



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:02 PM BST

PDB ID : 6DUK
Title : EGFR with an allosteric inhibitor
Authors : Park, E.; Eck, M.J.
Deposited on : 2018-06-21
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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 : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

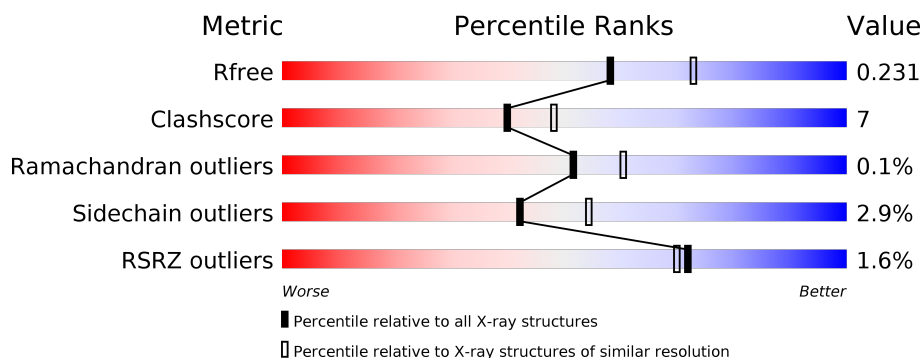
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	331	<div> <div>81%</div> <div>11% • 8%</div> </div>
1	B	331	<div> <div>%</div> <div>77%</div> <div>11% • 11%</div> </div>
1	C	331	<div> <div>2%</div> <div>69%</div> <div>19% • 11%</div> </div>
1	D	331	<div> <div>2%</div> <div>82%</div> <div>9% • 7%</div> </div>
1	E	331	<div> <div>%</div> <div>72%</div> <div>18% • 10%</div> </div>
1	F	331	<div> <div>3%</div> <div>68%</div> <div>22% • 10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15408 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	1	0
			2458	1579	415	446	18			
1	B	296	Total	C	N	O	S	0	1	0
			2355	1515	395	426	19			
1	C	295	Total	C	N	O	S	0	0	0
			2333	1499	395	420	19			
1	D	307	Total	C	N	O	S	0	0	0
			2449	1573	416	441	19			
1	E	298	Total	C	N	O	S	0	1	0
			2393	1539	404	431	19			
1	F	298	Total	C	N	O	S	0	1	0
			2350	1511	393	429	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533

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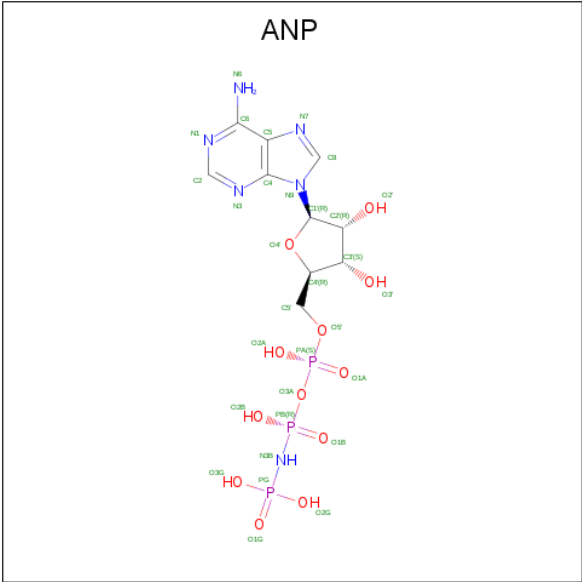
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Chain	Residue	Modelled	Actual	Comment	Reference
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
E	692	GLY	-	expression tag	UNP P00533
E	693	SER	-	expression tag	UNP P00533
E	694	THR	-	expression tag	UNP P00533
E	790	MET	THR	engineered mutation	UNP P00533
E	948	ARG	VAL	engineered mutation	UNP P00533
F	692	GLY	-	expression tag	UNP P00533
F	693	SER	-	expression tag	UNP P00533
F	694	THR	-	expression tag	UNP P00533
F	790	MET	THR	engineered mutation	UNP P00533
F	948	ARG	VAL	engineered mutation	UNP P00533

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

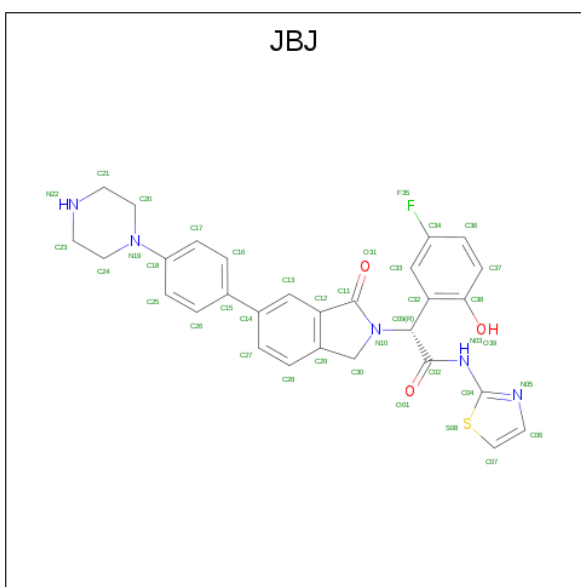
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 4 is (2R)-2-(5-fluoro-2-hydroxyphenyl)-2-{1-oxo-6-[4-(piperazin-1-yl)phenyl]-1,3-dihydro-2H-isoindol-2-yl}-N-(1,3-thiazol-2-yl)acetamide (three-letter code: JBJ) (formula: C₂₉H₂₆FN₅O₃S).

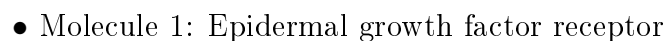


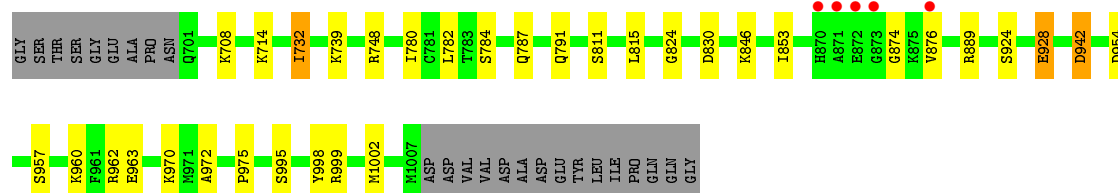
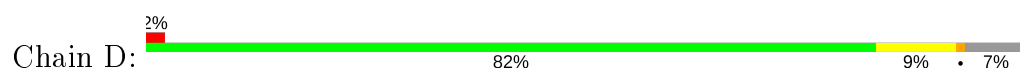
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	
			39	29	1	5	3	1	0
4	B	1	Total	C	F	N	O	S	
			39	29	1	5	3	1	0
4	C	1	Total	C	F	N	O	S	
			39	29	1	5	3	1	0
4	D	1	Total	C	F	N	O	S	
			39	29	1	5	3	1	0
4	E	1	Total	C	F	N	O	S	
			39	29	1	5	3	1	0
4	F	1	Total	C	F	N	O	S	
			39	29	1	5	3	1	0

- Molecule 5 is water.

