



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:12 PM UTC

PDB ID : 6H13 / pdb_00006h13
Title : Crystal structure of TcACHE complexed to 1-(4-((Methyl((1-(2-((1,2,3,4-tetrahydroacridin-9-yl)amino)ethyl)-1H-1,2,3-triazol-4-yl)methyl)amino)methyl)pyridin-2-yl)-3-(6-oxo-1,2,3,4,6,10b-hexahydropyrido[2,1-a]isoindol-10-yl)urea
Authors : Coquelle, N.; Colletier, J.P.
Deposited on : 2018-07-10
Resolution : 2.80 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

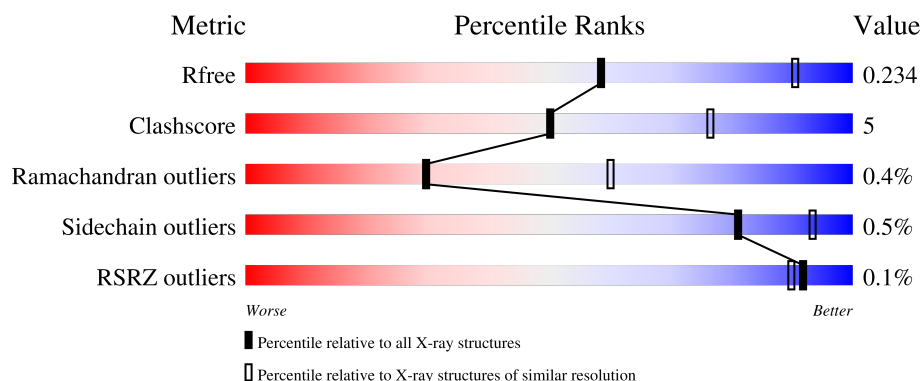
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	565	 81% 13% 6%
1	B	565	 83% 11% 6%

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	602	X	-	-	-
3	FJN	A	604	X	-	-	-
3	FJN	B	605	X	-	-	-
4	CL	B	612	-	-	X	-
7	MES	B	604	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9055 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	8	0
			4292	2753	732	785	22			
1	B	532	Total	C	N	O	S	0	8	0
			4290	2751	730	787	22			

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



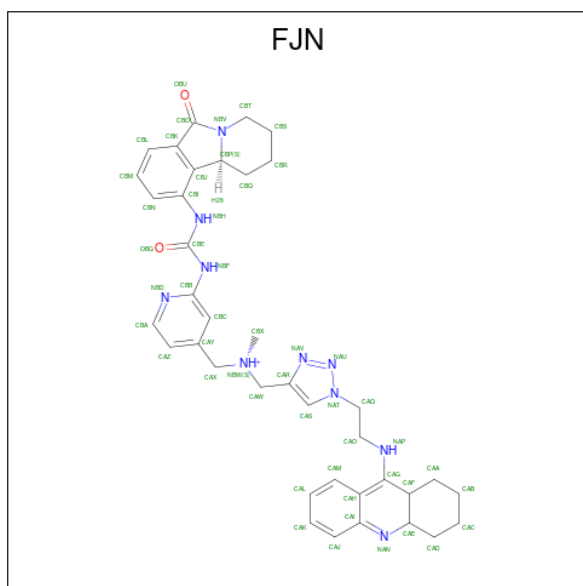
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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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		

- Molecule 3 is [1-[2-(1,2,3,4,4 {a},9 {a}-hexahydroacridin-9-ylamino)ethyl]-1,2,3-triazol-4-yl] methyl-[[2-[[[(10 {b} {S})-6-oxidanylidene-2,3,4,10 {b}-tetrahydro-1 {H}-pyrido[2,1-a]isoin dol-10-yl]carbamoylamino]pyridin-4-yl]methyl]-methyl-azanium (CCD ID: FJN) (formula: C₃₈H₄₅N₁₀O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			50	38	10	2		
3	B	1	Total	C	N	O	0	0
			50	38	10	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Cl	0	0
			5	5		
4	B	8	Total	Cl	0	0
			8	8		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



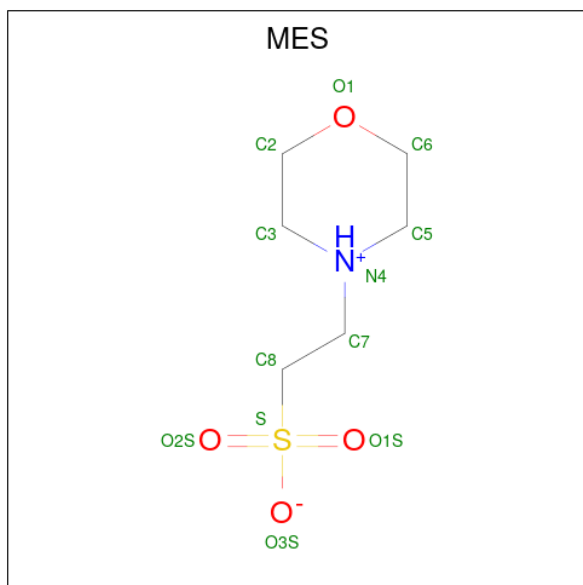
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

