



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:39 AM UTC

PDB ID : 9BJ1 / pdb_00009bj1
Title : Crystal structure of inhibitor GNE-6893 bound to HPK1
Authors : Kiefer, J.R.; Tellis, J.C.; Chan, B.K.; Wang, W.; Wu, P.; Choo, E.F.; Heffron, T.P.; Wei, B.; Siu, M.
Deposited on : 2024-04-24
Resolution : 2.18 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

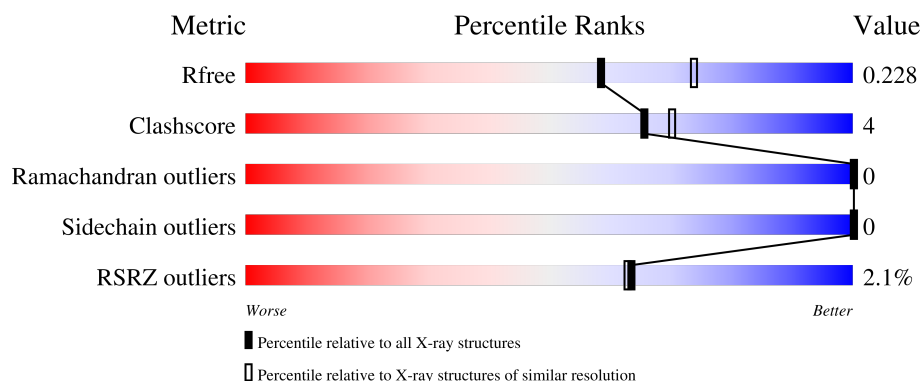
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

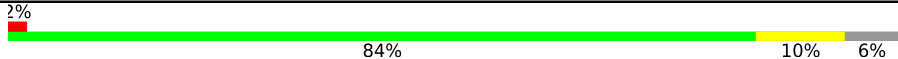
The reported resolution of this entry is 2.18 Å.

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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	311	
1	B	311	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9618 atoms, of which 4740 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 Mitogen-activated protein kinase kinase kinase kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	H	N	O	S	0	2	0
			4603	1470	2317	393	412	11			
1	B	290	Total	C	H	N	O	S	0	0	0
			4540	1453	2280	387	409	11			

There are 42 discrepancies between the modelled and reference sequences:

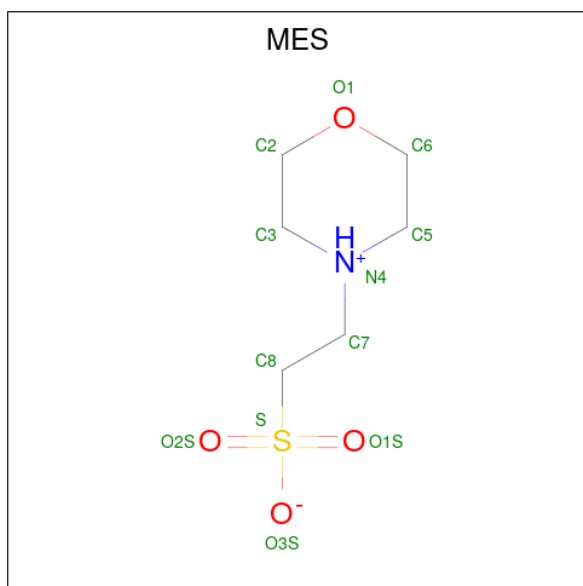
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP Q92918
A	-13	HIS	-	expression tag	UNP Q92918
A	-12	HIS	-	expression tag	UNP Q92918
A	-11	HIS	-	expression tag	UNP Q92918
A	-10	HIS	-	expression tag	UNP Q92918
A	-9	HIS	-	expression tag	UNP Q92918
A	-8	HIS	-	expression tag	UNP Q92918
A	-7	GLY	-	expression tag	UNP Q92918
A	-6	GLU	-	expression tag	UNP Q92918
A	-5	ASN	-	expression tag	UNP Q92918
A	-4	LEU	-	expression tag	UNP Q92918
A	-3	TYR	-	expression tag	UNP Q92918
A	-2	PHE	-	expression tag	UNP Q92918
A	-1	GLN	-	expression tag	UNP Q92918
A	0	GLY	-	expression tag	UNP Q92918
A	1	SER	-	expression tag	UNP Q92918
A	165	GLU	THR	conflict	UNP Q92918
A	171	GLU	SER	conflict	UNP Q92918
A	294	GLY	-	expression tag	UNP Q92918
A	295	ASN	-	expression tag	UNP Q92918
A	296	SER	-	expression tag	UNP Q92918
B	-14	MET	-	initiating methionine	UNP Q92918
B	-13	HIS	-	expression tag	UNP Q92918
B	-12	HIS	-	expression tag	UNP Q92918
B	-11	HIS	-	expression tag	UNP Q92918

