Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2023 – 04:25 PM EDT

PDB ID	:	4Q15
Title	:	Crystal Structure of Prolyl-tRNA synthetase (ProRS, Proline–tRNA ligase) from Plasmodium falciparum in complex with Halofuginone and AMPPNP in space group P212121 at 2.35 A
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2014-04-02
Resolution	:	2.35 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 (i) 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 (i)) were used in the production of this report:

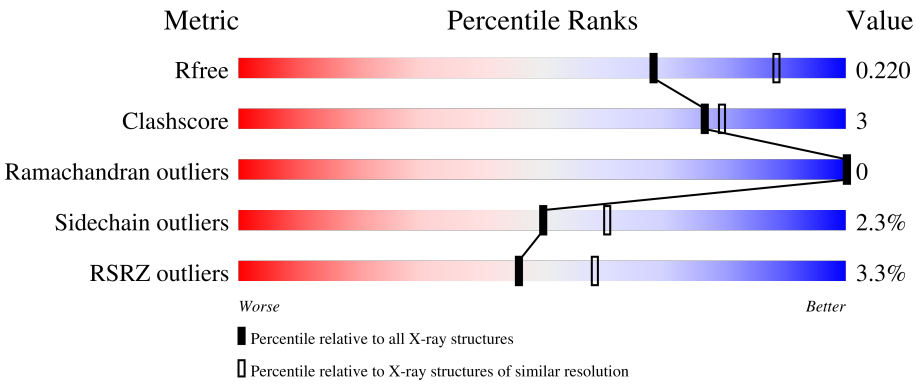
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	506	2% 84% 7% 9%
1	B	506	4% 83% 6% • 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7587 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 Proline–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	3572	2309	594	649	20	0	0	0
1	B	458	3618	2343	597	659	19	0	0	0

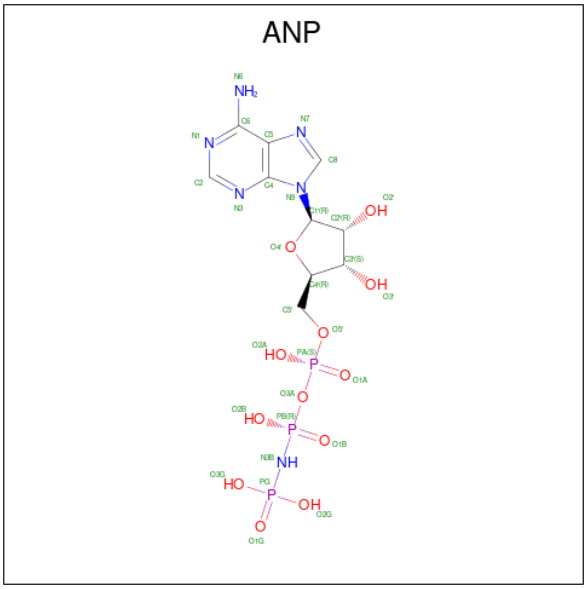
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	expression tag	UNP Q8I5R7
A	242	ALA	-	expression tag	UNP Q8I5R7
A	243	HIS	-	expression tag	UNP Q8I5R7
A	244	HIS	-	expression tag	UNP Q8I5R7
A	245	HIS	-	expression tag	UNP Q8I5R7
A	246	HIS	-	expression tag	UNP Q8I5R7
A	247	HIS	-	expression tag	UNP Q8I5R7
A	248	HIS	-	expression tag	UNP Q8I5R7
B	241	MET	-	expression tag	UNP Q8I5R7
B	242	ALA	-	expression tag	UNP Q8I5R7
B	243	HIS	-	expression tag	UNP Q8I5R7
B	244	HIS	-	expression tag	UNP Q8I5R7
B	245	HIS	-	expression tag	UNP Q8I5R7
B	246	HIS	-	expression tag	UNP Q8I5R7
B	247	HIS	-	expression tag	UNP Q8I5R7
B	248	HIS	-	expression tag	UNP Q8I5R7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

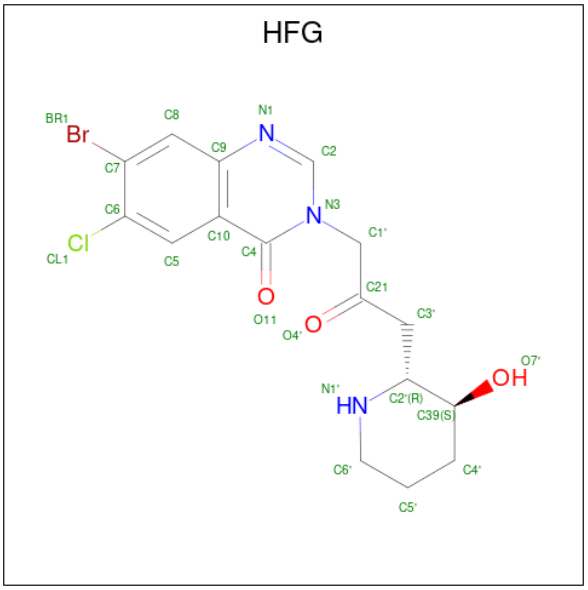
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