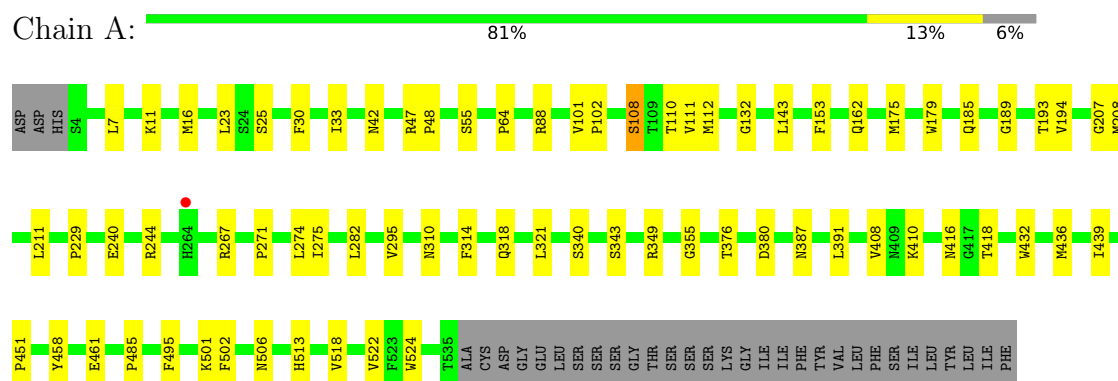
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	118	Total	O	0	0
			118	118		
8	B	102	Total	O	0	0
			102	102		

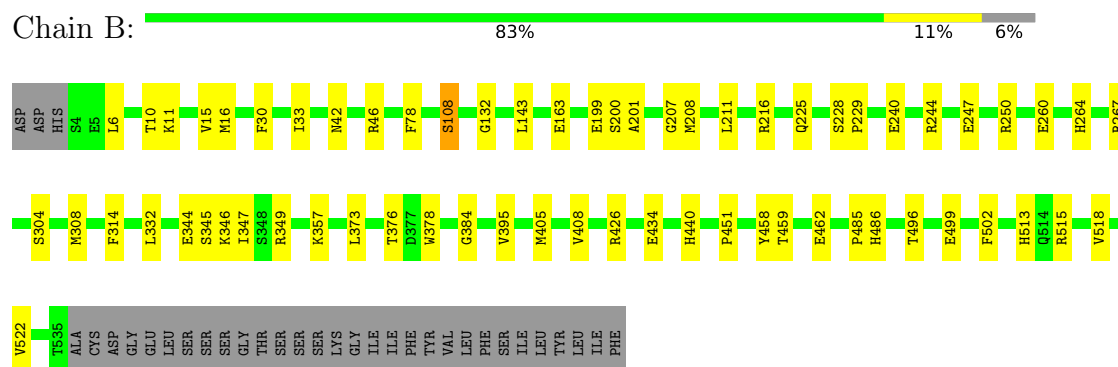
3 Residue-property plots [i](#)

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	91.74Å 105.46Å 150.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.80 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.93-2.80) 99.5 (19.93-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.79Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.197 , 0.234 0.198 , 0.234	Depositor DCC
R_{free} test set	737 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.919	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9055	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0079e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, MES, NAG, GOL, FJN, 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	0.30	0/4439	0.49	0/6025
1	B	0.30	0/4434	0.50	0/6019
All	All	0.30	0/8873	0.50	0/12044

