



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:14 PM UTC

PDB ID : 7QB4 / pdb_00007qb4
Title : Mus Musculus Acetylcholinesterase in complex with 7-[(1-benzylpiperidin-3-yl)methoxy]-3,4-dimethyl-2H-chromen-2-one
Authors : Ekstrom, F.J.; Forsgren, N.
Deposited on : 2021-11-18
Resolution : 2.50 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	:	2022.3.0, CSD as543be (2022)
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

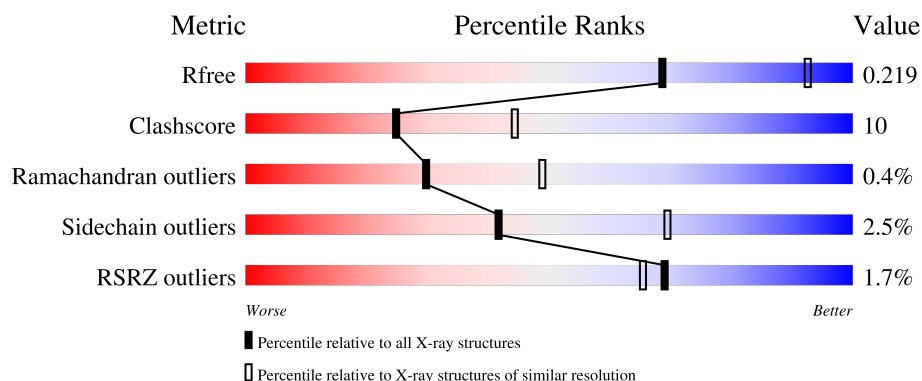
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 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	543	
1	B	543	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8802 atoms, of which 48 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	537	Total	C	N	O	S	0	1	0
			4196	2691	728	763	14			
1	B	535	Total	C	N	O	S	0	4	0
			4202	2697	729	761	15			

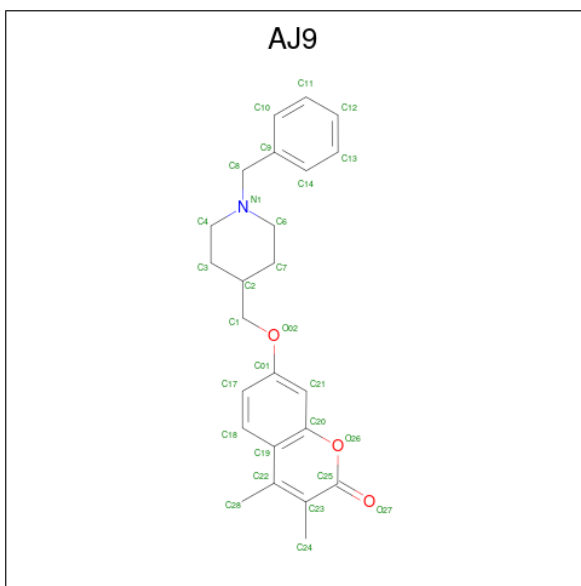
- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

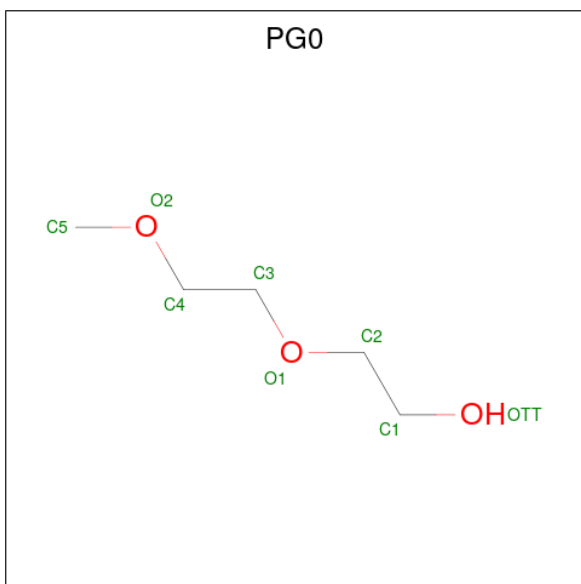
- Molecule 3 is 3,4-dimethyl-7-[[1-(phenylmethyl)piperidin-4-yl]methoxy]chromen-2-one (CCD

ID: AJ9) (formula: C₂₄H₂₇NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	11	3		
3	B	1	Total	C	O	0	0
			14	11	3		

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	5	3		

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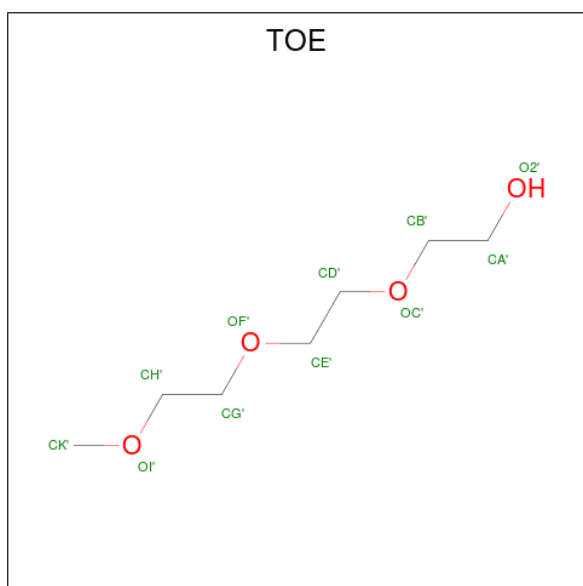
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			8	5	3			
4	A	1	Total	C	O		0	0
			5	3	2			
4	A	1	Total	C	O		0	0
			8	5	3			
4	A	1	Total	C	O		0	0
			8	5	3			
4	A	1	Total	C	O		0	0
			8	5	3			
4	A	1	Total	C	O		0	0
			8	5	3			
4	A	1	Total	C	O		0	0
			8	5	3			
4	A	1	Total	C	H	O	0	0
			20	5	12	3		
4	A	1	Total	C	H	O	0	0
			20	5	12	3		
4	B	1	Total	C	O		0	0
			8	5	3			
4	B	1	Total	C	O		0	0
			8	5	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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