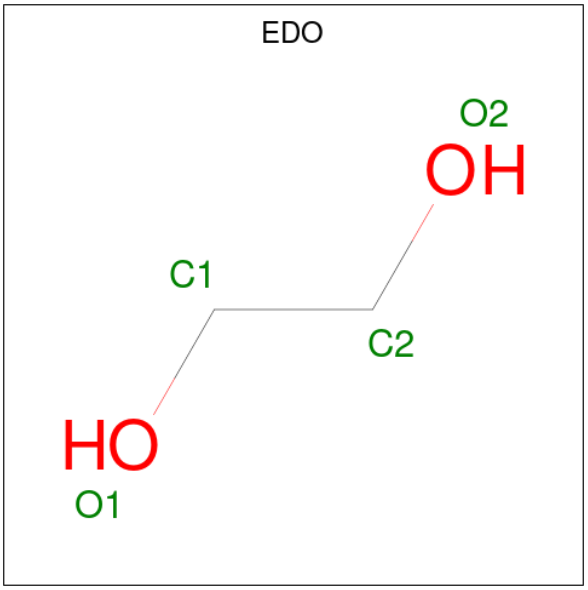
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	6	12	3	0	0

- Molecule 4 is 7-bromo-6-chloro-3-{3-[(2R,3S)-3-hydroxypiperidin-2-yl]-2-oxopropyl}quinazolin-4(3H)-one (three-letter code: HFG) (formula: $C_{16}H_{17}BrClN_3O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	Cl	N	O		
4	A	1	24	1	16	1	3	3	0	0
4	B	1	24	1	16	1	3	3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

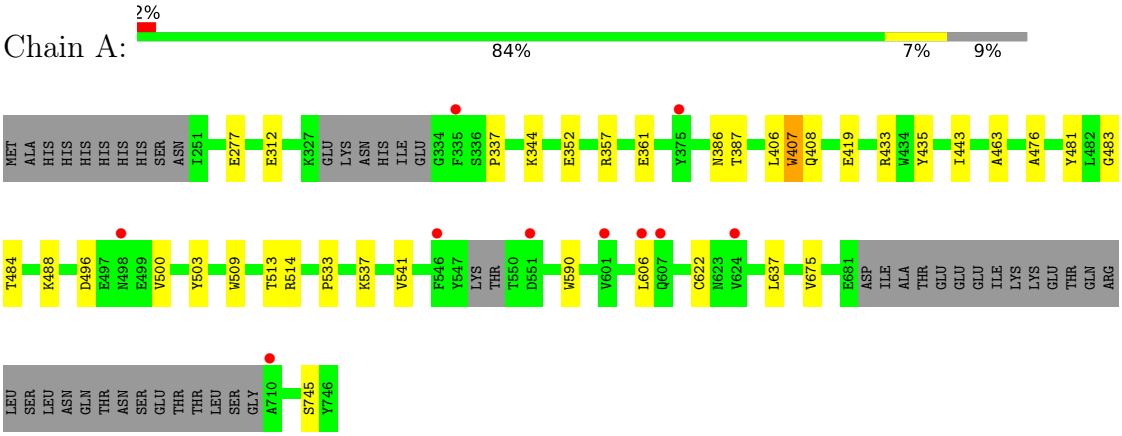
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	140	140	140	0	0
6	B	133	133	133	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

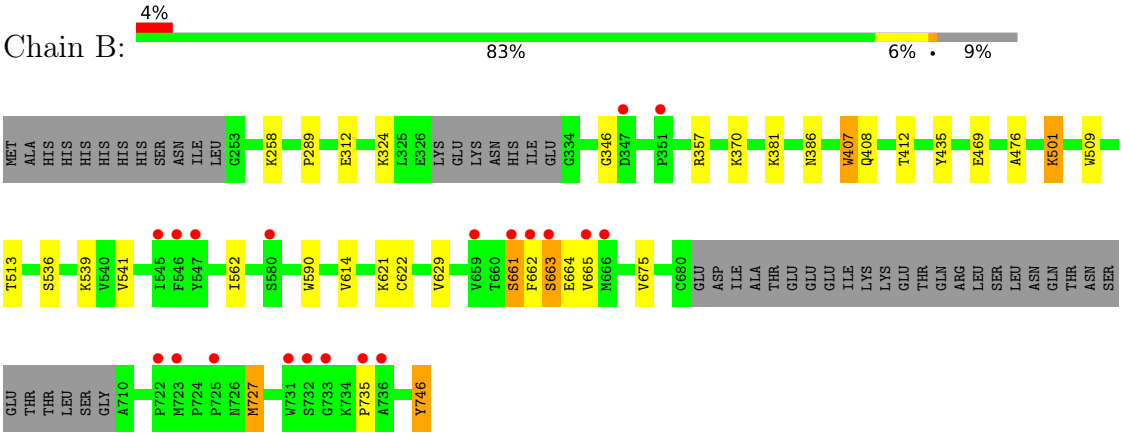
• Molecule 1: Proline–tRNA ligase

Chain A:



• Molecule 1: Proline–tRNA ligase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.58Å 78.09Å 167.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.33 – 2.35 45.81 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.33-2.35) 93.1 (45.81-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.34Å)	Xtriage
Refinement program	PHENIX dev_1659	Depositor
R, R_{free}	0.195 , 0.219 0.197 , 0.220	Depositor DCC
R_{free} test set	2117 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7587	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: HFG, MG, EDO, ANP

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	0.23	0/3668	0.41	0/4998
1	B	0.24	0/3717	0.44	0/5061
All	All	0.23	0/7385	0.42	0/10059

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	3572	0	3340	22	0
1	B	3618	0	3447	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	13	1	0
3	B	31	0	13	0	0
4	A	24	0	17	1	0
4	B	24	0	17	1	0
5	B	12	0	18	0	0
6	A	140	0	0	7	0
6	B	133	0	0	4	0
All	All	7587	0	6865	43	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 3.

