



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:13 PM BST

PDB ID : 6H12  
Title : Crystal structure of TcACHE complexed to 1-(6-Oxo-1,2,3,4,6,10b-hexahydro pyrido[2,1-a]isoindol-10-yl)-3-(4-(((1-(2-((1,2,3,4-tetrahydroacridin-9-yl)amino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)methyl)pyridin-2-yl)urea  
Authors : Coquelle, N.; Colletier, J.P.  
Deposited on : 2018-07-10  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

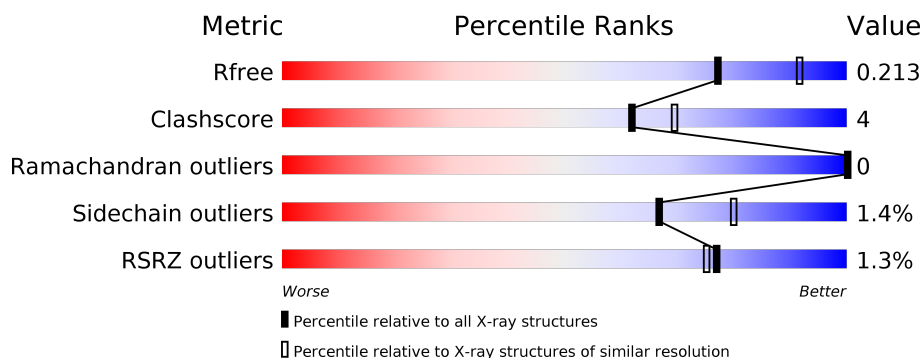
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 86%, green 8%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>8%</span> <span>6%</span> </div> </div>
1	B	565	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 87%, green 7%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>87%</span> <span>7%</span> <span>6%</span> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	FJK	A	626	X	-	-	-
10	FJK	B	619	X	-	-	-
2	MES	A	611	-	-	X	-
7	PEG	B	613	-	-	X	-

## 2 Entry composition [i](#)

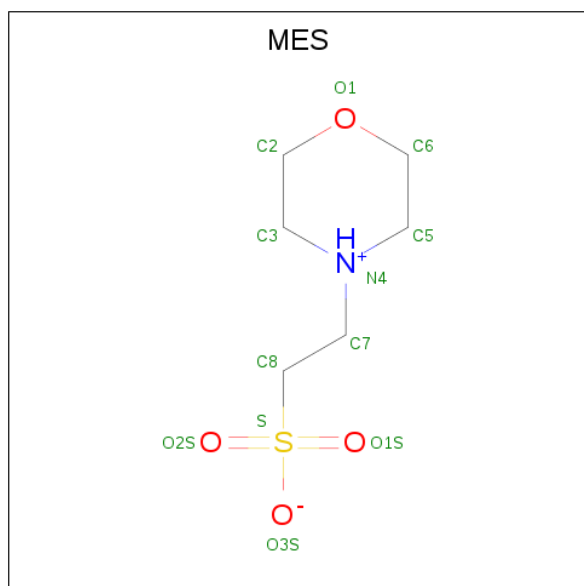
There are 11 unique types of molecules in this entry. The entry contains 9735 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	11	0
			4311	2765	736	788	22			
1	B	532	Total	C	N	O	S	0	9	0
			4295	2755	732	786	22			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



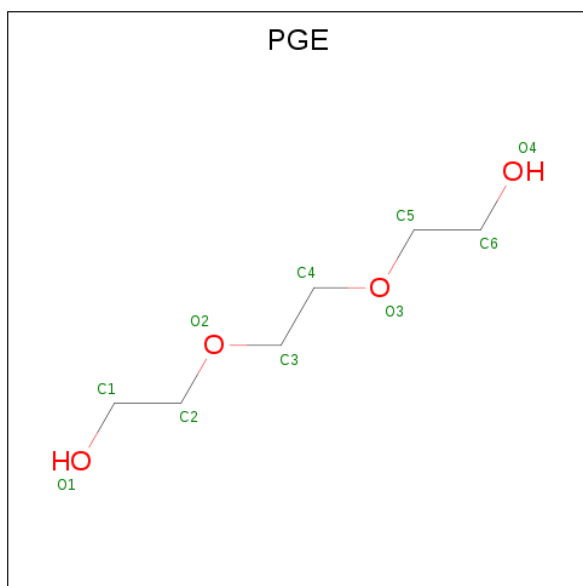
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



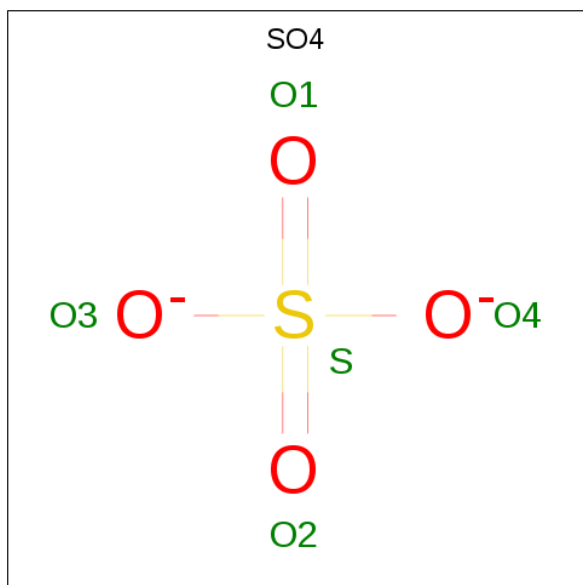
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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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 SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

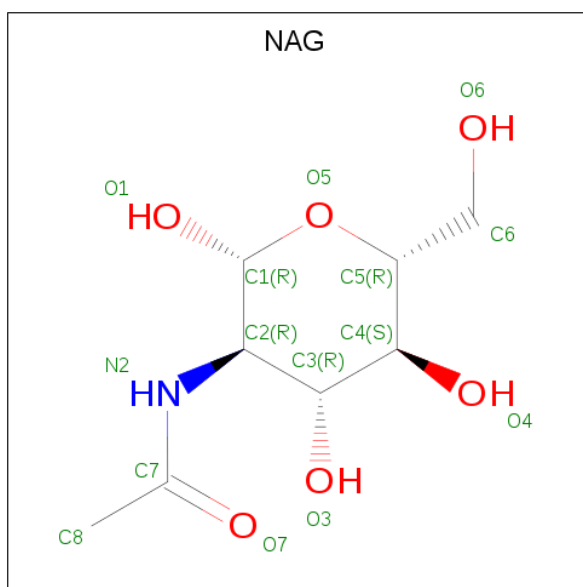
- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