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q92918
B	-9	HIS	-	expression tag	UNP Q92918
B	-8	HIS	-	expression tag	UNP Q92918
B	-7	GLY	-	expression tag	UNP Q92918
B	-6	GLU	-	expression tag	UNP Q92918
B	-5	ASN	-	expression tag	UNP Q92918
B	-4	LEU	-	expression tag	UNP Q92918
B	-3	TYR	-	expression tag	UNP Q92918
B	-2	PHE	-	expression tag	UNP Q92918
B	-1	GLN	-	expression tag	UNP Q92918
B	0	GLY	-	expression tag	UNP Q92918
B	1	SER	-	expression tag	UNP Q92918
B	165	GLU	THR	conflict	UNP Q92918
B	171	GLU	SER	conflict	UNP Q92918
B	294	GLY	-	expression tag	UNP Q92918
B	295	ASN	-	expression tag	UNP Q92918
B	296	SER	-	expression tag	UNP Q92918

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



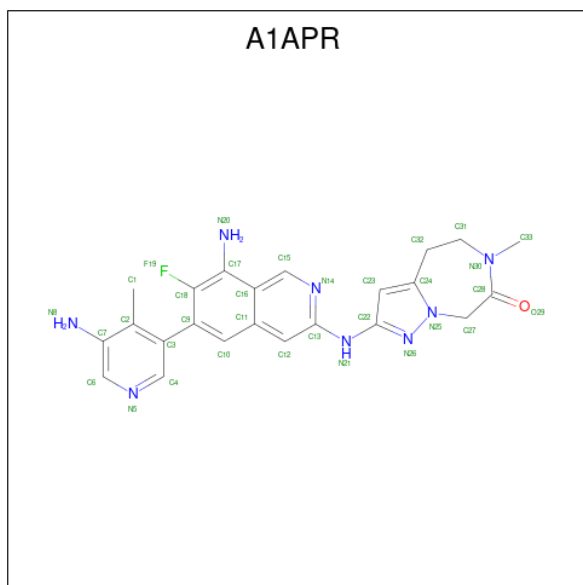
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
4	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
4	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 5 is (9S)-2-{[(6P)-8-amino-6-(5-amino-4-methylpyridin-3-yl)-7-fluoroisoquinolin-3-yl]amino}-6-methyl-5,6-dihydro-4H-pyrazolo[1,5-d][1,4]diazepin-7(8H)-one (CCD ID: A1APR) (formula: C₂₃H₂₃FN₈O) (labeled as "Ligand of Interest" by depositor).

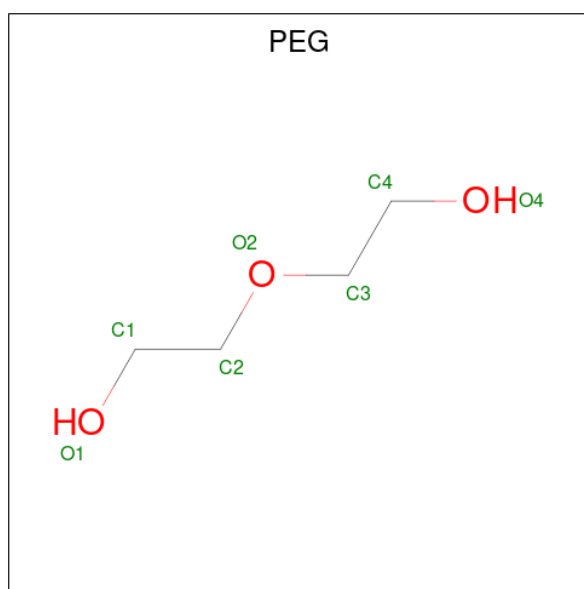


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	F	H	N	O	0	0
			56	23	1	23	8	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

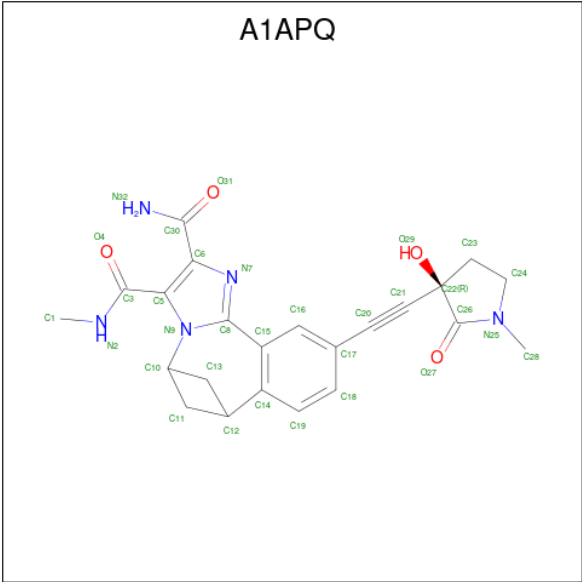
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 8 is (4S,5R,7R,11aP)-10-{[(3R)-3-hydroxy-1-methyl-2-oxopyrrolidin-3-yl]ethynyl}-N 3 -methyl-6,7-dihydro-5H-5,7-methanoimidazo[2,1-a][2]benzazepine-2,3-dicarboxamide (CCD ID: A1APQ) (formula: C₂₃H₂₃N₅O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			55	23	23	5	4		

