2	1:A:325:GLN:HE21	1.82	0.45
1:A:444:GLY:O	1:A:446:PRO:HD3	2.16	0.45
1:B:277:PRO:HG2	1:B:280:ASP:OD2	2.16	0.45
1:B:516:LYS:HB3	1:B:517:PRO:HD2	1.98	0.45
1:B:444:GLY:O	1:B:446:PRO:HD3	2.17	0.45
1:B:478:LYS:O	1:B:482:ASN:HB2	2.16	0.45
1:B:499:GLN:O	1:B:501:PRO:HD3	2.17	0.45
1:A:1:GLU:HA	1:A:4:GLU:HG3	1.98	0.45
1:A:208:SER:HA	1:A:211:MET:HG3	1.99	0.44
1:B:243:GLU:O	1:B:247:ARG:HG3	2.18	0.44
1:B:339:LEU:HD11	1:B:399:SER:HA	2.00	0.44
1:B:80:PHE:CE2	1:B:82:GLY:HA3	2.52	0.44
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.53	0.44
1:B:291:GLN:HE21	1:B:291:GLN:HB2	1.56	0.44
1:B:395:ARG:HD2	1:B:396:ASP:OD1	2.18	0.43
1:A:160:ALA:HB2	1:A:169:GLY:HA3	2.00	0.43
1:A:525:ARG:CG	1:A:525:ARG:HH11	2.30	0.43
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.84	0.43
1:A:45:ARG:HA	1:A:48:MET:HG3	2.01	0.43
1:A:219:ARG:HA	1:A:219:ARG:HD2	1.77	0.43
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.53	0.43
1:A:536:LEU:HD12	1:A:536:LEU:HA	1.65	0.43
1:A:468:GLU:N	1:A:468:GLU:OE1	2.45	0.43
1:B:89:ASN:O	1:B:90:ARG:HD3	2.19	0.42
1:B:38:ALA:HB2	1:B:178:LEU:HD23	2.01	0.42
1:B:122:GLY:O	1:B:123:PHE:HB2	2.20	0.42
1:A:243:GLU:OE2	1:A:246:ARG:NH1	2.52	0.42
1:B:83:THR:HG23	1:B:439:TRP:CH2	2.54	0.42
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.71	0.42
1:A:274:ARG:HD3	6:A:2019:HOH:O	2.19	0.42
1:A:319:GLY:O	1:A:421:GLN:HG2	2.20	0.42
1:A:38:ALA:HB2	1:A:178:LEU:HD23	2.02	0.42
1:A:466:THR:OG1	1:A:469:GLU:HG3	2.19	0.42
1:B:216:LEU:HB3	1:B:217:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:PHE:HB2	1:B:455:PHE:O	2.19	0.42
1:A:115:LEU:HD21	1:A:484:ALA:HB2	2.01	0.42
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.49	0.42
1:B:183:VAL:O	1:B:187:ILE:HB	2.19	0.42
1:B:291:GLN:HE22	1:B:369:GLN:HE21	1.66	0.42
1:A:300:VAL:HB	1:A:301:PRO:HD2	2.02	0.42
1:A:339:LEU:HD11	1:A:399:SER:HA	2.02	0.41
2:B:601:NAG:H61	6:B:2111:HOH:O	2.20	0.41
1:A:473:ALA:O	1:A:477:MET:HG3	2.20	0.41
1:A:453:PHE:HB3	1:A:476:LEU:HD12	2.01	0.41
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.21	0.41
1:A:525:ARG:HD3	4:A:1545:PG0:C5	2.50	0.41
1:B:166:GLU:CD	1:B:166:GLU:H	2.21	0.41
1:A:224:ARG:HD3	1:A:325:GLN:NE2	2.35	0.41
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.56	0.41
1:B:155:THR:HG22	1:B:299:PHE:CE2	2.56	0.41
1:B:245:ARG:O	1:B:249:THR:CG2	2.66	0.41
1:A:113:PRO:HG3	1:A:485:ARG:HG2	2.02	0.41
1:A:23:LYS:HB3	1:A:23:LYS:HE3	1.83	0.41
1:A:5:ASP:HB3	1:A:8:LEU:HD12	2.01	0.41
1:A:170:ASN:OD1	1:A:301:PRO:HA	2.21	0.40
1:B:68:VAL:HG22	1:B:127:ALA:CB	2.51	0.40