All (43) 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:663:SER:HA	1:B:665:VAL:H	1.33	0.93
1:A:484:THR:OG1	6:A:1006:HOH:O	2.01	0.77
1:A:361:GLU:OE1	6:A:992:HOH:O	2.04	0.74
1:B:661:SER:HB2	1:B:664:GLU:H	1.54	0.73
1:A:352:GLU:O	6:A:1015:HOH:O	2.11	0.67
1:B:746:TYR:OH	6:B:990:HOH:O	2.12	0.64
1:B:324:LYS:NZ	6:B:901:HOH:O	2.25	0.64
1:B:501:LYS:NZ	6:B:1022:HOH:O	2.09	0.64
1:B:614:VAL:HG22	1:B:621:LYS:HG2	1.81	0.62
1:B:661:SER:HB2	1:B:664:GLU:N	2.14	0.61
1:B:663:SER:HA	1:B:665:VAL:N	2.10	0.61
1:B:662:PHE:HA	1:B:665:VAL:HG23	1.83	0.60
1:B:663:SER:CA	1:B:665:VAL:H	2.13	0.58
1:A:537:LYS:NZ	1:B:312:GLU:OE2	2.27	0.56
1:A:435:TYR:CZ	1:A:476:ALA:HB1	2.41	0.55
1:A:277:GLU:OE2	1:B:370:LYS:NZ	2.37	0.55
1:A:407:TRP:CH2	4:A:803:HFG:H6	2.42	0.55
1:A:433:ARG:NH1	6:A:1014:HOH:O	2.38	0.53
1:B:407:TRP:CH2	4:B:803:HFG:H6	2.43	0.53
1:A:419:GLU:OE1	6:A:1011:HOH:O	2.19	0.50
1:A:387:THR:HG23	1:A:406:LEU:HD23	1.93	0.50
1:A:541:VAL:HG21	1:A:590:TRP:CD1	2.47	0.50
1:A:496:ASP:HB2	1:A:500:VAL:O	2.12	0.49
1:A:357:ARG:NH2	1:A:386:ASN:HB2	2.28	0.49
1:A:622:CYS:SG	6:A:1007:HOH:O	2.58	0.48
1:B:258:LYS:HG2	1:B:469:GLU:HG2	1.96	0.48
1:A:443:ILE:HD13	1:A:463:ALA:HB1	1.96	0.47
1:A:488:LYS:HG2	1:A:503:TYR:CE2	2.49	0.47
1:A:352:GLU:N	6:A:1015:HOH:O	2.17	0.47
1:B:357:ARG:NH2	1:B:386:ASN:HB2	2.30	0.46
1:B:435:TYR:CZ	1:B:476:ALA:HB1	2.50	0.46
1:B:536:SER:O	1:B:539:LYS:NZ	2.33	0.46
1:A:337:PRO:HA	1:B:346:GLY:HA3	1.99	0.43
1:B:381:LYS:HA	1:B:412:THR:HG22	2.01	0.43
1:A:533:PRO:HB3	1:A:637:LEU:HD22	2.01	0.42
1:B:622:CYS:SG	6:B:1015:HOH:O	2.62	0.42
1:A:312:GLU:HB3	1:B:289:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ARG:NH1	3:A:802:ANP:O2'	2.53	0.42
1:A:481:TYR:CZ	1:A:483:GLY:HA2	2.56	0.41
1:B:541:VAL:HG21	1:B:590:TRP:CD1	2.55	0.41
1:B:562:ILE:HG23	1:B:629:VAL:HG11	2.03	0.40
1:B:727:MET:O	1:B:735:PRO:HA	2.22	0.40
1:B:665:VAL:HG22	1:B:675:VAL:HG11	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	452/506 (89%)	443 (98%)	9 (2%)	0	100	100
1	B	452/506 (89%)	440 (97%)	12 (3%)	0	100	100
All	All	904/1012 (89%)	883 (98%)	21 (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	362/460 (79%)	354 (98%)	8 (2%)	52	63
1	B	378/460 (82%)	369 (98%)	9 (2%)	49	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	740/920 (80%)	723 (98%)	17 (2%)	50 61

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	LYS
1	A	407	TRP
1	A	408	GLN
1	A	509	TRP
1	A	513	THR
1	A	606	LEU
1	A	675	VAL
1	A	745	SER
1	B	407	TRP
1	B	408	GLN
1	B	501	LYS
1	B	509	TRP
1	B	513	THR
1	B	661	SER
1	B	663	SER
1	B	727	MET
1	B	746	TYR