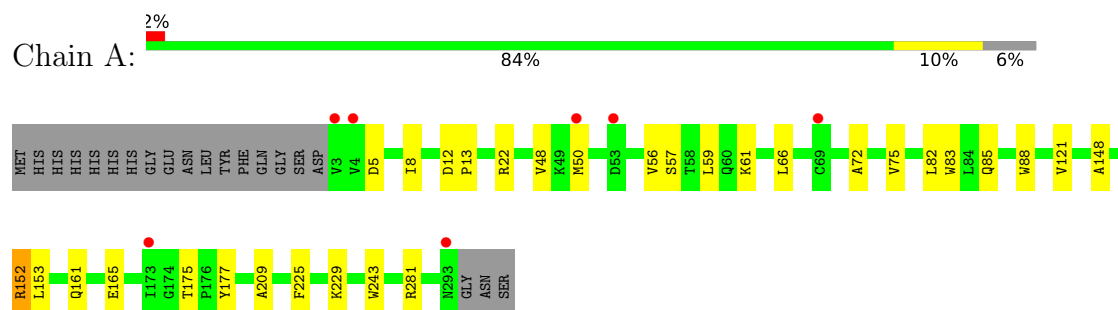
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	84	Total	O	0	0
			84	84		
9	B	107	Total	O	0	0
			107	107		

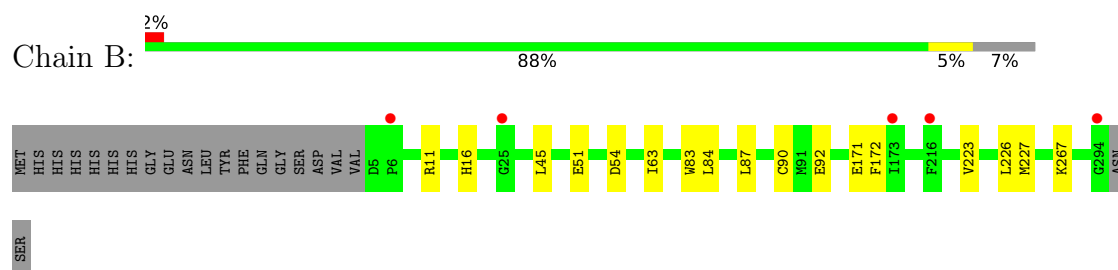
3 Residue-property plots [i](#)

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: Mitogen-activated protein kinase kinase kinase kinase 1



- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.48Å 57.00Å 61.53Å 86.67° 85.37° 66.70°	Depositor
Resolution (Å)	30.65 – 2.18 30.65 – 2.18	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.65-2.18) 95.7 (30.65-2.18)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.173 , 0.228 0.173 , 0.228	Depositor DCC
R_{free} test set	1568 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9618	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, DMS, PEG, A1APR, A1APQ, EDO, NA

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	0.26	0/2344	0.35	0/3174
1	B	0.22	0/2309	0.34	0/3128
All	All	0.24	0/4653	0.34	0/6302

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Sidechain
1	A	22	ARG	Sidechain