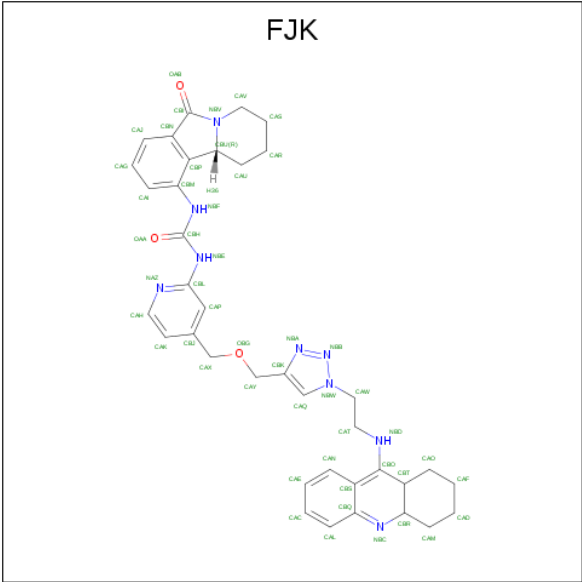


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cl	0	0
			1	1		
9	A	5	Total	Cl	0	0
			5	5		

- Molecule 10 is 1-[4-[[1-[2-(1,2,3,4,4 {a},9 {a})-hexahydroacridin-9-ylamino)ethyl]-1,2,3-triazol-4-yl]methoxymethyl]pyridin-2-yl]-3-[(10 {b} {R})-6-oxidanylidene-2,3,4,10 {b}-tetrahydro-1 {H}-pyrido[2,1-a]isoindol-10-yl]urea (three-letter code: FJK) (formula: C<sub>37</sub>H<sub>41</sub>N<sub>9</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			49	37	9	3		
10	B	1	Total	C	N	O	0	0
			49	37	9	3		

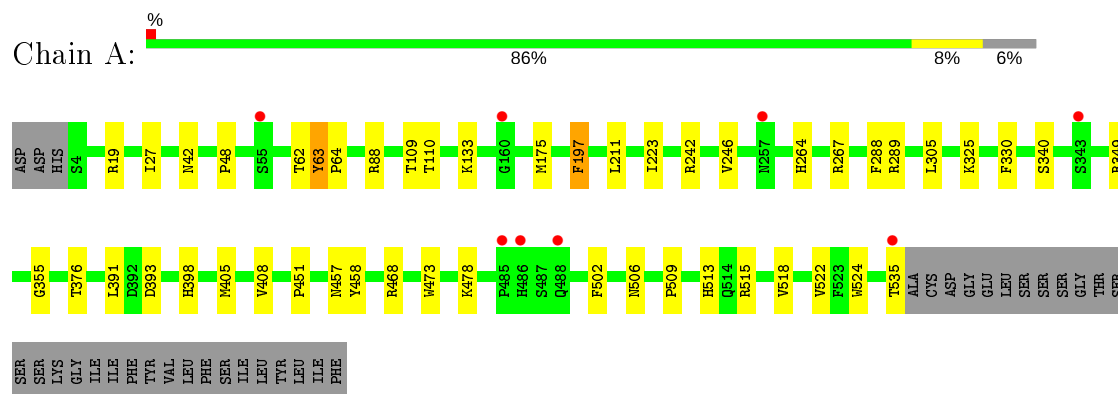
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	362	Total	O	0	0
			362	362		
11	B	384	Total	O	0	0
			384	384		

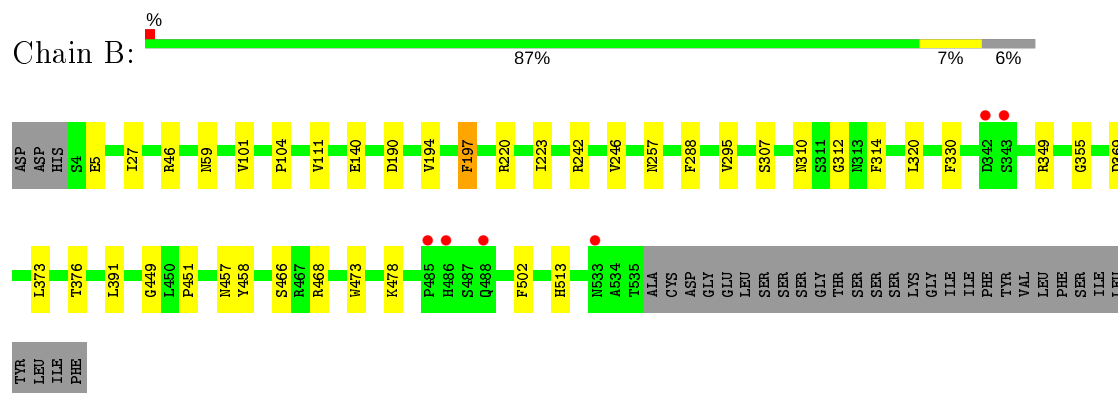
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	91.27Å 105.09Å 149.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 2.20 19.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.84-2.20) 99.9 (19.88-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.19Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.171 , 0.212 0.171 , 0.213	Depositor DCC
$R_{free}$ test set	2000 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 44.97 % 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 1.4139e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FJK, GOL, PGE, NAG, CL, EDO, SO4, MES, 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	0.39	0/4467	0.54	0/6061
1	B	0.41	0/4445	0.55	0/6033
All	All	0.40	0/8912	0.55	0/12094