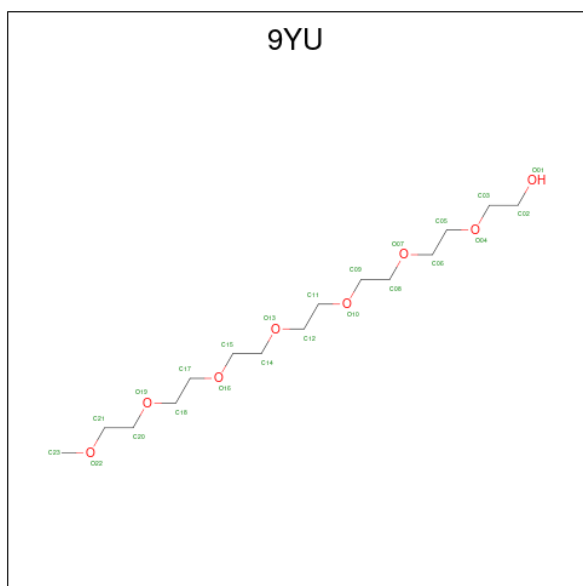
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (CCD ID: TOE) (formula: $C_7H_{16}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is 2-[2-[2-[2-[2-(2-methoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol (CCD ID: 9YU) (formula: C₁₅H₃₂O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			23	15	8		

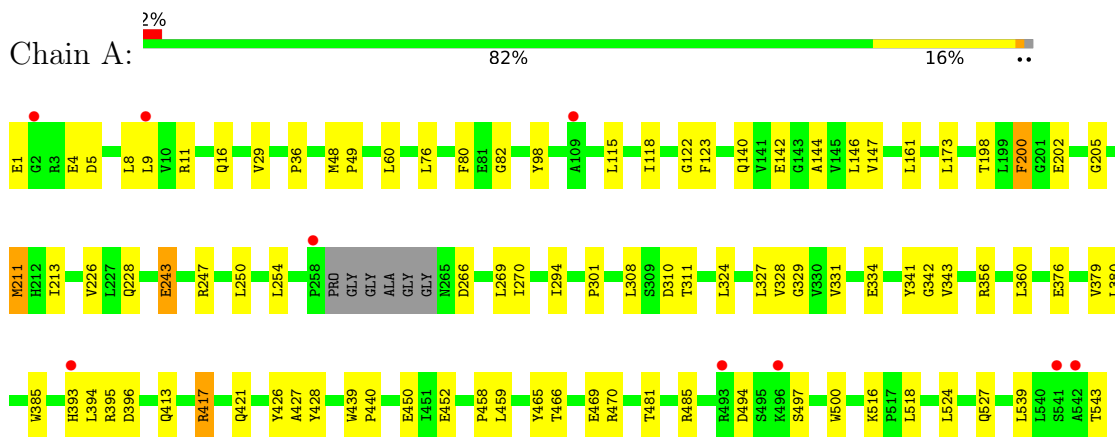
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	72	Total	O	0	0
			72	72		
8	B	51	Total	O	0	0
			51	51		

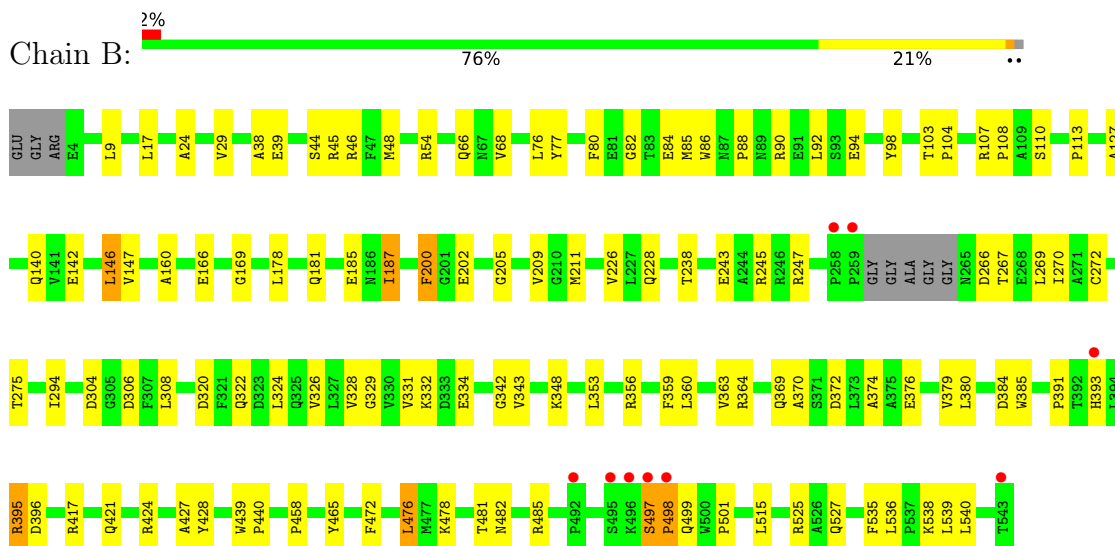
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.41Å 111.05Å 227.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 2.50 46.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.19-2.50) 99.5 (46.19-2.50)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.184 , 0.217 0.187 , 0.219	Depositor DCC
R_{free} test set	1410 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8802	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: EDO, TOE, PG0, AJ9, NAG, 9YU

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	0.22	0/4320	0.42	0/5904
1	B	0.20	0/4328	0.43	0/5917
All	All	0.21	0/8648	0.43	0/11821

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4196	0	4078	79	0
1	B	4202	0	4078	94	0
2	A	28	0	26	0	0
2	B	14	0	13	0	0
3	A	14	0	0	0	0
3	B	14	0	0	0	0
4	A	85	24	124	7	0
4	B	32	24	48	6	0
5	B	12	0	18	1	0
6	B	11	0	16	0	0
7	B	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	72	0	0	2	0
8	B	51	0	0	0	0
All	All	8754	48	8401	167	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 10.

