



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2026 – 02:33 pm BST

PDB ID : 9SCN / pdb_00009scn
Title : Crystal structure of Tc AChE with reactivator JDS364 Monoclinic
Authors : de la Mora, E.; De Sousa, J.; Weik, M.; Nachon, F.; Baati, R.; Dias, J.
Deposited on : 2025-08-11
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

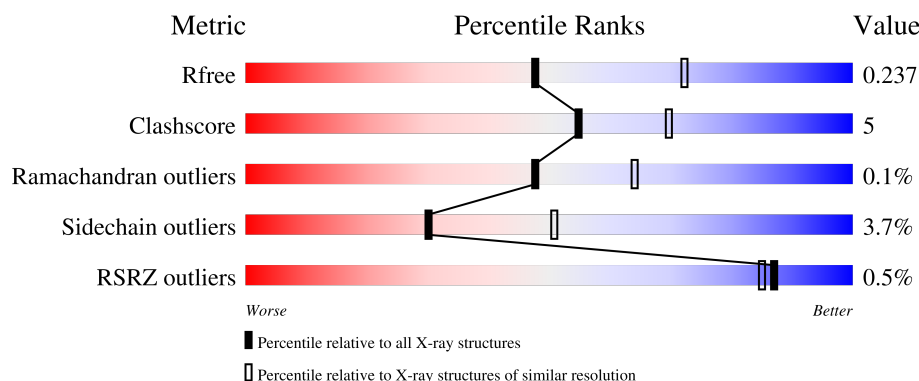
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	532	
1	B	532	
1	C	532	
1	D	532	

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	A1JM9	D	603	-	-	X	-

2 Entry composition [i](#)

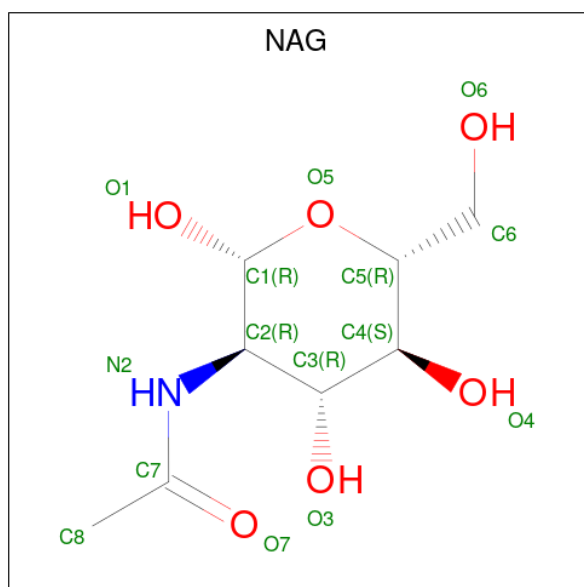
There are 5 unique types of molecules in this entry. The entry contains 17747 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	2	0
			4263	2731	726	784	22			
1	B	532	Total	C	N	O	S	0	3	0
			4247	2728	721	775	23			
1	C	532	Total	C	N	O	S	0	1	0
			4255	2727	724	782	22			
1	D	532	Total	C	N	O	S	0	2	0
			4255	2728	723	782	22			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



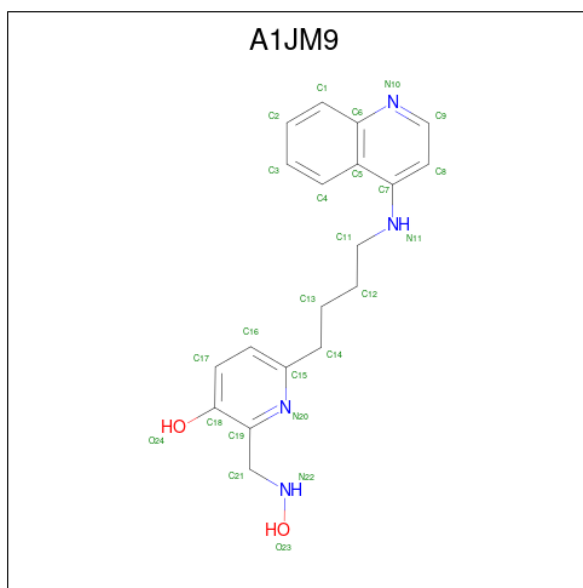
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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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	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-[(oxidanylamino)methyl]-6-[4-(quinolin-4-ylamino)butyl]pyridin-3-ol (CCD ID: A1JM9) (formula: C₁₉H₂₂N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	19	4	2		
3	D	1	Total	C	N	O	0	0
			25	19	4	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0

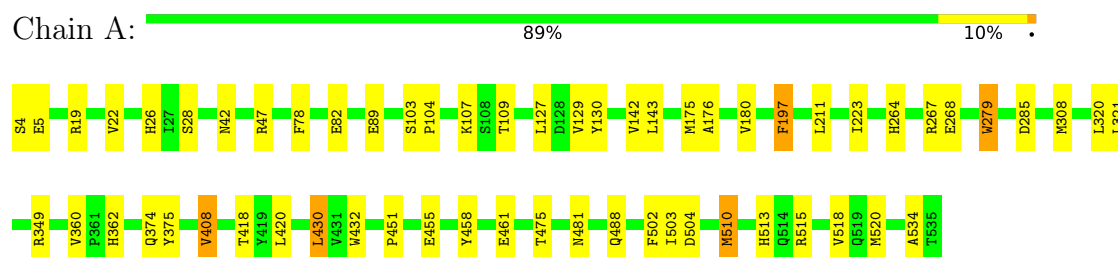
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total 189	O 189	0	0
5	B	147	Total 147	O 147	0	0
5	C	121	Total 121	O 121	0	0
5	D	90	Total 90	O 90	0	0