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	4292	0	4160	42	0
1	B	4290	0	4151	48	0
2	A	42	0	39	0	0
2	B	42	0	39	0	0
3	A	50	0	0	2	0
3	B	50	0	0	1	0
4	A	5	0	0	0	0
4	B	8	0	0	2	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
6	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	16	3	0
7	B	24	0	24	7	0
8	A	118	0	0	7	0
8	B	102	0	0	1	0
All	All	9055	0	8457	92	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 (92) 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:260:GLU:OE1	4:B:612:CL:CL	1.97	1.19
1:B:200[B]:SER:HG	1:B:440:HIS:HE2	1.00	0.92
1:A:432:TRP:HB3	1:A:436:MET:HE2	1.60	0.84
1:B:267:ARG:HD3	7:B:604:MES:H32	1.58	0.82
1:A:310:ASN:OD1	1:A:410:LYS:NZ	2.11	0.82
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.63	0.79
1:B:42:ASN:CB	7:B:604:MES:H31	2.16	0.76
1:B:46:ARG:NH1	1:B:163:GLU:OE2	2.19	0.76
1:A:47:ARG:NH1	1:A:162:GLN:OE1	2.19	0.76
3:A:604:FJN:NBD	3:A:604:FJN:NBH	2.31	0.75
1:B:264:HIS:HA	7:B:604:MES:H61	1.71	0.72
3:B:605:FJN:NBD	3:B:605:FJN:NBH	2.31	0.72
1:B:216:ARG:NH1	1:B:314:PHE:HA	2.06	0.70
1:B:485:PRO:O	1:B:486:HIS:HB2	1.94	0.67
1:B:260:GLU:O	1:B:260:GLU:OE2	2.11	0.67
1:B:11:LYS:HA	6:B:615:GOL:H11	1.77	0.67
1:A:318:GLN:HG3	1:A:416:ASN:O	1.95	0.67
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.79	0.65
1:A:7:LEU:HD13	1:A:16:MET:HE2	1.79	0.64
1:B:240:GLU:O	1:B:244:ARG:HG3	1.99	0.63
1:A:111:VAL:HB	1:A:194:VAL:HG22	1.84	0.60
1:B:108:SER:O	1:B:108:SER:OG	2.13	0.60
1:A:110:THR:HG23	1:A:193:THR:HG22	1.84	0.59
1:A:349:ARG:NH2	1:A:376:THR:OG1	2.36	0.58
1:B:373:LEU:HD12	1:B:378:TRP:HE1	1.68	0.58
1:B:30:PHE:HB3	1:B:33:ILE:HD11	1.84	0.57
1:A:349:ARG:NH1	1:A:387:ASN:OD1	2.37	0.57
1:B:247:GLU:OE2	1:B:250:ARG:NH1	2.38	0.57
1:B:451:PRO:HA	1:B:458:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PHE:HB3	1:A:33:ILE:HD11	1.86	0.56
1:A:461:GLU:N	1:A:461:GLU:OE2	2.37	0.55
1:B:349:ARG:NH2	1:B:376:THR:OG1	2.40	0.55
1:A:88[B]:ARG:NH1	8:A:709:HOH:O	2.41	0.54
1:A:321:LEU:HD11	1:A:408:VAL:HG23	1.89	0.54
1:A:506:ASN:HB2	8:A:742:HOH:O	2.07	0.53
1:B:199:GLU:OE1	1:B:200[B]:SER:HB2	2.08	0.53
1:A:451:PRO:HA	1:A:458:TYR:CD2	2.44	0.53
1:A:64:PRO:O	1:A:88[B]:ARG:HG2	2.09	0.53
1:B:200[B]:SER:HG	1:B:440:HIS:CE1	2.23	0.53
1:A:240:GLU:O	1:A:244:ARG:HG3	2.09	0.53
1:B:6:LEU:O	1:B:16:MET:HA	2.11	0.51
1:B:42:ASN:HB2	7:B:604:MES:H31	1.90	0.51
1:B:357:LYS:NZ	8:B:704:HOH:O	2.42	0.51
1:B:459:THR:OG1	1:B:462:GLU:HG3	2.12	0.50