All (167) 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:161:LEU:HD12	1:A:270:ILE:HD11	1.45	0.98
1:A:211:MET:HE1	1:A:301:PRO:HG2	1.54	0.90
1:B:320:ASP:OD1	1:B:322:GLN:HG3	1.78	0.82
1:A:459:LEU:HD23	1:A:470:ARG:HG3	1.62	0.81
1:A:380:LEU:HD12	1:B:535:PHE:HB2	1.63	0.81
1:B:324:LEU:HD21	1:B:326:VAL:CG2	2.11	0.79
1:B:324:LEU:HD21	1:B:326:VAL:HG23	1.65	0.78
1:B:103:THR:HG22	1:B:104:PRO:O	1.85	0.77
1:A:539:LEU:O	1:A:543:THR:HG22	1.84	0.77
1:A:211:MET:CE	1:A:301:PRO:HG2	2.16	0.75
1:A:161:LEU:HD12	1:A:270:ILE:CD1	2.16	0.74
1:A:376:GLU:HG3	1:B:538:LYS:HZ2	1.53	0.72
1:B:326:VAL:HG12	1:B:328:VAL:HG13	1.71	0.72
1:B:46:ARG:NH2	1:B:94:GLU:OE2	2.20	0.70
1:B:324:LEU:CD2	1:B:326:VAL:HG23	2.21	0.70
1:B:332:LYS:HE2	4:B:606:PG0:H53	1.74	0.69
1:B:364:ARG:NH2	1:B:372:ASP:OD1	2.29	0.66
1:A:485:ARG:HE	4:A:609:PG0:H32	1.61	0.66
1:B:272:CYS:O	1:B:275:THR:HB	1.97	0.65
1:A:60:LEU:HD11	4:A:614:PG0:H31	1.78	0.65
1:A:173:LEU:HD11	1:A:211:MET:HE2	1.77	0.65
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.32	0.64
1:A:328:VAL:O	1:A:427:ALA:HA	1.99	0.62
1:A:417:ARG:HE	4:A:611:PG0:H21	1.63	0.62
1:A:266:ASP:O	1:A:270:ILE:HD12	1.99	0.62
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.33	0.62
1:B:103:THR:HG23	1:B:108:PRO:HD3	1.80	0.62
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.35	0.62
1:A:516:LYS:HD2	1:A:516:LYS:N	2.15	0.60
1:B:395:ARG:HG3	1:B:396:ASP:N	2.16	0.60
1:A:48:MET:HG3	1:A:49:PRO:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:CD2	1:A:470:ARG:HG3	2.32	0.59
1:A:213:ILE:HD13	1:A:324:LEU:HD21	1.85	0.59
1:A:243:GLU:OE1	1:A:247:ARG:NE	2.35	0.59
1:B:113:PRO:HG2	4:B:609:PG0:C4	2.33	0.59
1:A:380:LEU:CD1	1:B:535:PHE:HB2	2.31	0.58
1:B:328:VAL:O	1:B:427:ALA:HA	2.03	0.57
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.39	0.57
1:B:142:GLU:HG3	1:B:481:THR:HG21	1.86	0.57
1:B:202:GLU:HA	1:B:228:GLN:O	2.04	0.57
1:A:393:HIS:HB2	8:A:752:HOH:O	2.04	0.56
1:B:104:PRO:HG2	1:B:108:PRO:HG3	1.88	0.55
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.42	0.55
1:B:360:LEU:HD23	1:B:379:VAL:HG21	1.88	0.55
1:B:166:GLU:HB2	1:B:270:ILE:HD12	1.88	0.55
1:A:385:TRP:HD1	1:B:527:GLN:OE1	1.90	0.55
1:B:515:LEU:H	5:B:604:EDO:H21	1.71	0.55
1:A:376:GLU:HG3	1:B:538:LYS:NZ	2.21	0.55
1:A:144:ALA:HA	4:A:609:PG0:H52	1.90	0.54
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.90	0.54
1:A:5:ASP:HB3	1:A:8:LEU:HD12	1.90	0.54
1:A:356:ARG:HA	1:A:394:LEU:HD13	1.90	0.54
1:B:360:LEU:C	1:B:360:LEU:HD13	2.33	0.54
1:B:269:LEU:C	1:B:269:LEU:HD23	2.33	0.53
1:B:200:PHE:CB	1:B:226:VAL:HB	2.38	0.53
1:B:9:LEU:HD23	1:B:17:LEU:O	2.09	0.53
1:B:103:THR:CG2	1:B:108:PRO:HD3	2.37	0.53
1:B:359:PHE:O	1:B:363:VAL:HG23	2.08	0.53
1:B:245:ARG:NH2	1:B:266:ASP:OD2	2.42	0.53
1:A:11:ARG:NH1	1:A:16:GLN:HG3	2.25	0.52
1:B:294:ILE:HD13	1:B:343:VAL:HG23	1.91	0.52
1:A:211:MET:CE	1:A:301:PRO:CG	2.85	0.51
1:B:211:MET:HE2	1:B:238:THR:HG22	1.90	0.51
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.92	0.51
1:A:29:VAL:CG1	1:A:140:GLN:HB2	2.40	0.51
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.45	0.51
1:B:331:VAL:HG22	1:B:334:GLU:OE2	2.09	0.51
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.93	0.51
1:A:142:GLU:HG3	1:A:481:THR:HG21	1.93	0.51
1:A:211:MET:HE1	1:A:301:PRO:CG	2.34	0.51
1:B:80:PHE:O	1:B:84:GLU:HG2	2.11	0.50
1:B:85:MET:HE2	1:B:86:TRP:CZ2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.46	0.50
1:B:77:TYR:CD1	1:B:348:LYS:HE3	2.47	0.50
1:B:166:GLU:OE1	1:B:166:GLU:N	2.41	0.50
1:A:202:GLU:HA	1:A:228:GLN:O	2.12	0.50
1:B:369:GLN:OE1	1:B:369:GLN:N	2.32	0.50
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.47	0.50
1:B:243:GLU:O	1:B:247:ARG:HG3	2.11	0.49
1:A:485:ARG:HE	4:A:609:PG0:C3	2.25	0.49
1:B:539:LEU:C	1:B:539:LEU:HD23	2.37	0.49
1:B:80:PHE:CE2	1:B:82:GLY:HA3	2.47	0.49
1:B:205:GLY:O	1:B:209:VAL:HG23	2.12	0.49
1:A:211:MET:HE3	1:A:301:PRO:CB	2.43	0.49
1:A:527:GLN:OE1	1:B:385:TRP:HD1	1.96	0.49
1:B:211:MET:HE2	1:B:238:THR:CG2	2.43	0.49
1:B:376:GLU:O	1:B:380:LEU:HG	2.13	0.49
1:B:181[A]:GLN:O	1:B:185:GLU:HG3	2.12	0.49
1:A:211:MET:CE	1:A:301:PRO:CB	2.90	0.48
1:A:331:VAL:HG22	1:A:334:GLU:OE2	2.13	0.48
1:A:450:GLU:OE1	1:A:450:GLU:N	2.37	0.48
1:A:417:ARG:HA	1:A:417:ARG:HD2	1.69	0.47
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.15	0.47
1:B:45:ARG:NH2	1:B:48:MET:HE3	2.29	0.47
1:A:327:LEU:HD11	1:A:500:TRP:CZ2	2.50	0.47
1:B:332:LYS:HE2	4:B:606:PG0:C5	2.42	0.47
1:B:481:THR:O	1:B:485:ARG:HG3	2.14	0.47
1:A:452:GLU:HG2	8:A:725:HOH:O	2.15	0.47
1:A:142:GLU:OE1	1:A:485:ARG:NH1	2.46	0.47
1:A:173:LEU:HD11	1:A:211:MET:CE	2.43	0.47
1:A:200:PHE:CB	1:A:226:VAL:HB	2.45	0.47
1:B:107:ARG:HE	1:B:107:ARG:HB2	1.58	0.47
1:B:38:ALA:HB2	1:B:178:LEU:HD23	1.96	0.46
1:B:374:ALA:HB2	1:B:539:LEU:HD22	1.97	0.46
1:B:478:LYS:O	1:B:482:ASN:HB2	2.15	0.46
1:B:160:ALA:HB2	1:B:169:GLY:CA	2.45	0.45
1:B:304:ASP:OD2	1:B:306:ASP:HB3	2.15	0.45
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.51	0.45
1:B:113:PRO:HG2	4:B:609:PG0:H41	1.98	0.45
1:A:60:LEU:C	1:A:60:LEU:HD23	2.42	0.45
1:A:115:LEU:HD23	1:A:198:THR:HB	1.99	0.45
1:B:269:LEU:HD23	1:B:269:LEU:O	2.17	0.45
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LEU:HD22	1:B:360:LEU:O	2.17	0.45
1:A:98:TYR:HE1	4:A:614:PG0:H32	1.82	0.44
1:A:466:THR:OG1	1:A:469:GLU:HG3	2.18	0.44
1:B:324:LEU:C	1:B:324:LEU:HD23	2.43	0.44
1:B:181[B]:GLN:O	1:B:185:GLU:HG3	2.17	0.44
1:A:36:PRO:HB3	1:A:98:TYR:CE1	2.52	0.44
1:B:68:VAL:HG23	1:B:90:ARG:HB2	2.00	0.44
1:B:113:PRO:HG2	4:B:609:PG0:H53	1.98	0.44
1:A:250:LEU:O	1:A:254:LEU:HG	2.18	0.43
1:A:122:GLY:O	1:A:123:PHE:HB2	2.19	0.43
1:B:68:VAL:HG13	1:B:127:ALA:HB2	2.00	0.43
1:A:29:VAL:HG11	1:A:140:GLN:HB2	2.00	0.43
1:B:146:LEU:HD13	1:B:147:VAL:N	2.34	0.43
1:B:211:MET:HG2	1:B:308:LEU:HD21	2.01	0.43
1:B:384:ASP:HB2	1:B:393[B]:HIS:NE2	2.32	0.43
1:B:275:THR:O	1:B:275:THR:CG2	2.66	0.43
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.77	0.43
1:A:360:LEU:HD22	1:A:379:VAL:HG21	2.00	0.43
1:B:166:GLU:OE2	1:B:267:THR:OG1	2.28	0.43
1:A:417:ARG:NH1	1:A:421:GLN:OE1	2.52	0.43
1:A:200:PHE:HB3	1:A:226:VAL:HB	2.00	0.42
1:B:294:ILE:HD13	1:B:343:VAL:CG2	2.49	0.42
1:A:516:LYS:HD2	1:A:516:LYS:H	1.83	0.42
1:B:200:PHE:HB2	1:B:226:VAL:HB	2.01	0.42
1:A:211:MET:HG3	1:A:308:LEU:HD21	2.01	0.42
1:B:39:GLU:OE1	1:B:54:ARG:HD3	2.19	0.42
1:A:310:ASP:OD1	1:A:311:THR:N	2.41	0.42
1:B:370:ALA:HA	1:B:540:LEU:HD21	2.02	0.42
1:B:439:TRP:HB3	1:B:440:PRO:HD2	2.01	0.42
1:A:439:TRP:HB3	1:A:440:PRO:HD2	2.01	0.42
1:B:499:GLN:O	1:B:501:PRO:HD3	2.18	0.42
1:B:39:GLU:CD	1:B:54:ARG:HD3	2.45	0.42
1:B:211:MET:CE	1:B:238:THR:HG22	2.50	0.42
1:B:497:SER:N	1:B:498:PRO:HD3	2.35	0.42
1:B:29:VAL:HG11	1:B:140:GLN:HB2	2.02	0.42
1:A:327:LEU:HD12	1:A:426:TYR:O	2.20	0.42
1:B:29:VAL:CG1	1:B:140:GLN:HB2	2.50	0.42
1:A:98:TYR:CE1	4:A:614:PG0:H32	2.55	0.41
1:A:118:ILE:O	1:A:205:GLY:HA3	2.21	0.41
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.87	0.41
1:A:494:ASP:OD2	1:A:497:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:VAL:HG22	1:B:334:GLU:CD	2.46	0.41
1:A:146:LEU:HD23	1:A:147:VAL:N	2.35	0.41
1:A:380:LEU:HD22	1:A:385:TRP:CZ2	2.56	0.40
1:A:518:LEU:HD12	1:A:518:LEU:HA	1.95	0.40
1:A:76:LEU:HD22	1:A:341:TYR:CD2	2.57	0.40
1:B:88:PRO:HG2	1:B:92:LEU:HD21	2.04	0.40
1:B:324:LEU:HD21	1:B:326:VAL:HG21	1.99	0.40
1:B:472:PHE:CZ	1:B:476:LEU:HD21	2.56	0.40
4:B:606:PG0:H31	4:B:606:PG0:H12	1.90	0.40
1:A:294:ILE:HD13	1:A:343:VAL:HG23	2.03	0.40
1:A:356:ARG:O	1:A:360:LEU:HG	2.22	0.40
1:A:385:TRP:CD1	1:B:527:GLN:OE1	2.74	0.40
1:B:76:LEU:HG	1:B:77:TYR:CD2	2.57	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	534/543 (98%)	515 (96%)	18 (3%)	1 (0%)	43	63
1	B	535/543 (98%)	508 (95%)	24 (4%)	3 (1%)	21	38
All	All	1069/1086 (98%)	1023 (96%)	42 (4%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	498	PRO
1	B	497	SER
1	A	342	GLY
1	B	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	441/443 (100%)	432 (98%)	9 (2%)	48	75
1	B	442/443 (100%)	429 (97%)	13 (3%)	37	65
All	All	883/886 (100%)	861 (98%)	22 (2%)	42	69