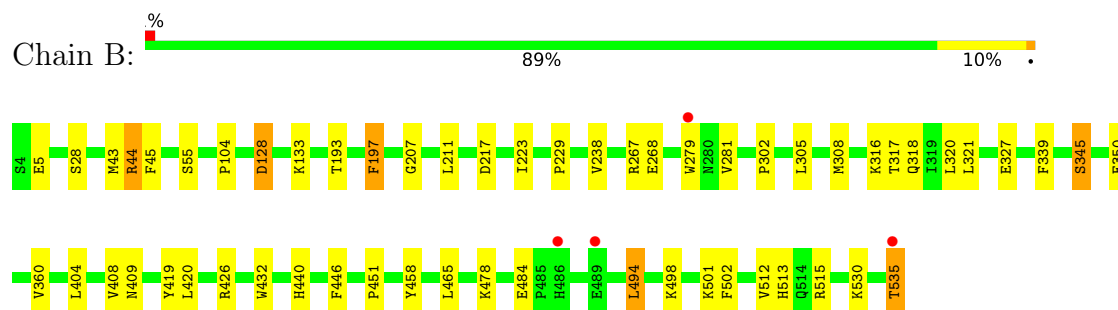
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

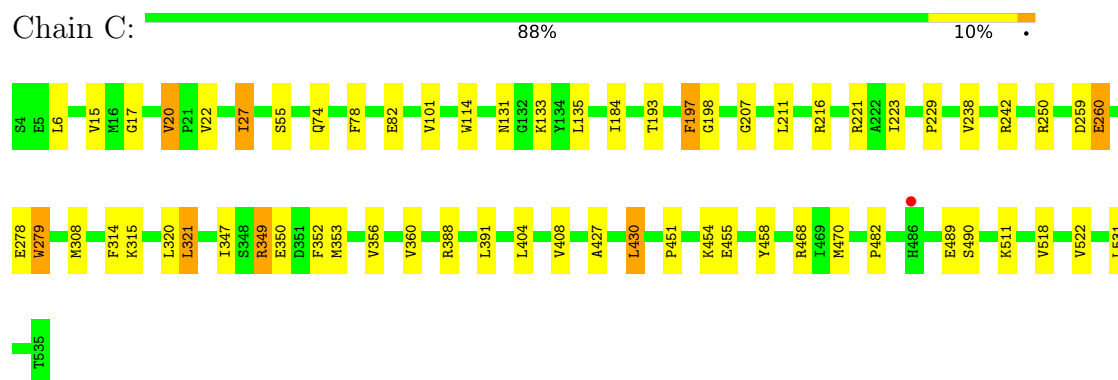
• Molecule 1: Acetylcholinesterase



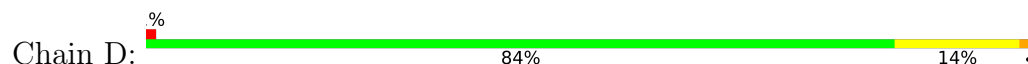
• Molecule 1: Acetylcholinesterase

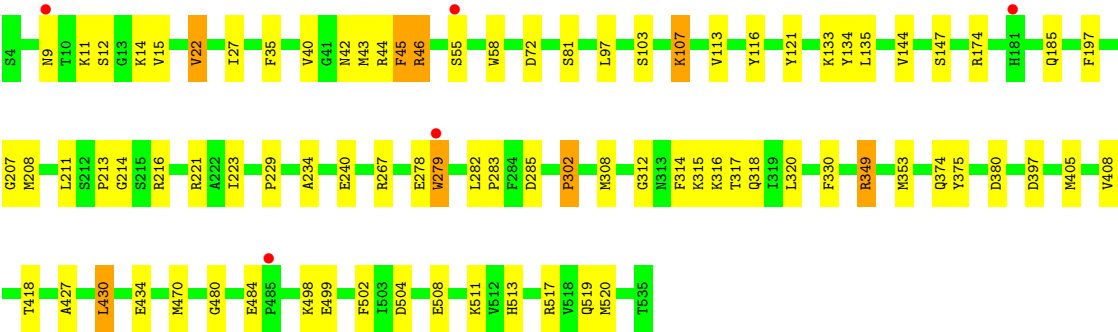


• Molecule 1: Acetylcholinesterase



• Molecule 1: Acetylcholinesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.51Å 121.96Å 123.00Å 90.00° 102.58° 90.00°	Depositor
Resolution (Å)	39.67 – 2.40 39.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.67-2.40) 98.4 (39.67-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.236 0.187 , 0.237	Depositor DCC
R_{free} test set	5748 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.7	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	0.95	EDS
Total number of atoms	17747	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 5.81% 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: A1JM9, MG, NAG

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	0.41	0/4386	0.58	0/5954
1	B	0.33	0/4376	0.53	2/5943 (0.0%)
1	C	0.31	0/4378	0.51	0/5943
1	D	0.31	0/4384	0.51	0/5952
All	All	0.34	0/17524	0.53	2/23792 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ARG	CA-C-N	5.02	130.74	121.70
1	B	44	ARG	C-N-CA	5.02	130.74	121.70

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	4263	0	4114	40	0
1	B	4247	0	4091	29	0
1	C	4255	0	4107	34	0
1	D	4255	0	4108	59	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	42	0	39	0	0
2	C	42	0	39	0	0
2	D	28	0	26	0	0
3	A	25	0	0	2	0
3	D	25	0	0	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	189	0	0	3	0
5	B	147	0	0	3	0
5	C	121	0	0	1	0
5	D	90	0	0	4	0
All	All	17747	0	16537	162	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 5.