1:B:207:GLY:HA3	1:B:229:PRO:HD3	1.92	0.50
1:B:260:GLU:CD	4:B:612:CL:CL	2.88	0.49
1:B:345:SER:O	1:B:347:ILE:HG23	2.13	0.49
1:B:496:THR:OG1	1:B:499:GLU:OE2	2.29	0.49
1:A:524:TRP:HB3	6:A:611:GOL:H2	1.95	0.48
1:B:42:ASN:HB3	7:B:604:MES:H31	1.93	0.48
1:A:11:LYS:NZ	8:A:714:HOH:O	2.45	0.48
1:B:200[B]:SER:OG	1:B:440:HIS:NE2	2.11	0.48
1:A:42:ASN:HA	1:A:267:ARG:HD3	1.96	0.47
1:B:267:ARG:CD	7:B:604:MES:H32	2.39	0.47
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.97	0.47
1:B:199:GLU:CD	1:B:200[B]:SER:HB2	2.42	0.45
1:A:185:GLN:HA	1:A:189:GLY:O	2.17	0.45
1:B:200[A]:SER:OG	1:B:201:ALA:N	2.50	0.45
1:A:501:LYS:NZ	8:A:701:HOH:O	2.27	0.45
1:B:10:THR:C	6:B:615:GOL:H31	2.42	0.45
1:B:228:SER:HB2	1:B:229:PRO:HD2	1.99	0.44
1:A:418:THR:HG22	1:A:495:PHE:HB3	2.00	0.44
1:A:153:PHE:CE1	1:A:274:LEU:HD12	2.52	0.44
1:B:405:MET:HA	1:B:408:VAL:HG12	1.99	0.44
1:B:518:VAL:O	1:B:522:VAL:HG23	2.18	0.44
1:B:211:LEU:HD23	1:B:314:PHE:HB3	1.99	0.43
1:A:436:MET:HE3	1:A:439:ILE:CD1	2.48	0.43
1:B:502:PHE:CZ	1:B:513:HIS:HB2	2.54	0.43
1:B:208:MET:HG3	1:B:229:PRO:HB3	2.01	0.43
1:A:112:MET:O	1:A:143:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD21	1:B:395:VAL:HG21	2.00	0.43
1:B:426:ARG:CZ	1:B:434:GLU:HA	2.49	0.43
1:B:132:GLY:CA	1:B:143:LEU:HD23	2.49	0.42
1:B:515:ARG:HB3	1:B:518:VAL:HB	2.01	0.42
1:A:101:VAL:HG12	1:A:102:PRO:O	2.20	0.42
1:A:179:TRP:HA	8:A:787:HOH:O	2.20	0.42
1:A:108:SER:O	1:A:108:SER:OG	2.19	0.42
1:A:208:MET:HG3	1:A:229:PRO:HB3	2.01	0.42
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.55	0.42
1:A:518:VAL:O	1:A:522:VAL:HG23	2.20	0.42
1:A:132:GLY:CA	1:A:143:LEU:HD23	2.50	0.42
1:B:304:SER:O	1:B:308:MET:HG3	2.20	0.41
1:A:55:SER:N	8:A:720:HOH:O	2.53	0.41
1:B:199:GLU:HA	1:B:225:GLN:O	2.20	0.41
1:A:458:TYR:HB2	8:A:752:HOH:O	2.19	0.41
1:A:271:PRO:O	1:A:275:ILE:HG13	2.21	0.41
1:A:48:PRO:HB2	1:A:175:MET:CE	2.50	0.41
1:A:340:SER:HB3	1:A:343:SER:HB3	2.03	0.41
1:B:346:LYS:HB3	1:B:384:GLY:HA3	2.03	0.40
1:A:282:LEU:HB2	3:A:604:FJN:CBR	2.52	0.40
1:B:78:PHE:CD1	7:B:617:MES:H21	2.55	0.40
1:B:10:THR:O	6:B:615:GOL:H31	2.21	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	538/565 (95%)	509 (95%)	26 (5%)	3 (1%)	21	51
1	B	538/565 (95%)	507 (94%)	30 (6%)	1 (0%)	43	72
All	All	1076/1130 (95%)	1016 (94%)	56 (5%)	4 (0%)	30	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	PRO
1	B	344	GLU
1	A	380	ASP
1	A	23	LEU