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	2286	2317	2303	20	0
1	B	2260	2280	2280	14	0
2	A	12	13	13	0	0
2	B	24	26	25	3	0
3	A	12	18	18	1	0
3	B	8	12	12	0	0
4	A	8	12	12	2	0
4	B	4	6	6	0	0
5	A	33	23	0	0	0
6	A	1	0	0	0	0
7	B	7	10	10	0	0
8	B	32	23	0	2	0
9	A	84	0	0	0	0
9	B	107	0	0	0	0
All	All	4878	4740	4679	36	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 (36) 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:223:VAL:HG12	1:B:227:MET:HE2	1.61	0.82
1:B:83:TRP:CD1	1:B:84:LEU:HD12	2.21	0.76
1:A:48:VAL:HG11	1:A:59:LEU:HD11	1.80	0.63
1:A:66:LEU:HD21	4:A:305:DMS:H13	1.80	0.63
1:B:63:ILE:HD11	1:B:87:LEU:HD21	1.84	0.60
3:A:303:EDO:O2	4:A:306:DMS:S	2.61	0.56
1:A:82:LEU:HD23	1:A:83:TRP:N	2.25	0.52
1:A:148:ALA:O	1:A:281:ARG:HD2	2.10	0.51
1:B:45:LEU:HD23	1:B:90:CYS:HA	1.93	0.50
1:A:50:MET:CE	1:A:56:VAL:HG12	2.42	0.50
8:B:307:A1APQ:O31	8:B:307:A1APQ:N2	2.45	0.49
1:A:121:VAL:HG13	1:A:153:LEU:HD21	1.94	0.49
1:B:63:ILE:HD11	1:B:87:LEU:CD2	2.41	0.49
1:A:175:THR:HG22	1:A:177:TYR:HE2	1.78	0.49
1:A:75:VAL:HA	1:A:152:ARG:HD2	1.95	0.48
1:A:5:ASP:HB3	1:A:8:ILE:HG12	1.96	0.48
1:A:50:MET:O	1:A:85:GLN:HB3	2.14	0.47
1:A:209:ALA:HB1	1:A:243:TRP:CZ2	2.50	0.47
1:B:171:GLU:OE1	1:B:172:PHE:CZ	2.68	0.46
1:A:161:GLN:O	1:A:165:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:VAL:HA	1:B:226:LEU:HD12	1.97	0.46
1:A:57:SER:O	1:A:61:LYS:HG2	2.17	0.45
1:B:267:LYS:HA	1:B:267:LYS:HE2	1.98	0.45
1:A:225:PHE:CZ	1:A:229:LYS:HD3	2.52	0.44
1:A:13:PRO:HG3	1:A:88:TRP:CG	2.53	0.44
1:B:171:GLU:OE1	1:B:172:PHE:CE1	2.70	0.44
1:A:72:ALA:O	1:A:152:ARG:NH1	2.49	0.44
1:B:16:HIS:CE1	2:B:302:MES:H52	2.53	0.43
1:A:12:ASP:HB2	1:A:83:TRP:CD1	2.54	0.43
1:A:50:MET:HE2	1:A:50:MET:HB3	1.90	0.42
1:B:51:GLU:O	1:B:54:ASP:HB2	2.19	0.42
1:A:82:LEU:HD23	1:A:82:LEU:C	2.44	0.42
1:B:92:GLU:O	8:B:307:A1APQ:N32	2.53	0.41
1:B:11:ARG:HH11	2:B:302:MES:H72	1.84	0.41
1:B:11:ARG:HD2	2:B:302:MES:O1S	2.21	0.41
1:A:48:VAL:CG1	1:A:59:LEU:HD11	2.49	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/311 (94%)	284 (98%)	7 (2%)	0	100	100
1	B	288/311 (93%)	281 (98%)	7 (2%)	0	100	100
All	All	579/622 (93%)	565 (98%)	14 (2%)	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	245/265 (92%)	245 (100%)	0	100	100
1	B	240/265 (91%)	240 (100%)	0	100	100
All	All	485/530 (92%)	485 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	21	GLN
1	B	212	GLN
1	B	293	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	B	301	-	12,12,12	2.34	1 (8%)	15,16,16	1.71	3 (20%)
3	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.43	0
8	A1APQ	B	307	-	34,36,36	7.27	24 (70%)	43,56,56	3.66	18 (41%)
4	DMS	A	306	-	3,3,3	0.68	0	3,3,3	0.51	0
5	A1APR	A	307	-	37,37,37	3.15	13 (35%)	40,55,55	2.56	11 (27%)
4	DMS	A	305	-	3,3,3	0.67	0	3,3,3	0.36	0
3	EDO	B	304	-	3,3,3	0.48	0	2,2,2	0.43	0
7	PEG	B	303	-	6,6,6	0.17	0	5,5,5	0.05	0
2	MES	A	301	-	12,12,12	2.23	1 (8%)	15,16,16	1.45	3 (20%)
3	EDO	A	303	-	3,3,3	0.51	0	2,2,2	0.31	0
3	EDO	A	302	-	3,3,3	0.67	0	2,2,2	0.26	0
4	DMS	B	306	-	3,3,3	0.69	0	3,3,3	0.48	0
3	EDO	B	305	-	3,3,3	0.51	0	2,2,2	0.35	0
2	MES	B	302	-	12,12,12	2.21	1 (8%)	15,16,16	1.49	2 (13%)