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

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	4311	0	4192	41	0
1	B	4295	0	4165	32	0
2	A	48	0	49	15	0
3	A	12	0	15	2	0
3	B	6	0	8	2	0
4	A	10	0	12	0	0
4	B	10	0	14	0	0
5	A	24	0	36	3	0
5	B	28	0	42	7	0
6	A	10	0	0	0	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	28	0	38	2	0
7	B	28	0	36	11	0
8	A	28	0	26	0	0
8	B	42	0	39	0	0
9	A	5	0	0	0	0
9	B	1	0	0	0	0
10	A	49	0	0	1	0
10	B	49	0	0	0	0
11	A	362	0	0	3	0
11	B	384	0	0	7	0
All	All	9735	0	8672	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (77) 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:398:HIS:HD1	5:A:610:EDO:H22	1.38	0.86
10:A:626:FJK:NAZ	10:A:626:FJK:NBF	2.17	0.85
1:A:242[A]:ARG:HH11	2:A:614:MES:H81	1.43	0.83
7:B:614:PEG:H12	11:B:735:HOH:O	1.79	0.83
1:B:242:ARG:HH11	7:B:611:PEG:H31	1.47	0.78
1:B:59:ASN:H	5:B:609:EDO:H11	1.49	0.77
1:A:478:LYS:HD2	2:A:611:MES:H32	1.69	0.74
1:A:478:LYS:HE3	2:A:611:MES:H72	1.71	0.71
1:A:267:ARG:HD2	2:A:601:MES:H21	1.75	0.67
1:B:373:LEU:HB2	5:B:607:EDO:H22	1.77	0.66
1:B:140:GLU:OE1	11:B:701:HOH:O	2.14	0.66
1:A:398:HIS:ND1	5:A:610:EDO:H22	2.10	0.65
1:B:310:ASN:HD22	7:B:613:PEG:H12	1.63	0.64
1:A:289:ARG:HE	3:A:609:GOL:H11	1.63	0.63
1:A:246:VAL:HG21	2:A:614:MES:H82	1.82	0.61
1:B:246:VAL:HG21	7:B:611:PEG:H41	1.82	0.60
1:A:349:ARG:NH2	1:A:376:THR:OG1	2.33	0.60
1:A:110:THR:OG1	2:A:611:MES:H71	2.03	0.59
1:A:242[A]:ARG:HG2	2:A:614:MES:H51	1.84	0.58
1:A:264:HIS:HA	2:A:601:MES:H22	1.86	0.57
1:A:62:THR:HG23	1:A:88[B]:ARG:NH2	2.21	0.56
1:A:506:ASN:HB2	3:A:602:GOL:H11	1.88	0.55
1:A:109:THR:HA	2:A:611:MES:H82	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ARG:NH2	1:B:376:THR:OG1	2.37	0.55
1:A:393:ASP:OD1	7:A:615:PEG:H31	2.07	0.55
1:B:307:SER:HB3	7:B:613:PEG:H11	1.89	0.54
1:A:524:TRP:HB3	5:A:610:EDO:H21	1.89	0.53
1:B:369:ASP:HB3	5:B:607:EDO:H12	1.91	0.53
1:B:59:ASN:N	5:B:609:EDO:H11	2.21	0.52
1:A:63:TYR:HB2	1:A:88[B]:ARG:HE	1.74	0.52
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.44	0.52
1:B:451:PRO:HA	1:B:458:TYR:CD2	2.45	0.52
3:B:604:GOL:H31	11:B:894:HOH:O	2.10	0.51
1:A:64:PRO:O	1:A:88[B]:ARG:HG2	2.10	0.51
1:A:246:VAL:HG11	2:A:614:MES:H21	1.91	0.50
1:A:48:PRO:HB2	1:A:175:MET:HE2	1.94	0.50
1:B:242:ARG:HD3	7:B:611:PEG:H42	1.93	0.50
1:B:197:PHE:HB3	1:B:223:ILE:HB	1.94	0.49
1:A:110:THR:HB	2:A:611:MES:H31	1.94	0.49
1:A:42:ASN:HB3	2:A:601:MES:H51	1.95	0.49
1:B:190:ASP:OD2	3:B:604:GOL:H12	2.12	0.49
1:A:468[A]:ARG:NH1	11:A:701:HOH:O	2.17	0.49
1:A:478:LYS:NZ	2:A:611:MES:H52	2.28	0.48
1:B:59:ASN:H	5:B:609:EDO:C1	2.23	0.48
1:A:355:GLY:HA3	1:A:391:LEU:HD21	1.95	0.48
1:B:5:GLU:OE2	1:B:104:PRO:HA	2.14	0.48
1:B:355:GLY:HA3	1:B:391:LEU:HD21	1.95	0.48
1:B:478:LYS:NZ	5:B:603:EDO:H22	2.28	0.48
1:A:325:LYS:HG3	7:A:615:PEG:H12	1.95	0.48
1:A:211:LEU:HD13	1:A:305:LEU:HD22	1.96	0.47
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.50	0.47
1:B:220:ARG:NH1	11:B:714:HOH:O	2.38	0.47
1:B:468[A]:ARG:NH2	11:B:708:HOH:O	2.33	0.47
5:B:606:EDO:O1	7:B:614:PEG:H22	2.15	0.46
1:A:457:ASN:ND2	11:A:724:HOH:O	2.48	0.46
1:A:509:PRO:HG2	1:B:46[B]:ARG:NH1	2.31	0.46
1:B:502:PHE:CZ	1:B:513:HIS:HB2	2.49	0.46
1:A:518:VAL:O	1:A:522:VAL:HG23	2.15	0.45
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.99	0.45
1:A:110:THR:CB	2:A:611:MES:H31	2.45	0.44