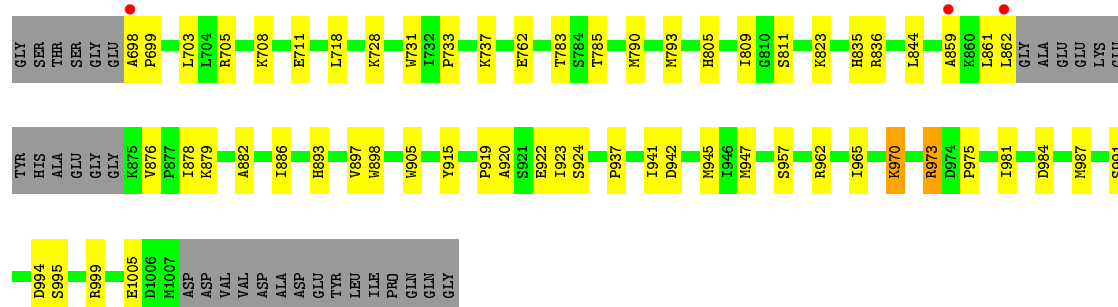
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total	O		
			179	179	0	0
5	B	99	Total	O		
			99	99	0	0
5	C	61	Total	O		
			61	61	0	0
5	D	145	Total	O		
			145	145	0	0
5	E	100	Total	O		
			100	100	0	0
5	F	60	Total	O		
			60	60	0	0

- Molecule 1: Epidermal growth factor receptor

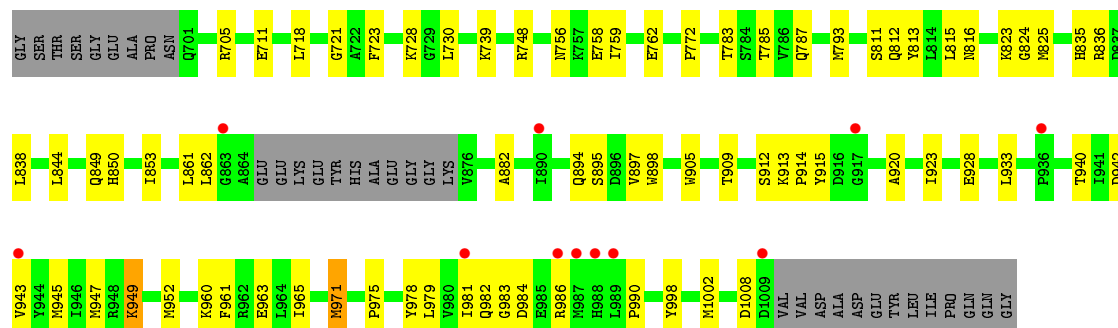




- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.48Å 94.71Å 97.40Å 70.38° 77.46° 79.14°	Depositor
Resolution (Å)	88.50 – 2.20 88.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (88.50-2.20) 98.1 (88.51-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.190 , 0.223 0.197 , 0.231	Depositor DCC
R_{free} test set	1725 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.075 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15408	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2817e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, JBJ

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	0.46	0/2516	0.60	0/3402
1	B	0.40	0/2410	0.58	0/3265
1	C	0.42	0/2385	0.56	0/3231
1	D	0.45	0/2504	0.60	0/3386
1	E	0.42	0/2449	0.55	0/3315
1	F	0.41	0/2404	0.57	0/3259
All	All	0.43	0/14668	0.58	0/19858

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	2458	0	2492	23	0
1	B	2355	0	2368	28	0
1	C	2333	0	2341	50	0
1	D	2449	0	2477	19	0
1	E	2393	0	2430	38	0
1	F	2350	0	2346	53	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0
3	C	31	0	13	0	0
3	D	31	0	13	0	0
3	E	31	0	13	0	0
3	F	31	0	13	0	0
4	A	39	0	0	1	0
4	B	39	0	0	1	0
4	C	39	0	0	1	0
4	D	39	0	0	0	0
4	E	39	0	0	3	0
4	F	39	0	0	0	0
5	A	179	0	0	3	0
5	B	99	0	0	2	0
5	C	61	0	0	1	0
5	D	145	0	0	2	0
5	E	100	0	0	4	0
5	F	60	0	0	1	0
All	All	15408	0	14532	214	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 7.