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	471/494 (95%)	468 (99%)	3 (1%)	78	92
1	B	471/494 (95%)	468 (99%)	3 (1%)	78	92
All	All	942/988 (95%)	936 (99%)	6 (1%)	81	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	108	SER
1	A	295	VAL
1	B	15[A]	VAL
1	B	15[B]	VAL
1	B	108	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	159	HIS
1	A	178	GLN
1	A	382	ASN
1	B	66	ASN
1	B	257	ASN

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 ⓘ

Of 28 ligands modelled in this entry, 13 are monoatomic - leaving 15 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$
5	PEG	A	610	-	6,6,6	0.53	0	5,5,5	0.31	0
5	PEG	B	614	-	6,6,6	0.50	0	5,5,5	0.39	0
7	MES	B	604	-	12,12,12	2.07	1 (8%)	15,16,16	2.53	7 (46%)
2	NAG	A	602	1	14,14,15	0.56	0	17,19,21	0.64	0
3	FJN	B	605	-	54,57,57	3.39	20 (37%)	64,81,81	3.00	30 (46%)
6	GOL	A	611	-	5,5,5	0.64	0	5,5,5	0.47	0
6	GOL	B	615	-	5,5,5	0.84	0	5,5,5	1.95	2 (40%)
2	NAG	A	603	1	14,14,15	0.44	0	17,19,21	0.48	0
2	NAG	A	601	1	14,14,15	1.79	2 (14%)	17,19,21	1.14	1 (5%)
7	MES	B	617	-	12,12,12	2.48	4 (33%)	15,16,16	2.93	6 (40%)
3	FJN	A	604	-	54,57,57	3.42	22 (40%)	64,81,81	2.96	31 (48%)
2	NAG	B	601	1	14,14,15	0.68	0	17,19,21	0.50	0
2	NAG	B	603	1	14,14,15	1.13	2 (14%)	17,19,21	0.70	0
2	NAG	B	602	1	14,14,15	0.99	2 (14%)	17,19,21	0.66	0
6	GOL	B	616	-	5,5,5	0.76	0	5,5,5	0.86	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
5	PEG	A	610	-	-	1/4/4/4	-
5	PEG	B	614	-	-	3/4/4/4	-
7	MES	B	604	-	-	3/6/14/14	0/1/1/1
2	NAG	A	602	1	1/1/5/7	0/6/23/26	0/1/1/1
6	GOL	A	611	-	-	4/4/4/4	-
6	GOL	B	615	-	-	0/4/4/4	-
2	NAG	A	603	1	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1	-	4/6/23/26	0/1/1/1
7	MES	B	617	-	-	5/6/14/14	0/1/1/1
3	FJN	A	604	-	2/2/8/11	6/22/68/68	0/7/8/8
3	FJN	B	605	-	2/2/8/11	6/22/68/68	0/7/8/8
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	603	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	-	0/6/23/26	0/1/1/1
6	GOL	B	616	-	-	4/4/4/4	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	FJN	CAF-CAE	-10.83	1.40	1.53
3	B	605	FJN	CAF-CAE	-10.76	1.40	1.53
3	B	605	FJN	CAE-NAN	-9.17	1.34	1.47
3	B	605	FJN	CBK-CBO	-8.90	1.34	1.48
3	A	604	FJN	CAE-NAN	-8.80	1.35	1.47
3	A	604	FJN	CBK-CBO	-8.79	1.34	1.48
3	B	605	FJN	CAA-CAF	-6.79	1.41	1.53
3	A	604	FJN	CAA-CAF	-6.75	1.41	1.53
7	B	604	MES	C8-S	-6.74	1.68	1.77
3	A	604	FJN	CAF-CAG	-6.71	1.40	1.50
3	A	604	FJN	CAI-NAN	6.69	1.35	1.29
3	B	605	FJN	CAF-CAG	-6.67	1.40	1.50
2	A	601	NAG	O5-C1	6.16	1.54	1.43
7	B	617	MES	C8-S	-5.85	1.69	1.77
3	B	605	FJN	CAI-NAN	5.81	1.34	1.29
3	B	605	FJN	CAX-CAY	-5.42	1.41	1.51
3	A	604	FJN	CAD-CAE	-5.29	1.42	1.53
3	B	605	FJN	CAD-CAE	-5.26	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	FJN	CBJ-CBP	-5.21	1.42	1.51
3	B	605	FJN	CBJ-CBP	-5.20	1.42	1.51
3	A	604	FJN	NAV-NAU	-4.90	1.24	1.32
3	A	604	FJN	CAX-CAY	-4.79	1.42	1.51
3	B	605	FJN	NAV-NAU	-4.73	1.24	1.32
7	B	617	MES	O1S-S	4.41	1.57	1.45
3	A	604	FJN	CAG-CAH	4.13	1.42	1.36
3	A	604	FJN	CBA-NBD	3.74	1.42	1.34
3	A	604	FJN	CBL-CBK	-3.62	1.34	1.39
3	B	605	FJN	CBL-CBK	-3.62	1.34	1.39
3	B	605	FJN	CAG-CAH	3.58	1.41	1.36
2	B	603	NAG	O5-C1	3.56	1.49	1.43
3	B	605	FJN	CBA-NBD	3.49	1.41	1.34
3	B	605	FJN	NAT-NAU	-3.25	1.29	1.34
3	B	605	FJN	CBO-NBV	-3.15	1.33	1.36
7	B	617	MES	O2S-S	3.12	1.53	1.45
3	A	604	FJN	CBO-NBV	-3.08	1.33	1.36
3	B	605	FJN	CBB-NBF	-2.79	1.34	1.40
3	A	604	FJN	CBB-NBF	-2.60	1.34	1.40
3	A	604	FJN	NAT-NAU	-2.59	1.30	1.34
2	B	602	NAG	O5-C1	2.54	1.48	1.43
2	A	601	NAG	C1-C2	2.54	1.55	1.52
3	B	605	FJN	CAS-CAR	-2.50	1.32	1.36
3	A	604	FJN	CBP-NBV	-2.47	1.44	1.47
3	A	604	FJN	CBK-CBJ	-2.47	1.36	1.39
2	B	602	NAG	C1-C2	2.45	1.55	1.52
7	B	617	MES	O3S-S	2.42	1.56	1.47
3	A	604	FJN	CAS-CAR	-2.34	1.32	1.36
3	B	605	FJN	CBK-CBJ	-2.34	1.36	1.39
3	A	604	FJN	CBT-NBV	2.33	1.50	1.47
3	A	604	FJN	CBI-NBH	-2.22	1.37	1.41
2	B	603	NAG	C1-C2	2.14	1.55	1.52
3	B	605	FJN	CBI-CBJ	-2.12	1.36	1.39
3	A	604	FJN	CBI-CBJ	-2.09	1.36	1.39
3	B	605	FJN	CAR-NAV	-2.01	1.32	1.36