1:B:27:ILE:HG12	1:B:101:VAL:O	2.17	0.44
1:B:197:PHE:CB	1:B:223:ILE:HB	2.48	0.44
1:B:310:ASN:ND2	7:B:613:PEG:H12	2.32	0.44
1:B:257:ASN:ND2	11:B:704:HOH:O	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ARG:HB3	1:A:518:VAL:HB	2.00	0.43
1:B:223:ILE:HA	1:B:320:LEU:O	2.18	0.43
1:A:197:PHE:CB	1:A:223:ILE:HB	2.49	0.42
1:B:111:VAL:HB	1:B:194:VAL:HG22	2.02	0.42
1:A:19[A]:ARG:NH1	11:A:704:HOH:O	2.27	0.42
1:B:307:SER:HA	7:B:613:PEG:H11	2.01	0.42
1:A:27:ILE:HD11	1:A:133:LYS:HB2	2.01	0.41
1:B:307:SER:CB	7:B:613:PEG:H11	2.49	0.41
7:B:613:PEG:H22	11:B:898:HOH:O	2.21	0.41
1:B:449:GLY:HA2	1:B:466:SER:OG	2.21	0.41
1:A:242[A]:ARG:NH1	2:A:614:MES:H81	2.23	0.41
1:B:312:GLY:HA2	1:B:314:PHE:CE2	2.55	0.41
1:A:405:MET:HA	1:A:408:VAL:HG12	2.03	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	541/565 (96%)	521 (96%)	20 (4%)	0	100	100
1	B	539/565 (95%)	519 (96%)	20 (4%)	0	100	100
All	All	1080/1130 (96%)	1040 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	475/494 (96%)	468 (98%)	7 (2%)	65	78
1	B	472/494 (96%)	466 (99%)	6 (1%)	69	81
All	All	947/988 (96%)	934 (99%)	13 (1%)	67	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	197	PHE
1	A	288	PHE
1	A	330	PHE
1	A	340	SER
1	A	473	TRP
1	A	535	THR
1	B	197	PHE
1	B	288	PHE
1	B	295	VAL
1	B	330	PHE
1	B	457	ASN
1	B	473	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 46 ligands modelled in this entry, 6 are monoatomic - leaving 40 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
6	SO4	B	608	-	4,4,4	0.19	0	6,6,6	0.11	0
2	MES	A	601	-	12,12,12	2.23	1 (8%)	14,16,16	1.82	4 (28%)
8	NAG	B	615	1	14,14,15	0.77	1 (7%)	17,19,21	0.69	1 (5%)
5	EDO	A	608	-	3,3,3	0.43	0	2,2,2	0.60	0
6	SO4	A	613	-	4,4,4	0.17	0	6,6,6	0.09	0
7	PEG	B	611	-	6,6,6	0.62	0	5,5,5	0.75	0
5	EDO	B	610	-	3,3,3	0.42	0	2,2,2	0.86	0
7	PEG	A	617	-	6,6,6	0.61	0	5,5,5	0.32	0
4	PGE	B	605	-	9,9,9	0.38	0	8,8,8	0.29	0
6	SO4	A	627	-	4,4,4	0.17	0	6,6,6	0.24	0
7	PEG	B	614	-	6,6,6	0.63	0	5,5,5	0.42	0
5	EDO	A	607	-	3,3,3	0.44	0	2,2,2	0.38	0
3	GOL	B	604	-	5,5,5	0.26	0	5,5,5	0.79	0
7	PEG	B	613	-	6,6,6	0.58	0	5,5,5	0.35	0
8	NAG	B	616	1	14,14,15	0.40	0	17,19,21	0.57	0
10	FJK	A	626	-	52,56,56	5.84	23 (44%)	57,79,79	2.88	22 (38%)
5	EDO	B	602	-	3,3,3	0.62	0	2,2,2	0.05	0
5	EDO	B	609	-	3,3,3	0.34	0	2,2,2	0.69	0
5	EDO	B	603	-	3,3,3	0.43	0	2,2,2	0.51	0
5	EDO	A	605	-	3,3,3	0.43	0	2,2,2	0.68	0
5	EDO	A	604	-	3,3,3	0.56	0	2,2,2	0.21	0
7	PEG	A	615	-	6,6,6	0.66	0	5,5,5	0.86	0
3	GOL	A	602	-	5,5,5	0.28	0	5,5,5	0.64	0
7	PEG	A	618	-	6,6,6	0.62	0	5,5,5	0.27	0
5	EDO	B	601	-	3,3,3	0.43	0	2,2,2	0.35	0
7	PEG	A	616	-	6,6,6	0.56	0	5,5,5	0.20	0
4	PGE	A	603	-	9,9,9	0.38	0	8,8,8	0.38	0
5	EDO	B	607	-	3,3,3	0.47	0	2,2,2	0.14	0
2	MES	A	614	-	12,12,12	2.25	1 (8%)	14,16,16	2.18	5 (35%)
3	GOL	A	609	-	5,5,5	0.45	0	5,5,5	0.81	0
8	NAG	B	617	-	14,14,15	0.70	1 (7%)	17,19,21	0.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MES	A	611	-	12,12,12	1.93	1 (8%)	14,16,16	2.01	3 (21%)
8	NAG	A	619	1	14,14,15	0.44	0	17,19,21	0.75	1 (5%)
5	EDO	B	606	-	3,3,3	0.39	0	2,2,2	0.40	0
5	EDO	A	606	-	3,3,3	0.51	0	2,2,2	0.11	0
7	PEG	B	612	-	6,6,6	0.59	0	5,5,5	0.35	0
5	EDO	A	610	-	3,3,3	0.50	0	2,2,2	0.36	0
2	MES	A	612	-	12,12,12	2.34	1 (8%)	14,16,16	1.85	3 (21%)
8	NAG	A	620	1	14,14,15	0.41	0	17,19,21	0.58	0
10	FJK	B	619	-	52,56,56	5.82	21 (40%)	57,79,79	2.53	21 (36%)

