



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:49 am BST

PDB ID : 6U1Y
Title : bcs1 AAA domain
Authors : Tang, W.K.; Xia, D.
Deposited on : 2019-08-17
Resolution : 2.17 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 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 : 2.11
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) : 2.11

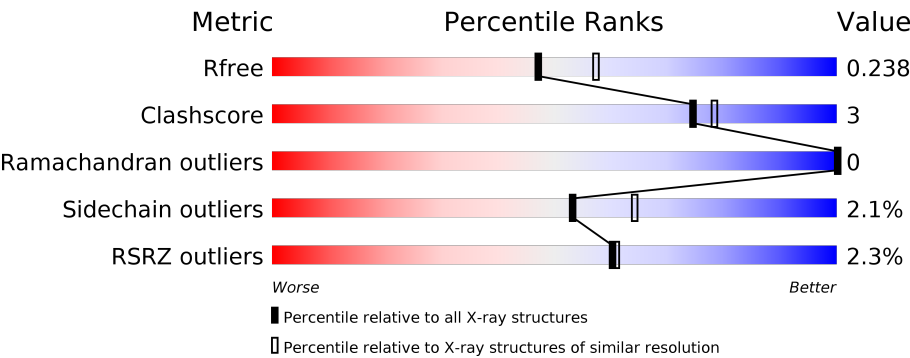
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (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 on 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	277	<div><div>%</div><div><div></div><div>80%</div><div>7%</div><div>12%</div></div></div>
1	B	277	<div><div>2%</div><div><div></div><div>80%</div><div>8%</div><div>12%</div></div></div>
1	C	277	<div><div>3%</div><div><div></div><div>78%</div><div>8%</div><div>13%</div></div></div>
1	D	277	<div><div>%</div><div><div></div><div>79%</div><div>8%</div><div>12%</div></div></div>
1	E	277	<div><div>3%</div><div><div></div><div>82%</div><div>6%</div><div>11%</div></div></div>
1	F	277	<div><div>3%</div><div><div></div><div>82%</div><div>6%</div><div>12%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	277	<div><div>%</div><div><div></div><div>82%</div><div>6%</div><div>12%</div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 29531 atoms, of which 13661 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 Mitochondrial chaperone BCS1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total	C	H	N	O	S	96	1	0
			3891	1245	1936	346	356	8			
1	B	245	Total	C	H	N	O	S	94	1	0
			3895	1246	1937	345	359	8			
1	C	242	Total	C	H	N	O	S	98	3	0
			3897	1247	1940	346	356	8			
1	D	244	Total	C	H	N	O	S	96	1	0
			3895	1246	1937	347	357	8			
1	E	246	Total	C	H	N	O	S	96	1	0
			3913	1252	1945	348	360	8			
1	F	244	Total	C	H	N	O	S	96	1	0
			3891	1245	1936	346	356	8			
1	G	244	Total	C	H	N	O	S	96	2	0
			3898	1247	1939	347	357	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	PRO	-	expression tag	UNP Q9CZP5
A	420	ARG	-	expression tag	UNP Q9CZP5
A	421	ASP	-	expression tag	UNP Q9CZP5
A	422	HIS	-	expression tag	UNP Q9CZP5
A	423	HIS	-	expression tag	UNP Q9CZP5
A	424	HIS	-	expression tag	UNP Q9CZP5
A	425	HIS	-	expression tag	UNP Q9CZP5
A	426	HIS	-	expression tag	UNP Q9CZP5
A	427	HIS	-	expression tag	UNP Q9CZP5
B	419	PRO	-	expression tag	UNP Q9CZP5
B	420	ARG	-	expression tag	UNP Q9CZP5
B	421	ASP	-	expression tag	UNP Q9CZP5
B	422	HIS	-	expression tag	UNP Q9CZP5
B	423	HIS	-	expression tag	UNP Q9CZP5
B	424	HIS	-	expression tag	UNP Q9CZP5

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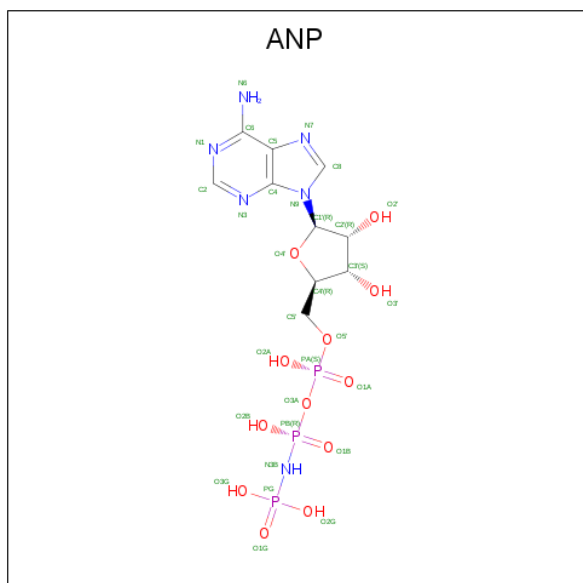
Chain	Residue	Modelled	Actual	Comment	Reference
B	425	HIS	-	expression tag	UNP Q9CZP5
B	426	HIS	-	expression tag	UNP Q9CZP5
B	427	HIS	-	expression tag	UNP Q9CZP5
C	419	PRO	-	expression tag	UNP Q9CZP5
C	420	ARG	-	expression tag	UNP Q9CZP5
C	421	ASP	-	expression tag	UNP Q9CZP5
C	422	HIS	-	expression tag	UNP Q9CZP5
C	423	HIS	-	expression tag	UNP Q9CZP5
C	424	HIS	-	expression tag	UNP Q9CZP5
C	425	HIS	-	expression tag	UNP Q9CZP5
C	426	HIS	-	expression tag	UNP Q9CZP5
C	427	HIS	-	expression tag	UNP Q9CZP5
D	419	PRO	-	expression tag	UNP Q9CZP5
D	420	ARG	-	expression tag	UNP Q9CZP5
D	421	ASP	-	expression tag	UNP Q9CZP5
D	422	HIS	-	expression tag	UNP Q9CZP5
D	423	HIS	-	expression tag	UNP Q9CZP5
D	424	HIS	-	expression tag	UNP Q9CZP5
D	425	HIS	-	expression tag	UNP Q9CZP5
D	426	HIS	-	expression tag	UNP Q9CZP5
D	427	HIS	-	expression tag	UNP Q9CZP5
E	419	PRO	-	expression tag	UNP Q9CZP5
E	420	ARG	-	expression tag	UNP Q9CZP5
E	421	ASP	-	expression tag	UNP Q9CZP5
E	422	HIS	-	expression tag	UNP Q9CZP5
E	423	HIS	-	expression tag	UNP Q9CZP5
E	424	HIS	-	expression tag	UNP Q9CZP5
E	425	HIS	-	expression tag	UNP Q9CZP5
E	426	HIS	-	expression tag	UNP Q9CZP5
E	427	HIS	-	expression tag	UNP Q9CZP5
F	419	PRO	-	expression tag	UNP Q9CZP5
F	420	ARG	-	expression tag	UNP Q9CZP5
F	421	ASP	-	expression tag	UNP Q9CZP5
F	422	HIS	-	expression tag	UNP Q9CZP5
F	423	HIS	-	expression tag	UNP Q9CZP5
F	424	HIS	-	expression tag	UNP Q9CZP5
F	425	HIS	-	expression tag	UNP Q9CZP5
F	426	HIS	-	expression tag	UNP Q9CZP5
F	427	HIS	-	expression tag	UNP Q9CZP5
G	419	PRO	-	expression tag	UNP Q9CZP5
G	420	ARG	-	expression tag	UNP Q9CZP5
G	421	ASP	-	expression tag	UNP Q9CZP5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	422	HIS	-	expression tag	UNP Q9CZP5
G	423	HIS	-	expression tag	UNP Q9CZP5
G	424	HIS	-	expression tag	UNP Q9CZP5
G	425	HIS	-	expression tag	UNP Q9CZP5
G	426	HIS	-	expression tag	UNP Q9CZP5
G	427	HIS	-	expression tag	UNP Q9CZP5

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	4	0
			44	10	13	6	12	3		
2	B	1	Total	C	H	N	O	P	4	0
			44	10	13	6	12	3		
2	C	1	Total	C	H	N	O	P	4	0
			44	10	13	6	12	3		
2	D	1	Total	C	H	N	O	P	4	0
			44	10	13	6	12	3		
2	E	1	Total	C	H	N	O	P	4	0
			44	10	13	6	12	3		
2	F	1	Total	C	H	N	O	P	4	0
			44	10	13	6	12	3		
2	G	1	Total	C	H	N	O	P	4	0
			44	10	13	6	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

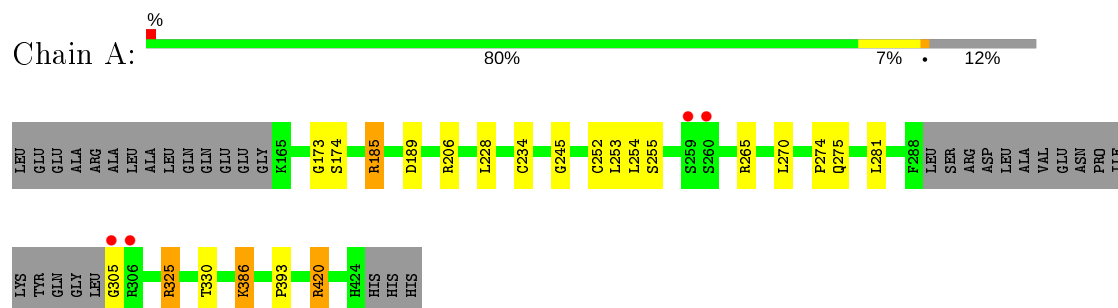
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	319	Total O 319 319	0	0
4	B	273	Total O 273 273	0	0
4	C	287	Total O 287 287	0	0
4	D	263	Total O 263 263	0	0
4	E	247	Total O 247 247	0	0
4	F	264	Total O 264 264	0	0
4	G	283	Total O 283 283	0	0