1:B:9:LEU:HD22	1:B:16:GLN:NE2	2.37	0.40
1:A:202:GLU:HA	1:A:228:GLN:O	2.21	0.40
1:B:66:GLN:HG3	1:B:98:TYR:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	532/548 (97%)	508 (96%)	23 (4%)	1 (0%)	51 63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	532/548 (97%)	507 (95%)	22 (4%)	3 (1%)	28	34
All	All	1064/1096 (97%)	1015 (95%)	45 (4%)	4 (0%)	38	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	GLN
1	B	497	SER
1	B	496	LYS
1	A	342	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	439/446 (98%)	424 (97%)	15 (3%)	42	57
1	B	437/446 (98%)	419 (96%)	18 (4%)	35	48
All	All	876/892 (98%)	843 (96%)	33 (4%)	38	52

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	70	TYR
1	A	187	ILE
1	A	200	PHE
1	A	211	MET
1	A	246	ARG
1	A	249	THR
1	A	285	GLU
1	A	295	PHE
1	A	356	ARG
1	A	386	LEU
1	A	421	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	480	TRP
1	A	524	LEU
1	A	525	ARG
1	B	4	GLU
1	B	9	LEU
1	B	11	ARG
1	B	136	ARG
1	B	181	GLN
1	B	200	PHE
1	B	246	ARG
1	B	249	THR
1	B	281	LEU
1	B	285	GLU
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	437	LEU
1	B	467	THR
1	B	491	ASP
1	B	494	ASP
1	B	525	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	325	GLN
1	B	16	GLN
1	B	291	GLN
1	B	413	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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$
3	GC8	A	1543	-	28,28,28	1.99	7 (25%)	37,37,37	1.68	9 (24%)
4	PG0	A	1544	-	7,7,7	0.58	0	6,6,6	0.82	0
4	PG0	A	1545	-	7,7,7	0.56	0	6,6,6	0.78	0
2	NAG	A	601	1	14,14,15	0.86	1 (7%)	15,19,21	0.63	0
2	NAG	A	701	1	14,14,15	0.56	0	15,19,21	0.64	0
3	GC8	B	1544	-	28,28,28	2.02	4 (14%)	37,37,37	1.91	10 (27%)
4	PG0	B	1545	-	7,7,7	0.46	0	6,6,6	0.69	0
4	PG0	B	1546	-	7,7,7	0.60	0	6,6,6	0.76	0
5	P15	B	1547	-	19,19,19	0.54	0	18,18,18	0.89	1 (5%)
2	NAG	B	601	1	14,14,15	0.70	0	15,19,21	0.57	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
3	GC8	A	1543	-	-	0/13/21/21	0/3/3/3
4	PG0	A	1544	-	-	0/5/5/5	0/0/0/0
4	PG0	A	1545	-	-	0/5/5/5	0/0/0/0
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	GC8	B	1544	-	-	0/13/21/21	0/3/3/3
4	PG0	B	1545	-	-	0/5/5/5	0/0/0/0
4	PG0	B	1546	-	-	0/5/5/5	0/0/0/0
5	P15	B	1547	-	-	0/17/17/17	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1543	GC8	O06-C07	-2.52	1.36	1.42
3	A	1543	GC8	C17-C14	-2.45	1.46	1.51
3	A	1543	GC8	C16-C11	2.26	1.43	1.39
3	A	1543	GC8	C07-C08	2.63	1.56	1.51
2	A	601	NAG	O5-C1	2.79	1.48	1.43
3	A	1543	GC8	C19-N18	2.96	1.55	1.47
3	B	1544	GC8	C07-C08	3.02	1.57	1.51
3	A	1543	GC8	C08-N10	3.74	1.44	1.35