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	4	GLU
1	A	9	LEU
1	A	200	PHE
1	A	211	MET
1	A	243	GLU
1	A	413	GLN
1	A	417	ARG
1	A	524	LEU
1	B	44	SER
1	B	110	SER
1	B	146	LEU
1	B	187	ILE
1	B	200	PHE
1	B	356	ARG
1	B	395	ARG
1	B	417	ARG
1	B	421	GLN
1	B	424	ARG
1	B	476	LEU
1	B	525	ARG
1	B	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	499	GLN
1	B	284	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 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	$\# Z > 2$
4	PG0	B	606	-	7,7,7	0.63	0	6,6,6	0.82	0
2	NAG	A	601	1	14,14,15	0.51	0	17,19,21	0.59	1 (5%)
4	PG0	A	607	-	7,7,7	0.58	0	6,6,6	0.74	0
5	EDO	B	603	-	3,3,3	0.39	0	2,2,2	0.44	0
3	AJ9	A	603	-	15,15,31	1.13	1 (6%)	19,22,43	1.90	5 (26%)
4	PG0	A	612	-	7,7,7	0.65	0	6,6,6	0.78	0
4	PG0	B	608	-	7,7,7	0.64	0	6,6,6	1.16	1 (16%)
4	PG0	A	608	-	7,7,7	0.59	0	6,6,6	0.75	0
4	PG0	A	609	-	7,7,7	0.61	0	6,6,6	0.77	0
2	NAG	A	602	1	14,14,15	0.43	0	17,19,21	0.58	0
2	NAG	B	601	1	14,14,15	0.63	0	17,19,21	0.69	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PG0	A	610	-	7,7,7	0.63	0	6,6,6	0.82	0
6	TOE	B	610	-	10,10,10	0.64	0	9,9,9	0.85	0
7	9YU	B	611	-	22,22,22	0.65	0	21,21,21	0.90	1 (4%)
4	PG0	B	609	-	7,7,7	0.68	0	6,6,6	1.08	1 (16%)
4	PG0	A	613	-	7,7,7	0.61	0	6,6,6	0.97	1 (16%)
4	PG0	B	607	-	7,7,7	0.63	0	6,6,6	0.80	0
4	PG0	A	614	-	7,7,7	0.56	0	6,6,6	0.83	0
4	PG0	A	611	-	7,7,7	0.59	0	6,6,6	0.80	0
4	PG0	A	604	-	7,7,7	0.62	0	6,6,6	0.76	0
4	PG0	A	605	-	7,7,7	0.62	0	6,6,6	0.73	0
4	PG0	A	606	-	4,4,7	0.55	0	3,3,6	0.68	0
5	EDO	B	604	-	3,3,3	0.44	0	2,2,2	0.29	0
3	AJ9	B	602	-	15,15,31	1.04	2 (13%)	19,22,43	1.89	6 (31%)
5	EDO	B	605	-	3,3,3	0.40	0	2,2,2	0.41	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
4	PG0	B	606	-	-	3/5/5/5	-
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	PG0	A	607	-	-	2/5/5/5	-
5	EDO	B	603	-	-	1/1/1/1	-
3	AJ9	A	603	-	-	-	0/2/2/4
4	PG0	A	612	-	-	4/5/5/5	-
4	PG0	B	608	-	-	3/5/5/5	-
4	PG0	A	608	-	-	4/5/5/5	-
4	PG0	A	609	-	-	3/5/5/5	-
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	PG0	A	610	-	-	2/5/5/5	-
6	TOE	B	610	-	-	7/8/8/8	-
7	9YU	B	611	-	-	11/20/20/20	-
4	PG0	B	609	-	-	3/5/5/5	-
4	PG0	A	613	-	-	1/5/5/5	-
4	PG0	B	607	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG0	A	614	-	-	1/5/5/5	-
4	PG0	A	611	-	-	4/5/5/5	-
4	PG0	A	604	-	-	4/5/5/5	-
4	PG0	A	605	-	-	1/5/5/5	-
4	PG0	A	606	-	-	1/2/2/5	-
5	EDO	B	604	-	-	1/1/1/1	-
3	AJ9	B	602	-	-	-	0/2/2/4
5	EDO	B	605	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	AJ9	C17-C01	2.83	1.44	1.39
3	B	602	AJ9	C17-C01	2.17	1.43	1.39
3	B	602	AJ9	C21-C20	2.13	1.42	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	AJ9	O26-C25-O27	-3.70	111.35	116.22
3	B	602	AJ9	C17-C01-C21	-3.57	116.27	120.19
3	A	603	AJ9	C17-C01-C21	-3.41	116.44	120.19
3	B	602	AJ9	O26-C25-O27	-3.26	111.93	116.22
3	B	602	AJ9	C18-C19-C20	-3.18	114.04	118.21
3	A	603	AJ9	C18-C19-C20	-3.02	114.25	118.21
3	A	603	AJ9	C18-C19-C22	2.87	127.14	122.75
3	B	602	AJ9	C18-C19-C22	2.66	126.82	122.75
2	B	601	NAG	C1-O5-C5	2.46	115.48	112.19
3	B	602	AJ9	C28-C22-C19	2.44	121.27	118.49
4	B	609	PG0	C2-O1-C3	2.19	122.83	113.26
4	B	608	PG0	C2-O1-C3	2.15	122.69	113.26
3	A	603	AJ9	C28-C22-C19	2.15	120.93	118.49
7	B	611	9YU	C14-O13-C12	2.12	122.52	113.26
4	A	613	PG0	C2-O1-C3	2.04	122.19	113.26
2	A	601	NAG	C1-O5-C5	2.03	114.91	112.19
3	B	602	AJ9	O02-C01-C21	2.03	125.16	119.85