Sometimes 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 (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
4	HFG	A	803	-	25,26,26	3.12	12 (48%)	27,37,37	2.41	3 (11%)
3	ANP	B	802	2	29,33,33	1.08	4 (13%)	31,52,52	1.06	2 (6%)
5	EDO	B	804	-	3,3,3	0.50	0	2,2,2	0.20	0
5	EDO	B	806	-	3,3,3	0.53	0	2,2,2	0.28	0
5	EDO	B	805	-	3,3,3	0.44	0	2,2,2	0.45	0
3	ANP	A	802	2	29,33,33	1.08	5 (17%)	31,52,52	1.08	4 (12%)
4	HFG	B	803	-	25,26,26	3.12	12 (48%)	27,37,37	2.36	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HFG	A	803	-	-	0/8/19/19	1/3/3/3
3	ANP	B	802	2	-	7/14/38/38	0/3/3/3
5	EDO	B	804	-	-	0/1/1/1	-
5	EDO	B	806	-	-	1/1/1/1	-
5	EDO	B	805	-	-	1/1/1/1	-
3	ANP	A	802	2	-	9/14/38/38	0/3/3/3
4	HFG	B	803	-	-	0/8/19/19	1/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	HFG	C4'-C39	-7.02	1.41	1.52
4	B	803	HFG	C4'-C39	-6.97	1.41	1.52
4	B	803	HFG	C1'-N3	5.45	1.53	1.46
4	A	803	HFG	C1'-N3	5.41	1.53	1.46
4	B	803	HFG	C10-C4	-5.22	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	HFG	C10-C4	-5.22	1.37	1.47
4	A	803	HFG	C2'-N1'	-5.11	1.40	1.47
4	B	803	HFG	C2'-N1'	-4.99	1.40	1.47
4	A	803	HFG	C2-N1	4.57	1.34	1.29
4	B	803	HFG	C2-N1	4.48	1.34	1.29
4	B	803	HFG	O7'-C39	4.43	1.52	1.43
4	A	803	HFG	O7'-C39	4.42	1.52	1.43
4	A	803	HFG	C2-N3	-3.68	1.32	1.36
4	A	803	HFG	C5'-C4'	-3.67	1.43	1.53
4	B	803	HFG	C2-N3	-3.61	1.32	1.36
4	B	803	HFG	C5'-C4'	-3.59	1.43	1.53
4	A	803	HFG	C5-C10	3.13	1.44	1.39
4	B	803	HFG	C5-C10	3.09	1.44	1.39
4	B	803	HFG	BR1-C7	2.89	1.96	1.89
4	B	803	HFG	C3'-C21	2.81	1.55	1.51
4	A	803	HFG	C3'-C21	2.74	1.55	1.51
4	A	803	HFG	BR1-C7	2.68	1.95	1.89
3	B	802	ANP	PG-N3B	2.61	1.70	1.63
3	A	802	ANP	PG-N3B	2.55	1.70	1.63
3	A	802	ANP	PG-O1G	2.52	1.50	1.46
3	B	802	ANP	PG-O1G	2.49	1.50	1.46
4	B	803	HFG	C39-C2'	2.38	1.55	1.52
3	A	802	ANP	PB-O1B	2.35	1.49	1.46
3	B	802	ANP	PB-O1B	2.29	1.49	1.46
4	A	803	HFG	C39-C2'	2.29	1.55	1.52
3	B	802	ANP	PB-N3B	2.05	1.68	1.63
3	A	802	ANP	PB-O3A	-2.03	1.56	1.59
3	A	802	ANP	PB-N3B	2.02	1.68	1.63

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	HFG	C10-C4-N3	10.03	119.65	113.80
4	B	803	HFG	C10-C4-N3	9.97	119.61	113.80
4	A	803	HFG	N3-C2-N1	-5.31	121.72	126.34
4	B	803	HFG	N3-C2-N1	-5.09	121.91	126.34
3	B	802	ANP	PB-O3A-PA	-3.08	121.78	132.62
4	A	803	HFG	C9-N1-C2	2.86	119.44	116.62
4	B	803	HFG	C9-N1-C2	2.77	119.35	116.62
3	A	802	ANP	O1G-PG-N3B	-2.62	107.91	111.77
3	A	802	ANP	PB-O3A-PA	-2.27	124.64	132.62
3	A	802	ANP	C5-C6-N6	2.25	123.77	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	ANP	C5-C6-N6	2.24	123.76	120.35
3	A	802	ANP	O2B-PB-O3A	2.13	111.74	104.64
4	B	803	HFG	C2-N3-C4	-2.08	120.28	121.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	ANP	PG-N3B-PB-O1B
3	A	802	ANP	C5'-O5'-PA-O2A
3	B	802	ANP	PB-N3B-PG-O1G
3	B	802	ANP	PG-N3B-PB-O1B
3	B	802	ANP	C5'-O5'-PA-O2A
3	B	802	ANP	O4'-C4'-C5'-O5'
3	B	802	ANP	C3'-C4'-C5'-O5'
3	A	802	ANP	O4'-C4'-C5'-O5'
5	B	806	EDO	O1-C1-C2-O2
3	A	802	ANP	C3'-C4'-C5'-O5'
3	A	802	ANP	PB-O3A-PA-O1A
3	A	802	ANP	C5'-O5'-PA-O3A
3	B	802	ANP	C5'-O5'-PA-O3A
3	A	802	ANP	C5'-O5'-PA-O1A
3	B	802	ANP	C5'-O5'-PA-O1A
5	B	805	EDO	O1-C1-C2-O2
3	A	802	ANP	PB-O3A-PA-O2A
3	A	802	ANP	PB-N3B-PG-O1G

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803	HFG	C2'-C39-C4'-C5'-C6'-N1'
4	A	803	HFG	C2'-C39-C4'-C5'-C6'-N1'