3	B	1544	GC8	C08-N10	4.15	1.45	1.35
3	B	1544	GC8	C19-N18	4.93	1.60	1.47
3	B	1544	GC8	C17-N18	5.66	1.58	1.47
3	A	1543	GC8	C17-N18	6.38	1.59	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1544	GC8	C17-N18-C19	-3.35	103.97	111.08
3	A	1543	GC8	C17-C14-C13	-3.32	114.46	120.78
3	A	1543	GC8	C17-N18-C19	-3.16	104.38	111.08
3	B	1544	GC8	C17-C14-C13	-3.11	114.86	120.78
3	A	1543	GC8	O09-C08-N10	-2.50	118.96	123.67
3	B	1544	GC8	O09-C08-N10	-2.49	118.98	123.67
3	B	1544	GC8	C04-C05-C24	-2.40	114.97	118.80
3	A	1543	GC8	C16-C11-C12	-2.04	116.19	119.04
3	A	1543	GC8	C04-C05-C24	-2.02	115.57	118.80
3	B	1544	GC8	C22-C23-N18	-2.00	108.06	111.40
3	B	1544	GC8	C26-C24-C05	2.11	123.93	121.02
3	A	1543	GC8	C26-C24-C05	2.11	123.94	121.02
5	B	1547	P15	C10-O5-C11	2.32	123.36	113.30
3	A	1543	GC8	C14-C17-N18	2.42	117.83	113.17
3	B	1544	GC8	C14-C17-N18	2.72	118.41	113.17
3	B	1544	GC8	C20-C19-N18	2.88	116.21	111.40
3	A	1543	GC8	C17-C14-C15	3.68	127.77	120.78
3	B	1544	GC8	C17-C14-C15	3.77	127.95	120.78
3	A	1543	GC8	O06-C05-C24	4.37	121.77	116.38
3	B	1544	GC8	O06-C05-C24	5.56	123.23	116.38

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	1545	PG0	2	0
5	B	1547	P15	2	0
2	B	601	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	535/548 (97%)	-0.22	14 (2%) 56 63	26, 39, 65, 120	0
1	B	534/548 (97%)	-0.09	10 (1%) 67 73	28, 46, 71, 151	0
All	All	1069/1096 (97%)	-0.15	24 (2%) 62 69	26, 42, 69, 151	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	ALA	20.1
1	B	543	THR	8.9
1	A	493	ARG	5.5
1	B	497	SER	4.6
1	A	495	SER	4.3
1	B	542	ALA	4.1
1	A	496	LYS	3.9
1	A	540	LEU	3.3
1	A	203	SER	3.0
1	A	322	GLN	2.8
1	A	494	ASP	2.8
1	B	541	SER	2.7
1	A	165	ARG	2.5
1	B	109	ALA	2.5
1	A	206	ALA	2.4
1	B	540	LEU	2.2
1	A	226	VAL	2.2
1	B	118	ILE	2.2
1	A	204	ALA	2.1
1	B	4	GLU	2.1
1	B	463	LEU	2.1
1	A	454	ILE	2.1
1	A	497	SER	2.1
1	A	227	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](#)

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
2	NAG	A	601	14/15	0.80	0.29	9.00	65,77,83,88	0
4	PG0	A	1544	8/8	0.90	0.23	6.17	66,80,91,91	0
4	PG0	B	1546	8/8	0.84	0.22	4.52	68,82,91,91	20
4	PG0	A	1545	8/8	0.85	0.22	3.58	48,81,109,109	0
5	P15	B	1547	20/20	0.87	0.17	1.87	29,71,113,116	0
4	PG0	B	1545	8/8	0.73	0.16	0.87	53,70,84,84	0
3	GC8	A	1543	26/26	0.87	0.16	0.09	34,48,63,80	0
3	GC8	B	1544	26/26	0.90	0.15	0.05	27,47,97,110	0
2	NAG	B	601	14/15	0.69	0.41	-	57,88,100,100	0
2	NAG	A	701	14/15	0.86	0.27	-	77,87,96,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.