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	PG0	C1-C2-O1-C3
2	B	601	NAG	O5-C5-C6-O6
4	A	604	PG0	O1-C3-C4-O2
6	B	610	TOE	OF'-CG'-CH'-OI'
4	B	608	PG0	OTT-C1-C2-O1
2	B	601	NAG	C4-C5-C6-O6
2	A	602	NAG	O5-C5-C6-O6
4	B	609	PG0	O1-C3-C4-O2
2	A	602	NAG	C4-C5-C6-O6
7	B	611	9YU	O10-C11-C12-O13
4	A	608	PG0	O1-C3-C4-O2
2	A	601	NAG	O5-C5-C6-O6
4	A	607	PG0	O1-C3-C4-O2
2	A	601	NAG	C4-C5-C6-O6
4	B	609	PG0	OTT-C1-C2-O1
4	A	611	PG0	C1-C2-O1-C3
4	B	608	PG0	O1-C3-C4-O2
4	A	604	PG0	OTT-C1-C2-O1
7	B	611	9YU	O04-C05-C06-O07
4	A	605	PG0	OTT-C1-C2-O1
4	A	606	PG0	O1-C3-C4-O2
4	A	610	PG0	OTT-C1-C2-O1
4	A	608	PG0	OTT-C1-C2-O1
4	A	609	PG0	O1-C3-C4-O2
5	B	604	EDO	O1-C1-C2-O2
6	B	610	TOE	CG'-CH'-OI'-CK'
4	A	607	PG0	OTT-C1-C2-O1
4	B	606	PG0	O1-C3-C4-O2
4	A	611	PG0	C3-C4-O2-C5
6	B	610	TOE	CH'-CG'-OF'-CE'
4	B	607	PG0	OTT-C1-C2-O1
6	B	610	TOE	CD'-CE'-OF'-CG'
7	B	611	9YU	C09-C08-O07-C06
4	B	607	PG0	O1-C3-C4-O2
4	A	604	PG0	C3-C4-O2-C5
7	B	611	9YU	C14-C15-O16-C17
4	B	607	PG0	C4-C3-O1-C2
4	A	608	PG0	C3-C4-O2-C5
4	A	612	PG0	C1-C2-O1-C3
6	B	610	TOE	O2'-CA'-CB'-OC'
4	A	611	PG0	C4-C3-O1-C2
4	A	612	PG0	C4-C3-O1-C2
6	B	610	TOE	CA'-CB'-OC'-CD'