All (214) 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:932:ARG:CZ	1:C:951:TRP:O	2.08	1.01
1:E:859:ALA:O	1:E:862:LEU:O	1.76	1.00
1:C:932:ARG:NH2	1:C:951:TRP:O	2.04	0.91
1:F:940:THR:HG22	1:F:943:VAL:HG23	1.58	0.85
1:F:783:THR:HG21	1:F:787:GLN:HE21	1.42	0.84
1:D:714:LYS:NZ	1:D:787:GLN:OE1	2.12	0.82
1:F:812:GLN:O	1:F:816:ASN:ND2	2.14	0.80
1:C:923:ILE:HA	1:C:926:ILE:CG1	2.14	0.78
1:F:721:GLY:O	1:F:748:ARG:NH2	2.17	0.77
1:B:991:SER:HB3	1:B:994:ASP:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:999:ARG:HH22	1:C:1007:MET:HB2	1.54	0.72
1:C:923:ILE:HA	1:C:926:ILE:HG12	1.69	0.72
1:C:878:ILE:HG21	1:C:920:ALA:HB1	1.73	0.70
1:F:913:LYS:HE3	1:F:914:PRO:HD2	1.72	0.70
1:E:991:SER:HB3	1:E:994:ASP:HB2	1.73	0.69
1:F:945:MET:O	1:F:949:LYS:HD2	1.92	0.69
1:E:920:ALA:HA	1:E:923:ILE:HD13	1.75	0.69
1:E:762:GLU:HG3	1:E:861:LEU:HD11	1.75	0.68
1:B:829:GLU:O	1:B:832:ARG:NH2	2.27	0.68
1:D:830:ASP:OD1	1:D:962:ARG:NH2	2.27	0.67
1:F:783:THR:HG23	1:F:785:THR:O	1.96	0.66
1:E:905:TRP:HD1	1:E:947:MET:HE1	1.61	0.66
1:E:783:THR:HG23	1:E:785:THR:O	1.94	0.66
1:E:699:PRO:HD2	5:E:1208:HOH:O	1.96	0.65
1:C:783:THR:HB	1:C:785:THR:O	1.97	0.65
1:C:923:ILE:HA	1:C:926:ILE:CD1	2.27	0.64
1:B:944:TYR:CE2	1:B:948:ARG:HD2	2.32	0.64
1:C:923:ILE:HA	1:C:926:ILE:HD11	1.79	0.64
1:E:879:LYS:HG2	1:E:915:TYR:HD2	1.64	0.62
1:F:813:TYR:OH	1:F:990:PRO:HG3	1.99	0.62
1:E:984:ASP:HA	1:E:987:MET:HE2	1.82	0.61
1:F:815:LEU:HD11	1:F:979:LEU:HD13	1.83	0.61
1:B:886:ILE:O	1:B:889:ARG:NH2	2.33	0.61
1:C:768:SER:OG	1:C:831:ARG:NH2	2.28	0.60
1:C:734:GLU:H	1:C:734:GLU:CD	2.04	0.59
1:B:879:LYS:NZ	1:B:915:TYR:O	2.33	0.59
1:F:894:GLN:O	1:F:897:VAL:HG22	2.02	0.59
1:A:737:LYS:NZ	5:A:1201:HOH:O	2.33	0.59
1:F:940:THR:HG23	1:F:942:ASP:H	1.68	0.59
1:C:999:ARG:NH2	1:C:1007:MET:HB2	2.17	0.58
1:C:932:ARG:NH1	1:C:951:TRP:O	2.36	0.58
1:E:718:LEU:HD13	1:E:728:LYS:H	1.67	0.58
1:F:811:SER:OG	1:F:975:PRO:HB2	2.03	0.58
1:A:968:PHE:HA	1:A:971:MET:HE3	1.86	0.58
1:B:748:ARG:NH1	5:B:1208:HOH:O	2.37	0.57
1:D:995:SER:O	1:D:999:ARG:HG3	2.05	0.57
1:C:943:VAL:O	1:C:947:MET:HG3	2.04	0.57
1:E:920:ALA:HA	1:E:923:ILE:CD1	2.34	0.57
1:C:977:ARG:NH1	1:C:978:TYR:OH	2.37	0.56
1:A:836:ARG:O	1:A:836:ARG:HG2	2.04	0.56
1:C:892:THR:HG23	1:C:895:SER:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:LYS:HB3	1:C:710:THR:HG22	1.87	0.56
1:E:805:HIS:HB2	1:E:809:ILE:HD11	1.88	0.56
1:E:970:LYS:O	1:E:973:ARG:HG3	2.06	0.55
1:B:968:PHE:HA	1:B:971:MET:HE3	1.88	0.55
1:B:879:LYS:HD3	1:B:915:TYR:HB2	1.87	0.55
1:F:949:LYS:O	1:F:952:MET:HG3	2.06	0.55
1:F:758:GLU:HG2	1:F:861:LEU:CD1	2.36	0.55
1:C:808:ASN:HA	1:C:987:MET:CE	2.36	0.55
1:A:960:LYS:N	1:A:960:LYS:HD2	2.23	0.54
1:C:888:HIS:HB2	1:C:890:ILE:HG13	1.90	0.54
1:F:705:ARG:NH1	1:F:711:GLU:OE2	2.40	0.54
1:E:762:GLU:HG3	1:E:861:LEU:CD1	2.37	0.54
1:F:983:GLY:O	1:F:986:ARG:N	2.41	0.53
1:F:730:LEU:HD22	1:F:739:LYS:HB3	1.91	0.53
1:B:858:LEU:O	1:B:862:LEU:HG	2.09	0.53
1:C:878:ILE:HG21	1:C:920:ALA:CB	2.39	0.53
1:C:922:GLU:O	1:C:926:ILE:HG12	2.09	0.53
1:A:989:LEU:HD12	1:A:989:LEU:N	2.24	0.52
1:C:977:ARG:HD2	1:C:978:TYR:CZ	2.44	0.52
1:C:879:LYS:HE3	1:C:923:ILE:HD11	1.90	0.52
1:F:920:ALA:HA	1:F:923:ILE:CD1	2.40	0.52
1:D:815:LEU:HD23	1:D:972:ALA:HA	1.90	0.52
1:E:981:ILE:HG21	1:E:987:MET:HE1	1.91	0.51
1:F:758:GLU:HG3	5:F:1232:HOH:O	2.09	0.51
1:D:708:LYS:HE2	5:D:1260:HOH:O	2.10	0.51
1:D:732:ILE:HD13	1:D:739:LYS:HG2	1.92	0.51
1:C:877:PRO:O	1:C:881:MET:HG3	2.11	0.51
1:F:940:THR:HG23	1:F:942:ASP:N	2.25	0.51
1:A:908:MET:HG3	1:A:939:CYS:SG	2.51	0.51
1:B:752:SER:H	1:B:755:ALA:HB3	1.76	0.51
1:D:960:LYS:HB2	1:D:963:GLU:HG3	1.92	0.51
1:E:941:ILE:O	1:E:945:MET:HG2	2.11	0.51
1:F:723:PHE:CZ	1:F:862:LEU:HD11	2.45	0.51
1:A:987:MET:O	1:A:989:LEU:HD12	2.10	0.50
1:E:705:ARG:NH2	1:E:711:GLU:OE1	2.44	0.50
1:D:954:ASP:OD2	1:D:957:SER:OG	2.25	0.50
1:C:811:SER:OG	1:C:975:PRO:HB2	2.11	0.50
1:F:943:VAL:O	1:F:947:MET:HG3	2.11	0.50
1:C:923:ILE:CA	1:C:926:ILE:HG12	2.41	0.50
1:B:762:GLU:HG3	1:B:861:LEU:HD11	1.94	0.49
1:F:825:MET:HE3	1:F:838:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:MET:HG3	1:A:844:LEU:HB3	1.94	0.49
1:F:825:MET:HE3	1:F:835:HIS:HD2	1.77	0.49
1:C:808:ASN:HA	1:C:987:MET:HE1	1.93	0.49
1:F:783:THR:HG21	1:F:787:GLN:NE2	2.21	0.49
1:C:974:ASP:OD2	1:C:977:ARG:NE	2.46	0.49
1:D:824:GLY:HA3	1:D:853:ILE:HD12	1.95	0.49
1:D:811:SER:OG	1:D:975:PRO:HB2	2.13	0.49
1:C:923:ILE:HG13	1:C:926:ILE:HD11	1.95	0.48
1:E:882:ALA:HA	1:E:898:TRP:CD2	2.49	0.48
1:F:960:LYS:HB2	1:F:963:GLU:HG3	1.94	0.48
1:A:943:VAL:O	1:A:947:MET:HG3	2.13	0.48
4:A:1103:JBJ:O01	4:A:1103:JBJ:S08	2.72	0.48
1:C:859:ALA:O	1:C:861:LEU:N	2.47	0.48
1:E:970:LYS:NZ	5:E:1206:HOH:O	2.46	0.48
1:A:962:ARG:NH1	5:A:1210:HOH:O	2.47	0.47
1:C:953:ILE:HD12	1:C:953:ILE:H	1.78	0.47
1:D:889:ARG:HD3	1:D:889:ARG:HA	1.64	0.47
1:F:718:LEU:HD13	1:F:728:LYS:H	1.79	0.47
1:A:815:LEU:HD12	1:A:975:PRO:HB3	1.96	0.47
1:F:756:ASN:HA	1:F:759:ILE:HB	1.96	0.47
1:B:939:CYS:HA	1:B:979:LEU:HD23	1.95	0.47
1:C:829:GLU:HG3	1:C:893:HIS:CG	2.50	0.47
1:E:924:SER:HB3	5:E:1247:HOH:O	2.14	0.47
1:B:811:SER:OG	1:B:975:PRO:HB2	2.14	0.46
1:F:723:PHE:CE2	1:F:862:LEU:HD11	2.51	0.46
1:E:893:HIS:O	1:E:897:VAL:HG23	2.16	0.46
1:B:806:LYS:HE2	1:B:806:LYS:HB3	1.59	0.46
1:C:963:GLU:O	1:C:967:GLU:HG3	2.15	0.46
1:E:876:VAL:O	1:E:878:ILE:N	2.47	0.46
1:F:825:MET:HE2	1:F:853:ILE:HG12	1.98	0.46
1:F:882:ALA:HA	1:F:898:TRP:CD2	2.50	0.46
1:F:971:MET:HG3	1:F:978:TYR:CD2	2.50	0.46
1:C:967:GLU:O	1:C:971:MET:HG3	2.16	0.46
1:F:824:GLY:HA3	1:F:853:ILE:HD12	1.97	0.46
1:F:909:THR:HG22	1:F:912:SER:H	1.81	0.46
1:F:979:LEU:HD23	1:F:981:ILE:HD11	1.98	0.46
1:B:788:LEU:C	1:B:789:ILE:HD12	2.36	0.46
1:C:744:ILE:HG12	1:C:789:ILE:HD13	1.98	0.46
1:A:778:LEU:HD22	1:A:790:MET:HA	1.98	0.45
1:A:889:ARG:HA	1:A:889:ARG:HD3	1.76	0.45
1:B:748:ARG:HG2	1:B:748:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1103:JBJ:S08	4:C:1103:JBJ:O01	2.74	0.45
1:E:995:SER:O	1:E:999:ARG:HG3	2.16	0.45
1:B:766:MET:HB3	1:B:766:MET:HE2	1.83	0.45
1:D:791:GLN:NE2	1:D:846:LYS:HE3	2.32	0.45
1:C:708:LYS:O	1:C:711:GLU:HG2	2.16	0.45
1:B:938:ILE:HD12	1:B:979:LEU:HD22	1.99	0.45
1:B:815:LEU:CD1	1:B:979:LEU:HD12	2.47	0.45
1:B:832:ARG:HA	1:B:832:ARG:HD3	1.72	0.45
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.51	0.45
1:B:752:SER:O	1:B:756:ASN:N	2.43	0.45
1:D:942:ASP:OD1	1:D:942:ASP:N	2.50	0.45
1:E:698:ALA:N	1:E:699:PRO:HD3	2.32	0.45
1:E:835:HIS:O	1:E:836:ARG:HB2	2.17	0.45
1:C:960:LYS:HE2	1:C:962:ARG:HH12	1.82	0.45
1:C:981:ILE:O	1:C:984:ASP:HB2	2.17	0.45
1:E:790:MET:HG2	4:E:1103:JBJ:C07	2.47	0.45
1:A:893:HIS:HD2	5:A:1267:HOH:O	1.99	0.45
1:C:836:ARG:HG2	1:C:836:ARG:O	2.17	0.45
1:F:849:GLN:OE1	1:F:990:PRO:HG2	2.16	0.45
1:A:798:LEU:O	1:A:802:VAL:HG13	2.17	0.44
1:E:861:LEU:HD22	4:E:1103:JBJ:C26	2.47	0.44
1:E:823:LYS:HA	1:E:965:ILE:HD11	1.99	0.44
1:F:823:LYS:HA	1:F:965:ILE:HD11	1.99	0.44
1:C:892:THR:H	1:C:895:SER:HB3	1.83	0.44
1:F:943:VAL:HG22	1:F:971:MET:CE	2.47	0.44
1:D:780:ILE:HG12	1:D:782:LEU:HD13	2.00	0.44
1:F:813:TYR:OH	1:F:990:PRO:CG	2.65	0.44
1:F:793:MET:HG3	1:F:844:LEU:HD13	1.99	0.44
1:C:731:TRP:CZ3	1:C:733:PRO:HG3	2.53	0.44
1:E:919:PRO:O	1:E:923:ILE:HD12	2.18	0.44
1:B:974:ASP:OD2	1:B:977:ARG:HB2	2.17	0.44
1:A:944:TYR:CZ	1:A:948:ARG:HD3	2.54	0.43
1:D:960:LYS:HA	1:D:960:LYS:HD2	1.80	0.43
1:C:894:GLN:HB3	1:C:955:ALA:HB1	2.00	0.43
1:F:825:MET:CE	1:F:835:HIS:HD2	2.31	0.43
1:C:858:LEU:HD22	5:C:1206:HOH:O	2.19	0.43
1:F:762:GLU:HG3	1:F:861:LEU:CD2	2.48	0.43
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.83	0.43
1:A:806:LYS:HB3	1:A:806:LYS:HE3	1.71	0.43
1:A:905:TRP:CD1	1:A:947:MET:HE1	2.54	0.43
1:E:886:ILE:HG21	1:E:924:SER:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:703:LEU:HD23	1:E:703:LEU:HA	1.72	0.43
1:E:937:PRO:HD2	5:E:1246:HOH:O	2.19	0.43
1:C:760:LEU:HD11	1:C:782:LEU:HD11	2.01	0.42
1:F:825:MET:HE3	1:F:835:HIS:CD2	2.53	0.42
1:C:825:MET:CE	1:C:838:LEU:HD13	2.50	0.42
1:F:905:TRP:HD1	1:F:947:MET:HE1	1.83	0.42
1:D:846:LYS:HE2	1:D:1002:MET:O	2.18	0.42
1:F:909:THR:HG21	1:F:912:SER:HB2	2.00	0.42
1:B:803:ARG:O	1:B:806:LYS:HE2	2.20	0.42
1:F:772:PRO:O	1:F:850:HIS:NE2	2.53	0.42
1:C:939:CYS:HA	1:C:979:LEU:HD23	2.00	0.42
1:F:705:ARG:HH12	1:F:711:GLU:CD	2.23	0.42
1:A:701:GLN:HA	1:A:764:TYR:CE1	2.54	0.42
1:B:766:MET:H	1:B:766:MET:HG2	1.56	0.42
1:D:924:SER:O	1:D:928:GLU:HG2	2.19	0.42
1:E:984:ASP:HA	1:E:987:MET:CE	2.50	0.42
1:F:762:GLU:HG3	1:F:861:LEU:HD22	2.00	0.42
1:A:705:ARG:NH1	1:B:994:ASP:OD1	2.53	0.42
1:C:808:ASN:HA	1:C:987:MET:HE2	2.01	0.42
1:E:793:MET:HG3	1:E:844:LEU:HB3	2.00	0.42
1:F:915:TYR:CZ	1:F:933:LEU:HG	2.55	0.42
1:C:707:LEU:HD13	1:C:789:ILE:HG13	2.01	0.42
1:E:941:ILE:HA	1:E:941:ILE:HD12	1.98	0.42
1:E:811:SER:OG	1:E:975:PRO:HB2	2.20	0.41
4:E:1103:JBJ:O01	4:E:1103:JBJ:S08	2.78	0.41
1:A:824:GLY:HA3	1:A:853:ILE:HD12	2.01	0.41
1:F:835:HIS:O	1:F:836:ARG:HB3	2.21	0.41
1:F:971:MET:HG3	1:F:978:TYR:CG	2.56	0.41
1:B:815:LEU:O	1:B:819:VAL:HG23	2.20	0.41
1:E:731:TRP:CH2	1:E:733:PRO:HG3	2.55	0.41
4:B:1103:JBJ:O01	4:B:1103:JBJ:S08	2.79	0.41
1:F:978:TYR:O	1:F:979:LEU:HD12	2.21	0.41
1:D:874:GLY:C	1:D:876:VAL:H	2.23	0.41
1:C:825:MET:HE3	1:C:838:LEU:HD13	2.03	0.40
1:D:748:ARG:HD3	5:D:1267:HOH:O	2.21	0.40
1:F:897:VAL:HG12	1:F:961:PHE:CZ	2.56	0.40
1:E:905:TRP:CD1	1:E:947:MET:HE1	2.49	0.40
1:A:850:HIS:ND1	1:A:1003:ASP:OD2	2.54	0.40
1:B:953:ILE:HG12	5:B:1256:HOH:O	2.22	0.40
1:C:774:VAL:HG22	1:C:853:ILE:HD11	2.03	0.40