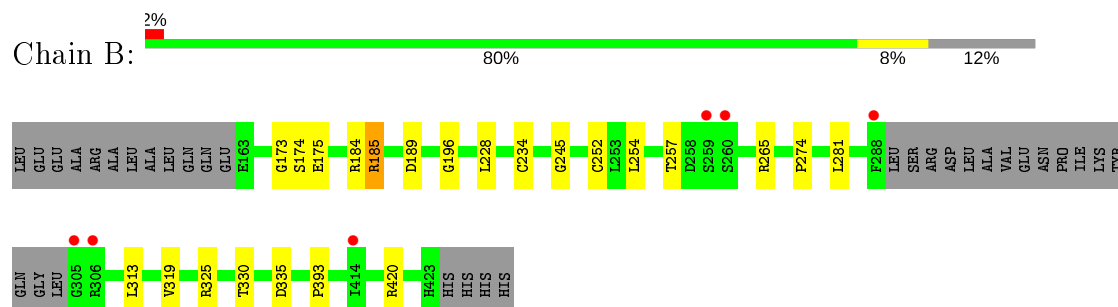
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

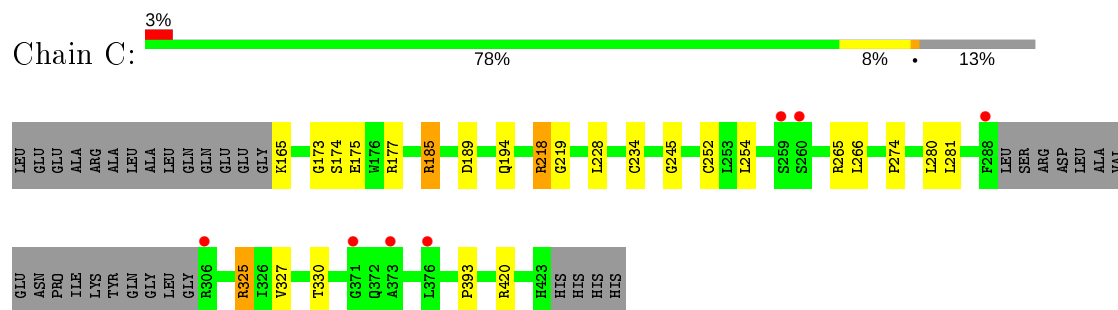
- Molecule 1: Mitochondrial chaperone BCS1



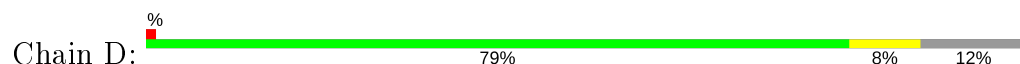
- Molecule 1: Mitochondrial chaperone BCS1



- Molecule 1: Mitochondrial chaperone BCS1

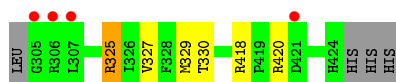
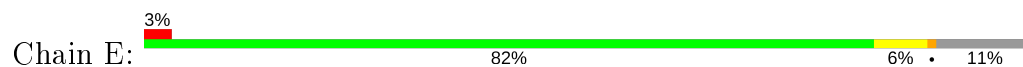


- Molecule 1: Mitochondrial chaperone BCS1

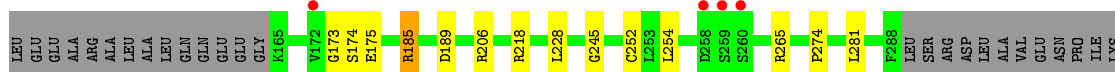
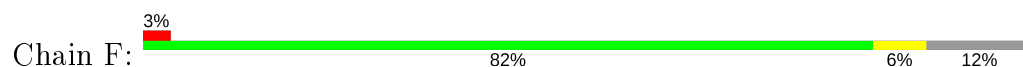




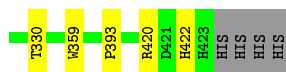
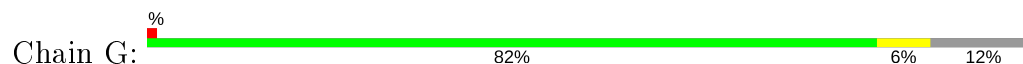
• Molecule 1: Mitochondrial chaperone BCS1



• Molecule 1: Mitochondrial chaperone BCS1



• Molecule 1: Mitochondrial chaperone BCS1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.21Å 207.25Å 116.61Å 90.00° 95.98° 90.00°	Depositor
Resolution (Å)	44.46 – 2.17 44.42 – 2.17	Depositor EDS
% Data completeness (in resolution range)	86.9 (44.46-2.17) 86.9 (44.42-2.17)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.181 , 0.235 0.187 , 0.238	Depositor DCC
R_{free} test set	4596 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29531	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 4.55% 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: MG, 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	0.69	0/2007	0.82	1/2723 (0.0%)
1	B	0.67	0/2009	0.81	2/2725 (0.1%)
1	C	0.67	0/2012	0.80	2/2730 (0.1%)
1	D	0.69	0/2007	0.83	2/2723 (0.1%)
1	E	0.69	0/2020	0.81	2/2740 (0.1%)
1	F	0.68	0/2007	0.80	0/2723
1	G	0.68	0/2011	0.81	0/2728
All	All	0.68	0/14073	0.81	9/19092 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	D	325	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	E	325	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	325	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	325	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	E	325	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	C	325	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	A	325	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	C	325	ARG	NE-CZ-NH2	5.59	123.09	120.30