All (162) 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:D:279:TRP:CE3	3:D:603:A1JM9:C3	2.55	0.89
1:D:278:GLU:OE1	3:D:603:A1JM9:C2	2.31	0.79
1:D:279:TRP:CE3	3:D:603:A1JM9:C2	2.68	0.76
1:D:279:TRP:CZ3	3:D:603:A1JM9:C3	2.68	0.76
1:D:375:TYR:CZ	1:D:520:MET:HE2	2.23	0.74
1:D:216:ARG:HG3	1:D:315:LYS:HB2	1.70	0.73
1:A:375:TYR:CZ	1:A:520:MET:HE2	2.24	0.73
1:B:44:ARG:O	1:B:267:ARG:NE	2.21	0.71
1:C:321:LEU:HD11	1:C:408:VAL:HG12	1.74	0.70
1:D:330:PHE:CD1	3:D:603:A1JM9:C17	2.77	0.68
1:A:78:PHE:O	1:A:82:GLU:HG2	1.94	0.67
1:B:321:LEU:HD11	1:B:408:VAL:HG12	1.77	0.65
1:B:478:LYS:NZ	5:B:703:HOH:O	2.30	0.64
1:D:374:GLN:CG	1:D:520:MET:HE1	2.28	0.63
1:D:427:ALA:HB3	1:D:430:LEU:HD23	1.81	0.63
1:A:504:ASP:OD2	1:A:513:HIS:NE2	2.32	0.62
1:A:430:LEU:HD23	1:A:432:TRP:H	1.64	0.61
1:A:4:SER:OG	1:A:5:GLU:N	2.34	0.61
1:C:427:ALA:HB3	1:C:430:LEU:HD23	1.83	0.61
1:D:135:LEU:HD13	1:D:470:MET:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9[B]:ASN:OD1	1:D:14:LYS:NZ	2.34	0.60
1:A:374:GLN:HG2	1:A:520:MET:HE1	1.82	0.60
1:D:520:MET:HE3	1:D:520:MET:HA	1.82	0.60
1:B:419:TYR:CZ	1:B:494:LEU:HD13	2.38	0.58
1:C:207:GLY:HA3	1:C:229:PRO:HD3	1.84	0.58
1:D:405:MET:HA	1:D:408:VAL:HG12	1.85	0.58
1:D:374:GLN:HG2	1:D:520:MET:HE1	1.84	0.58
1:D:43:MET:O	1:D:46:ARG:N	2.31	0.57
1:A:420:LEU:HD23	1:A:502:PHE:HB3	1.86	0.57
1:C:451:PRO:HA	1:C:458:TYR:CD1	2.40	0.56
1:C:404:LEU:O	1:C:408:VAL:HG13	2.06	0.56
1:B:484[B]:GLU:OE1	1:B:484[B]:GLU:N	2.38	0.56
1:C:216:ARG:HD2	1:C:315:LYS:HB2	1.88	0.56
1:D:221:ARG:HD3	1:D:480:GLY:HA2	1.87	0.56
1:D:397:ASP:OD2	1:D:517:ARG:NH1	2.39	0.56
1:C:278:GLU:HG3	1:C:279:TRP:HE3	1.71	0.55
1:D:174:ARG:NE	1:D:214:GLY:O	2.39	0.55
1:D:312:GLY:O	1:D:316:LYS:NZ	2.38	0.55
1:D:216:ARG:NH1	5:D:703:HOH:O	2.40	0.55
1:A:211:LEU:O	1:A:308:MET:HE1	2.07	0.55
1:D:279:TRP:CE2	3:D:603:A1JM9:C4	2.89	0.55
1:B:207:GLY:HA3	1:B:229:PRO:HD3	1.87	0.55
1:D:317:THR:OG1	1:D:318:GLN:N	2.42	0.53
1:D:42:ASN:O	1:D:267:ARG:NH1	2.42	0.53
1:B:211:LEU:HD13	1:B:305:LEU:HD22	1.91	0.53
1:D:208:MET:HE1	1:D:234:ALA:O	2.08	0.53
1:A:375:TYR:OH	1:A:520:MET:HE2	2.09	0.52
1:D:279:TRP:CD2	3:D:603:A1JM9:C3	2.92	0.52
1:A:520:MET:HA	1:A:520:MET:HE3	1.91	0.52
1:D:499:GLU:HB2	5:D:730:HOH:O	2.09	0.52
1:D:519:GLN:OE1	5:D:701:HOH:O	2.19	0.51
1:A:374:GLN:CG	1:A:520:MET:HE1	2.39	0.51
1:C:197:PHE:CB	1:C:223:ILE:HB	2.41	0.51
1:D:318:GLN:HE21	1:D:480:GLY:HA3	1.75	0.51
1:C:347:ILE:HG12	1:C:388:ARG:HB2	1.93	0.51
1:C:221:ARG:NH2	5:C:703:HOH:O	2.36	0.51
1:D:113:VAL:HG22	1:D:144:VAL:HB	1.93	0.50
1:C:135:LEU:HD13	1:C:470:MET:HG2	1.94	0.49
1:D:374:GLN:HG3	1:D:520:MET:HE1	1.92	0.49
1:C:211:LEU:HD23	1:C:314:PHE:HB3	1.95	0.49
1:A:47:ARG:NE	5:A:703:HOH:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ILE:HG12	1:C:101:VAL:O	2.13	0.47
1:C:211:LEU:O	1:C:308:MET:HE1	2.13	0.47
1:A:461:GLU:H	1:A:461:GLU:CD	2.23	0.47
1:D:45:PHE:CD1	1:D:45:PHE:N	2.82	0.47
1:D:279:TRP:CD2	3:D:603:A1JM9:C4	2.98	0.47
1:A:109:THR:CG2	1:A:142:VAL:HG23	2.44	0.47
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.50	0.47
1:D:27:ILE:HD11	1:D:133:LYS:HB2	1.97	0.47
1:D:107:LYS:HA	1:D:107:LYS:HD3	1.64	0.46
1:D:511:LYS:HE2	1:D:511:LYS:HB3	1.71	0.46
1:A:534:ALA:HB1	1:B:535:THR:HG21	1.97	0.46
1:B:197:PHE:CB	1:B:223:ILE:HB	2.44	0.46
1:B:43:MET:HE2	1:B:43:MET:HB3	1.88	0.46
1:A:503:ILE:HD13	1:A:510:MET:HE2	1.97	0.46
1:B:404:LEU:O	1:B:408:VAL:HG13	2.16	0.46
1:A:375:TYR:CE2	1:A:520:MET:HE2	2.51	0.45
1:B:446:PHE:CE2	1:B:465:LEU:HD23	2.52	0.45
1:D:35:PHE:CD2	1:D:97:LEU:HD23	2.51	0.45
1:D:349:ARG:HD3	1:D:353:MET:HE2	1.97	0.45
1:A:321:LEU:O	1:A:420:LEU:HA	2.17	0.45
1:B:133:LYS:NZ	5:B:714:HOH:O	2.48	0.45
1:D:27:ILE:HA	1:D:103:SER:HB2	1.98	0.45
1:D:408:VAL:HG23	1:D:418:THR:HG21	1.99	0.45