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	B	301	-	-	4/6/14/14	0/1/1/1
3	EDO	A	304	-	-	1/1/1/1	-
8	A1APQ	B	307	-	-	0/13/52/52	0/4/5/5
5	A1APR	A	307	-	-	2/8/30/30	0/4/5/5
3	EDO	B	304	-	-	1/1/1/1	-
7	PEG	B	303	-	-	0/4/4/4	-
2	MES	A	301	-	-	1/6/14/14	0/1/1/1
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	B	305	-	-	0/1/1/1	-
2	MES	B	302	-	-	5/6/14/14	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	307	A1APQ	C26-N25	23.31	1.60	1.34
8	B	307	A1APQ	C22-C26	-14.92	1.30	1.54
8	B	307	A1APQ	C11-C12	-14.42	1.29	1.56
5	A	307	A1APR	C22-N26	14.22	1.52	1.33
8	B	307	A1APQ	C11-C10	-14.20	1.32	1.53
8	B	307	A1APQ	C23-C24	-13.07	1.29	1.52
8	B	307	A1APQ	C23-C22	9.69	1.71	1.54
8	B	307	A1APQ	C10-N9	8.39	1.55	1.48
8	B	307	A1APQ	C3-N2	7.92	1.44	1.33
2	B	301	MES	C8-S	-7.78	1.66	1.77
2	B	302	MES	C8-S	-7.43	1.67	1.77
2	A	301	MES	C8-S	-7.38	1.67	1.77
8	B	307	A1APQ	C15-C14	-6.11	1.33	1.40
8	B	307	A1APQ	C13-C12	-4.93	1.47	1.56
5	A	307	A1APR	C31-C32	-4.86	1.44	1.52
5	A	307	A1APR	C17-C16	-4.77	1.38	1.44
5	A	307	A1APR	C22-N21	4.69	1.45	1.37
8	B	307	A1APQ	C30-N32	4.58	1.46	1.33
8	B	307	A1APQ	C24-N25	4.42	1.59	1.46
8	B	307	A1APQ	C15-C8	-4.15	1.36	1.48
8	B	307	A1APQ	C13-C10	-4.14	1.47	1.53
8	B	307	A1APQ	C5-C3	4.03	1.55	1.46
8	B	307	A1APQ	C17-C20	3.85	1.53	1.44
5	A	307	A1APR	C32-C24	-3.83	1.45	1.50
8	B	307	A1APQ	C5-N9	-3.34	1.33	1.41
5	A	307	A1APR	C17-N20	3.29	1.45	1.36
8	B	307	A1APQ	C14-C12	-3.11	1.49	1.52
5	A	307	A1APR	N25-N26	-3.11	1.31	1.36
5	A	307	A1APR	C16-C11	-2.87	1.37	1.43
5	A	307	A1APR	C15-C16	-2.67	1.39	1.42
8	B	307	A1APQ	C8-N9	-2.59	1.34	1.39
8	B	307	A1APQ	O4-C3	-2.52	1.18	1.23
5	A	307	A1APR	C7-N8	2.48	1.46	1.38
5	A	307	A1APR	C13-N21	2.37	1.45	1.40
8	B	307	A1APQ	C6-C30	2.34	1.54	1.47
5	A	307	A1APR	C15-N14	2.16	1.36	1.32
8	B	307	A1APQ	O31-C30	-2.15	1.19	1.24
5	A	307	A1APR	C9-C3	-2.05	1.45	1.49
8	B	307	A1APQ	C6-N7	-2.04	1.34	1.38
8	B	307	A1APQ	O27-C26	-2.00	1.19	1.22