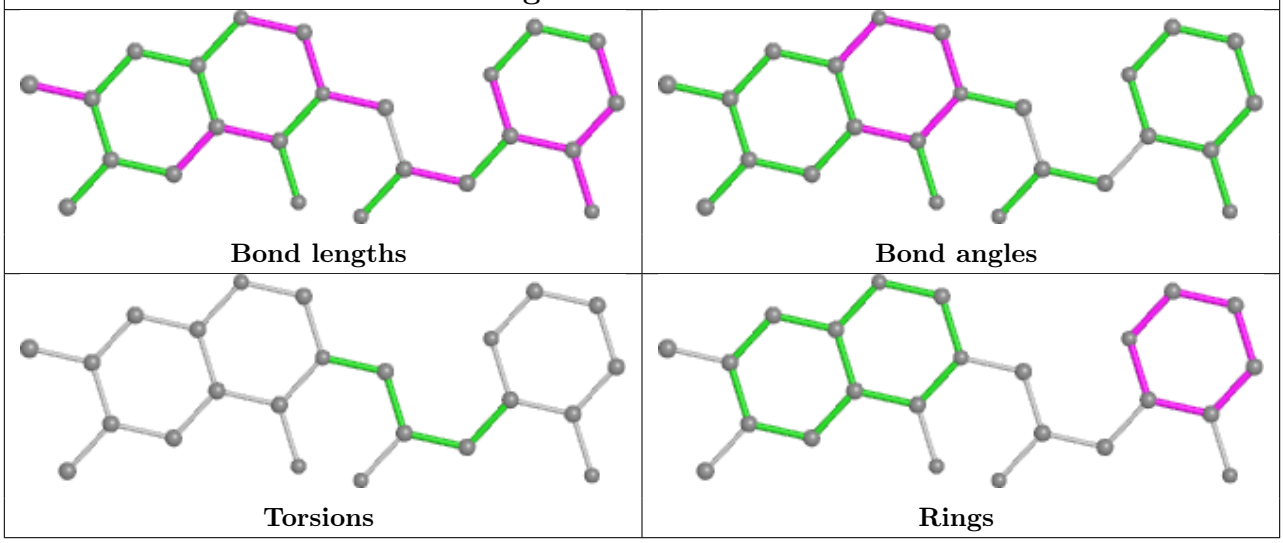
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	HFG	1	0
3	A	802	ANP	1	0
4	B	803	HFG	1	0

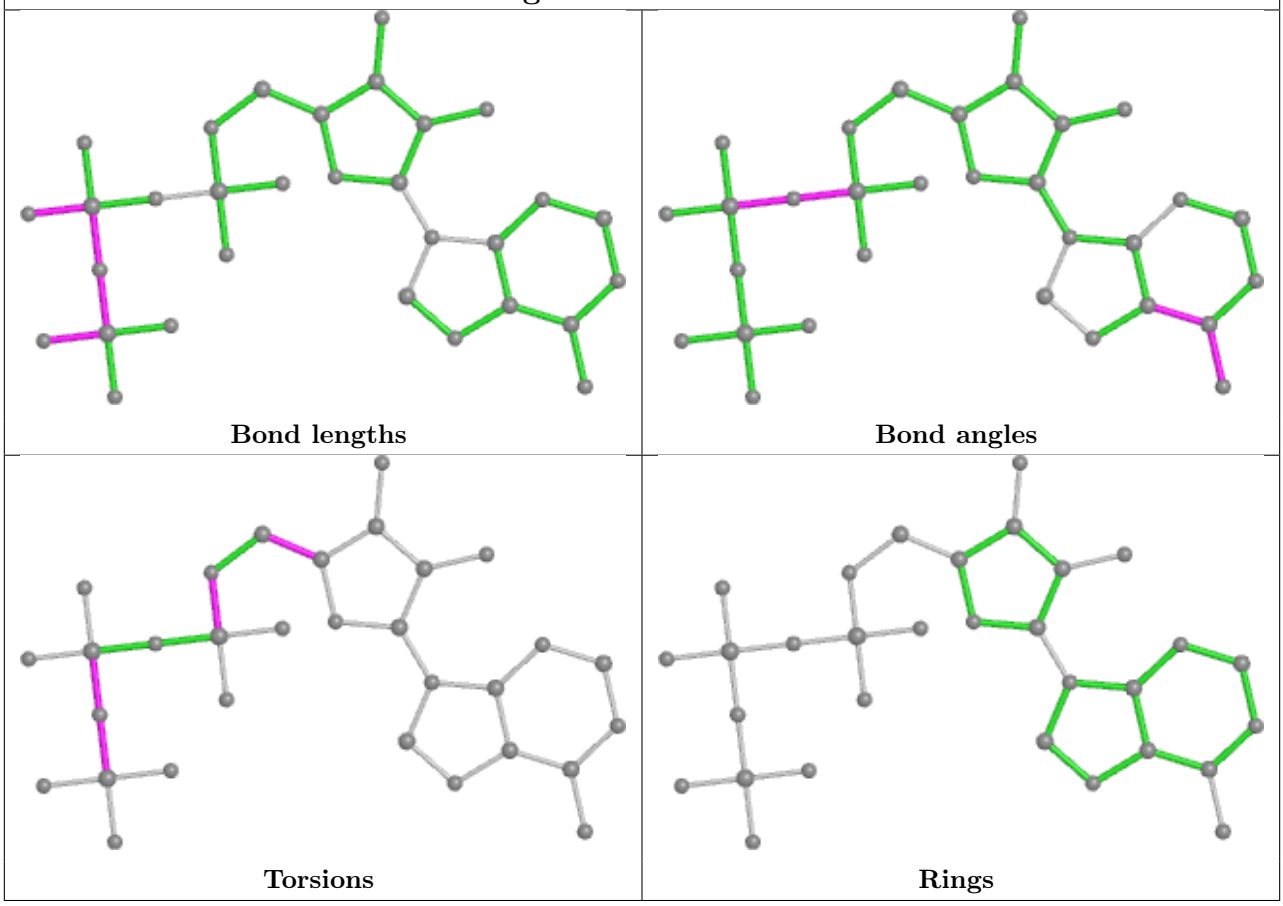
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