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	1955	1936	1925	16	0
1	B	1958	1937	1927	13	0
1	C	1957	1940	1930	16	0
1	D	1958	1937	1924	16	0
1	E	1968	1945	1935	10	0
1	F	1955	1936	1925	11	0
1	G	1959	1939	1927	9	0
2	A	31	13	13	1	0
2	B	31	13	13	0	0
2	C	31	13	13	0	0
2	D	31	13	13	0	0
2	E	31	13	13	0	0
2	F	31	13	13	0	0
2	G	31	13	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	319	0	0	8	0
4	B	273	0	0	5	0
4	C	287	0	0	9	0
4	D	263	0	0	8	0
4	E	247	0	0	4	0
4	F	264	0	0	3	0
4	G	283	0	0	4	0
All	All	15870	13661	13584	89	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 (89) 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:C:165:LYS:N	4:C:901:HOH:O	1.77	1.17
1:E:217:ASP:OD1	4:E:901:HOH:O	2.03	0.76
1:B:257:THR:OG1	4:B:901:HOH:O	2.05	0.72
1:G:359:TRP:HZ3	4:G:960:HOH:O	1.75	0.69
1:E:418:ARG:NH2	4:E:904:HOH:O	2.25	0.67
1:D:325:ARG:HD2	4:D:1025:HOH:O	1.94	0.66
1:B:313:LEU:HD12	4:C:1043:HOH:O	1.95	0.66
1:A:325:ARG:HD2	4:A:1031:HOH:O	1.96	0.66
1:A:305:GLY:N	1:D:259:SER:HB2	2.16	0.60
1:B:184:ARG:NH1	4:B:902:HOH:O	2.24	0.60
1:D:288:PHE:HA	4:D:974:HOH:O	2.02	0.59
1:B:175:GLU:HG2	4:B:977:HOH:O	2.04	0.57
1:D:218:ARG:NH1	4:D:904:HOH:O	2.37	0.57
1:C:219:GLY:HA2	4:C:1117:HOH:O	2.03	0.57
1:E:267:ASN:OD1	4:E:902:HOH:O	2.17	0.57
4:A:906:HOH:O	1:D:184:ARG:NH2	2.39	0.55
1:B:335:ASP:HB2	4:B:989:HOH:O	2.06	0.55
4:D:909:HOH:O	1:F:422:HIS:HD2	1.89	0.55
1:E:173:GLY:O	1:E:265:ARG:HD3	2.07	0.55
1:G:173:GLY:O	1:G:265:ARG:HD3	2.07	0.55
1:F:175:GLU:OE1	4:F:901:HOH:O	2.18	0.55
1:A:173:GLY:O	1:A:265:ARG:HD3	2.08	0.54
1:C:173:GLY:O	1:C:265:ARG:HD3	2.08	0.54
1:F:173:GLY:O	1:F:265:ARG:HD3	2.08	0.54
1:B:173:GLY:O	1:B:265:ARG:HD3	2.09	0.53
1:D:359:TRP:HZ3	4:D:923:HOH:O	1.90	0.53
1:D:173:GLY:O	1:D:265:ARG:HD3	2.09	0.52
4:D:909:HOH:O	1:F:422:HIS:CD2	2.64	0.51
1:A:386:LYS:NZ	4:A:910:HOH:O	2.42	0.50
1:A:206:ARG:NH1	4:A:912:HOH:O	2.43	0.50
1:A:270:LEU:O	4:A:901:HOH:O	2.19	0.50
1:A:420:ARG:HD3	4:A:1096:HOH:O	2.12	0.49
1:C:194[B]:GLN:HG3	4:C:933:HOH:O	2.13	0.49
1:F:218:ARG:NH1	4:F:912:HOH:O	2.46	0.48
1:C:325:ARG:HD3	1:C:327:VAL:HG23	1.96	0.47
1:E:228:LEU:O	1:E:330:THR:HA	2.15	0.47
1:E:252:CYS:SG	1:E:274:PRO:HD2	2.55	0.47
1:A:305:GLY:N	1:D:259:SER:CB	2.77	0.47
1:G:252:CYS:SG	1:G:274:PRO:HD2	2.54	0.47
1:B:252:CYS:SG	1:B:274:PRO:HD2	2.55	0.47
1:A:252:CYS:SG	1:A:274:PRO:HD2	2.55	0.47
1:D:228:LEU:O	1:D:330:THR:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:CYS:SG	1:C:274:PRO:HD2	2.55	0.46
1:F:206:ARG:NE	4:F:909:HOH:O	2.45	0.46
1:A:228:LEU:O	1:A:330:THR:HA	2.15	0.46
1:C:228:LEU:O	1:C:330:THR:HA	2.16	0.46
1:B:254:LEU:HD23	1:B:281:LEU:HD21	1.98	0.46
1:B:228:LEU:O	1:B:330:THR:HA	2.16	0.45
1:G:228:LEU:O	1:G:330:THR:HA	2.16	0.45
1:F:252:CYS:SG	1:F:274:PRO:HD2	2.56	0.45
1:D:325:ARG:HD3	1:D:327:VAL:HG23	1.99	0.45
1:G:206:ARG:HD3	4:G:1044:HOH:O	2.16	0.45
1:F:228:LEU:O	1:F:330:THR:HA	2.16	0.45
1:D:252:CYS:SG	1:D:274:PRO:HD2	2.56	0.45
1:A:254:LEU:HD23	1:A:281:LEU:HD21	1.98	0.44
1:D:200:ARG:HD2	4:D:912:HOH:O	2.16	0.44
1:E:325:ARG:HD3	1:E:327:VAL:HG23	1.99	0.44
4:C:903:HOH:O	1:G:422:HIS:HB2	2.18	0.44
1:A:275:GLN:HG2	4:A:1137:HOH:O	2.18	0.44
1:G:175:GLU:HG3	4:G:1054:HOH:O	2.16	0.44
1:F:185:ARG:HD2	1:F:245:GLY:CA	2.48	0.43
1:D:424:HIS:CD2	4:D:1034:HOH:O	2.70	0.43
1:A:255:SER:OG	4:A:902:HOH:O	2.21	0.43
1:C:177:ARG:HD2	4:C:924:HOH:O	2.17	0.43
1:E:185:ARG:HD2	1:E:245:GLY:CA	2.48	0.43
1:B:196:GLY:C	4:B:936:HOH:O	2.57	0.43
1:C:254:LEU:HD23	1:C:281:LEU:HD21	2.01	0.42
1:F:254:LEU:HD23	1:F:281:LEU:HD21	2.00	0.42
1:B:234:CYS:HA	1:B:393:PRO:HD2	2.01	0.42
1:D:188:LEU:HA	1:D:188:LEU:HD12	1.93	0.42
1:C:185:ARG:HD2	1:C:245:GLY:CA	2.49	0.42
1:D:254:LEU:HD23	1:D:281:LEU:HD21	2.01	0.42
1:F:423:HIS:O	1:F:423:HIS:CD2	2.73	0.41
1:A:234:CYS:HA	1:A:393:PRO:HD2	2.01	0.41
1:C:254:LEU:HD21	1:C:266:LEU:CD1	2.50	0.41
1:B:185:ARG:HD2	1:B:245:GLY:CA	2.50	0.41
1:C:234:CYS:HA	1:C:393:PRO:HD2	2.02	0.41
1:A:185:ARG:HD2	1:A:245:GLY:CA	2.51	0.41
1:C:175:GLU:HG2	4:C:947:HOH:O	2.20	0.41
1:D:234:CYS:HA	1:D:393:PRO:HD2	2.02	0.41
1:G:188:LEU:HA	1:G:188:LEU:HD12	1.93	0.41
1:B:319:VAL:HG21	1:C:280:LEU:CD2	2.50	0.41
1:C:325:ARG:HD2	4:C:976:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD12	4:G:1122:HOH:O	2.21	0.41
1:E:254:LEU:HD23	1:E:281:LEU:HD21	2.02	0.40
2:A:800:ANP:O5'	2:A:800:ANP:H8	2.22	0.40
1:C:218:ARG:NH1	4:C:919:HOH:O	2.54	0.40
1:E:329:MET:SD	4:E:1140:HOH:O	2.61	0.40
1:G:234:CYS:HA	1:G:393:PRO:HD2	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	241/277 (87%)	237 (98%)	4 (2%)	0	100	100
1	B	242/277 (87%)	240 (99%)	2 (1%)	0	100	100
1	C	241/277 (87%)	238 (99%)	3 (1%)	0	100	100
1	D	241/277 (87%)	239 (99%)	2 (1%)	0	100	100
1	E	243/277 (88%)	240 (99%)	3 (1%)	0	100	100
1	F	241/277 (87%)	236 (98%)	5 (2%)	0	100	100
1	G	242/277 (87%)	239 (99%)	3 (1%)	0	100	100
All	All	1691/1939 (87%)	1669 (99%)	22 (1%)	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	211/237 (89%)	206 (98%)	5 (2%)	49	59
1	B	211/237 (89%)	207 (98%)	4 (2%)	57	68
1	C	212/237 (90%)	207 (98%)	5 (2%)	49	59
1	D	211/237 (89%)	207 (98%)	4 (2%)	57	68
1	E	212/237 (90%)	208 (98%)	4 (2%)	57	68
1	F	211/237 (89%)	207 (98%)	4 (2%)	57	68
1	G	211/237 (89%)	206 (98%)	5 (2%)	49	59
All	All	1479/1659 (89%)	1448 (98%)	31 (2%)	53	64

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	SER
1	A	185	ARG
1	A	189	ASP
1	A	386	LYS
1	A	420	ARG
1	B	174	SER
1	B	185	ARG
1	B	189	ASP
1	B	420	ARG
1	C	174	SER
1	C	185	ARG
1	C	189	ASP
1	C	218	ARG
1	C	420	ARG
1	D	174	SER
1	D	185	ARG
1	D	189	ASP
1	D	420	ARG
1	E	174	SER
1	E	185	ARG
1	E	189	ASP
1	E	420	ARG
1	F	174	SER
1	F	185	ARG
1	F	189	ASP
1	F	420	ARG

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Mol	Chain	Res	Type
1	G	174	SER
1	G	185	ARG
1	G	189	ASP
1	G	218	ARG
1	G	420	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	B	195	GLN
1	C	195	GLN
1	D	195	GLN
1	E	195	GLN
1	F	405	ASN
1	F	423	HIS
1	G	195	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 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	$\# Z > 2$
2	ANP	E	800	3	29,33,33	1.40	4 (13%)	31,52,52	1.52	4 (12%)
2	ANP	C	800	3	29,33,33	1.39	5 (17%)	31,52,52	1.33	3 (9%)
2	ANP	G	800	3	29,33,33	1.11	2 (6%)	31,52,52	1.40	5 (16%)
2	ANP	A	800	3	29,33,33	1.21	2 (6%)	31,52,52	1.73	7 (22%)
2	ANP	B	800	3	29,33,33	1.14	4 (13%)	31,52,52	1.49	4 (12%)
2	ANP	F	800	3	29,33,33	1.42	5 (17%)	31,52,52	1.49	4 (12%)
2	ANP	D	800	3	29,33,33	1.20	5 (17%)	31,52,52	1.49	3 (9%)

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	ANP	E	800	3	-	4/14/38/38	0/3/3/3
2	ANP	C	800	3	-	4/14/38/38	0/3/3/3
2	ANP	G	800	3	-	4/14/38/38	0/3/3/3
2	ANP	A	800	3	-	4/14/38/38	0/3/3/3
2	ANP	B	800	3	-	4/14/38/38	0/3/3/3
2	ANP	F	800	3	-	4/14/38/38	0/3/3/3
2	ANP	D	800	3	-	4/14/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	ANP	PG-O1G	3.97	1.52	1.46
2	A	800	ANP	PB-O3A	3.96	1.64	1.59
2	F	800	ANP	PG-O1G	3.78	1.52	1.46
2	E	800	ANP	PB-O1B	3.59	1.51	1.46
2	C	800	ANP	PB-O3A	3.39	1.63	1.59
2	G	800	ANP	PB-O1B	3.39	1.51	1.46
2	C	800	ANP	PB-O1B	3.37	1.51	1.46
2	D	800	ANP	PG-O1G	3.11	1.51	1.46
2	F	800	ANP	PB-O3A	3.10	1.63	1.59
2	C	800	ANP	PG-O1G	2.85	1.50	1.46
2	E	800	ANP	PB-O3A	2.79	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	ANP	PG-O2G	-2.78	1.49	1.56
2	F	800	ANP	PB-O1B	2.71	1.50	1.46
2	E	800	ANP	PB-O2B	-2.68	1.49	1.56
2	F	800	ANP	PG-O3G	-2.64	1.49	1.56
2	D	800	ANP	PG-O3G	-2.63	1.49	1.56
2	B	800	ANP	PB-O3A	2.53	1.62	1.59
2	B	800	ANP	PG-O1G	2.51	1.50	1.46
2	F	800	ANP	PB-O2B	-2.51	1.50	1.56
2	G	800	ANP	PB-O2B	-2.48	1.50	1.56
2	D	800	ANP	PB-O2B	-2.43	1.50	1.56
2	A	800	ANP	PB-O1B	2.33	1.49	1.46
2	D	800	ANP	PB-O1B	2.33	1.49	1.46
2	B	800	ANP	PB-O1B	2.27	1.49	1.46
2	B	800	ANP	PB-O2B	-2.23	1.50	1.56
2	C	800	ANP	PG-O3G	-2.16	1.50	1.56
2	D	800	ANP	C8-N7	-2.02	1.31	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	ANP	O2B-PB-O1B	5.11	120.63	109.92
2	B	800	ANP	O2B-PB-O1B	4.96	120.32	109.92
2	D	800	ANP	O2B-PB-O1B	4.96	120.32	109.92
2	E	800	ANP	O1G-PG-N3B	-4.93	104.51	111.77
2	E	800	ANP	O2B-PB-O1B	4.13	118.59	109.92
2	A	800	ANP	O2G-PG-O1G	-4.12	103.10	113.45
2	C	800	ANP	O2B-PB-O1B	4.08	118.48	109.92
2	D	800	ANP	O3A-PB-N3B	-3.62	96.54	106.59
2	G	800	ANP	O3A-PB-N3B	-3.62	96.55	106.59
2	F	800	ANP	O1B-PB-N3B	3.57	117.03	111.77
2	B	800	ANP	O1G-PG-N3B	-3.50	106.61	111.77
2	F	800	ANP	O2B-PB-O1B	3.37	116.98	109.92
2	C	800	ANP	O2G-PG-O1G	-3.30	105.16	113.45
2	G	800	ANP	O2B-PB-O1B	3.30	116.84	109.92
2	F	800	ANP	O3A-PB-N3B	-3.18	97.78	106.59
2	A	800	ANP	O1B-PB-N3B	-3.08	107.24	111.77
2	F	800	ANP	O3G-PG-O2G	2.97	115.54	107.64
2	G	800	ANP	O3G-PG-O2G	2.80	115.10	107.64
2	A	800	ANP	O3G-PG-O1G	-2.79	106.43	113.45
2	G	800	ANP	O3G-PG-O1G	-2.68	106.70	113.45
2	D	800	ANP	C5-C6-N6	2.52	124.17	120.35
2	E	800	ANP	C3'-C2'-C1'	2.50	104.74	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	ANP	C3'-C2'-C1'	2.48	104.71	100.98
2	A	800	ANP	C5-C6-N6	2.41	124.02	120.35
2	E	800	ANP	C5-C6-N6	2.36	123.93	120.35
2	B	800	ANP	C5-C6-N6	2.29	123.83	120.35
2	G	800	ANP	C5-C6-N6	2.19	123.68	120.35
2	A	800	ANP	C3'-C2'-C1'	2.11	104.16	100.98
2	B	800	ANP	C3'-C2'-C1'	2.10	104.14	100.98
2	A	800	ANP	C5-C6-N1	-2.03	115.75	120.35