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	305/331 (92%)	296 (97%)	9 (3%)	0	100	100
1	B	293/331 (88%)	284 (97%)	9 (3%)	0	100	100
1	C	291/331 (88%)	277 (95%)	13 (4%)	1 (0%)	41	46
1	D	305/331 (92%)	298 (98%)	7 (2%)	0	100	100
1	E	295/331 (89%)	281 (95%)	14 (5%)	0	100	100
1	F	295/331 (89%)	284 (96%)	10 (3%)	1 (0%)	41	46
All	All	1784/1986 (90%)	1720 (96%)	62 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	982	GLN
1	C	859	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/290 (93%)	262 (97%)	7 (3%)	46	58
1	B	257/290 (89%)	250 (97%)	7 (3%)	44	57
1	C	253/290 (87%)	245 (97%)	8 (3%)	39	50
1	D	266/290 (92%)	260 (98%)	6 (2%)	50	63
1	E	264/290 (91%)	254 (96%)	10 (4%)	33	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	253/290 (87%)	245 (97%)	8 (3%)	39 50
All	All	1562/1740 (90%)	1516 (97%)	46 (3%)	42 54

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	737	LYS
1	A	867	LYS
1	A	942	ASP
1	A	970	LYS
1	A	989	LEU
1	A	995	SER
1	A	998	TYR
1	B	737	LYS
1	B	766	MET
1	B	889	ARG
1	B	921	SER
1	B	942	ASP
1	B	970	LYS
1	B	994	ASP
1	C	708	LYS
1	C	749	GLU
1	C	768	SER
1	C	776	ARG
1	C	861	LEU
1	C	931	GLU
1	C	945	MET
1	C	982	GLN
1	D	732	ILE
1	D	784	SER
1	D	928	GLU
1	D	942	ASP
1	D	970	LYS
1	D	998	TYR
1	E	708	LYS
1	E	737	LYS
1	E	922[A]	GLU
1	E	922[B]	GLU
1	E	942	ASP
1	E	957	SER
1	E	962	ARG
1	E	970	LYS

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Mol	Chain	Res	Type
1	E	973	ARG
1	E	1005	GLU
1	F	895	SER
1	F	928	GLU
1	F	949	LYS
1	F	971	MET
1	F	984	ASP
1	F	998	TYR
1	F	1002	MET
1	F	1008	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	988	HIS
1	C	812	GLN
1	E	805	HIS

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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	JBJ	A	1103	-	42,44,44	2.41	9 (21%)	52,63,63	3.26	8 (15%)
4	JBJ	B	1103	-	42,44,44	2.75	10 (23%)	52,63,63	3.07	11 (21%)
4	JBJ	E	1103	-	42,44,44	2.54	9 (21%)	52,63,63	3.34	13 (25%)
4	JBJ	F	1103	-	42,44,44	2.69	9 (21%)	52,63,63	3.17	7 (13%)
3	ANP	E	1102	2	29,33,33	2.29	12 (41%)	31,52,52	2.88	8 (25%)
3	ANP	C	1102	2	29,33,33	2.44	11 (37%)	31,52,52	2.55	10 (32%)
3	ANP	A	1102	2	29,33,33	2.45	12 (41%)	31,52,52	2.37	10 (32%)
3	ANP	B	1102	2	29,33,33	2.17	10 (34%)	31,52,52	2.81	11 (35%)
3	ANP	F	1102	2	29,33,33	2.17	8 (27%)	31,52,52	3.08	8 (25%)
3	ANP	D	1102	2	29,33,33	2.23	12 (41%)	31,52,52	2.93	8 (25%)
4	JBJ	C	1103	-	42,44,44	2.65	10 (23%)	52,63,63	3.56	13 (25%)
4	JBJ	D	1103	-	42,44,44	2.77	10 (23%)	52,63,63	2.85	8 (15%)