1:A:264:HIS:O	1:A:268:GLU:HG2	2.17	0.45
1:B:223:ILE:HA	1:B:320:LEU:O	2.17	0.45
1:B:339:PHE:HA	1:B:345:SER:HB3	1.97	0.45
1:C:242:ARG:NH2	1:C:259:ASP:OD2	2.50	0.45
1:D:133:LYS:HE2	1:D:134:TYR:CZ	2.51	0.45
1:D:302:PRO:HD2	1:D:308:MET:SD	2.57	0.45
1:B:530:LYS:HB2	1:B:530:LYS:HE3	1.79	0.44
1:C:20:VAL:HG22	1:C:27:ILE:HG22	1.99	0.44
1:B:5:GLU:OE2	1:B:104:PRO:HA	2.17	0.44
1:D:15:VAL:HG12	1:D:58:TRP:HB3	1.98	0.44
1:A:19[B]:ARG:NH1	1:A:26:HIS:HB2	2.32	0.44
1:D:504:ASP:O	5:D:702:HOH:O	2.21	0.44
1:B:409:ASN:HB3	5:B:793:HOH:O	2.18	0.44
1:A:127:LEU:HD12	1:A:130:TYR:CE2	2.53	0.44
1:A:197:PHE:HB3	1:A:223:ILE:HB	2.00	0.44
1:D:44:ARG:HA	1:D:45:PHE:HA	1.80	0.44
1:D:116:TYR:CE2	1:D:147:SER:HA	2.53	0.44
1:A:475:THR:HG22	1:A:481:ASN:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ILE:HA	1:C:320:LEU:O	2.18	0.43
1:A:455:GLU:CD	1:A:455:GLU:H	2.25	0.43
1:B:197:PHE:HB3	1:B:223:ILE:HB	1.99	0.43
1:B:45:PHE:CD1	1:B:45:PHE:N	2.86	0.43
1:A:223:ILE:HA	1:A:320:LEU:O	2.19	0.43
1:D:375:TYR:OH	1:D:520:MET:HE2	2.17	0.43
1:B:451:PRO:HA	1:B:458:TYR:CD1	2.54	0.43
1:C:197:PHE:HB3	1:C:223:ILE:HB	1.99	0.43
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.54	0.43
1:C:6:LEU:O	1:C:17:GLY:N	2.40	0.43
1:C:131:ASN:OD1	1:C:133:LYS:HG2	2.19	0.43
1:D:279:TRP:HB2	3:D:603:A1JM9:C1	2.49	0.43
1:C:511:LYS:HA	1:C:511:LYS:HD3	1.75	0.43
3:A:602:A1JM9:O24	3:A:602:A1JM9:N22	2.52	0.42
1:B:321:LEU:O	1:B:420:LEU:HA	2.19	0.42
1:C:114:TRP:CZ3	1:C:198:GLY:HA2	2.54	0.42
1:A:42:ASN:HA	1:A:267:ARG:HD3	2.02	0.42
1:C:78:PHE:O	1:C:82:GLU:HG3	2.19	0.42
1:A:515:ARG:CZ	5:A:732:HOH:O	2.67	0.42
1:B:502:PHE:CZ	1:B:513:HIS:HB2	2.54	0.42
1:C:22:VAL:HB	1:C:133:LYS:HD2	2.00	0.42
1:D:216:ARG:NH2	1:D:314:PHE:HA	2.34	0.42
1:A:103:SER:HA	1:A:104:PRO:C	2.44	0.42
1:D:213:PRO:HD3	1:D:302:PRO:HD3	2.00	0.42
1:A:5:GLU:OE2	1:A:103:SER:OG	2.36	0.42
1:A:408:VAL:HG22	1:A:418:THR:HG21	2.02	0.42
1:B:501:LYS:HD3	1:B:512:VAL:HG11	2.01	0.42
1:A:279:TRP:HB2	3:A:602:A1JM9:C1	2.50	0.42
1:D:223:ILE:HA	1:D:320:LEU:O	2.19	0.42
1:A:175:MET:HE3	5:A:738:HOH:O	2.20	0.42
1:C:320:LEU:HD12	1:C:482:PRO:HG3	2.01	0.41
1:D:211:LEU:O	1:D:308:MET:HE1	2.20	0.41
1:C:184:ILE:HD12	1:C:184:ILE:HA	1.86	0.41
1:A:129:VAL:HG13	1:A:130:TYR:CD1	2.56	0.41
1:B:327:GLU:OE1	1:B:440:HIS:ND1	2.40	0.41
1:D:216:ARG:HH21	1:D:314:PHE:HA	1.85	0.41
1:C:518:VAL:O	1:C:522:VAL:HG23	2.21	0.41
1:B:128:ASP:OD1	1:B:128:ASP:N	2.42	0.41
1:B:302:PRO:HD2	1:B:308:MET:SD	2.61	0.41
1:B:426:ARG:NH2	1:B:432:TRP:O	2.46	0.41
1:D:121:TYR:OH	3:D:603:A1JM9:N20	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASP:OD2	1:D:81:SER:HB2	2.20	0.41
1:A:176:ALA:O	1:A:180:VAL:HG23	2.21	0.41
1:C:260:GLU:CD	1:C:260:GLU:H	2.29	0.41
1:C:349:ARG:O	1:C:353:MET:HG2	2.20	0.41
1:C:352:PHE:HA	1:C:391:LEU:HD11	2.03	0.41
1:D:207:GLY:HA3	1:D:229:PRO:HD3	2.02	0.41
1:A:197:PHE:CB	1:A:223:ILE:HB	2.51	0.41
1:A:321:LEU:HD21	1:A:408:VAL:CG2	2.51	0.41
1:C:308:MET:HE2	1:C:308:MET:HB3	1.96	0.41
1:A:362:HIS:H	1:A:362:HIS:HD1	1.69	0.40
1:A:515:ARG:HB3	1:A:518:VAL:HB	2.02	0.40
1:B:317:THR:OG1	1:B:318:GLN:N	2.54	0.40
1:C:250:ARG:HE	1:C:250:ARG:HB2	1.56	0.40
1:C:489:GLU:OE2	1:C:490:SER:N	2.47	0.40
1:D:240:GLU:OE2	1:D:283:PRO:HG3	2.22	0.40
1:D:502:PHE:CZ	1:D:513:HIS:HB2	2.57	0.40
1:D:282:LEU:HA	1:D:282:LEU:HD23	1.86	0.40
1:C:352:PHE:O	1:C:356:VAL:HG23	2.21	0.40
1:D:375:TYR:CE1	1:D:520:MET:HE2	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	532/532 (100%)	508 (96%)	24 (4%)	0	100	100
1	B	533/532 (100%)	507 (95%)	26 (5%)	0	100	100
1	C	531/532 (100%)	505 (95%)	26 (5%)	0	100	100
1	D	532/532 (100%)	497 (93%)	32 (6%)	3 (1%)	21	32
All	All	2128/2128 (100%)	2017 (95%)	108 (5%)	3 (0%)	48	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	302	PRO
1	D	380	ASP
1	D	22	VAL