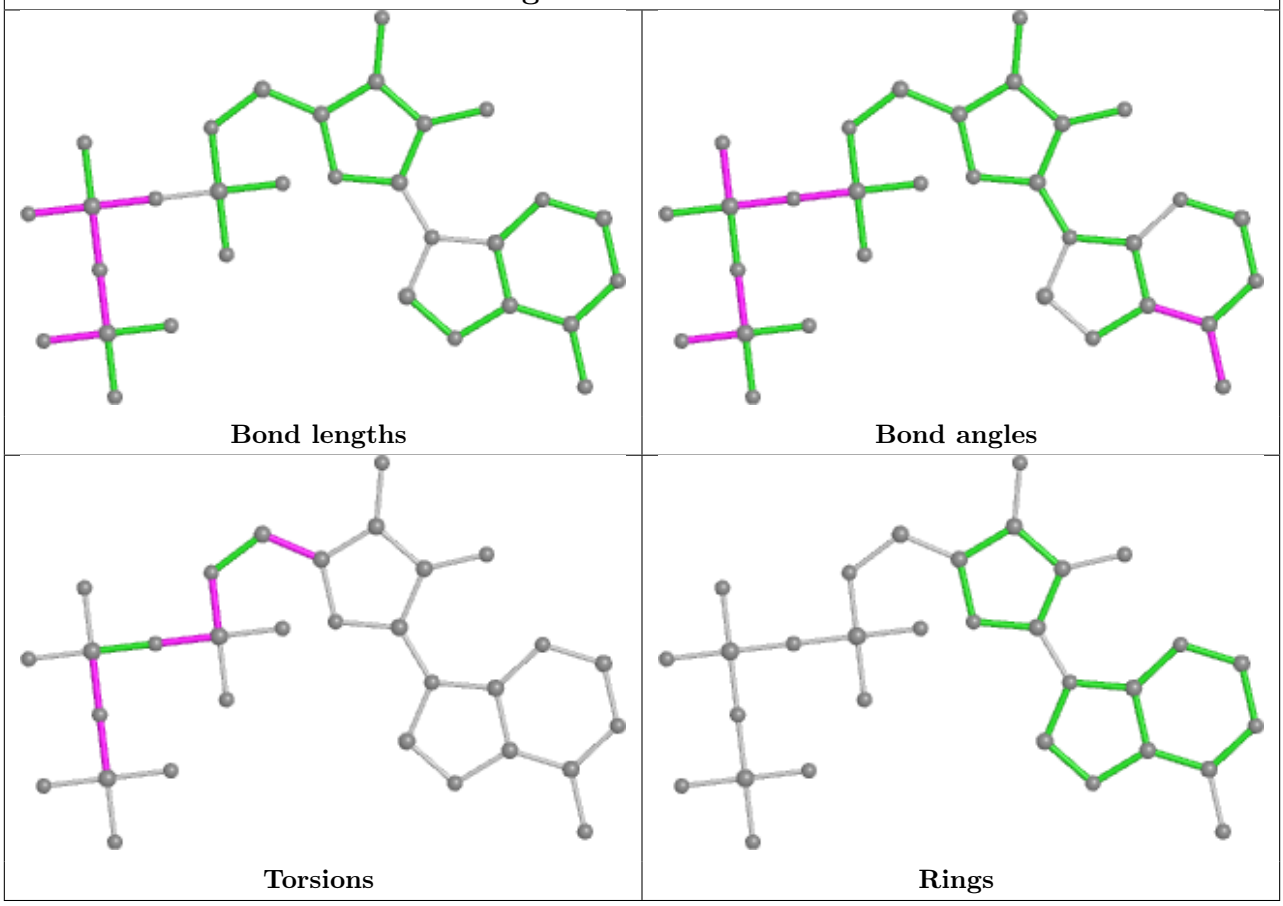
Ligand HFG A 803



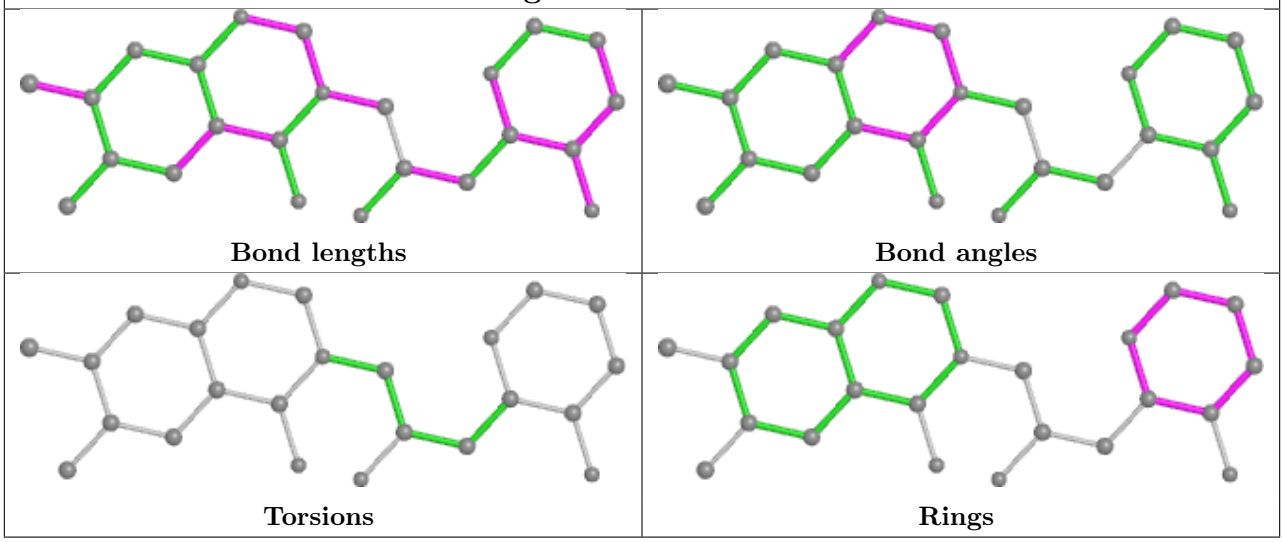
Ligand ANP B 802



Ligand ANP A 802



Ligand HFG B 803



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	460/506 (90%)	0.08	10 (2%)	62	72	27, 42, 72, 92	0
1	B	458/506 (90%)	0.14	20 (4%)	34	46	28, 42, 73, 96	0
All	All	918/1012 (90%)	0.11	30 (3%)	46	59	27, 42, 73, 96	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	PHE	5.8
1	B	733	GLY	5.2
1	B	351	PRO	4.7
1	B	663	SER	4.1
1	B	659	VAL	4.0
1	B	665	VAL	3.7
1	B	723	MET	3.4
1	B	735	PRO	3.3
1	B	662	PHE	3.2
1	B	666	MET	3.1
1	A	601	VAL	3.1
1	B	736	ALA	3.1
1	B	547	TYR	2.9
1	A	335	PHE	2.9
1	A	607	GLN	2.7
1	B	546	PHE	2.6
1	B	661	SER	2.6
1	A	624	VAL	2.6
1	B	722	PRO	2.5
1	B	731	TRP	2.5