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	307	A1APQ	C24-N25-C26	-12.83	106.53	114.38
5	A	307	A1APR	C23-C22-N26	-10.05	105.14	112.34
8	B	307	A1APQ	C13-C10-C11	-8.64	75.02	88.87
8	B	307	A1APQ	C12-C11-C10	8.62	106.67	83.51
5	A	307	A1APR	C16-C15-N14	-7.02	119.14	124.70
8	B	307	A1APQ	C6-C5-C3	-6.42	128.71	137.17
8	B	307	A1APQ	C13-C12-C11	-6.35	76.20	86.58
8	B	307	A1APQ	C13-C12-C14	-5.82	105.37	122.04
8	B	307	A1APQ	C23-C24-N25	4.38	107.45	103.54
2	B	301	MES	C6-C5-N4	-3.85	104.27	110.12
8	B	307	A1APQ	C22-C26-N25	-3.78	106.95	108.81
5	A	307	A1APR	C15-N14-C13	3.61	121.20	117.81
5	A	307	A1APR	N21-C22-N26	3.58	129.51	119.67
8	B	307	A1APQ	O4-C3-N2	-3.51	116.91	122.84
5	A	307	A1APR	C24-C23-C22	3.30	107.88	104.89
8	B	307	A1APQ	C19-C14-C12	-3.24	113.54	120.32
5	A	307	A1APR	C15-C16-C17	-3.21	117.59	121.86
5	A	307	A1APR	C3-C2-C7	3.13	120.03	117.41
8	B	307	A1APQ	N9-C8-N7	-3.09	108.85	112.16
8	B	307	A1APQ	C15-C8-N9	2.98	131.20	125.23
2	B	302	MES	C5-N4-C3	2.86	115.01	108.84
5	A	307	A1APR	C27-N25-N26	2.86	126.59	120.77
8	B	307	A1APQ	C12-C13-C10	2.81	91.05	83.51
8	B	307	A1APQ	C28-N25-C26	2.76	126.67	123.24
2	B	301	MES	C7-N4-C5	2.70	118.42	111.24
2	B	302	MES	O1S-S-C8	2.60	110.65	106.73
8	B	307	A1APQ	C16-C15-C8	-2.51	111.76	119.55
2	A	301	MES	C2-C3-N4	-2.48	106.35	110.12
8	B	307	A1APQ	C6-N7-C8	2.45	108.94	104.85
5	A	307	A1APR	C3-C9-C18	-2.30	118.75	121.11
8	B	307	A1APQ	C30-C6-N7	2.21	125.18	122.27
2	A	301	MES	O1S-S-C8	2.19	110.03	106.73
8	B	307	A1APQ	C19-C14-C15	2.19	121.36	118.78
2	B	301	MES	O2S-S-C8	2.17	110.01	106.73
2	A	301	MES	C5-N4-C3	2.16	113.49	108.84
5	A	307	A1APR	C17-C16-C11	2.09	121.19	119.50
5	A	307	A1APR	C10-C9-C18	2.01	119.58	117.44

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	MES	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
2	B	301	MES	C7-C8-S-O1S
2	B	301	MES	C7-C8-S-O3S
2	B	302	MES	C7-C8-S-O2S
2	B	302	MES	C7-C8-S-O3S
2	B	302	MES	C8-C7-N4-C3
2	B	302	MES	C8-C7-N4-C5
5	A	307	A1APR	C23-C22-N21-C13
5	A	307	A1APR	N26-C22-N21-C13
2	B	301	MES	C7-C8-S-O2S
2	B	302	MES	C7-C8-S-O1S
3	A	303	EDO	O1-C1-C2-O2
3	A	304	EDO	O1-C1-C2-O2
2	A	301	MES	C7-C8-S-O2S
3	B	304	EDO	O1-C1-C2-O2

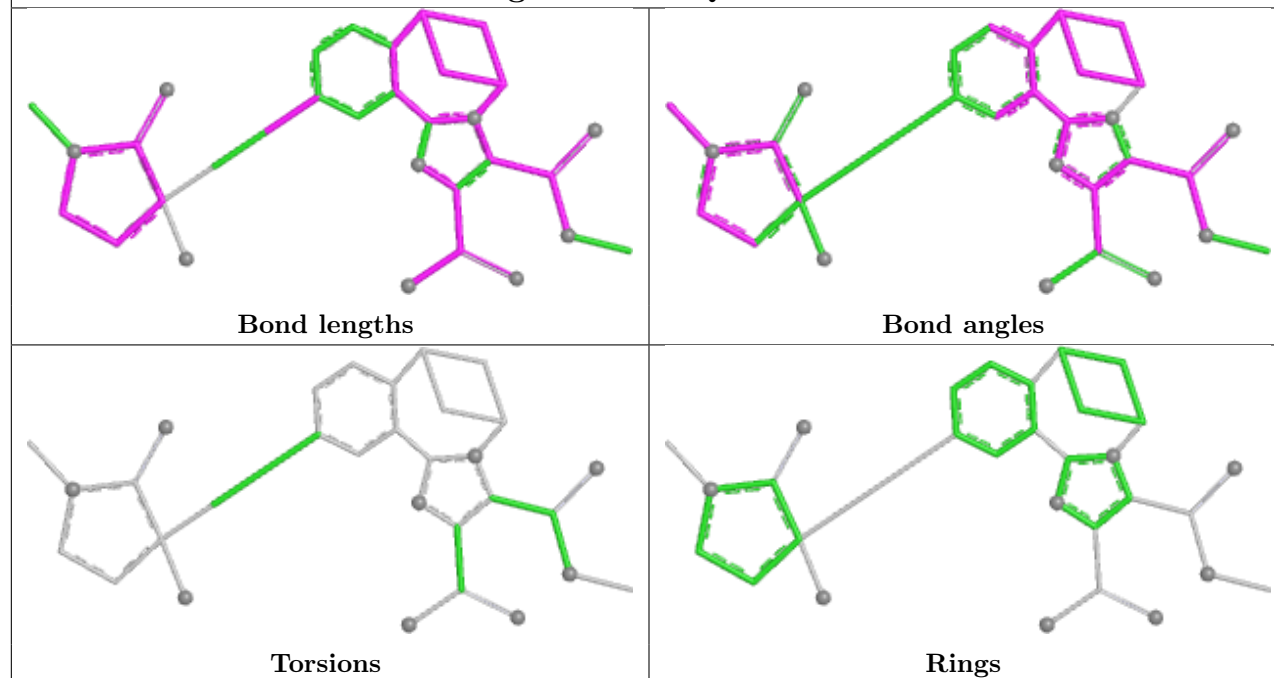
There are no ring outliers.