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	467/465 (100%)	453 (97%)	14 (3%)	36	58
1	B	460/465 (99%)	441 (96%)	19 (4%)	27	46
1	C	466/465 (100%)	446 (96%)	20 (4%)	26	44
1	D	466/465 (100%)	448 (96%)	18 (4%)	28	48
All	All	1859/1860 (100%)	1788 (96%)	71 (4%)	30	49

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	28	SER
1	A	89	GLU
1	A	107	LYS
1	A	143	LEU
1	A	197	PHE
1	A	279	TRP
1	A	285	ASP
1	A	349	ARG
1	A	360	VAL
1	A	408	VAL
1	A	430	LEU
1	A	488	GLN
1	A	510	MET
1	B	28	SER
1	B	55	SER
1	B	128	ASP

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Mol	Chain	Res	Type
1	B	193	THR
1	B	197	PHE
1	B	217	ASP
1	B	238	VAL
1	B	268	GLU
1	B	279	TRP
1	B	281	VAL
1	B	316	LYS
1	B	345	SER
1	B	350	GLU
1	B	360	VAL
1	B	494	LEU
1	B	498	LYS
1	B	515[A]	ARG
1	B	515[B]	ARG
1	B	535	THR
1	C	15	VAL
1	C	20	VAL
1	C	27	ILE
1	C	55	SER
1	C	74	GLN
1	C	193	THR
1	C	197	PHE
1	C	238	VAL
1	C	260	GLU
1	C	279	TRP
1	C	321	LEU
1	C	349	ARG
1	C	350	GLU
1	C	360	VAL
1	C	430	LEU
1	C	454	LYS
1	C	455	GLU
1	C	468[A]	ARG
1	C	468[B]	ARG
1	C	531	LEU
1	D	11	LYS
1	D	12	SER
1	D	22	VAL
1	D	40	VAL
1	D	45	PHE
1	D	46	ARG