1	B	347	ASP	2.4
1	A	498	ASN	2.3
1	A	375	TYR	2.2
1	B	580	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	732	SER	2.2
1	B	545	ILE	2.2
1	A	710	ALA	2.2
1	B	725	PRO	2.1
1	A	551	ASP	2.1
1	A	606	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

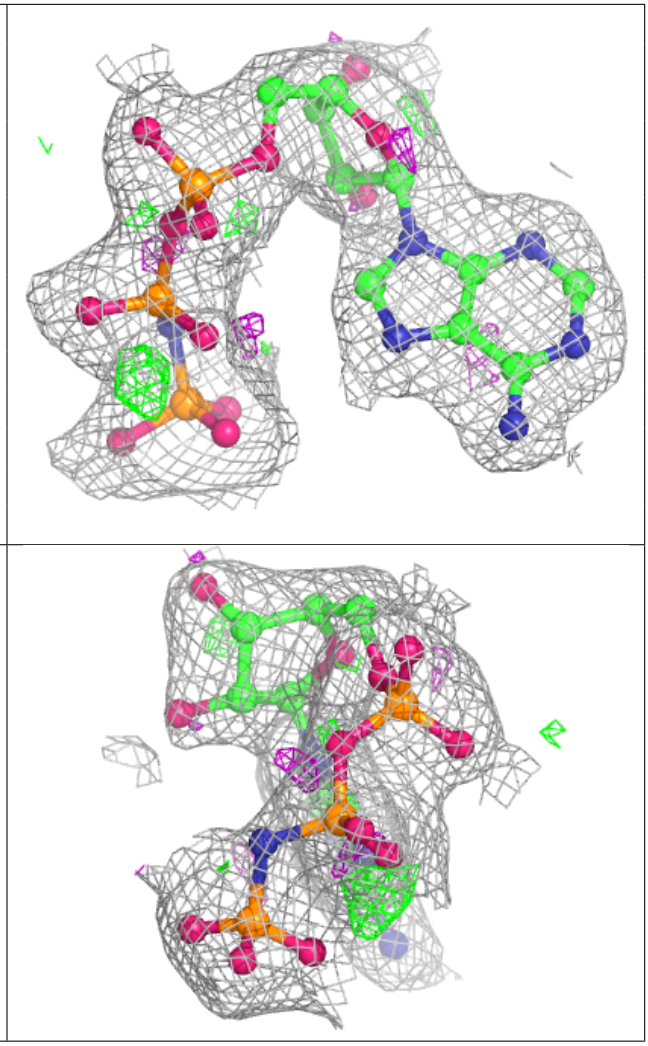
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	804	4/4	0.74	0.30	63,64,64,65	0
5	EDO	B	805	4/4	0.83	0.21	65,65,65,65	0
2	MG	B	801	1/1	0.88	0.14	38,38,38,38	0
5	EDO	B	806	4/4	0.93	0.19	49,49,49,50	0
3	ANP	A	802	31/31	0.96	0.13	29,37,44,68	0
4	HFG	A	803	24/24	0.96	0.11	32,35,36,60	0
4	HFG	B	803	24/24	0.96	0.10	29,33,36,58	0
3	ANP	B	802	31/31	0.97	0.16	31,39,48,86	0
2	MG	A	801	1/1	0.97	0.08	38,38,38,38	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.