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Mol	Chain	Res	Type	Atoms
7	B	611	9YU	O13-C14-C15-O16
4	A	610	PG0	O1-C3-C4-O2
7	B	611	9YU	C15-C14-O13-C12
4	A	612	PG0	C3-C4-O2-C5
4	B	607	PG0	C3-C4-O2-C5
4	B	609	PG0	C3-C4-O2-C5
4	A	609	PG0	C4-C3-O1-C2
4	A	612	PG0	OTT-C1-C2-O1
4	B	606	PG0	C1-C2-O1-C3
7	B	611	9YU	C21-C20-O19-C18
4	A	608	PG0	C1-C2-O1-C3
4	B	606	PG0	C4-C3-O1-C2
5	B	603	EDO	O1-C1-C2-O2
5	B	605	EDO	O1-C1-C2-O2
4	A	613	PG0	O1-C3-C4-O2
7	B	611	9YU	C11-C12-O13-C14
4	A	614	PG0	O1-C3-C4-O2
4	B	608	PG0	C4-C3-O1-C2
7	B	611	9YU	C12-C11-O10-C09
6	B	610	TOE	CE'-CD'-OC'-CB'
4	A	611	PG0	O1-C3-C4-O2
7	B	611	9YU	O16-C17-C18-O19
7	B	611	9YU	C08-C09-O10-C11
4	A	604	PG0	C4-C3-O1-C2

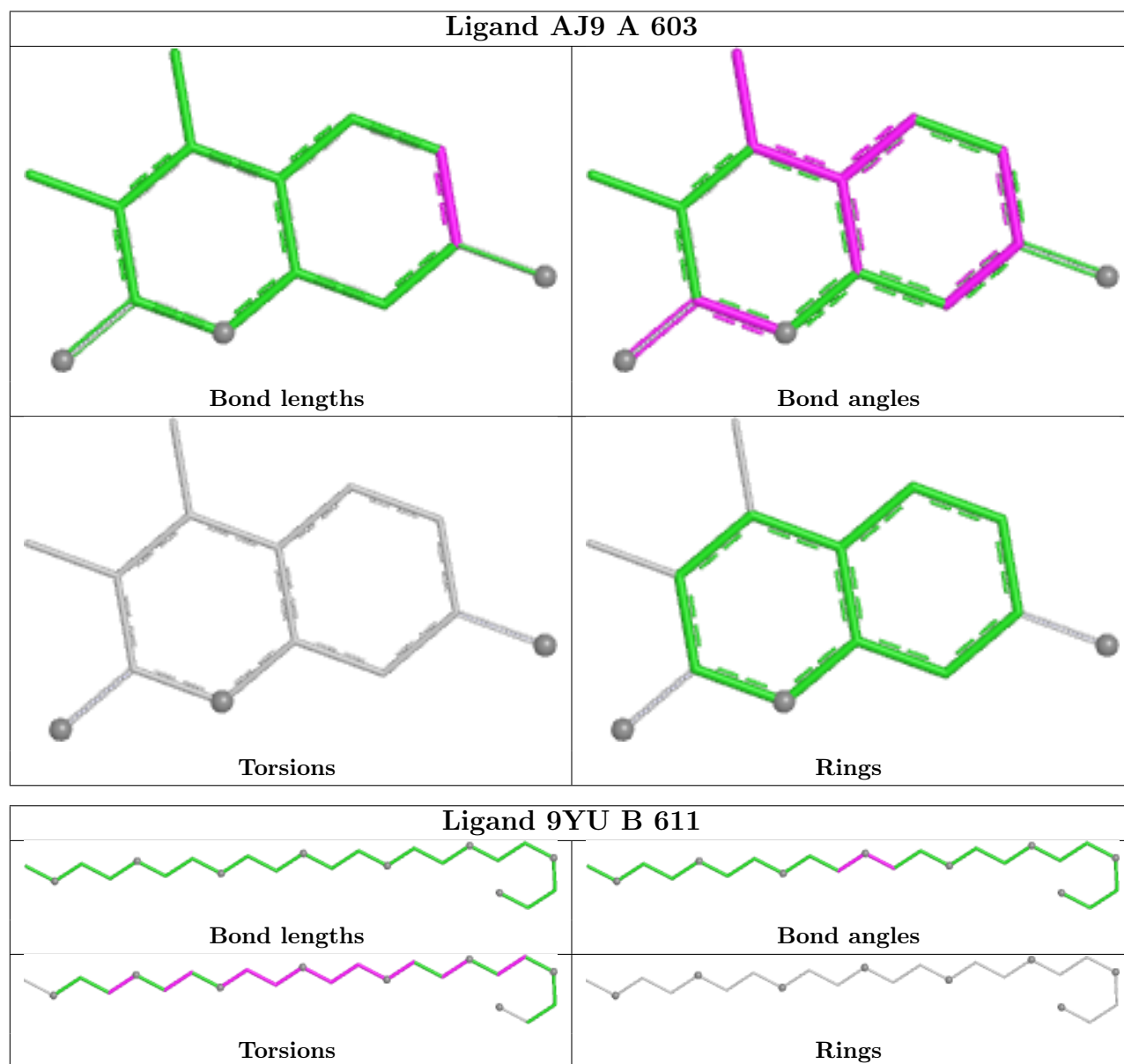
There are no ring outliers.