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	605	FJN	CBK-CBO-NBV	9.31	112.34	106.42
3	A	604	FJN	CBK-CBO-NBV	8.75	111.98	106.42
3	B	605	FJN	CBX-NBW-CAX	7.85	122.71	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	617	MES	C5-N4-C3	7.05	124.03	108.84
3	A	604	FJN	CBT-NBV-CBO	6.94	134.94	124.50
3	B	605	FJN	CBT-NBV-CBO	6.58	134.40	124.50
3	A	604	FJN	CAY-CBC-CBB	6.48	123.69	118.14
3	A	604	FJN	CBX-NBW-CAX	6.14	120.06	110.53
3	B	605	FJN	CAY-CBC-CBB	5.88	123.18	118.14
3	B	605	FJN	CBB-NBF-CBE	-5.84	119.00	129.91
3	B	605	FJN	CBP-NBV-CBO	-5.71	105.13	112.86
3	A	604	FJN	CBB-NBF-CBE	-5.67	119.32	129.91
3	A	604	FJN	CBP-NBV-CBO	-5.62	105.26	112.86
7	B	604	MES	O1-C6-C5	4.93	122.39	111.77
7	B	617	MES	O2S-S-C8	-4.90	99.32	106.73
3	A	604	FJN	CBJ-CBP-NBV	4.75	106.82	102.08
3	B	605	FJN	CBJ-CBP-NBV	4.74	106.81	102.08
7	B	604	MES	O1-C2-C3	-4.56	101.96	111.77
3	A	604	FJN	CAX-NBW-CAW	-4.55	103.25	110.94
7	B	617	MES	O1S-S-C8	4.45	113.45	106.73
3	B	605	FJN	NAT-NAU-NAV	4.36	110.94	107.02
3	B	605	FJN	CBI-NBH-CBE	4.33	135.43	125.34
3	A	604	FJN	CAY-CAX-NBW	4.28	121.06	113.29
3	B	605	FJN	CAY-CAX-NBW	4.26	121.02	113.29
3	A	604	FJN	CBI-NBH-CBE	4.15	135.00	125.34
7	B	604	MES	O1S-S-C8	4.14	112.98	106.73
3	A	604	FJN	NAT-NAU-NAV	4.01	110.63	107.02
2	A	601	NAG	C1-O5-C5	3.84	117.33	112.19
3	A	604	FJN	CAD-CAE-NAN	3.83	118.08	110.47
7	B	617	MES	O3S-S-C8	3.82	113.48	106.00
3	A	604	FJN	CBN-CBI-NBH	-3.72	113.20	121.82
3	B	605	FJN	CAD-CAE-NAN	3.55	117.52	110.47
3	B	605	FJN	NBF-CBB-NBD	3.51	125.41	114.87
3	A	604	FJN	NBF-CBB-NBD	3.50	125.36	114.87
3	B	605	FJN	CAA-CAF-CAG	3.48	119.90	112.04
3	A	604	FJN	CAO-NAP-CAG	3.47	129.96	125.66
3	B	605	FJN	CBN-CBI-NBH	-3.46	113.79	121.82
3	A	604	FJN	OBG-CBE-NBF	-3.46	117.50	123.64
3	B	605	FJN	OBG-CBE-NBF	-3.45	117.50	123.64
3	B	605	FJN	CAX-NBW-CAW	-3.37	105.25	110.94
3	A	604	FJN	CAA-CAF-CAG	3.30	119.50	112.04
3	B	605	FJN	CAZ-CBA-NBD	-3.15	120.11	123.97
3	A	604	FJN	CBX-NBW-CAW	-3.06	101.90	110.18
3	A	604	FJN	CBJ-CBI-NBH	3.01	126.81	119.89
3	A	604	FJN	CAZ-CBA-NBD	-3.00	120.29	123.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	605	FJN	CAR-CAW-NBW	-2.95	105.66	112.56
3	B	605	FJN	CBJ-CBI-NBH	2.93	126.62	119.89
3	A	604	FJN	CBN-CBM-CBL	-2.90	116.52	120.24
6	B	615	GOL	C3-C2-C1	-2.87	101.27	111.80
7	B	617	MES	C7-N4-C5	2.83	118.79	111.24
3	B	605	FJN	CAW-CAR-CAS	-2.80	125.06	129.89
3	A	604	FJN	CBC-CBB-NBD	-2.80	119.25	122.92
7	B	604	MES	O3S-S-C8	2.80	111.48	106.00
3	B	605	FJN	CBN-CBM-CBL	-2.78	116.67	120.24
3	B	605	FJN	CBC-CBB-NBD	-2.77	119.28	122.92
3	B	605	FJN	OBG-CBE-NBH	2.77	128.56	123.64
3	B	605	FJN	CBC-CBB-NBF	-2.72	115.25	122.53
3	A	604	FJN	OBG-CBE-NBH	2.68	128.41	123.64
3	A	604	FJN	CBC-CBB-NBF	-2.67	115.36	122.53
3	B	605	FJN	OBU-CBO-CBK	-2.57	123.69	128.66
7	B	604	MES	C7-N4-C5	2.47	117.81	111.24
3	A	604	FJN	OBU-CBO-CBK	-2.45	123.92	128.66
6	B	615	GOL	O2-C2-C1	2.39	119.06	109.18
7	B	617	MES	C2-C3-N4	2.38	113.73	110.12
3	A	604	FJN	CAW-CAR-CAS	-2.33	125.88	129.89
3	A	604	FJN	CBK-CBJ-CBI	-2.30	118.63	120.88
7	B	604	MES	C5-N4-C3	2.27	113.74	108.84
3	A	604	FJN	CAS-NAT-NAU	-2.25	108.57	110.75
3	A	604	FJN	CAQ-NAT-NAU	2.21	125.22	120.78
3	B	605	FJN	CBK-CBJ-CBI	-2.19	118.74	120.88
3	B	605	FJN	CAR-NAV-NAU	-2.15	106.69	109.01
3	B	605	FJN	CAB-CAC-CAD	-2.14	107.02	111.42
7	B	604	MES	O2S-S-O1S	-2.12	106.93	113.82
3	B	605	FJN	CAO-NAP-CAG	2.07	128.22	125.66
3	B	605	FJN	CBA-NBD-CBB	2.07	120.16	117.21
3	A	604	FJN	CAB-CAC-CAD	-2.04	107.23	111.42
3	A	604	FJN	OBU-CBO-NBV	-2.00	123.75	125.34