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	MES	A	601	-	-	5/6/14/14	0/1/1/1
8	NAG	B	615	1	-	2/6/23/26	0/1/1/1
5	EDO	A	608	-	-	1/1/1/1	-
7	PEG	B	611	-	-	1/4/4/4	-
5	EDO	B	610	-	-	1/1/1/1	-
7	PEG	A	617	-	-	2/4/4/4	-
4	PGE	B	605	-	-	4/7/7/7	-
10	FJK	B	619	-	2/2/7/10	5/17/66/66	0/7/8/8
5	EDO	A	607	-	-	1/1/1/1	-
3	GOL	B	604	-	-	0/4/4/4	-
7	PEG	B	613	-	-	1/4/4/4	-
8	NAG	B	616	1	-	0/6/23/26	0/1/1/1
10	FJK	A	626	-	2/2/7/10	2/17/66/66	0/7/8/8
5	EDO	B	602	-	-	0/1/1/1	-
5	EDO	B	609	-	-	0/1/1/1	-
5	EDO	B	603	-	-	0/1/1/1	-
5	EDO	A	605	-	-	1/1/1/1	-
5	EDO	A	604	-	-	0/1/1/1	-
7	PEG	A	615	-	-	3/4/4/4	-
3	GOL	A	602	-	-	4/4/4/4	-
7	PEG	A	618	-	-	1/4/4/4	-
5	EDO	B	601	-	-	1/1/1/1	-
7	PEG	A	616	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	A	603	-	-	4/7/7/7	-
5	EDO	B	607	-	-	0/1/1/1	-
2	MES	A	614	-	-	3/6/14/14	0/1/1/1
3	GOL	A	609	-	-	3/4/4/4	-
8	NAG	B	617	-	-	2/6/23/26	0/1/1/1
2	MES	A	611	-	-	3/6/14/14	0/1/1/1
8	NAG	A	619	1	-	2/6/23/26	0/1/1/1
5	EDO	B	606	-	-	0/1/1/1	-
5	EDO	A	606	-	-	0/1/1/1	-
7	PEG	B	612	-	-	1/4/4/4	-
5	EDO	A	610	-	-	1/1/1/1	-
2	MES	A	612	-	-	4/6/14/14	0/1/1/1
8	NAG	A	620	1	-	0/6/23/26	0/1/1/1
7	PEG	B	614	-	-	3/4/4/4	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	626	FJK	CAO-CBT	-20.80	1.15	1.53
10	B	619	FJK	CAO-CBT	-20.68	1.15	1.53
10	B	619	FJK	CAM-CBR	-18.83	1.16	1.53
10	A	626	FJK	CAM-CBR	-17.97	1.18	1.53
10	B	619	FJK	CAF-CAO	-13.79	1.16	1.53
10	A	626	FJK	CAF-CAO	-13.44	1.17	1.53
10	B	619	FJK	CAD-CAM	-13.15	1.18	1.53
10	A	626	FJK	CAD-CAM	-13.12	1.18	1.53
10	B	619	FJK	CBT-CBR	-12.99	1.35	1.53
10	A	626	FJK	CBT-CBR	-12.85	1.35	1.53
10	A	626	FJK	CBN-CBI	-9.16	1.34	1.48
10	B	619	FJK	CBN-CBI	-9.14	1.34	1.48
10	B	619	FJK	CBR-NBC	-8.34	1.35	1.47
10	B	619	FJK	CAF-CAD	-8.19	1.19	1.51
10	A	626	FJK	CBR-NBC	-8.10	1.35	1.47
10	A	626	FJK	CAF-CAD	-8.02	1.19	1.51
2	A	612	MES	C8-S	-7.83	1.66	1.77
2	A	614	MES	C8-S	-7.50	1.66	1.77
2	A	601	MES	C8-S	-7.40	1.67	1.77
10	B	619	FJK	CBT-CBO	-6.75	1.40	1.50
2	A	611	MES	C8-S	-6.42	1.68	1.77
10	A	626	FJK	CBT-CBO	-6.16	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	626	FJK	CBN-CBP	-5.59	1.32	1.39
10	A	626	FJK	CBM-CBP	-5.43	1.32	1.39
10	A	626	FJK	CAX-CBJ	-5.15	1.38	1.50
10	B	619	FJK	CAX-CBJ	-5.00	1.38	1.50
10	A	626	FJK	CBU-NBV	-4.89	1.40	1.47
10	B	619	FJK	CBM-NBF	-4.77	1.32	1.41
10	A	626	FJK	CBM-NBF	-4.75	1.32	1.41
10	A	626	FJK	NBA-NBB	-4.44	1.26	1.34
10	B	619	FJK	NBA-NBB	-4.30	1.26	1.34
10	B	619	FJK	CAJ-CBN	-4.01	1.33	1.39
10	B	619	FJK	CBS-CBO	3.86	1.41	1.36
10	A	626	FJK	CBI-NBV	-3.77	1.32	1.36
10	B	619	FJK	CBI-NBV	-3.63	1.32	1.36
10	A	626	FJK	NBB-NBW	-3.50	1.27	1.34
10	A	626	FJK	CBS-CBO	3.43	1.41	1.36
10	A	626	FJK	CAJ-CBN	-3.37	1.34	1.39
10	B	619	FJK	CBN-CBP	-3.25	1.35	1.39
10	B	619	FJK	CAH-NAZ	3.16	1.41	1.34
10	B	619	FJK	CBM-CBP	-3.04	1.36	1.39
10	A	626	FJK	CBL-NBE	-3.03	1.33	1.40
10	A	626	FJK	CAH-NAZ	2.98	1.40	1.34
10	B	619	FJK	CBL-NBE	-2.68	1.34	1.40
8	B	615	NAG	O5-C1	2.49	1.47	1.43
10	B	619	FJK	CAQ-NBW	-2.40	1.32	1.35
10	A	626	FJK	CAQ-CBK	-2.30	1.32	1.36
8	B	617	NAG	O5-C1	2.26	1.47	1.43
10	B	619	FJK	CAY-CBK	2.08	1.55	1.50
10	A	626	FJK	CBH-NBE	-2.07	1.33	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	626	FJK	CBN-CBI-NBV	11.18	113.04	106.44
10	A	626	FJK	CBL-NBE-CBH	-9.90	116.51	130.41
10	B	619	FJK	CBN-CBI-NBV	7.86	111.08	106.44
10	B	619	FJK	CBL-NBE-CBH	-7.20	120.31	130.41
10	B	619	FJK	CBM-NBF-CBH	-5.49	113.20	125.39
10	A	626	FJK	CBU-NBV-CBI	-5.03	105.83	112.87
10	B	619	FJK	CAM-CBR-NBC	5.01	121.46	110.60
10	A	626	FJK	CAM-CBR-NBC	4.96	121.37	110.60
2	A	612	MES	C5-N4-C3	4.95	119.97	108.83
10	A	626	FJK	OAB-CBI-NBV	-4.89	121.57	125.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	614	MES	C5-N4-C3	4.70	119.40	108.83
10	A	626	FJK	CAO-CBT-CBO	4.69	122.83	111.75
10	B	619	FJK	CAO-CBT-CBO	4.47	122.32	111.75
2	A	614	MES	O2S-S-C8	4.21	111.98	106.92
2	A	611	MES	O3S-S-C8	4.11	112.41	105.77
10	A	626	FJK	CAV-NBV-CBI	4.04	134.69	124.49
2	A	611	MES	C5-N4-C3	3.96	117.75	108.83
10	B	619	FJK	CBU-NBV-CBI	-3.89	107.43	112.87
10	B	619	FJK	NBA-NBB-NBW	3.71	110.11	107.31
10	A	626	FJK	NBA-NBB-NBW	3.57	110.01	107.31
10	B	619	FJK	CAK-CAH-NAZ	-3.44	119.69	123.96
10	B	619	FJK	CAV-NBV-CBI	3.30	132.82	124.49
10	A	626	FJK	CAK-CAH-NAZ	-3.29	119.87	123.96
10	B	619	FJK	NBE-CBL-NAZ	3.28	125.26	115.06
10	A	626	FJK	CBP-CBU-NBV	3.25	104.76	101.92
2	A	601	MES	C5-N4-C3	3.24	116.12	108.83
10	B	619	FJK	CBJ-CAP-CBL	3.02	120.73	118.17
10	A	626	FJK	CAY-OBG-CAX	-2.93	105.86	112.69
10	B	619	FJK	CAW-NBW-CAQ	-2.93	122.94	129.82
10	B	619	FJK	NBF-CBH-NBE	2.92	117.58	112.49
2	A	601	MES	O3S-S-C8	2.77	110.25	105.77
10	B	619	FJK	CAP-CBL-NBE	-2.75	115.13	122.66
2	A	601	MES	O2S-S-C8	2.73	110.20	106.92
10	A	626	FJK	CAJ-CBN-CBI	2.63	133.91	129.63
10	B	619	FJK	CAH-NAZ-CBL	2.59	120.90	117.22
10	A	626	FJK	CAH-NAZ-CBL	2.58	120.88	117.22
10	B	619	FJK	CAS-CAV-NBV	-2.54	106.69	110.67
10	A	626	FJK	CBJ-CAP-CBL	2.54	120.32	118.17
2	A	614	MES	C7-N4-C5	2.52	117.68	111.23
10	A	626	FJK	CAI-CBM-NBF	2.49	127.58	121.80
10	B	619	FJK	OAA-CBH-NBF	-2.47	119.45	123.62
10	B	619	FJK	CAY-OBG-CAX	2.44	118.39	112.69
8	A	619	NAG	C1-O5-C5	2.41	115.45	112.19
2	A	614	MES	C7-N4-C3	2.41	117.39	111.23
2	A	601	MES	C6-C5-N4	-2.40	106.46	110.10
10	B	619	FJK	CBP-CBU-NBV	2.38	104.00	101.92
2	A	611	MES	O1S-S-C8	2.34	109.73	106.92
10	A	626	FJK	CAW-NBW-CAQ	-2.33	124.34	129.82
10	A	626	FJK	NBE-CBL-NAZ	2.31	122.25	115.06
10	B	619	FJK	CAP-CBL-NAZ	-2.29	119.56	122.75
2	A	612	MES	O3S-S-C8	2.26	109.42	105.77
10	A	626	FJK	CAT-CAW-NBW	-2.19	107.35	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	619	FJK	CAF-CAD-CAM	2.19	115.87	111.42
8	B	617	NAG	C1-O5-C5	2.18	115.15	112.19
2	A	614	MES	O1S-S-C8	2.13	109.48	106.92
8	B	615	NAG	C1-O5-C5	2.13	115.08	112.19
10	A	626	FJK	CAP-CBL-NAZ	-2.13	119.78	122.75
10	A	626	FJK	CAF-CAD-CAM	2.11	115.73	111.42
10	A	626	FJK	CAD-CAM-CBR	2.08	114.69	111.32
10	A	626	FJK	CBM-NBF-CBH	-2.06	120.81	125.39
2	A	612	MES	O1S-S-C8	2.01	109.34	106.92