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	JBJ	A	1103	-	-	3/22/44/44	0/6/6/6
4	JBJ	B	1103	-	-	2/22/44/44	0/6/6/6
4	JBJ	E	1103	-	-	4/22/44/44	0/6/6/6
4	JBJ	F	1103	-	-	1/22/44/44	0/6/6/6
3	ANP	E	1102	2	-	3/14/38/38	0/3/3/3
3	ANP	C	1102	2	-	4/14/38/38	0/3/3/3
3	ANP	A	1102	2	-	2/14/38/38	0/3/3/3
3	ANP	B	1102	2	-	3/14/38/38	0/3/3/3
3	ANP	F	1102	2	-	2/14/38/38	0/3/3/3
3	ANP	D	1102	2	-	1/14/38/38	0/3/3/3
4	JBJ	C	1103	-	-	3/22/44/44	1/6/6/6
4	JBJ	D	1103	-	-	2/22/44/44	0/6/6/6

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	JBj	C12-C11	-9.75	1.33	1.48
4	C	1103	JBj	C12-C11	-9.74	1.33	1.48
4	E	1103	JBj	C12-C11	-9.70	1.33	1.48
4	F	1103	JBj	C12-C11	-9.35	1.33	1.48
4	D	1103	JBj	C12-C11	-9.12	1.34	1.48
4	D	1103	JBj	C32-C09	-9.07	1.41	1.52
4	A	1103	JBj	C12-C11	-8.94	1.34	1.48
4	B	1103	JBj	C32-C09	-8.60	1.42	1.52
4	F	1103	JBj	C32-C09	-8.51	1.42	1.52
4	D	1103	JBj	C30-C29	-7.58	1.40	1.50
4	C	1103	JBj	C30-C29	-7.31	1.40	1.50
4	C	1103	JBj	C32-C09	-7.27	1.43	1.52
4	F	1103	JBj	C30-C29	-7.23	1.40	1.50
4	B	1103	JBj	C30-C29	-7.11	1.40	1.50
4	A	1103	JBj	C30-C29	-6.95	1.41	1.50
4	E	1103	JBj	C32-C09	-6.76	1.44	1.52
4	A	1103	JBj	C32-C09	-6.67	1.44	1.52
4	E	1103	JBj	C30-C29	-6.31	1.41	1.50
3	C	1102	ANP	PG-N3B	5.78	1.78	1.63
3	A	1102	ANP	C2-N3	5.64	1.41	1.32
3	C	1102	ANP	C2-N3	5.59	1.41	1.32
3	C	1102	ANP	PB-O3A	4.94	1.65	1.59
3	A	1102	ANP	PB-O3A	4.90	1.65	1.59
3	B	1102	ANP	C2-N3	4.78	1.39	1.32
3	D	1102	ANP	O4'-C1'	4.67	1.47	1.41
3	E	1102	ANP	C2-N3	4.61	1.39	1.32
3	E	1102	ANP	PG-N3B	4.50	1.75	1.63
3	D	1102	ANP	C2-N3	4.42	1.39	1.32
4	B	1103	JBj	C13-C12	-4.42	1.32	1.39
3	F	1102	ANP	O4'-C1'	4.39	1.47	1.41
4	F	1103	JBj	F35-C34	4.33	1.46	1.36
3	F	1102	ANP	PG-N3B	4.33	1.74	1.63
4	D	1103	JBj	C13-C12	-4.05	1.33	1.39
4	D	1103	JBj	C11-N10	-4.03	1.32	1.36
3	B	1102	ANP	PG-N3B	4.02	1.73	1.63
3	A	1102	ANP	PG-O3G	-4.00	1.46	1.56
4	E	1103	JBj	C13-C12	-4.00	1.33	1.39
4	B	1103	JBj	C15-C14	-3.99	1.39	1.49
4	C	1103	JBj	C12-C29	-3.95	1.34	1.39
4	C	1103	JBj	C13-C12	-3.93	1.33	1.39
4	E	1103	JBj	C12-C29	-3.92	1.34	1.39
3	F	1102	ANP	C2-N3	3.90	1.38	1.32
3	D	1102	ANP	PG-O3G	-3.82	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	ANP	C2-N1	3.82	1.41	1.33
3	E	1102	ANP	O4'-C1'	3.82	1.46	1.41
3	D	1102	ANP	PB-O2B	-3.79	1.46	1.56
3	A	1102	ANP	PB-N3B	3.77	1.73	1.63
3	A	1102	ANP	PG-N3B	3.72	1.73	1.63
3	F	1102	ANP	C2-N1	3.71	1.40	1.33
4	D	1103	JBj	C12-C29	-3.71	1.34	1.39
4	C	1103	JBj	C15-C14	-3.69	1.39	1.49
4	B	1103	JBj	C11-N10	-3.68	1.32	1.36
4	D	1103	JBj	C28-C29	-3.66	1.33	1.39
4	F	1103	JBj	C15-C14	-3.63	1.40	1.49
3	B	1102	ANP	PG-O2G	-3.61	1.47	1.56
3	C	1102	ANP	C2-N1	3.60	1.40	1.33
4	E	1103	JBj	C15-C14	-3.58	1.40	1.49
4	D	1103	JBj	C15-C14	-3.58	1.40	1.49
3	E	1102	ANP	PB-O3A	3.56	1.63	1.59
4	F	1103	JBj	C28-C29	-3.54	1.33	1.39
3	E	1102	ANP	C2-N1	3.52	1.40	1.33
3	F	1102	ANP	PB-O2B	-3.52	1.47	1.56
3	C	1102	ANP	PB-O2B	-3.51	1.47	1.56
3	B	1102	ANP	PG-O3G	-3.51	1.47	1.56
3	D	1102	ANP	PB-N3B	3.47	1.72	1.63
4	F	1103	JBj	C13-C12	-3.43	1.34	1.39
3	E	1102	ANP	PB-O2B	-3.42	1.47	1.56
4	B	1103	JBj	C12-C29	-3.40	1.35	1.39
3	B	1102	ANP	C2-N1	3.39	1.40	1.33
4	C	1103	JBj	C09-N10	3.36	1.50	1.46
3	A	1102	ANP	PG-O2G	-3.32	1.47	1.56
3	F	1102	ANP	PG-O2G	-3.32	1.47	1.56
3	B	1102	ANP	PB-O2B	-3.32	1.47	1.56
4	F	1103	JBj	C11-N10	-3.30	1.32	1.36
3	C	1102	ANP	PG-O3G	-3.29	1.47	1.56
3	F	1102	ANP	PG-O3G	-3.28	1.47	1.56
3	E	1102	ANP	PG-O3G	-3.25	1.48	1.56
3	B	1102	ANP	PB-O3A	3.23	1.63	1.59
4	A	1103	JBj	C28-C29	-3.23	1.34	1.39
4	A	1103	JBj	C15-C14	-3.20	1.41	1.49
4	C	1103	JBj	C28-C29	-3.20	1.34	1.39
4	F	1103	JBj	C12-C29	-3.17	1.35	1.39
4	A	1103	JBj	C09-N10	3.15	1.50	1.46
3	D	1102	ANP	C2-N1	3.14	1.39	1.33
3	C	1102	ANP	O4'-C1'	3.09	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	JBj	C28-C29	-3.07	1.34	1.39
3	A	1102	ANP	PB-O2B	-3.05	1.48	1.56
3	E	1102	ANP	PG-O2G	-2.97	1.48	1.56
4	E	1103	JBj	C28-C29	-2.91	1.34	1.39
3	B	1102	ANP	O4'-C1'	2.88	1.45	1.41
3	C	1102	ANP	PG-O2G	-2.88	1.49	1.56
4	A	1103	JBj	C13-C12	-2.79	1.35	1.39
4	E	1103	JBj	C11-N10	-2.78	1.33	1.36
4	E	1103	JBj	C30-N10	2.77	1.49	1.46
3	A	1102	ANP	C5-C4	-2.73	1.33	1.40
3	D	1102	ANP	PG-N3B	2.73	1.70	1.63
4	D	1103	JBj	F35-C34	-2.72	1.29	1.36
4	A	1103	JBj	C12-C29	-2.65	1.36	1.39
3	D	1102	ANP	C2'-C1'	2.65	1.57	1.53
4	B	1103	JBj	F35-C34	-2.60	1.30	1.36
3	E	1102	ANP	C6-C5	-2.53	1.33	1.43
3	E	1102	ANP	C5-C4	-2.53	1.34	1.40
3	C	1102	ANP	C5-C4	-2.52	1.34	1.40
3	E	1102	ANP	PB-N3B	2.52	1.70	1.63
3	D	1102	ANP	PG-O2G	-2.50	1.50	1.56
3	F	1102	ANP	C5-C4	-2.50	1.34	1.40
3	A	1102	ANP	O4'-C1'	2.47	1.44	1.41
4	B	1103	JBj	C30-N10	2.46	1.48	1.46
3	B	1102	ANP	C5-C4	-2.46	1.34	1.40
3	D	1102	ANP	C5-C4	-2.42	1.34	1.40
3	D	1102	ANP	O3'-C3'	2.31	1.48	1.43
3	C	1102	ANP	C6-C5	-2.28	1.34	1.43
4	A	1103	JBj	C09-C02	-2.26	1.52	1.54
3	C	1102	ANP	PB-N3B	2.22	1.69	1.63
3	A	1102	ANP	C6-C5	-2.18	1.35	1.43
3	E	1102	ANP	C2'-C3'	-2.16	1.47	1.53
4	D	1103	JBj	C30-N10	2.11	1.48	1.46
4	C	1103	JBj	C33-C34	2.10	1.41	1.37
3	D	1102	ANP	C6-C5	-2.05	1.35	1.43
3	B	1102	ANP	C6-C5	-2.04	1.35	1.43
4	C	1103	JBj	C11-N10	-2.02	1.34	1.36
3	A	1102	ANP	O4'-C4'	2.01	1.49	1.45