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	602	NAG	C1
3	A	604	FJN	CAF
3	A	604	FJN	CAE
3	B	605	FJN	CAF
3	B	605	FJN	CAE

All (36) torsion outliers are listed below:

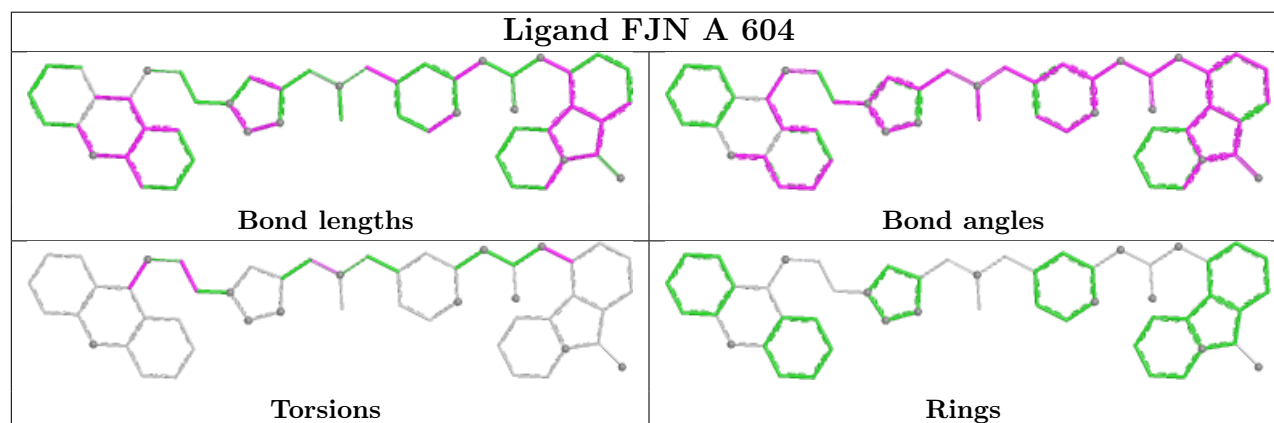
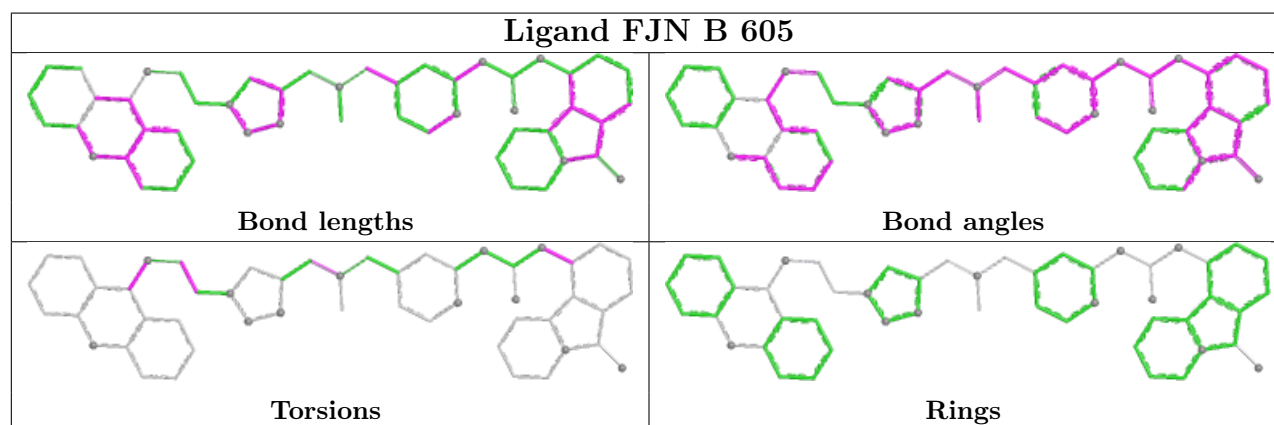
Mol	Chain	Res	Type	Atoms
3	A	604	FJN	CAF-CAG-NAP-CAO
3	A	604	FJN	CAR-CAW-NBW-CAX
3	A	604	FJN	CAR-CAW-NBW-CBX
3	A	604	FJN	CBJ-CBI-NBH-CBE
3	B	605	FJN	CAF-CAG-NAP-CAO
3	B	605	FJN	CAR-CAW-NBW-CAX
3	B	605	FJN	CAR-CAW-NBW-CBX
3	B	605	FJN	CBJ-CBI-NBH-CBE
6	A	611	GOL	O1-C1-C2-C3
6	A	611	GOL	C1-C2-C3-O3
7	B	604	MES	C7-C8-S-O1S
7	B	604	MES	C7-C8-S-O3S
7	B	617	MES	C8-C7-N4-C5
7	B	617	MES	N4-C7-C8-S
7	B	617	MES	C7-C8-S-O2S
7	B	617	MES	C7-C8-S-O3S
2	A	601	NAG	O5-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
3	A	604	FJN	CBN-CBI-NBH-CBE
3	B	605	FJN	CBN-CBI-NBH-CBE
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
3	B	605	FJN	NAP-CAO-CAQ-NAT
6	B	616	GOL	O1-C1-C2-C3
6	B	616	GOL	C1-C2-C3-O3
5	A	610	PEG	O1-C1-C2-O2
6	A	611	GOL	O1-C1-C2-O2
6	A	611	GOL	O2-C2-C3-O3
6	B	616	GOL	O1-C1-C2-O2
6	B	616	GOL	O2-C2-C3-O3
5	B	614	PEG	O2-C3-C4-O4
5	B	614	PEG	O1-C1-C2-O2
3	A	604	FJN	NAP-CAO-CAQ-NAT
7	B	604	MES	C7-C8-S-O2S
7	B	617	MES	C7-C8-S-O1S
5	B	614	PEG	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	604	MES	6	0
3	B	605	FJN	1	0
6	A	611	GOL	1	0
6	B	615	GOL	3	0
7	B	617	MES	1	0
3	A	604	FJN	2	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	532/565 (94%)	-0.48	1 (0%) 91 88	21, 38, 61, 110	11 (2%)
1	B	532/565 (94%)	-0.48	0 100 100	15, 39, 61, 105	8 (1%)
All	All	1064/1130 (94%)	-0.48	1 (0%) 92 90	15, 39, 61, 110	19 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	HIS	2.2