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Mol	Chain	Res	Type
1	D	55	SER
1	D	107	LYS
1	D	185	GLN
1	D	197	PHE
1	D	279	TRP
1	D	285	ASP
1	D	349	ARG
1	D	430	LEU
1	D	434	GLU
1	D	484	GLU
1	D	498	LYS
1	D	508	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	C	66	ASN
1	C	185	GLN
1	C	264	HIS
1	C	514	GLN
1	D	98	ASN
1	D	162	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	D	601	1	14,14,15	1.09	1 (7%)	17,19,21	0.71	1 (5%)
2	NAG	C	603	1	14,14,15	0.81	1 (7%)	17,19,21	0.70	1 (5%)
2	NAG	B	603	1	14,14,15	0.32	0	17,19,21	0.49	0
2	NAG	C	602	1	14,14,15	0.47	0	17,19,21	0.45	0
2	NAG	D	602	1	14,14,15	0.50	0	17,19,21	0.54	0
3	A1JM9	A	602	-	26,27,27	1.77	4 (15%)	28,35,35	1.59	7 (25%)
3	A1JM9	D	603	-	26,27,27	1.82	4 (15%)	28,35,35	1.85	7 (25%)
2	NAG	A	601	1	14,14,15	0.73	1 (7%)	17,19,21	0.79	1 (5%)
2	NAG	C	601	1	14,14,15	0.75	1 (7%)	17,19,21	0.81	1 (5%)
2	NAG	B	601	1	14,14,15	0.91	1 (7%)	17,19,21	0.82	1 (5%)
2	NAG	B	602	1	14,14,15	0.57	0	17,19,21	0.82	1 (5%)

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	D	601	1	-	2/6/23/26	0/1/1/1
2	NAG	C	603	1	-	2/6/23/26	0/1/1/1
2	NAG	B	603	1	-	2/6/23/26	0/1/1/1
2	NAG	C	602	1	-	2/6/23/26	0/1/1/1
2	NAG	D	602	1	-	0/6/23/26	0/1/1/1
3	A1JM9	A	602	-	-	4/10/11/11	0/3/3/3
3	A1JM9	D	603	-	-	7/10/11/11	0/3/3/3
2	NAG	A	601	1	-	4/6/23/26	0/1/1/1
2	NAG	C	601	1	-	4/6/23/26	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
2	NAG	B	602	1	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	603	A1JM9	C5-C6	-5.75	1.33	1.42
3	A	602	A1JM9	C7-N11	4.72	1.47	1.36
3	D	603	A1JM9	C21-C19	4.58	1.60	1.51
3	D	603	A1JM9	C7-N11	4.17	1.46	1.36
3	A	602	A1JM9	C5-C6	-3.87	1.36	1.42
2	D	601	NAG	O5-C1	3.78	1.49	1.43
3	A	602	A1JM9	C21-C19	3.56	1.58	1.51
2	B	601	NAG	O5-C1	3.20	1.48	1.43
2	C	603	NAG	O5-C1	2.65	1.48	1.43
2	C	601	NAG	O5-C1	2.60	1.47	1.43
2	A	601	NAG	O5-C1	2.60	1.47	1.43
3	D	603	A1JM9	C14-C15	2.45	1.56	1.51
3	A	602	A1JM9	O24-C18	2.41	1.41	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	603	A1JM9	C14-C15-N20	3.84	121.67	115.95
3	D	603	A1JM9	C9-N10-C6	3.69	122.65	116.93
3	A	602	A1JM9	C7-C5-C6	3.25	120.11	118.06
3	D	603	A1JM9	C7-C5-C6	3.15	120.06	118.06
3	A	602	A1JM9	C9-N10-C6	3.15	121.81	116.93
2	B	602	NAG	C1-O5-C5	2.94	116.17	112.19
2	B	601	NAG	C1-O5-C5	2.88	116.10	112.19
2	C	601	NAG	C1-O5-C5	2.76	115.94	112.19
3	A	602	A1JM9	C5-C6-N10	-2.72	119.94	122.83
2	A	601	NAG	C1-O5-C5	2.61	115.72	112.19
3	D	603	A1JM9	C8-C9-N10	-2.58	120.59	124.58
3	D	603	A1JM9	C15-N20-C19	2.56	121.27	118.16
3	D	603	A1JM9	C5-C6-N10	-2.50	120.17	122.83
3	A	602	A1JM9	C8-C9-N10	-2.38	120.89	124.58
3	A	602	A1JM9	C16-C17-C18	-2.21	118.23	120.50
3	A	602	A1JM9	C15-N20-C19	2.20	120.83	118.16
3	A	602	A1JM9	C4-C5-C7	-2.19	119.51	123.00
2	C	603	NAG	C1-O5-C5	2.19	115.16	112.19
2	D	601	NAG	C1-O5-C5	2.14	115.09	112.19
3	D	603	A1JM9	C4-C5-C7	-2.08	119.69	123.00