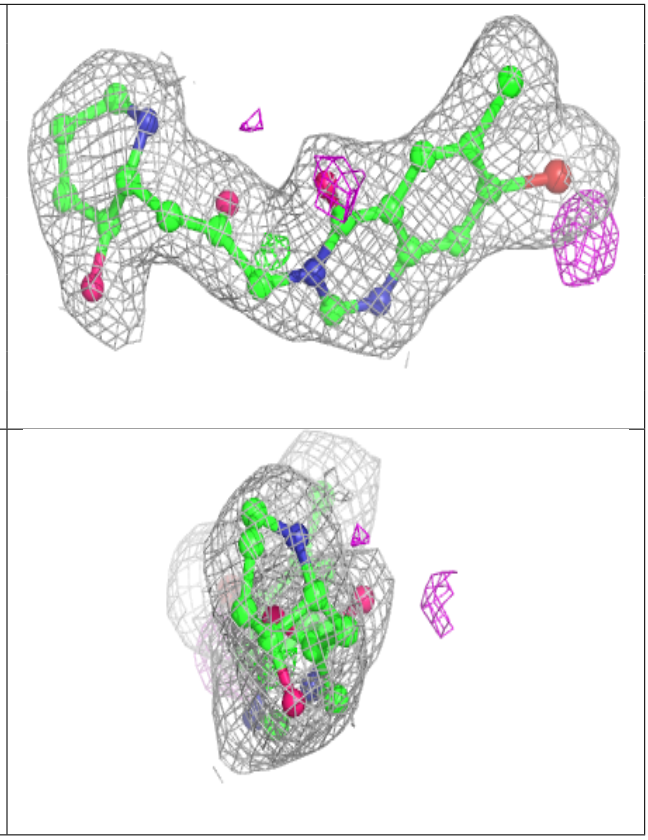
Electron density around ANP A 802:

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



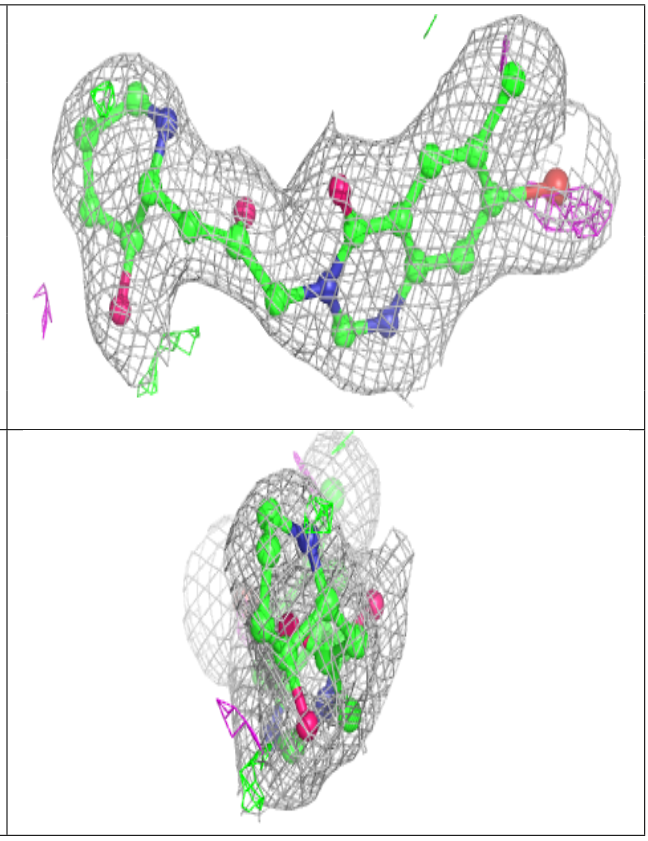
Electron density around HFG A 803:

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



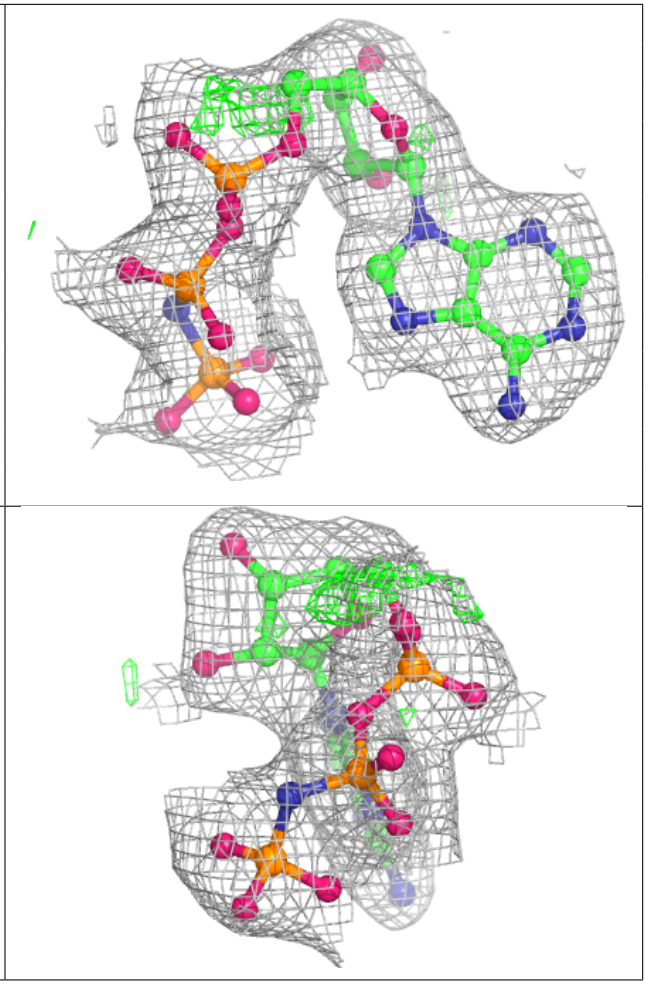
Electron density around HFG B 803:

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



Electron density around ANP B 802:

$2mF_o$-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.