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 [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. 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	603	14/15	0.49	0.15	79,96,105,106	0
2	NAG	A	603	14/15	0.64	0.12	55,74,82,86	0
2	NAG	B	601	14/15	0.71	0.13	57,70,77,80	0
6	GOL	B	616	6/6	0.71	0.16	41,45,57,63	0

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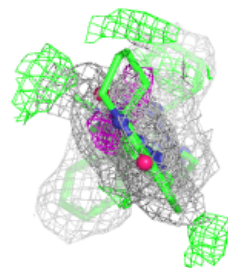
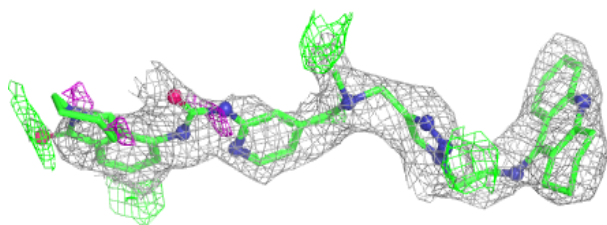
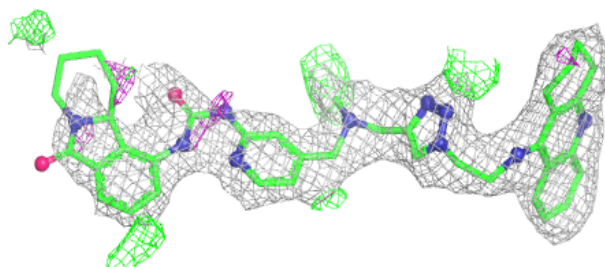
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	B	615	6/6	0.72	0.21	43,49,53,59	0
3	FJN	A	604	50/50	0.75	0.15	34,65,96,103	0
2	NAG	A	601	14/15	0.77	0.12	58,80,86,87	0
7	MES	B	604	12/12	0.81	0.13	66,76,88,91	0
2	NAG	A	602	14/15	0.82	0.09	45,58,68,72	0
4	CL	B	611	1/1	0.82	0.10	61,61,61,61	0
5	PEG	B	614	7/7	0.82	0.12	45,50,64,66	0
7	MES	B	617	12/12	0.82	0.15	60,74,99,120	0
2	NAG	B	602	14/15	0.83	0.09	37,55,62,65	0
3	FJN	B	605	50/50	0.83	0.16	36,62,100,109	50
5	PEG	A	610	7/7	0.84	0.11	44,52,61,62	0
4	CL	A	608	1/1	0.84	0.13	58,58,58,58	0
4	CL	B	612	1/1	0.85	0.10	77,77,77,77	0
4	CL	A	607	1/1	0.88	0.07	59,59,59,59	0
6	GOL	A	611	6/6	0.88	0.17	36,46,49,52	0
4	CL	A	605	1/1	0.89	0.09	58,58,58,58	0
4	CL	A	609	1/1	0.91	0.05	53,53,53,53	0
4	CL	B	608	1/1	0.92	0.11	74,74,74,74	0
4	CL	A	606	1/1	0.92	0.06	45,45,45,45	0
4	CL	B	613	1/1	0.93	0.09	57,57,57,57	0
4	CL	B	610	1/1	0.95	0.15	50,50,50,50	0
4	CL	B	606	1/1	0.96	0.07	55,55,55,55	0
4	CL	B	609	1/1	0.97	0.09	52,52,52,52	0
4	CL	B	607	1/1	0.97	0.03	53,53,53,53	0

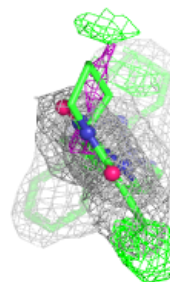
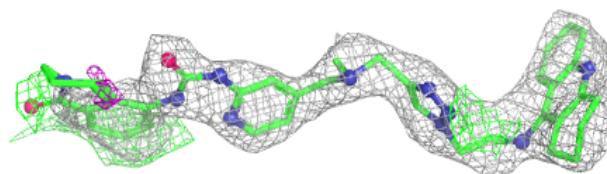
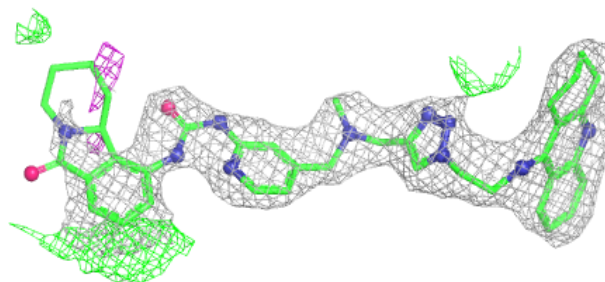
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FJN A 604:

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

**Electron density around FJN B 605:**

$2mF_o-DF_c$ (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.