5 monomers are involved in 7 short contacts:

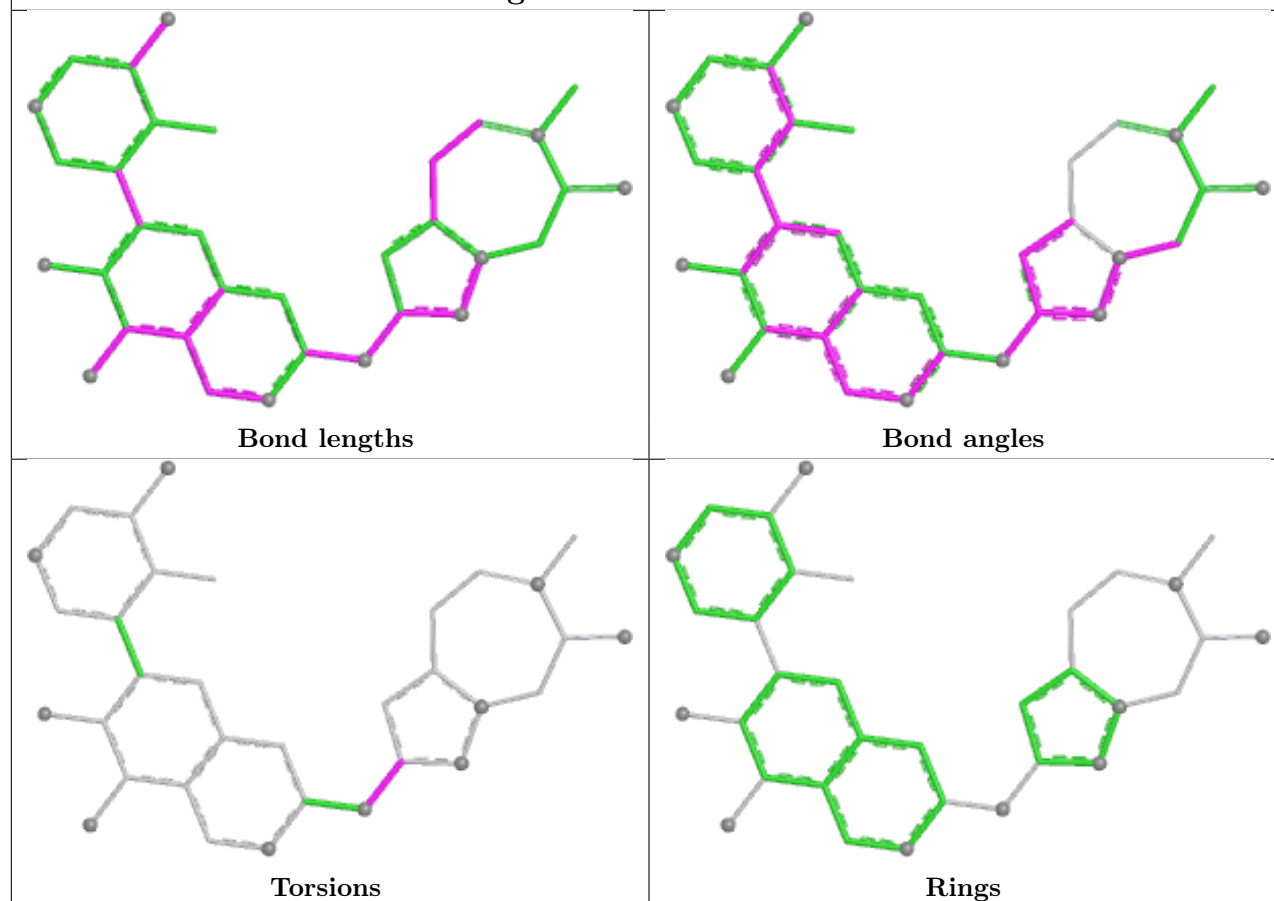
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	307	A1APQ	2	0
4	A	306	DMS	1	0
4	A	305	DMS	1	0
3	A	303	EDO	1	0
2	B	302	MES	3	0

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.