There are no chirality outliers.

All (28) torsion outliers are listed below:

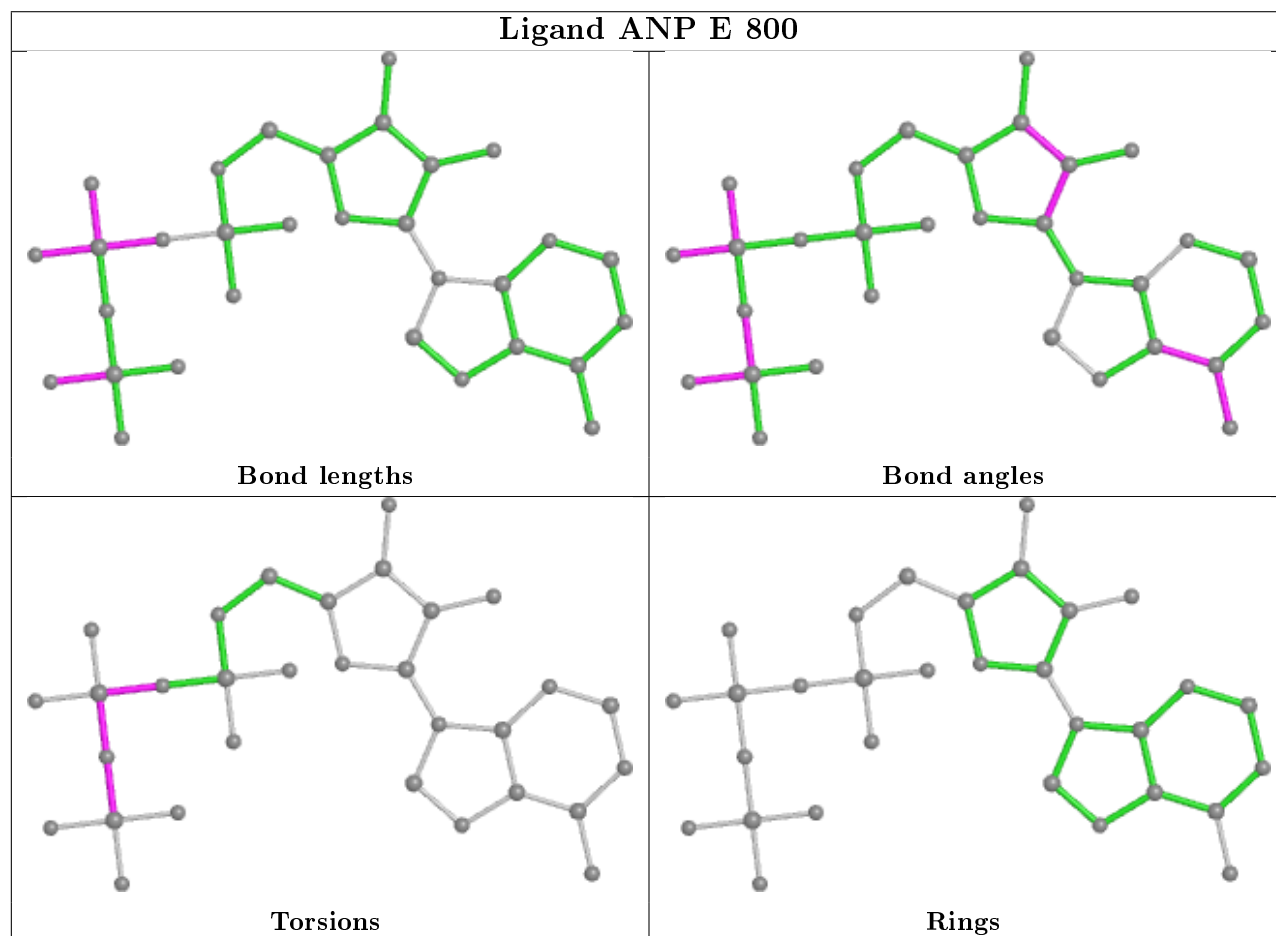
Mol	Chain	Res	Type	Atoms
2	E	800	ANP	PB-N3B-PG-O1G
2	E	800	ANP	PG-N3B-PB-O1B
2	E	800	ANP	PA-O3A-PB-O1B
2	E	800	ANP	PA-O3A-PB-O2B
2	C	800	ANP	PB-N3B-PG-O1G
2	C	800	ANP	PG-N3B-PB-O1B
2	C	800	ANP	PA-O3A-PB-O1B
2	C	800	ANP	PA-O3A-PB-O2B
2	G	800	ANP	PB-N3B-PG-O1G
2	G	800	ANP	PG-N3B-PB-O1B
2	G	800	ANP	PA-O3A-PB-O1B
2	G	800	ANP	PA-O3A-PB-O2B
2	A	800	ANP	PB-N3B-PG-O1G
2	A	800	ANP	PG-N3B-PB-O1B
2	A	800	ANP	PA-O3A-PB-O1B
2	A	800	ANP	PA-O3A-PB-O2B
2	B	800	ANP	PB-N3B-PG-O1G
2	B	800	ANP	PG-N3B-PB-O1B
2	B	800	ANP	PA-O3A-PB-O1B
2	B	800	ANP	PA-O3A-PB-O2B
2	F	800	ANP	PB-N3B-PG-O1G
2	F	800	ANP	PG-N3B-PB-O1B
2	F	800	ANP	PA-O3A-PB-O1B
2	F	800	ANP	PA-O3A-PB-O2B
2	D	800	ANP	PB-N3B-PG-O1G
2	D	800	ANP	PG-N3B-PB-O1B
2	D	800	ANP	PA-O3A-PB-O1B
2	D	800	ANP	PA-O3A-PB-O2B