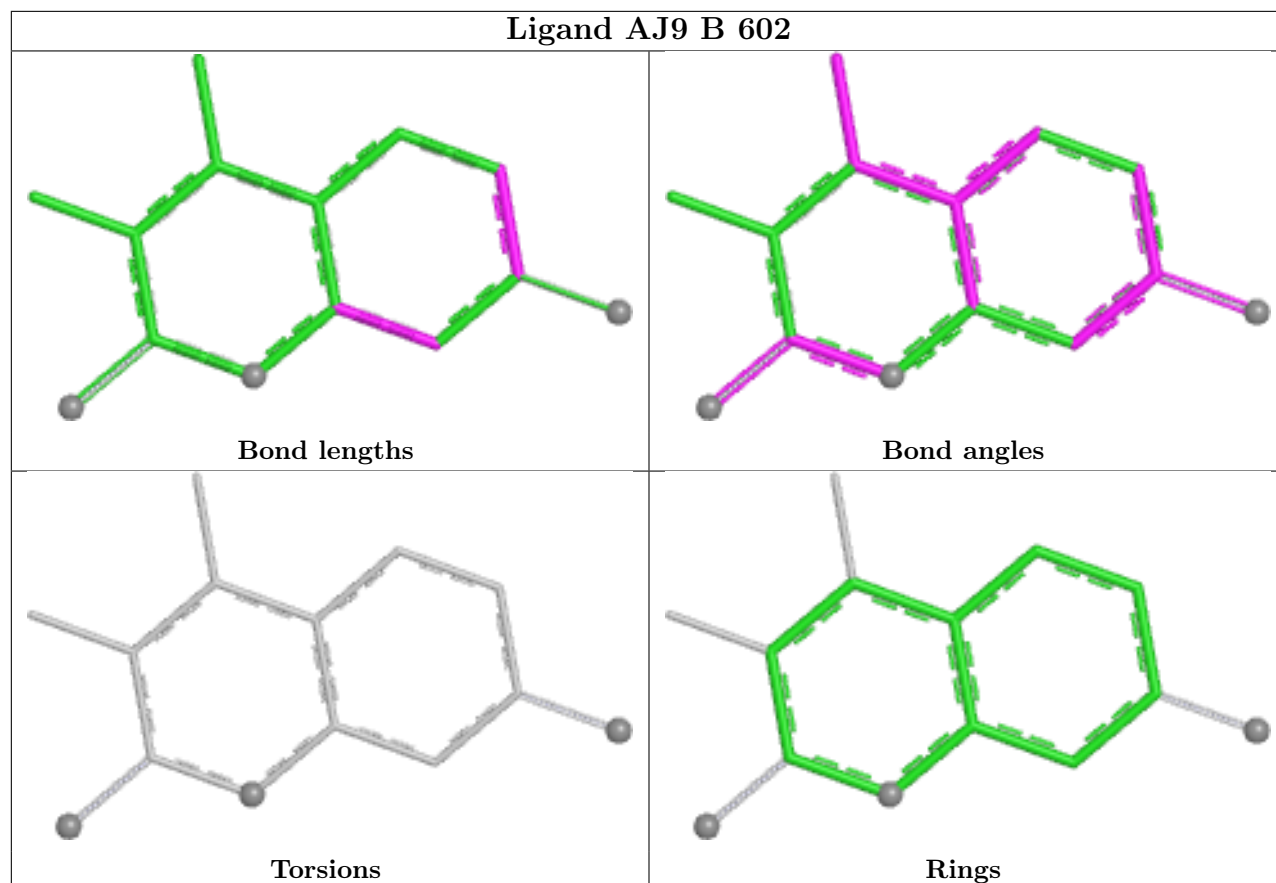
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	606	PG0	3	0
4	A	609	PG0	3	0
4	B	609	PG0	3	0
4	A	614	PG0	3	0
4	A	611	PG0	1	0
5	B	604	EDO	1	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 [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 [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	537/543 (98%)	-0.03	9 (1%) 69 65	28, 63, 92, 159	1 (0%)
1	B	535/543 (98%)	0.06	9 (1%) 69 65	29, 67, 96, 137	4 (0%)
All	All	1072/1086 (98%)	0.01	18 (1%) 69 65	28, 65, 94, 159	5 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	PRO	5.4
1	B	497	SER	4.5
1	B	498	PRO	4.4
1	B	543	THR	3.6
1	B	496	LYS	3.3
1	B	492	PRO	3.3
1	B	495	SER	3.0
1	A	493	ARG	2.9
1	B	393[A]	HIS	2.7
1	B	258	PRO	2.7
1	A	9	LEU	2.6
1	A	496	LYS	2.6
1	B	259	PRO	2.5
1	A	109	ALA	2.3
1	A	541	SER	2.2
1	A	2	GLY	2.1
1	A	393	HIS	2.1
1	A	542	ALA	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