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1103	JBj	C30-N10-C11	-19.37	105.15	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	JB	C30-N10-C11	-17.23	106.03	113.12
4	E	1103	JB	C30-N10-C11	-17.13	106.07	113.12
4	F	1103	JB	C30-N10-C11	-16.07	106.51	113.12
4	B	1103	JB	C30-N10-C11	-15.94	106.56	113.12
4	D	1103	JB	C30-N10-C11	-14.70	107.07	113.12
3	F	1102	AN	O1G-PG-N3B	-12.32	93.63	111.77
3	D	1102	AN	O1G-PG-N3B	-11.06	95.48	111.77
3	E	1102	AN	O1G-PG-N3B	-10.21	96.74	111.77
4	E	1103	JB	C30-N10-C09	10.18	133.38	123.86
4	F	1103	JB	C30-N10-C09	9.99	133.20	123.86
4	A	1103	JB	C12-C11-N10	9.31	111.94	106.44
4	F	1103	JB	C12-C11-N10	9.10	111.81	106.44
4	C	1103	JB	C12-C11-N10	9.07	111.80	106.44
3	B	1102	AN	O1G-PG-N3B	-8.73	98.91	111.77
4	E	1103	JB	C12-C11-N10	8.68	111.56	106.44
4	D	1103	JB	C30-N10-C09	8.40	131.71	123.86
4	B	1103	JB	C12-C11-N10	8.33	111.36	106.44
4	B	1103	JB	C30-N10-C09	8.13	131.46	123.86
4	C	1103	JB	C30-N10-C09	7.57	130.93	123.86
4	D	1103	JB	C12-C11-N10	7.55	110.90	106.44
3	E	1102	AN	N3-C2-N1	-7.43	117.06	128.68
4	A	1103	JB	C30-N10-C09	7.39	130.77	123.86
3	B	1102	AN	N3-C2-N1	-7.26	117.33	128.68
4	C	1103	JB	C29-C30-N10	7.17	104.57	102.18
3	D	1102	AN	N3-C2-N1	-7.11	117.57	128.68
3	A	1102	AN	N3-C2-N1	-7.03	117.69	128.68
3	C	1102	AN	N3-C2-N1	-6.54	118.46	128.68
4	A	1103	JB	C29-C30-N10	6.40	104.31	102.18
3	F	1102	AN	N3-C2-N1	-6.37	118.72	128.68
3	C	1102	AN	C1'-N9-C4	-6.14	115.85	126.64
3	C	1102	AN	O1G-PG-N3B	-5.84	103.16	111.77
3	A	1102	AN	O1G-PG-N3B	-5.22	104.09	111.77
3	E	1102	AN	O2B-PB-O1B	4.86	120.11	109.92
3	B	1102	AN	C1'-N9-C4	-4.72	118.35	126.64
4	A	1103	JB	C04-N03-C02	-4.70	118.56	129.02
4	C	1103	JB	C04-N03-C02	-4.55	118.89	129.02
3	C	1102	AN	O2B-PB-O1B	4.37	119.08	109.92
3	F	1102	AN	O2B-PB-O1B	4.31	118.95	109.92
3	A	1102	AN	O2B-PB-O1B	4.29	118.91	109.92
3	B	1102	AN	O3G-PG-O2G	4.18	118.78	107.64
3	D	1102	AN	O3G-PG-O2G	4.12	118.60	107.64
3	F	1102	AN	O3G-PG-O2G	4.09	118.52	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1102	ANP	C1'-N9-C4	-4.05	119.52	126.64
3	C	1102	ANP	O3G-PG-O2G	4.03	118.38	107.64
3	D	1102	ANP	O2B-PB-O1B	4.01	118.34	109.92
4	F	1103	JBj	C29-C30-N10	4.00	103.51	102.18
4	D	1103	JBj	C04-N03-C02	-3.89	120.36	129.02
4	F	1103	JBj	C04-N03-C02	-3.83	120.50	129.02
4	E	1103	JBj	C29-C30-N10	3.82	103.45	102.18
3	A	1102	ANP	O3G-PG-O2G	3.75	117.64	107.64
4	E	1103	JBj	C04-N03-C02	-3.74	120.69	129.02
4	B	1103	JBj	C29-C30-N10	3.68	103.40	102.18
4	B	1103	JBj	C04-N03-C02	-3.65	120.90	129.02
3	E	1102	ANP	C1'-N9-C4	-3.63	120.27	126.64
3	B	1102	ANP	O2B-PB-O1B	3.62	117.52	109.92
3	E	1102	ANP	O3G-PG-O2G	3.45	116.82	107.64
3	B	1102	ANP	O2B-PB-O3A	3.42	116.04	104.64
3	D	1102	ANP	C1'-N9-C4	-3.36	120.75	126.64
3	A	1102	ANP	C1'-N9-C4	-3.27	120.90	126.64
4	E	1103	JBj	C17-C18-N19	-3.24	116.92	121.38
3	A	1102	ANP	O2B-PB-O3A	3.23	115.42	104.64
3	B	1102	ANP	C2'-C3'-C4'	-3.01	96.79	102.64
4	A	1103	JBj	O31-C11-C12	-2.97	122.90	128.68
4	D	1103	JBj	C17-C18-N19	-2.95	117.31	121.38
4	C	1103	JBj	O31-C11-C12	-2.95	122.95	128.68
3	C	1102	ANP	O1B-PB-N3B	-2.81	107.63	111.77
3	F	1102	ANP	O3G-PG-O1G	2.78	120.44	113.45
3	E	1102	ANP	O3G-PG-O1G	2.76	120.40	113.45
3	E	1102	ANP	O1B-PB-N3B	-2.76	107.70	111.77
3	D	1102	ANP	O3A-PB-N3B	-2.75	98.96	106.59
3	C	1102	ANP	O3G-PG-O1G	2.71	120.26	113.45
4	E	1103	JBj	C16-C15-C14	-2.70	116.68	121.36
4	B	1103	JBj	C28-C27-C14	-2.69	117.26	121.13
4	E	1103	JBj	O31-C11-C12	-2.66	123.50	128.68
3	F	1102	ANP	C4-C5-N7	-2.64	106.65	109.40
3	A	1102	ANP	O3A-PB-N3B	-2.63	99.30	106.59
3	B	1102	ANP	O3A-PB-N3B	-2.57	99.46	106.59
3	F	1102	ANP	C2'-C3'-C4'	-2.56	97.68	102.64
4	D	1103	JBj	F35-C34-C33	2.53	121.87	118.25
4	E	1103	JBj	C02-C09-N10	-2.53	106.54	110.16
3	B	1102	ANP	C4-C5-N7	-2.52	106.77	109.40
4	B	1103	JBj	O31-C11-C12	-2.51	123.81	128.68
4	E	1103	JBj	C36-C34-C33	-2.47	120.09	123.29
4	B	1103	JBj	C24-N19-C18	-2.45	111.47	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	JB	C29-C12-C11	-2.42	107.65	108.94
4	C	1103	JB	C20-N19-C18	-2.41	111.57	118.09
4	D	1103	JB	C16-C15-C14	-2.41	117.18	121.36
3	A	1102	ANP	O4'-C4'-C3'	-2.36	100.45	105.11
4	C	1103	JB	C24-N19-C18	-2.35	111.74	118.09
3	C	1102	ANP	C4-C5-N7	-2.34	106.96	109.40
4	C	1103	JB	C28-C27-C14	-2.33	117.78	121.13
4	F	1103	JB	O31-C11-C12	-2.32	124.16	128.68
4	C	1103	JB	C17-C18-N19	-2.32	118.18	121.38
4	F	1103	JB	C36-C34-C33	-2.31	120.28	123.29
4	E	1103	JB	C29-C12-C11	2.28	110.16	108.94
4	C	1103	JB	C32-C33-C34	2.26	121.53	118.59
3	A	1102	ANP	C4-C5-N7	-2.26	107.05	109.40
4	A	1103	JB	C02-C09-N10	-2.25	106.94	110.16
3	A	1102	ANP	O3G-PG-O1G	2.22	119.03	113.45
4	D	1103	JB	C29-C30-N10	2.21	102.92	102.18
4	B	1103	JB	C16-C15-C14	-2.18	117.58	121.36
3	E	1102	ANP	C5-C6-N6	-2.18	117.05	120.35
4	E	1103	JB	C32-C33-C34	2.17	121.41	118.59
4	B	1103	JB	C20-N19-C18	-2.15	112.28	118.09
3	B	1102	ANP	PA-O3A-PB	-2.12	125.14	132.62
4	B	1103	JB	C38-C32-C09	2.12	123.65	120.58
4	E	1103	JB	C28-C27-C14	-2.11	118.10	121.13
3	D	1102	ANP	C2'-C3'-C4'	-2.11	98.55	102.64
4	C	1103	JB	C37-C38-C32	2.06	122.29	120.41
3	D	1102	ANP	C4-C5-N7	-2.06	107.26	109.40
4	C	1103	JB	C16-C15-C14	-2.04	117.81	121.36
3	C	1102	ANP	O2'-C2'-C3'	-2.04	105.21	111.82
3	C	1102	ANP	C5-C6-N6	-2.04	117.25	120.35
3	B	1102	ANP	O3G-PG-O1G	2.04	118.58	113.45