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	626	FJK	CBR
10	A	626	FJK	CBT
10	B	619	FJK	CBR
10	B	619	FJK	CBT

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MES	C8-C7-N4-C5
10	A	626	FJK	NBD-CAT-CAW-NBW
3	A	602	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
2	A	614	MES	N4-C7-C8-S
3	A	609	GOL	C1-C2-C3-O3
2	A	611	MES	C7-C8-S-O1S
2	A	611	MES	C7-C8-S-O3S
2	A	612	MES	C8-C7-N4-C5
2	A	612	MES	C7-C8-S-O2S
2	A	612	MES	C7-C8-S-O3S
10	B	619	FJK	NBD-CAT-CAW-NBW
10	B	619	FJK	CBK-CAY-OBG-CAX
8	B	617	NAG	O5-C5-C6-O6
4	A	603	PGE	O2-C3-C4-O3
8	B	615	NAG	C8-C7-N2-C2
8	B	615	NAG	O7-C7-N2-C2
8	A	619	NAG	C8-C7-N2-C2
8	A	619	NAG	O7-C7-N2-C2
8	B	617	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	605	PGE	O3-C5-C6-O4
7	B	614	PEG	O1-C1-C2-O2
7	B	613	PEG	O2-C3-C4-O4
7	A	615	PEG	O1-C1-C2-O2
3	A	609	GOL	O1-C1-C2-C3
3	A	609	GOL	O2-C2-C3-O3
5	B	601	EDO	O1-C1-C2-O2
4	A	603	PGE	O3-C5-C6-O4
7	B	612	PEG	O2-C3-C4-O4
7	A	617	PEG	O1-C1-C2-O2
7	A	618	PEG	O2-C3-C4-O4
7	A	616	PEG	O2-C3-C4-O4
10	B	619	FJK	CBJ-CAX-OBG-CAY
3	A	602	GOL	O2-C2-C3-O3
5	A	607	EDO	O1-C1-C2-O2
10	B	619	FJK	CAI-CBM-NBF-CBH
2	A	614	MES	C8-C7-N4-C3
2	A	614	MES	C8-C7-N4-C5
2	A	601	MES	C7-C8-S-O3S
10	B	619	FJK	CBP-CBM-NBF-CBH
7	B	611	PEG	O1-C1-C2-O2
4	B	605	PGE	O2-C3-C4-O3
4	B	605	PGE	C3-C4-O3-C5
7	A	616	PEG	C4-C3-O2-C2
4	A	603	PGE	C3-C4-O3-C5
4	A	603	PGE	C6-C5-O3-C4
7	A	615	PEG	O2-C3-C4-O4
2	A	601	MES	C7-C8-S-O1S
2	A	601	MES	C7-C8-S-O2S
2	A	611	MES	C7-C8-S-O2S
2	A	612	MES	C7-C8-S-O1S
7	B	614	PEG	C4-C3-O2-C2
4	B	605	PGE	C4-C3-O2-C2
7	B	614	PEG	C1-C2-O2-C3
7	A	615	PEG	C1-C2-O2-C3
5	B	610	EDO	O1-C1-C2-O2
7	A	616	PEG	O1-C1-C2-O2
2	A	601	MES	C8-C7-N4-C3
10	A	626	FJK	CBS-CBO-NBD-CAT
5	A	605	EDO	O1-C1-C2-O2
5	A	608	EDO	O1-C1-C2-O2
5	A	610	EDO	O1-C1-C2-O2