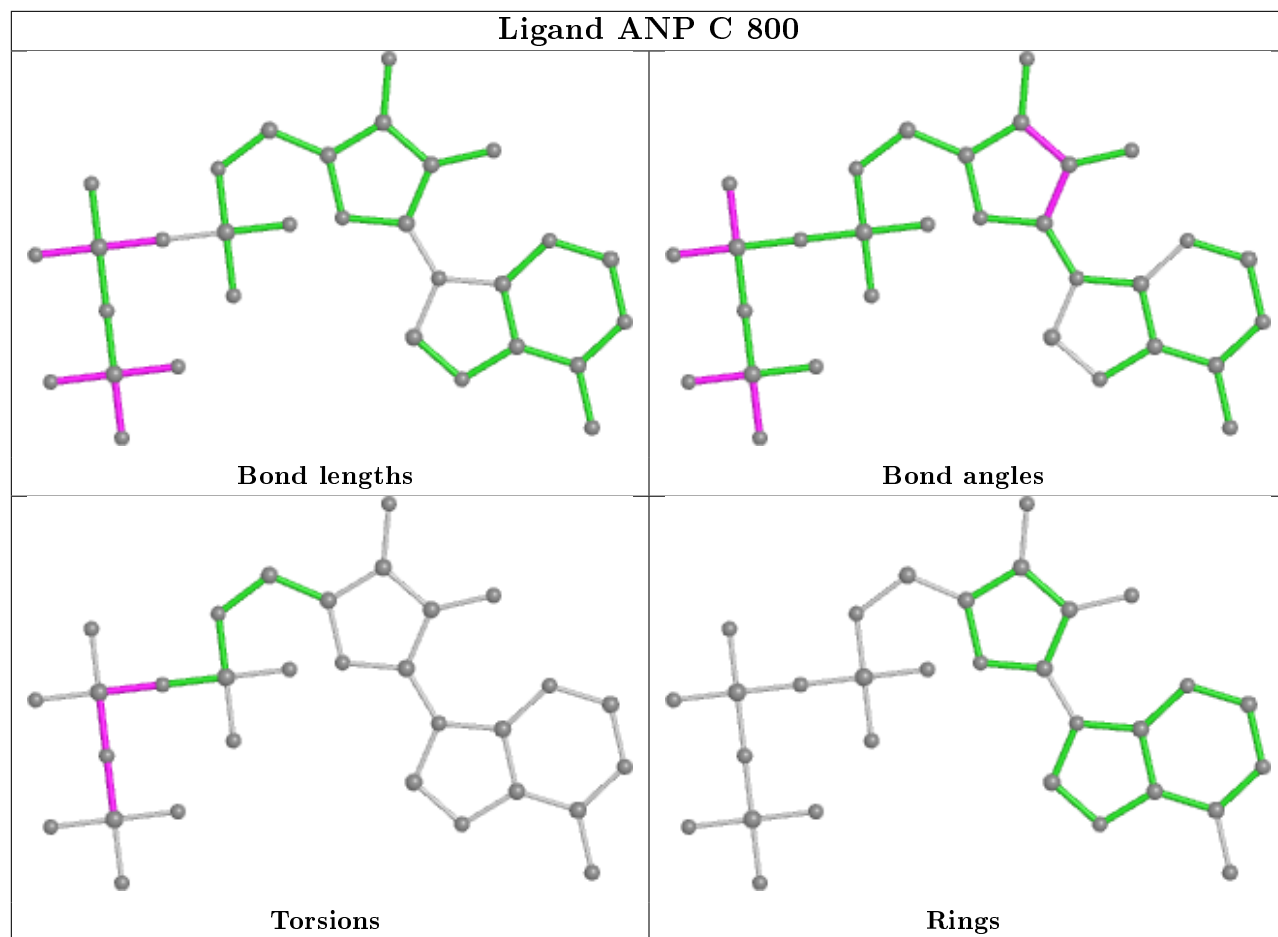
There are no ring outliers.

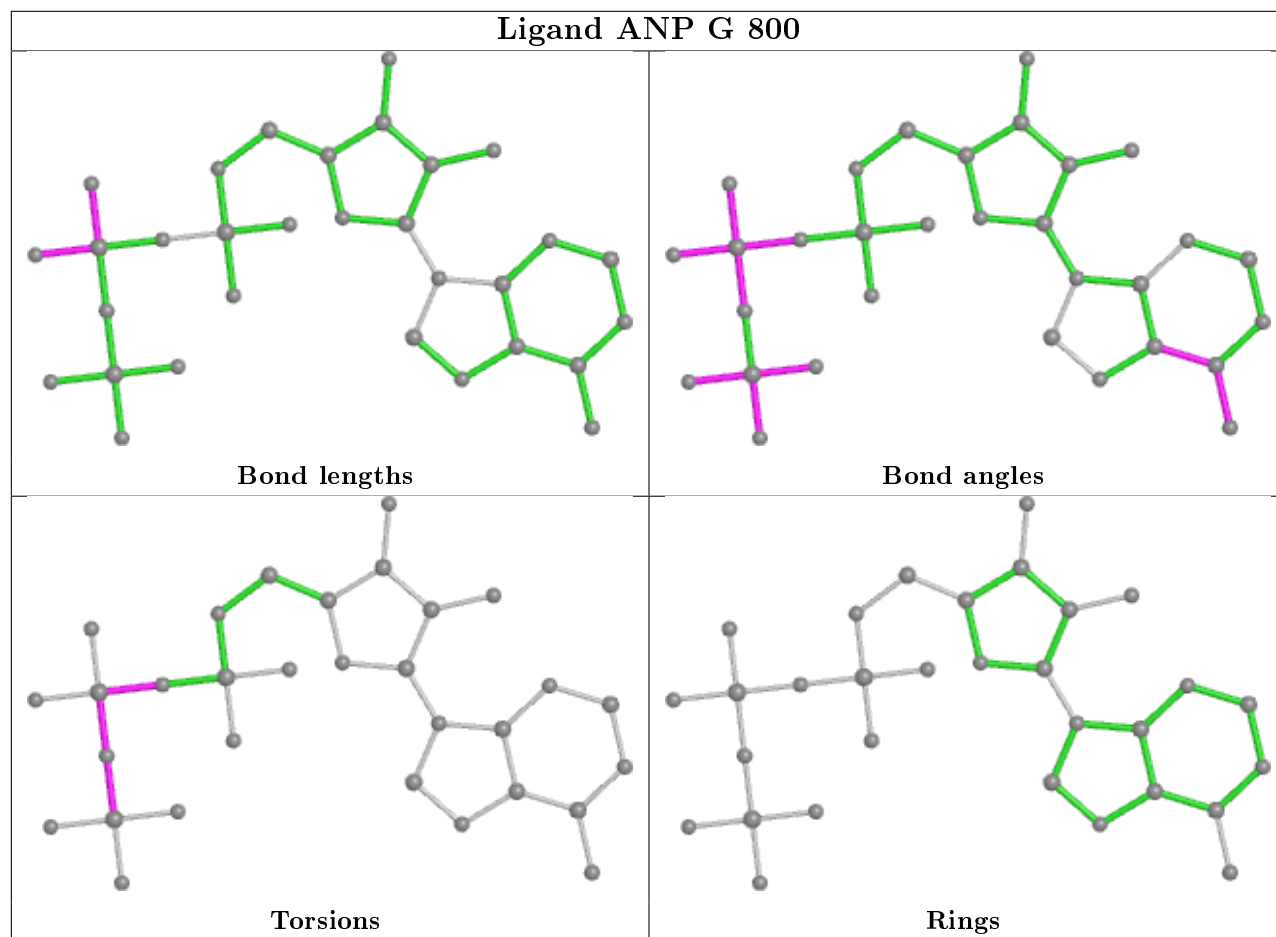
1 monomer is involved in 1 short contact:

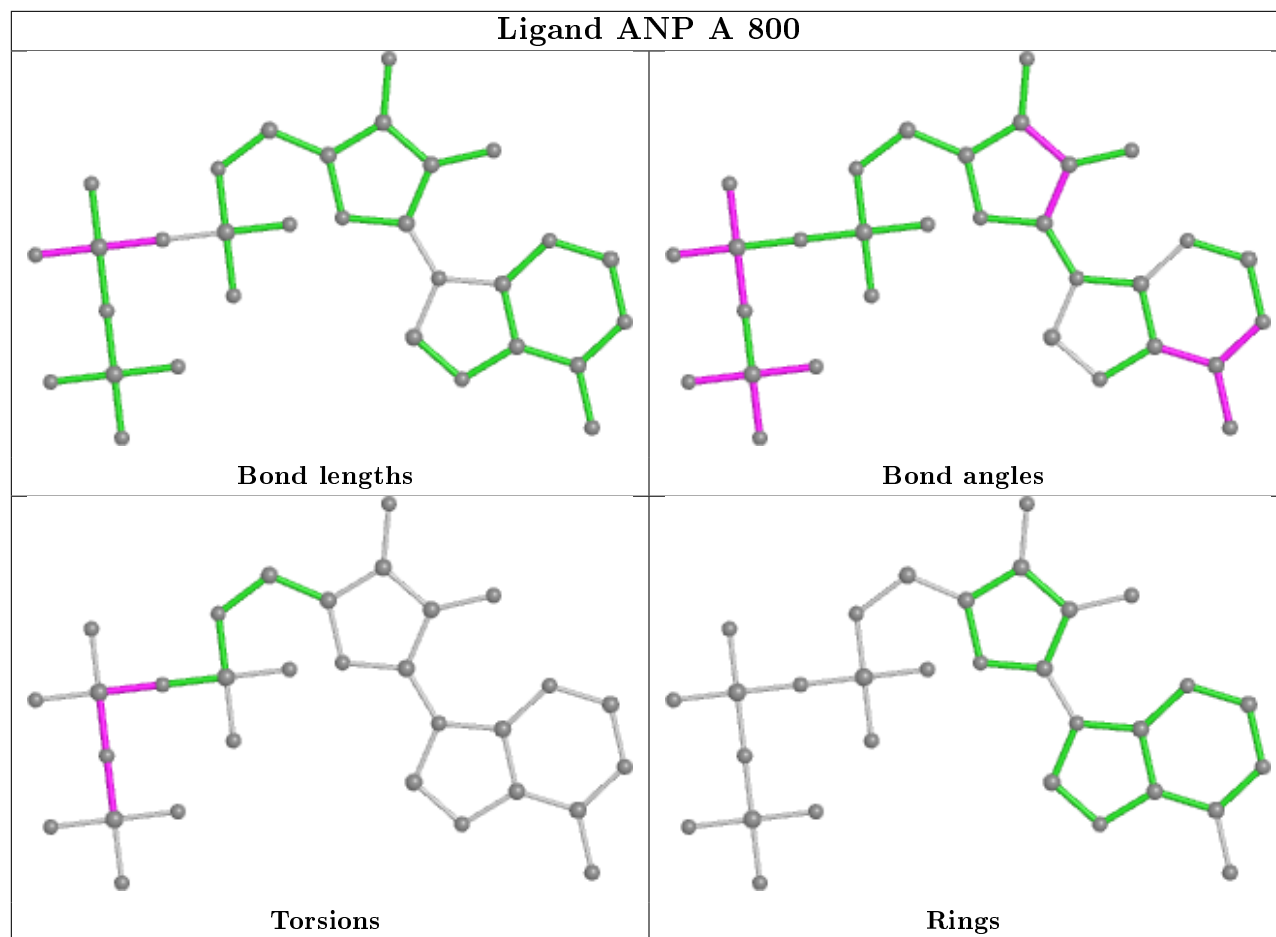
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	ANP	1	0