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1102	ANP	PG-N3B-PB-O3A
3	E	1102	ANP	PA-O3A-PB-O1B
3	E	1102	ANP	PA-O3A-PB-O2B
3	C	1102	ANP	PB-N3B-PG-O1G
3	C	1102	ANP	PG-N3B-PB-O3A
3	C	1102	ANP	PA-O3A-PB-O1B
3	C	1102	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	A	1102	ANP	PB-N3B-PG-O1G
3	B	1102	ANP	PB-N3B-PG-O1G
3	B	1102	ANP	PA-O3A-PB-O1B
3	B	1102	ANP	PA-O3A-PB-O2B
3	F	1102	ANP	PB-N3B-PG-O1G
3	D	1102	ANP	PG-N3B-PB-O3A
4	C	1103	JBj	C17-C18-N19-C20
4	C	1103	JBj	C25-C18-N19-C20
4	A	1103	JBj	N10-C09-C32-C33
3	A	1102	ANP	PG-N3B-PB-O3A
4	B	1103	JBj	C02-C09-C32-C38
4	C	1103	JBj	C02-C09-C32-C38
4	E	1103	JBj	C25-C18-N19-C24
4	E	1103	JBj	C17-C18-N19-C24
4	D	1103	JBj	N10-C09-C32-C33
4	A	1103	JBj	N10-C09-C32-C38
4	D	1103	JBj	N10-C09-C32-C38
4	B	1103	JBj	C02-C09-C32-C33
4	E	1103	JBj	C02-C09-C32-C33
3	F	1102	ANP	PG-N3B-PB-O3A
4	A	1103	JBj	C02-C09-C32-C38
4	F	1103	JBj	C02-C09-C32-C38
4	E	1103	JBj	C02-C09-C32-C38

All (1) ring outliers are listed below:

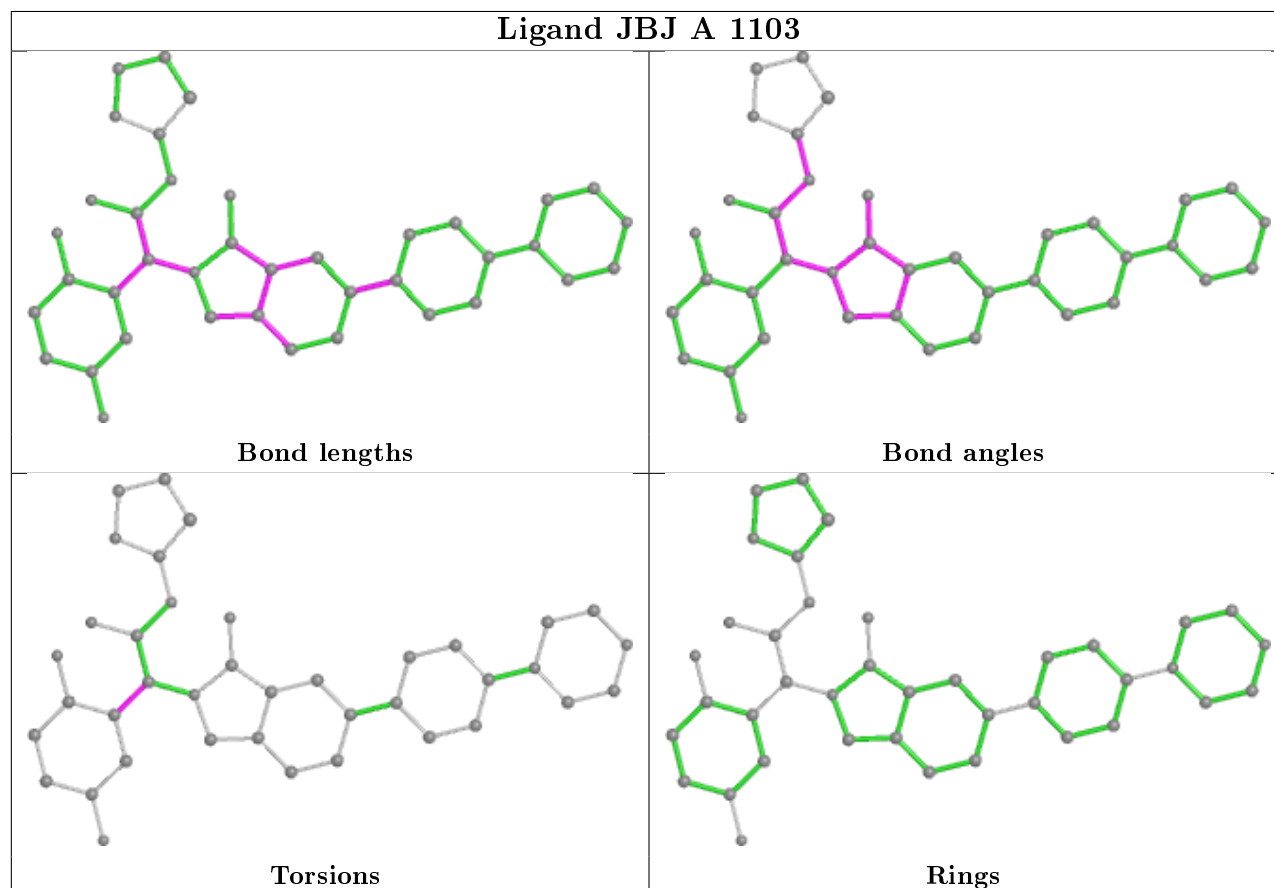
Mol	Chain	Res	Type	Atoms
4	C	1103	JBj	C20-C21-C23-C24-N19-N22