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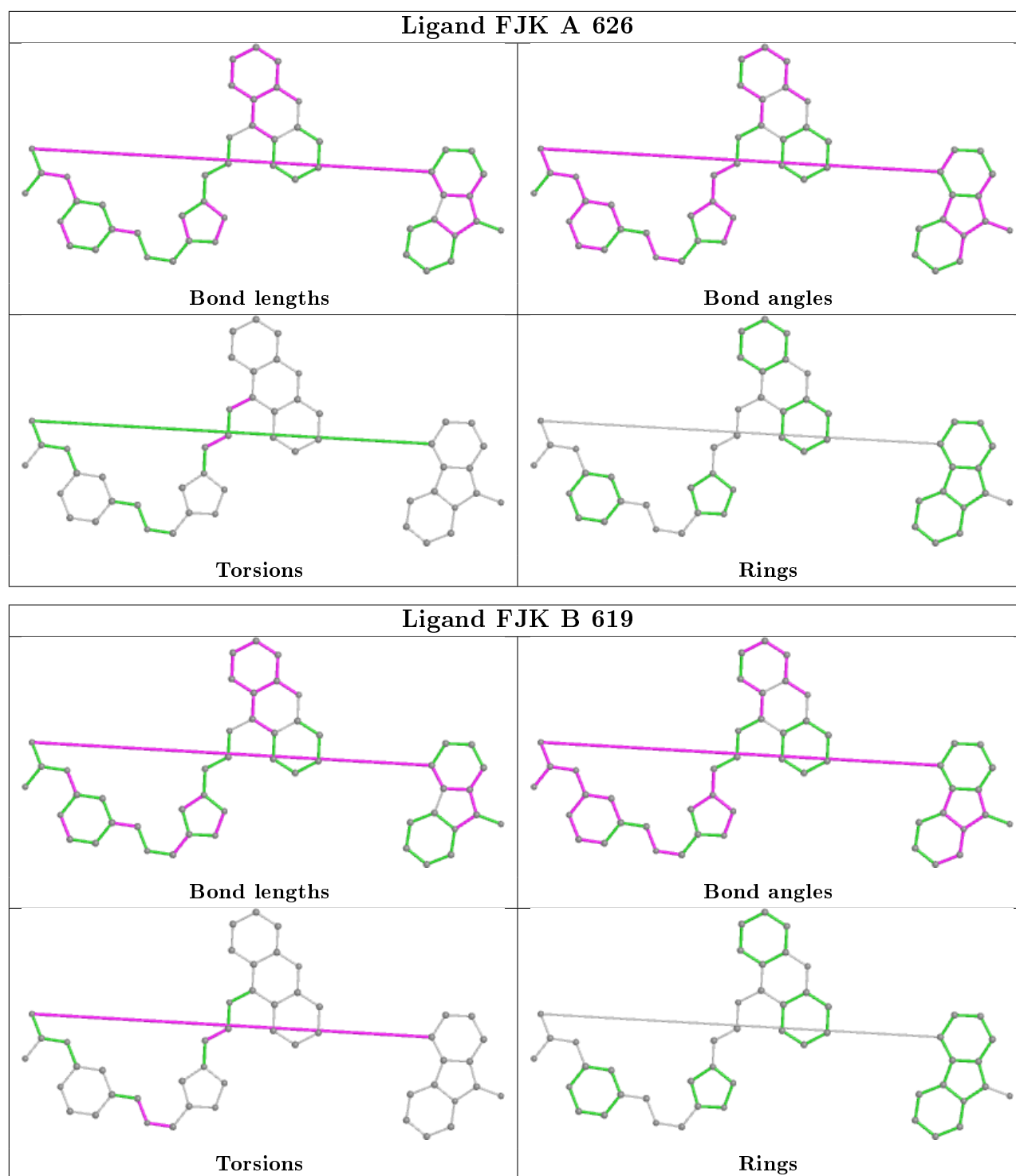
Mol	Chain	Res	Type	Atoms
7	A	617	PEG	O2-C3-C4-O4

There are no ring outliers.

16 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	MES	3	0
7	B	611	PEG	3	0
7	B	614	PEG	2	0
3	B	604	GOL	2	0
7	B	613	PEG	6	0
10	A	626	FJK	1	0
5	B	609	EDO	3	0
5	B	603	EDO	1	0
7	A	615	PEG	2	0
3	A	602	GOL	1	0
5	B	607	EDO	2	0
2	A	614	MES	5	0
3	A	609	GOL	1	0
2	A	611	MES	7	0
5	B	606	EDO	1	0
5	A	610	EDO	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	532/565 (94%)	-0.59	8 (1%) 73 72	18, 28, 46, 80	2 (0%)
1	B	532/565 (94%)	-0.61	6 (1%) 80 79	17, 27, 45, 88	3 (0%)
All	All	1064/1130 (94%)	-0.60	14 (1%) 77 75	17, 28, 46, 88	5 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	THR	5.3
1	B	486	HIS	4.8
1	B	485	PRO	4.4
1	A	488	GLN	4.1
1	A	486	HIS	3.6
1	B	343	SER	3.1
1	A	257	ASN	3.1
1	B	488	GLN	2.9
1	A	485	PRO	2.9
1	B	533	ASN	2.6
1	A	160	GLY	2.5
1	B	342	ASP	2.0
1	A	55	SER	2.0
1	A	343	SER	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	EDO	B	602	4/4	0.55	0.23	48,50,52,54	0
7	PEG	B	614	7/7	0.61	0.19	46,52,58,59	0
10	FJK	B	619	49/49	0.63	0.32	21,44,58,62	49
8	NAG	B	617	14/15	0.65	0.30	55,68,72,73	0
4	PGE	A	603	10/10	0.67	0.26	52,58,63,67	0
10	FJK	A	626	49/49	0.73	0.32	18,42,58,60	49
5	EDO	A	604	4/4	0.75	0.19	48,49,51,53	0
7	PEG	A	617	7/7	0.78	0.29	45,56,59,60	0
2	MES	A	614	12/12	0.78	0.38	45,54,64,64	12
3	GOL	A	609	6/6	0.80	0.24	49,51,53,58	0
7	PEG	A	616	7/7	0.82	0.23	39,49,54,56	0
7	PEG	A	615	7/7	0.83	0.19	34,38,48,49	0
7	PEG	B	612	7/7	0.83	0.16	39,46,51,55	0
7	PEG	A	618	7/7	0.83	0.22	38,45,49,50	0
7	PEG	B	613	7/7	0.84	0.43	48,51,60,68	0
8	NAG	A	619	14/15	0.84	0.26	48,54,60,70	0
2	MES	A	611	12/12	0.86	0.23	38,42,48,49	12
2	MES	A	612	12/12	0.86	0.31	38,56,65,65	12
5	EDO	B	607	4/4	0.86	0.18	36,42,43,50	0
5	EDO	B	609	4/4	0.87	0.18	35,39,46,55	0
3	GOL	B	604	6/6	0.87	0.26	39,43,45,54	0
8	NAG	B	615	14/15	0.87	0.27	50,57,67,68	0
9	CL	A	624	1/1	0.88	0.07	63,63,63,63	0
5	EDO	B	603	4/4	0.88	0.13	41,46,47,51	0
5	EDO	A	606	4/4	0.88	0.18	42,47,47,52	0
4	PGE	B	605	10/10	0.89	0.16	36,41,52,53	0
3	GOL	A	602	6/6	0.89	0.23	30,41,44,62	0
5	EDO	B	606	4/4	0.90	0.16	38,43,51,52	0
5	EDO	A	610	4/4	0.90	0.17	35,38,39,41	0
9	CL	A	623	1/1	0.91	0.09	69,69,69,69	0
7	PEG	B	611	7/7	0.91	0.15	32,36,45,46	0
8	NAG	A	620	14/15	0.92	0.22	30,41,55,59	0
5	EDO	A	605	4/4	0.92	0.14	29,42,43,44	0
2	MES	A	601	12/12	0.93	0.31	54,59,67,70	0
5	EDO	B	610	4/4	0.93	0.10	41,42,44,57	0
8	NAG	B	616	14/15	0.93	0.20	37,46,54,61	0
5	EDO	A	608	4/4	0.93	0.29	47,50,51,61	0