Ligand A1APQ B 307



Ligand A1APR A 307



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	291/311 (93%)	-0.02	7 (2%) 59 59	27, 50, 79, 119	1 (0%)
1	B	290/311 (93%)	-0.12	5 (1%) 69 68	34, 46, 73, 99	0
All	All	581/622 (93%)	-0.07	12 (2%) 63 63	27, 48, 76, 119	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	VAL	3.4
1	A	53	ASP	3.0
1	A	4	VAL	2.8
1	B	6	PRO	2.8
1	B	294	GLY	2.7
1	B	173	ILE	2.7
1	A	69	CYS	2.5
1	B	216	PHE	2.3
1	A	50	MET	2.1
1	A	293	ASN	2.0
1	A	173	ILE	2.0
1	B	25	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

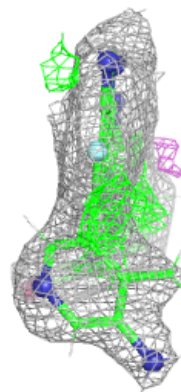
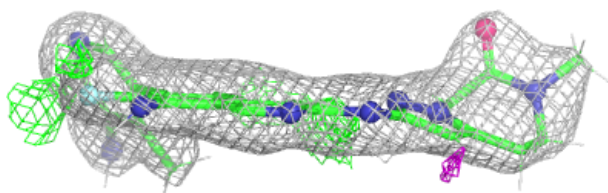
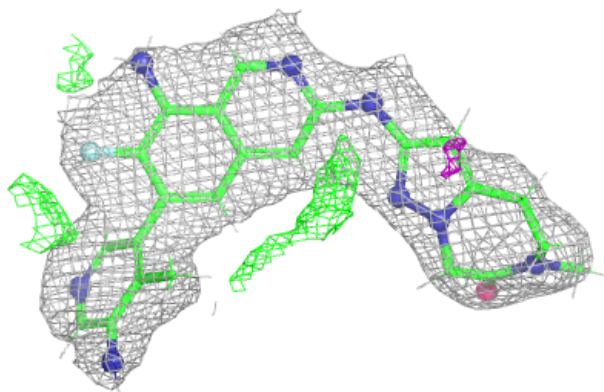
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	304	4/4	0.72	0.13	57,75,78,90	0
4	DMS	A	306	4/4	0.77	0.17	61,81,98,98	0
3	EDO	A	303	4/4	0.80	0.17	58,69,83,83	0
3	EDO	A	302	4/4	0.82	0.12	40,49,59,59	0
4	DMS	B	306	4/4	0.85	0.20	52,66,79,91	0
7	PEG	B	303	7/7	0.86	0.10	49,66,89,97	0
2	MES	B	301	12/12	0.88	0.09	48,67,84,84	0
4	DMS	A	305	4/4	0.89	0.14	48,60,62,71	0
2	MES	B	302	12/12	0.91	0.09	60,75,86,92	0
5	A1APR	A	307	33/33	0.91	0.10	38,55,72,74	0
2	MES	A	301	12/12	0.91	0.08	46,57,71,76	0
3	EDO	B	304	4/4	0.92	0.10	50,60,71,71	0
8	A1APQ	B	307	32/32	0.93	0.10	33,41,53,55	0
3	EDO	B	305	4/4	0.94	0.09	48,60,71,72	0
6	NA	A	308	1/1	0.94	0.10	65,65,65,65	0

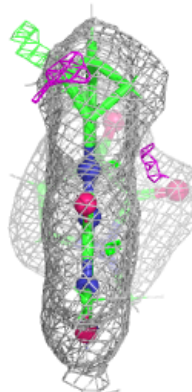
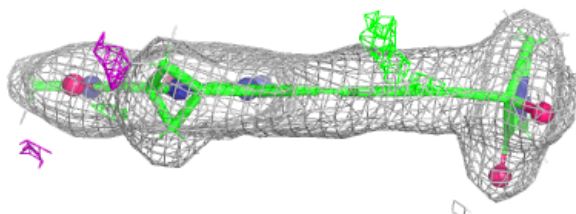
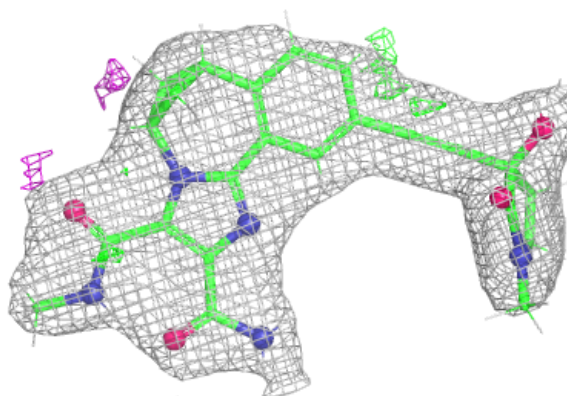
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1APR A 307:

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

**Electron density around A1APQ B 307:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.