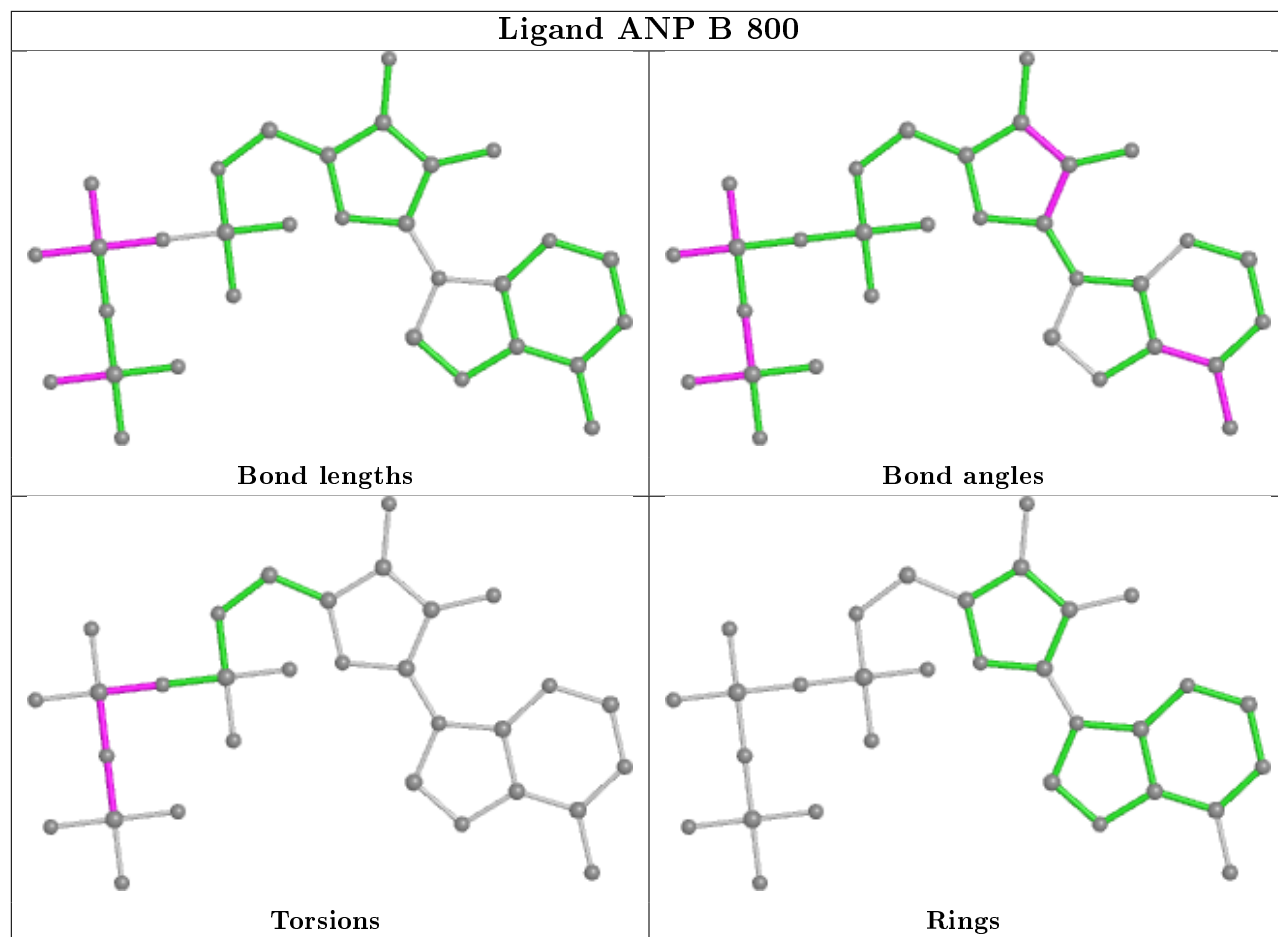
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