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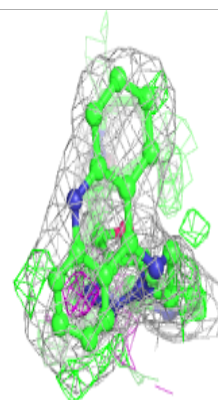
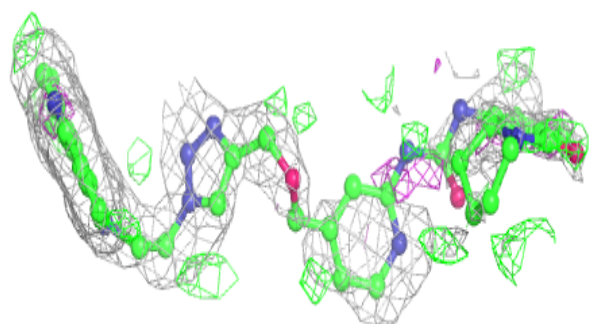
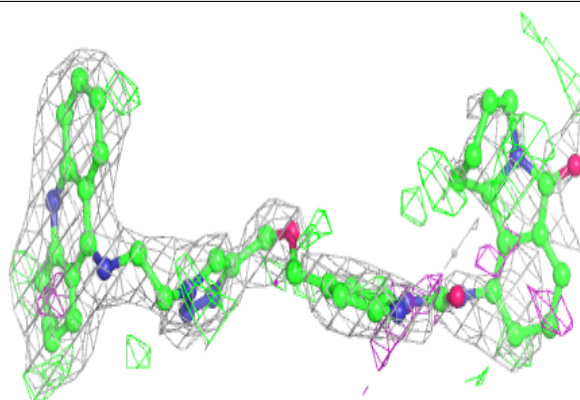
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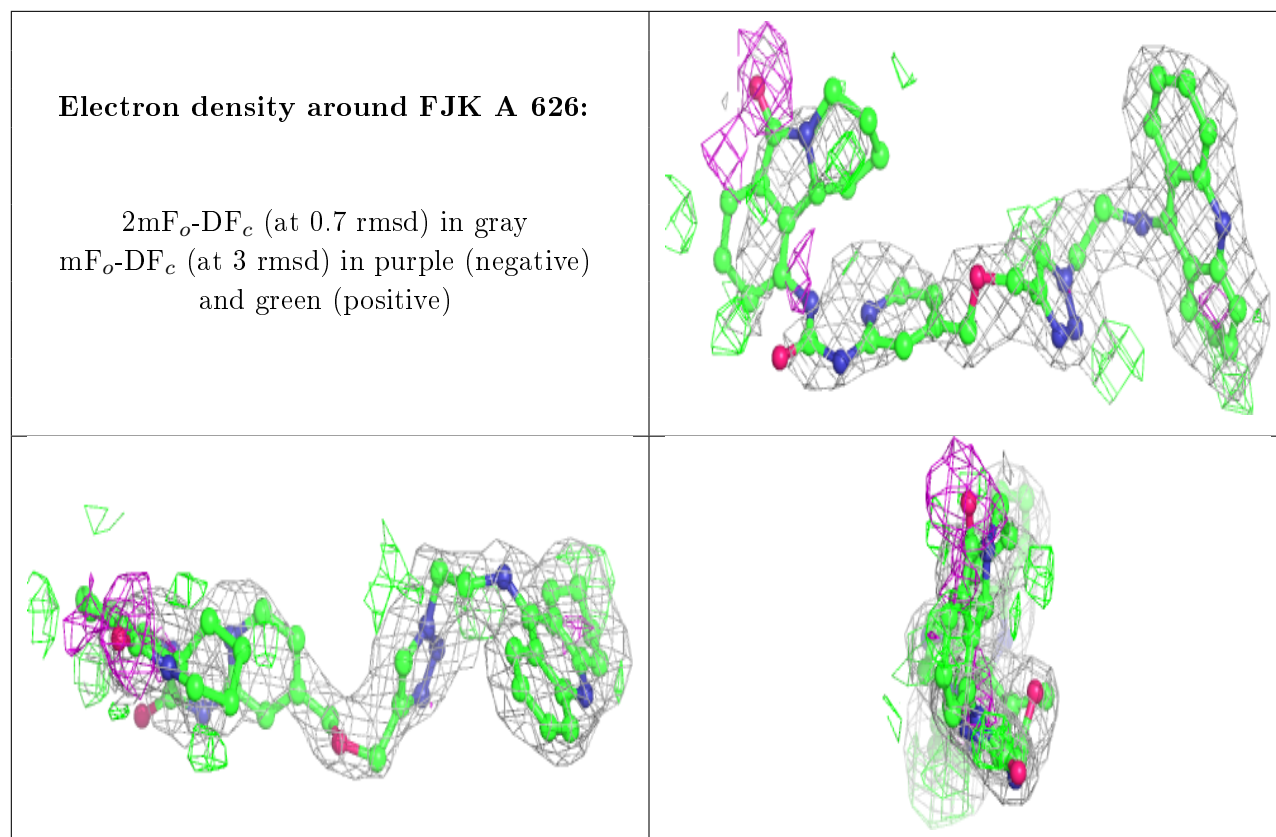
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	B	601	4/4	0.94	0.10	31,36,41,46	0
6	SO4	A	627	5/5	0.95	0.19	35,39,46,53	5
9	CL	A	621	1/1	0.95	0.07	57,57,57,57	0
5	EDO	A	607	4/4	0.95	0.09	36,38,45,48	0
9	CL	A	622	1/1	0.95	0.06	63,63,63,63	0
6	SO4	B	608	5/5	0.96	0.19	51,59,66,71	0
9	CL	A	625	1/1	0.96	0.05	55,55,55,55	0
9	CL	B	618	1/1	0.97	0.06	50,50,50,50	0
6	SO4	A	613	5/5	0.99	0.20	50,50,61,62	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 FJK B 619:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.