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	603	A1JM9	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
3	D	603	A1JM9	C5-C7-N11-C11
3	D	603	A1JM9	C8-C7-N11-C11
2	B	603	NAG	O5-C5-C6-O6
2	C	601	NAG	O5-C5-C6-O6
2	C	602	NAG	O5-C5-C6-O6
2	B	603	NAG	C4-C5-C6-O6
2	B	602	NAG	C4-C5-C6-O6
2	B	601	NAG	O5-C5-C6-O6
2	D	601	NAG	O5-C5-C6-O6
2	B	601	NAG	C4-C5-C6-O6
2	D	601	NAG	C4-C5-C6-O6
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	C	601	NAG	C8-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	A	601	NAG	O5-C5-C6-O6
2	B	602	NAG	O5-C5-C6-O6
2	C	603	NAG	O5-C5-C6-O6
2	C	601	NAG	C4-C5-C6-O6
2	C	602	NAG	C4-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
3	D	603	A1JM9	N11-C11-C12-C13
3	D	603	A1JM9	C11-C12-C13-C14
3	A	602	A1JM9	C12-C11-N11-C7
3	D	603	A1JM9	C13-C14-C15-N20
3	A	602	A1JM9	N11-C11-C12-C13
3	D	603	A1JM9	C13-C14-C15-C16
2	C	603	NAG	C4-C5-C6-O6
3	A	602	A1JM9	C18-C19-C21-N22
3	A	602	A1JM9	C5-C7-N11-C11

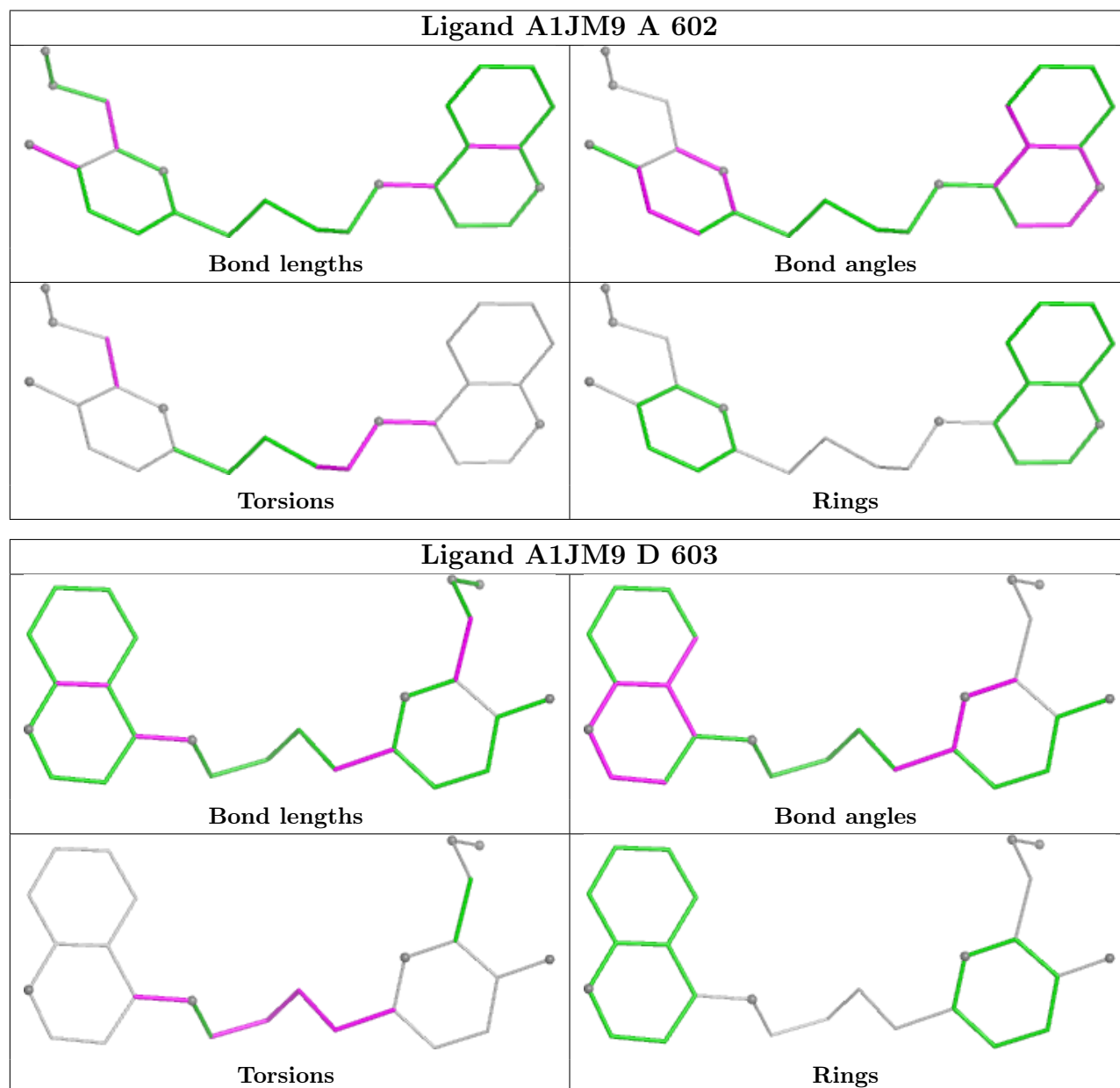
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	A1JM9	2	0
3	D	603	A1JM9	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	532/532 (100%)	-0.41	0 100 100	22, 36, 54, 90	2 (0%)
1	B	532/532 (100%)	-0.21	4 (0%) 82 80	23, 44, 63, 89	3 (0%)
1	C	532/532 (100%)	-0.16	1 (0%) 91 89	20, 46, 64, 85	1 (0%)
1	D	532/532 (100%)	0.13	5 (0%) 81 78	24, 51, 77, 103	2 (0%)
All	All	2128/2128 (100%)	-0.16	10 (0%) 87 85	20, 44, 69, 103	8 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	485	PRO	3.1
1	B	535	THR	2.6
1	D	279	TRP	2.6
1	D	9[A]	ASN	2.4
1	B	489	GLU	2.3
1	D	55	SER	2.2
1	B	486	HIS	2.2
1	C	486	HIS	2.1
1	D	181	HIS	2.1
1	B	279	TRP	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