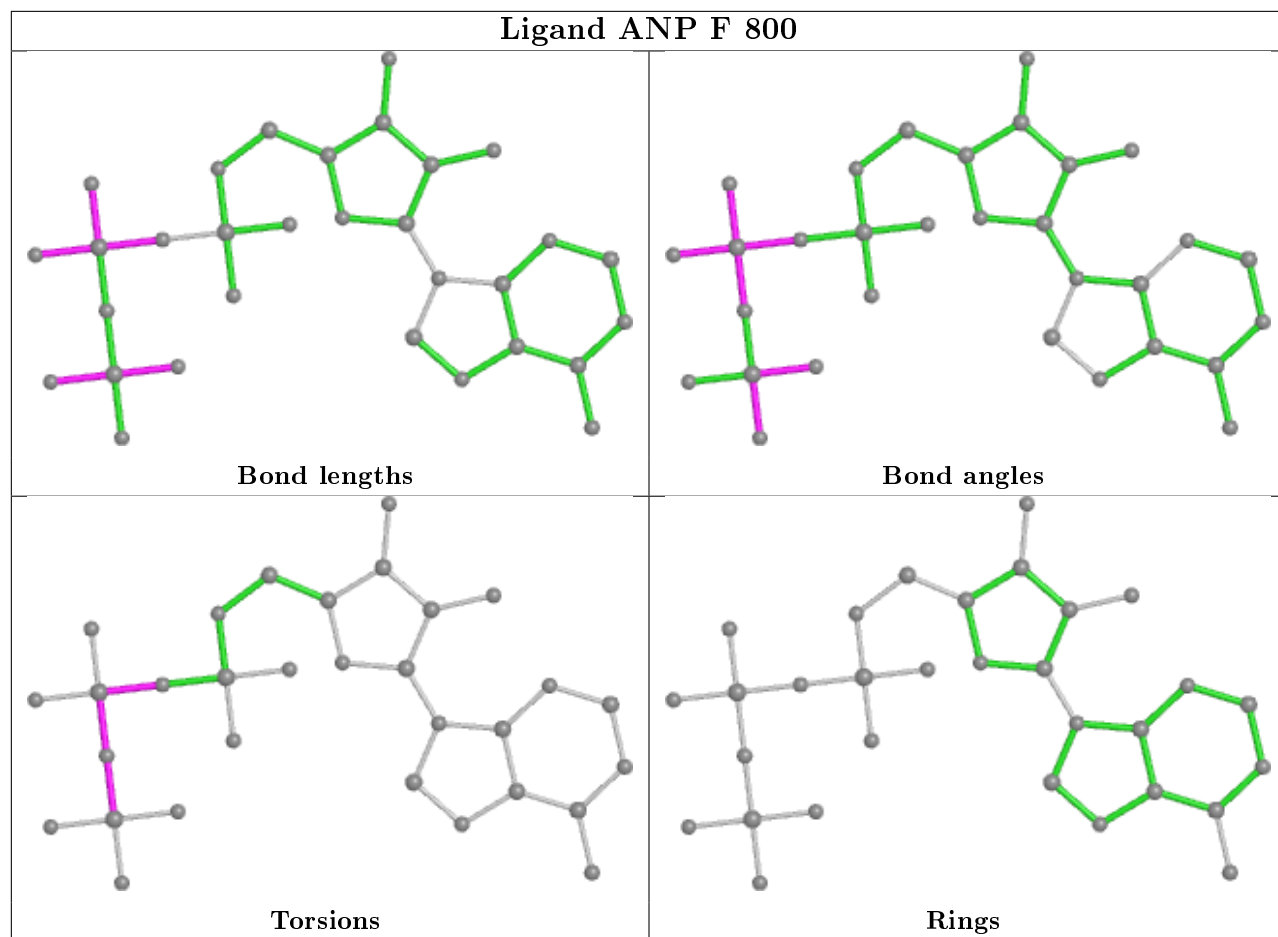


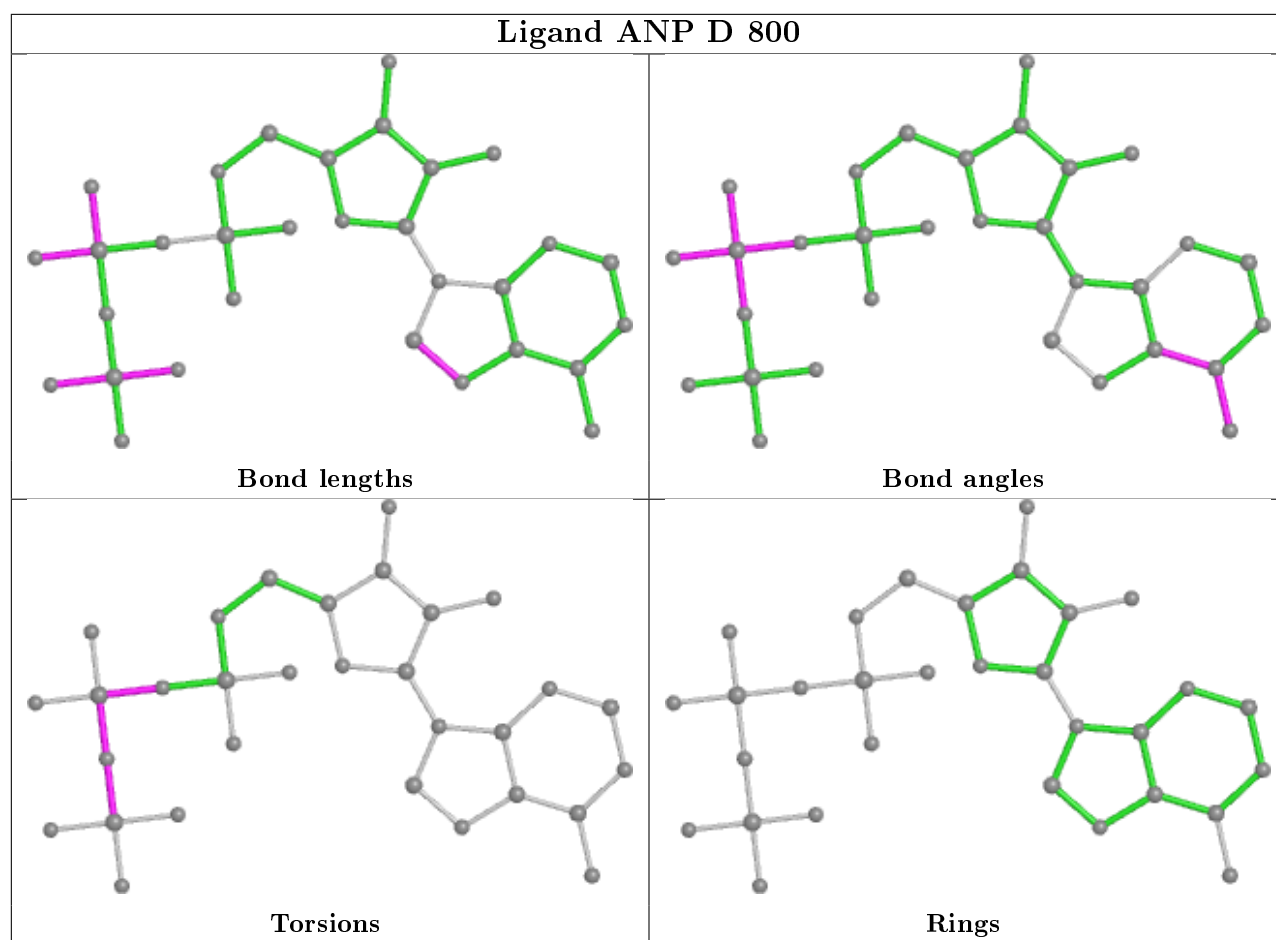












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	244/277 (88%)	-0.03	4 (1%) 72 72	24, 37, 58, 96	0
1	B	245/277 (88%)	0.11	6 (2%) 59 59	29, 44, 68, 96	0
1	C	242/277 (87%)	0.02	7 (2%) 51 52	26, 40, 64, 87	0
1	D	244/277 (88%)	-0.11	3 (1%) 79 79	26, 40, 64, 85	0
1	E	246/277 (88%)	0.12	8 (3%) 46 47	29, 43, 72, 119	0
1	F	244/277 (88%)	-0.04	8 (3%) 46 47	28, 42, 69, 111	0
1	G	244/277 (88%)	-0.05	4 (1%) 72 72	25, 37, 64, 101	0
All	All	1709/1939 (88%)	0.00	40 (2%) 60 61	24, 41, 67, 119	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	305	GLY	7.9
1	E	305	GLY	7.7
1	F	259	SER	7.1
1	A	305	GLY	6.4
1	B	305	GLY	5.2
1	E	421	ASP	5.1
1	A	306	ARG	4.8
1	E	259	SER	4.7
1	E	306	ARG	4.4
1	D	305	GLY	4.1
1	D	259	SER	3.9
1	A	259	SER	3.6
1	C	306	ARG	3.5
1	C	259	SER	3.5
1	D	306	ARG	3.3
1	G	306	ARG	3.2
1	B	414	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	306	ARG	3.1
1	E	257	THR	3.1
1	E	288	PHE	3.0
1	C	288	PHE	3.0
1	B	260	SER	2.9
1	F	260	SER	2.9
1	C	371	GLY	2.9
1	B	306	ARG	2.7
1	F	258	ASP	2.7
1	G	259	SER	2.7
1	E	260	SER	2.6
1	F	420	ARG	2.5
1	F	424	HIS	2.5
1	G	260	SER	2.3
1	B	259	SER	2.3
1	F	305	GLY	2.3
1	C	260	SER	2.2
1	C	376	LEU	2.2
1	A	260	SER	2.1
1	B	288	PHE	2.1
1	F	172	VAL	2.1
1	E	307	LEU	2.0
1	C	373	ALA	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 carbohydrates 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.

Continued on next page...

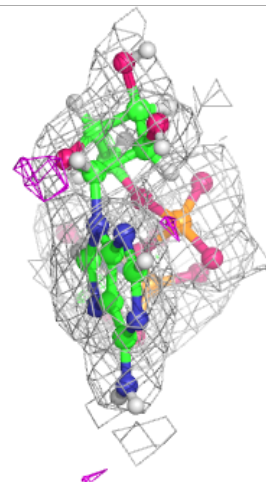
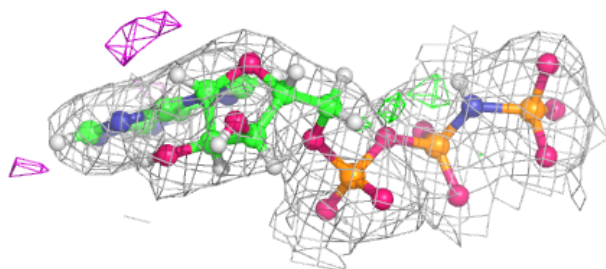
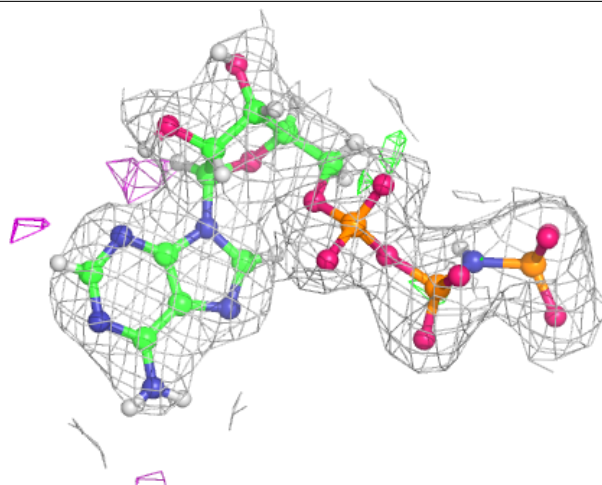
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	801	1/1	0.96	0.11	34,34,34,34	0
3	MG	E	801	1/1	0.97	0.14	32,32,32,32	0
3	MG	D	801	1/1	0.97	0.13	28,28,28,28	0
3	MG	C	801	1/1	0.97	0.09	35,35,35,35	0
3	MG	G	801	1/1	0.98	0.11	30,30,30,30	0
2	ANP	B	800	31/31	0.98	0.11	29,33,35,38	4
2	ANP	G	800	31/31	0.99	0.12	23,27,29,31	4
2	ANP	A	800	31/31	0.99	0.12	23,28,30,31	4
3	MG	A	801	1/1	0.99	0.09	23,23,23,23	0
2	ANP	E	800	31/31	0.99	0.11	27,32,33,36	4
3	MG	F	801	1/1	0.99	0.10	28,28,28,28	0
2	ANP	C	800	31/31	0.99	0.11	28,30,32,33	4
2	ANP	F	800	31/31	0.99	0.09	25,29,36,37	4
2	ANP	D	800	31/31	0.99	0.11	25,28,30,30	4

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.

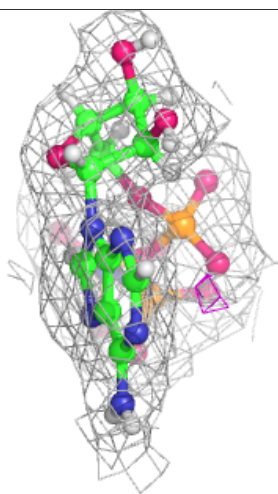
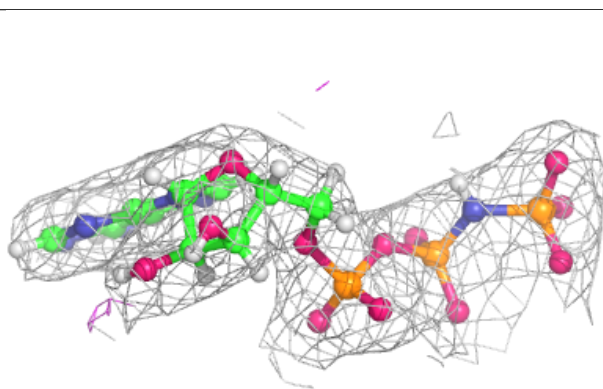
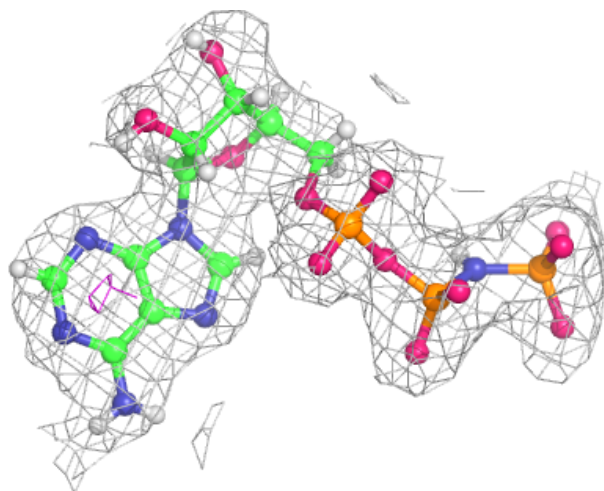
Electron density around ANP B 800:

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



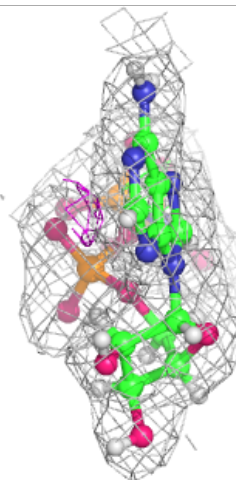
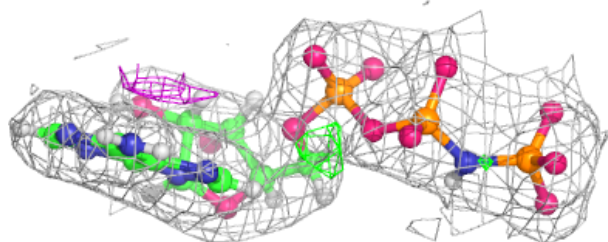
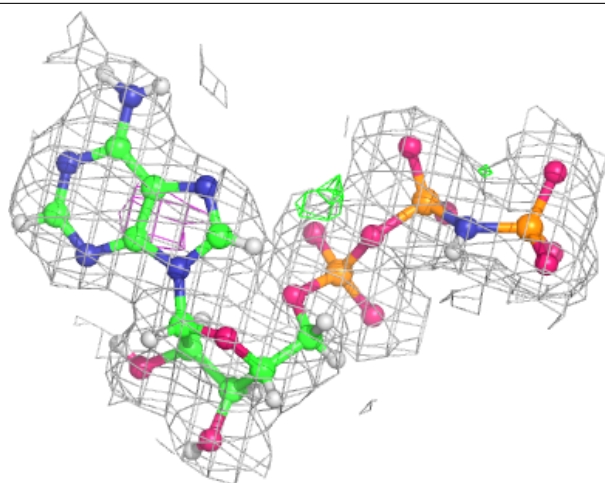
Electron density around ANP G 800:

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



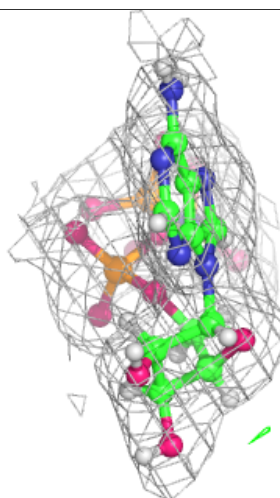
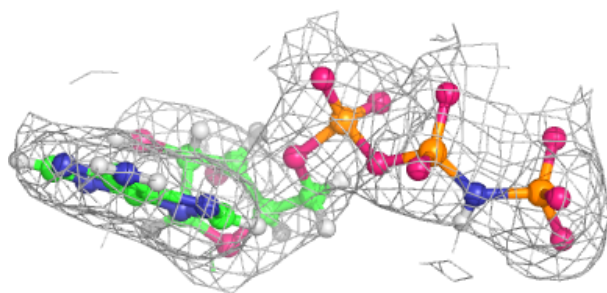
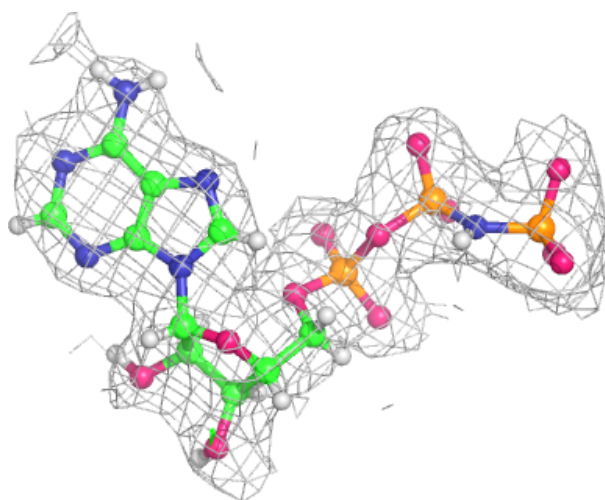
Electron density around ANP A 800:

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



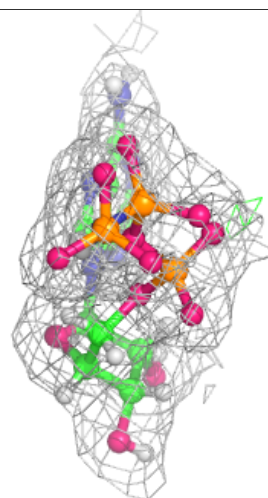
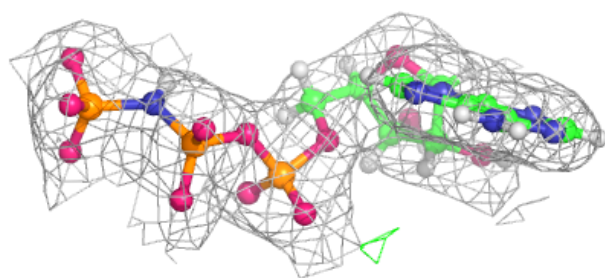
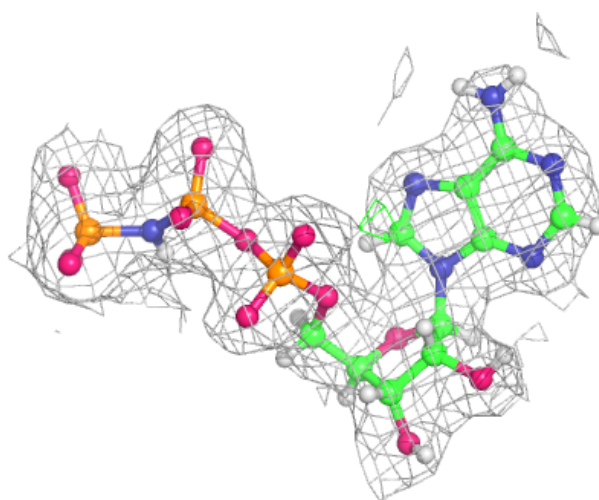
Electron density around ANP E 800:

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



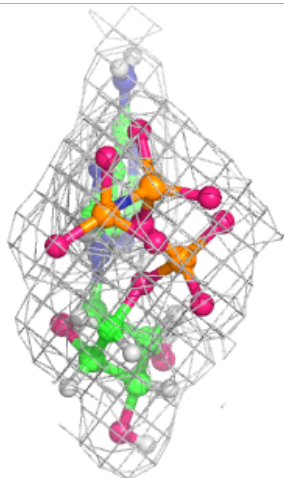
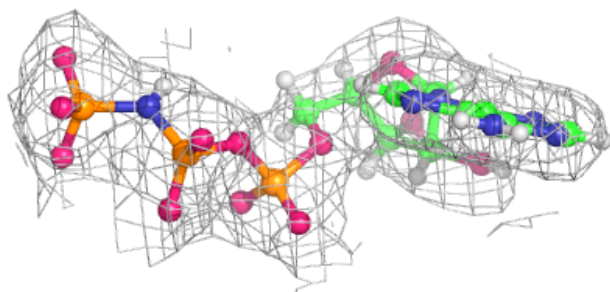
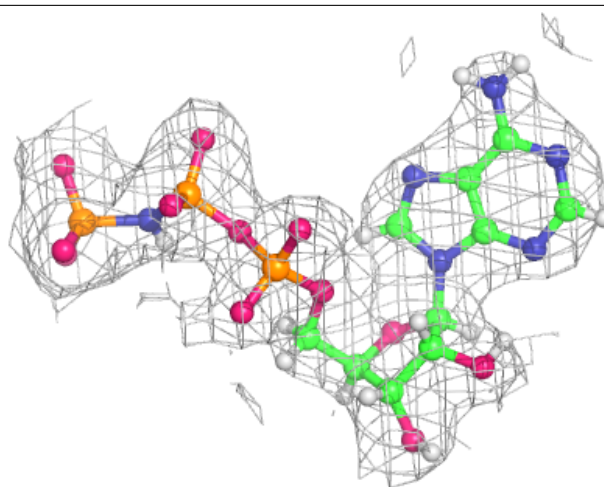
Electron density around ANP C 800:

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



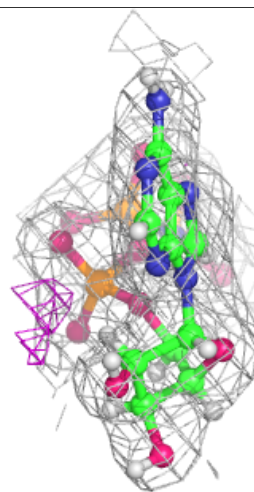
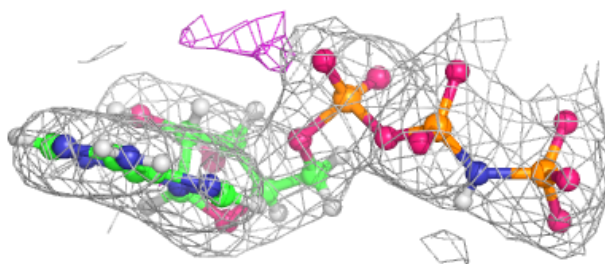
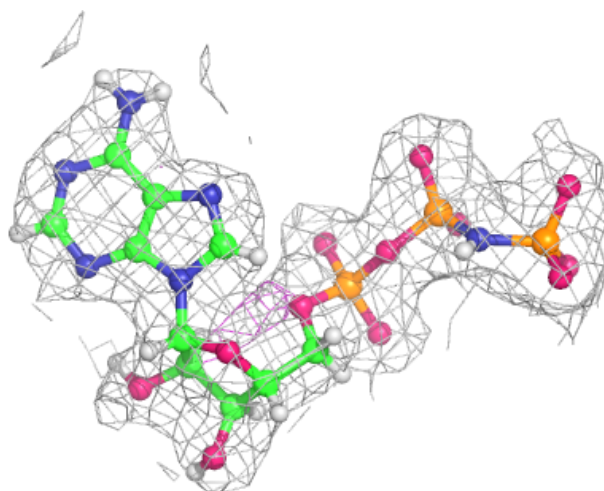
Electron density around ANP F 800:

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



Electron density around ANP D 800:

$2mF_o-DF_c$ (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.