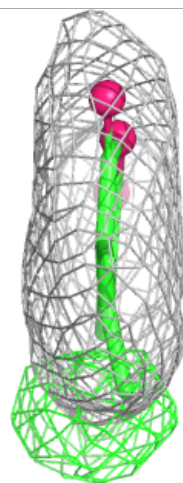
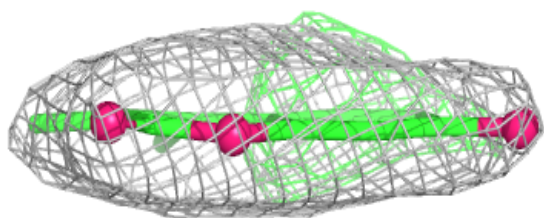
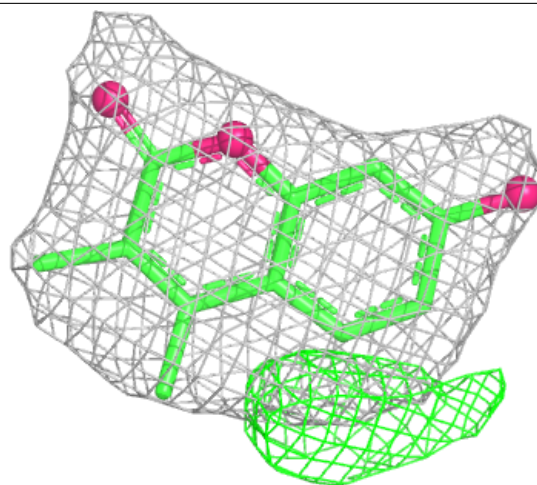
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	601	14/15	0.47	0.23	90,108,119,122	0
4	PG0	A	614	8/8	0.58	0.32	106,128,133,133	0
4	PG0	A	613	8/8	0.69	0.20	105,127,135,135	0
2	NAG	A	601	14/15	0.69	0.18	84,99,114,114	0
2	NAG	A	602	14/15	0.73	0.15	111,120,123,123	0
4	PG0	B	607	8/8	0.78	0.23	92,93,96,96	0
4	PG0	A	612	8/8	0.79	0.23	91,93,107,108	0
4	PG0	A	611	8/8	0.79	0.23	91,95,97,98	0
4	PG0	B	608	8/8	0.79	0.17	87,109,130,130	0
5	EDO	B	603	4/4	0.79	0.22	93,94,96,101	0
4	PG0	A	606	5/8	0.80	0.23	89,89,91,91	0
4	PG0	A	607	8/8	0.81	0.27	82,90,97,98	0
6	TOE	B	610	11/11	0.82	0.25	87,89,101,102	0
4	PG0	A	610	8/8	0.83	0.29	94,100,108,109	0
4	PG0	B	606	8/8	0.83	0.21	78,86,91,94	0
4	PG0	A	604	8/8	0.85	0.17	80,85,92,96	0
5	EDO	B	604	4/4	0.85	0.22	104,109,115,118	0
4	PG0	A	609	8/8	0.85	0.20	88,92,101,103	0
4	PG0	A	605	8/8	0.86	0.19	90,97,99,99	0
4	PG0	A	608	8/8	0.86	0.20	80,84,87,88	0
4	PG0	B	609	8/8	0.88	0.15	93,112,123,123	0
3	AJ9	A	603	14/28	0.88	0.18	79,92,101,103	0
7	9YU	B	611	23/23	0.88	0.17	58,80,92,95	0
3	AJ9	B	602	14/28	0.92	0.16	85,93,103,104	0
5	EDO	B	605	4/4	0.92	0.33	120,123,123,125	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.

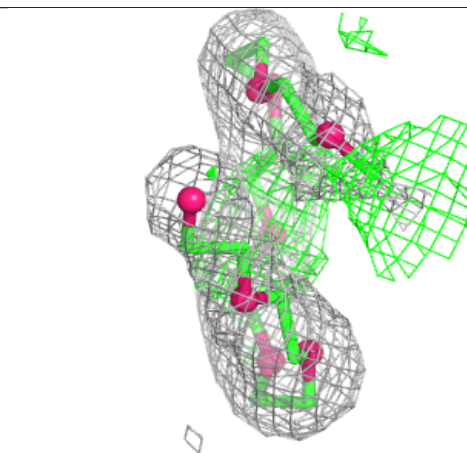
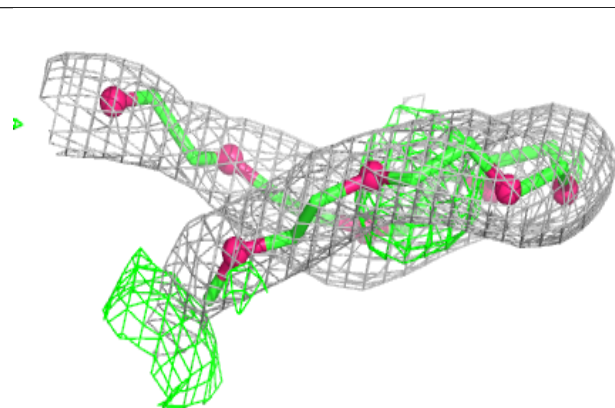
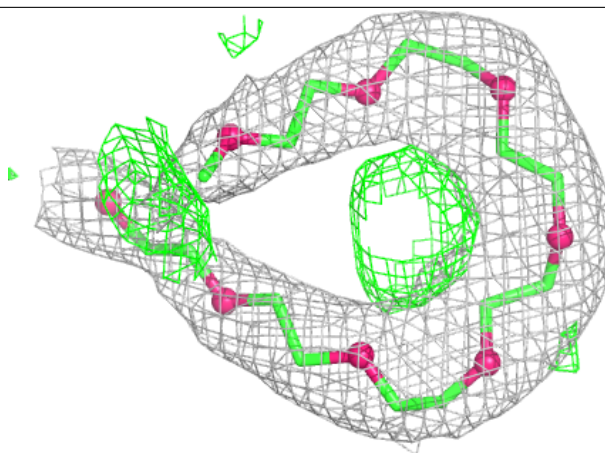
Electron density around AJ9 A 603:

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

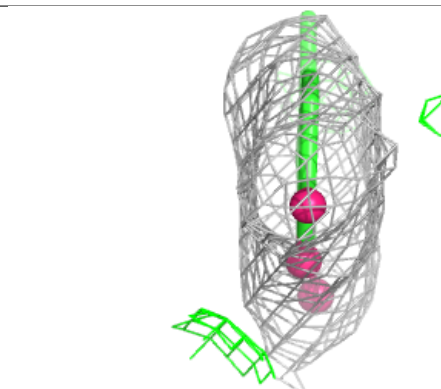
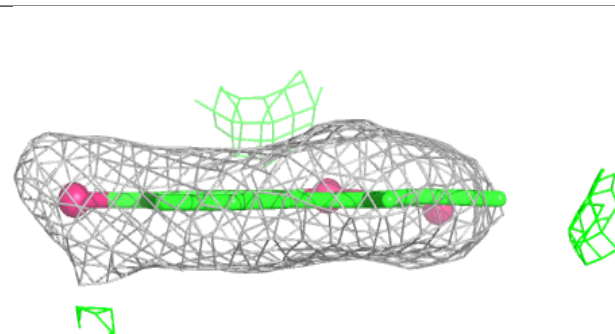
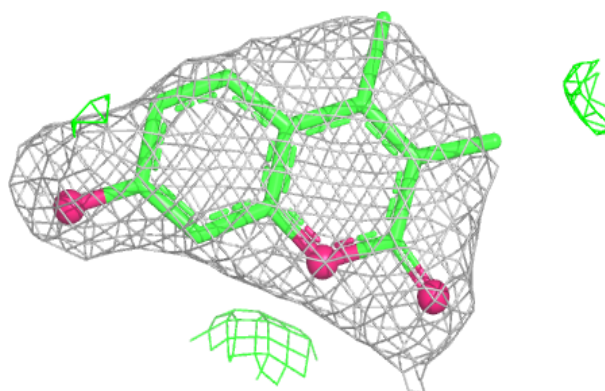


Electron density around 9YU B 611:

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

**Electron density around AJ9 B 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.