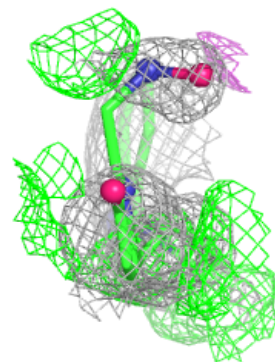
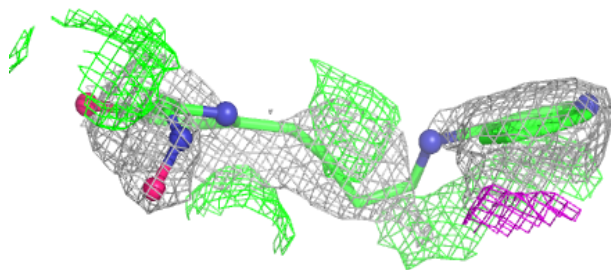
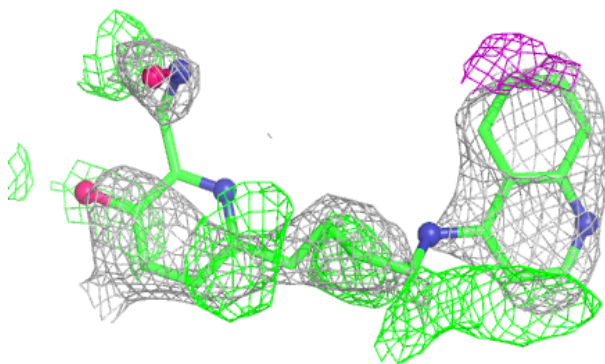
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	601	14/15	0.58	0.15	74,79,84,86	0
2	NAG	C	603	14/15	0.63	0.15	66,81,93,94	0
2	NAG	B	603	14/15	0.67	0.12	77,92,99,99	0
2	NAG	A	601	14/15	0.70	0.15	65,73,77,78	0
2	NAG	D	602	14/15	0.73	0.12	66,76,82,82	0
2	NAG	D	601	14/15	0.74	0.13	74,83,88,89	0
2	NAG	B	601	14/15	0.77	0.12	50,63,69,72	0
3	A1JM9	D	603	25/25	0.77	0.26	47,55,62,64	25
2	NAG	B	602	14/15	0.78	0.11	70,78,81,85	0
2	NAG	C	602	14/15	0.78	0.11	71,79,87,88	0
4	MG	B	604	1/1	0.79	0.23	53,53,53,53	0
3	A1JM9	A	602	25/25	0.81	0.21	46,53,62,65	25
4	MG	D	604	1/1	0.83	0.26	56,56,56,56	0
4	MG	C	604	1/1	0.85	0.26	51,51,51,51	0
4	MG	A	603	1/1	0.87	0.25	61,61,61,61	0

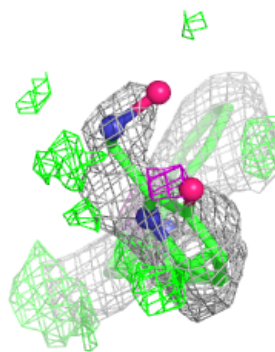
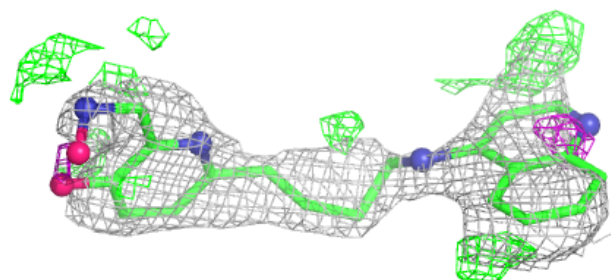
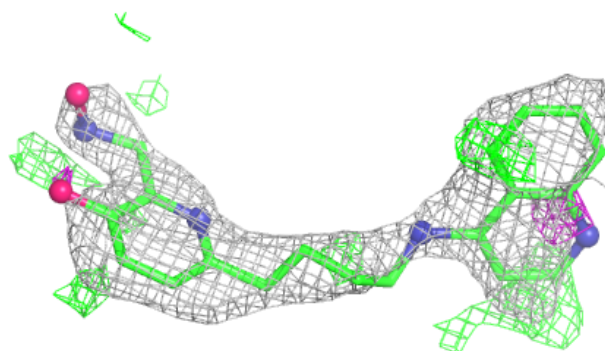
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1JM9 D 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around A1JM9 A 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.