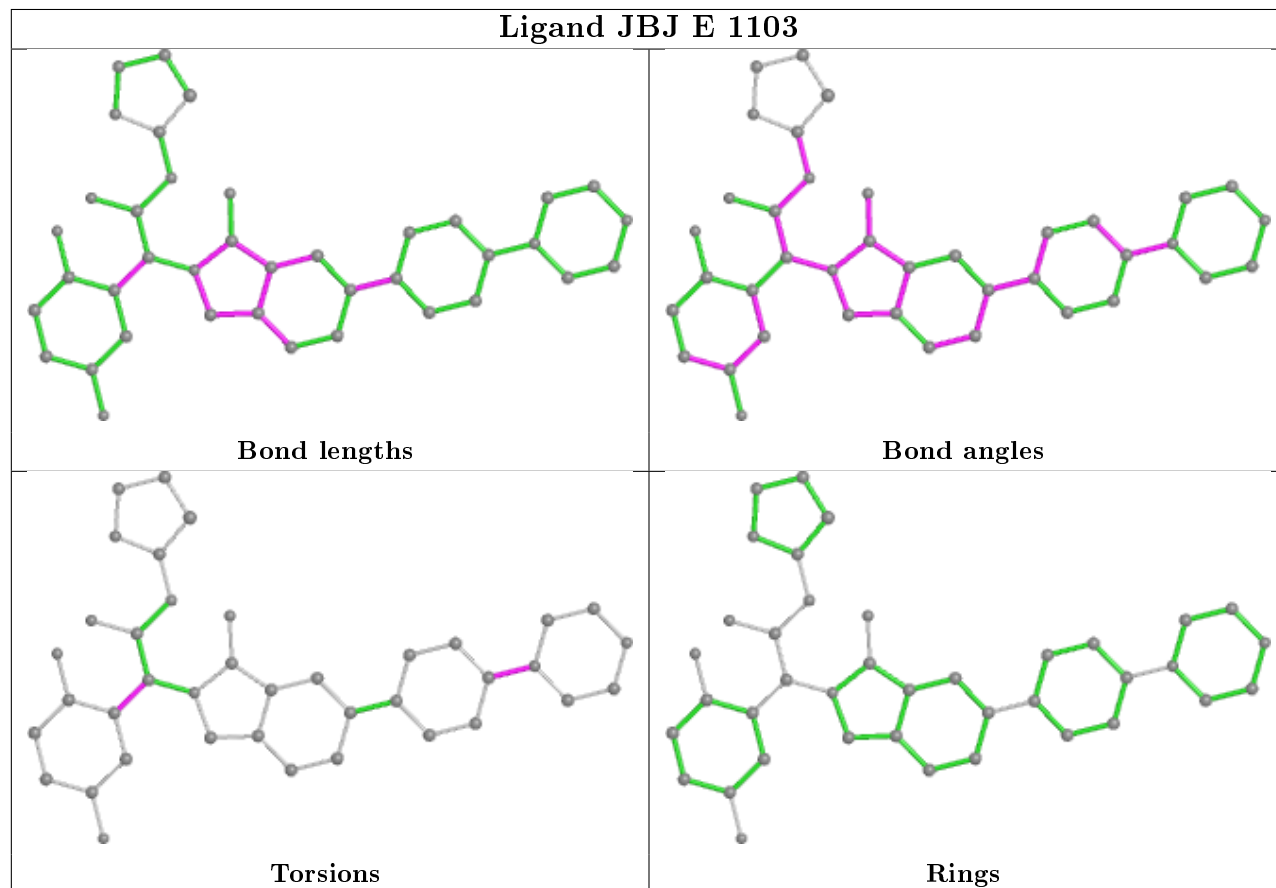
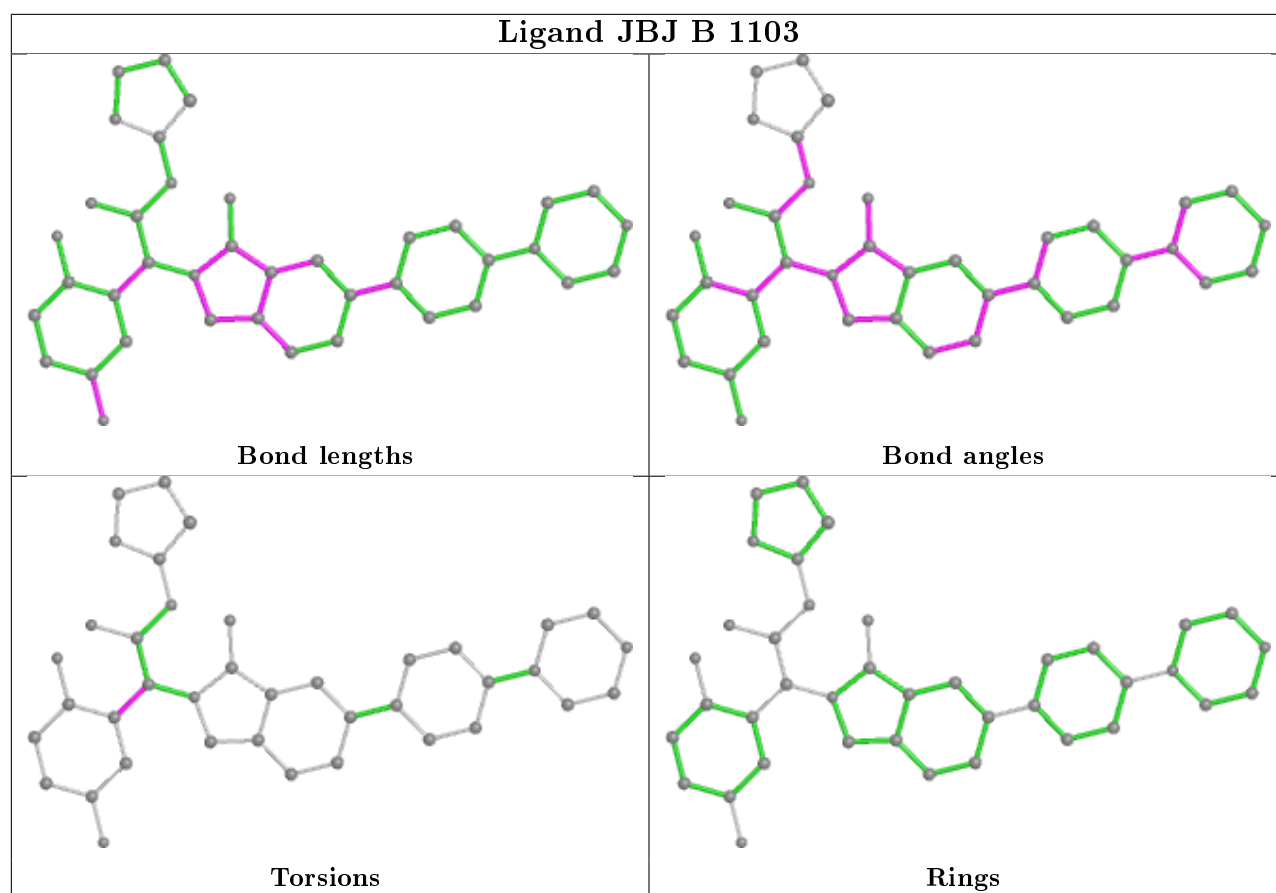
4 monomers are involved in 6 short contacts:

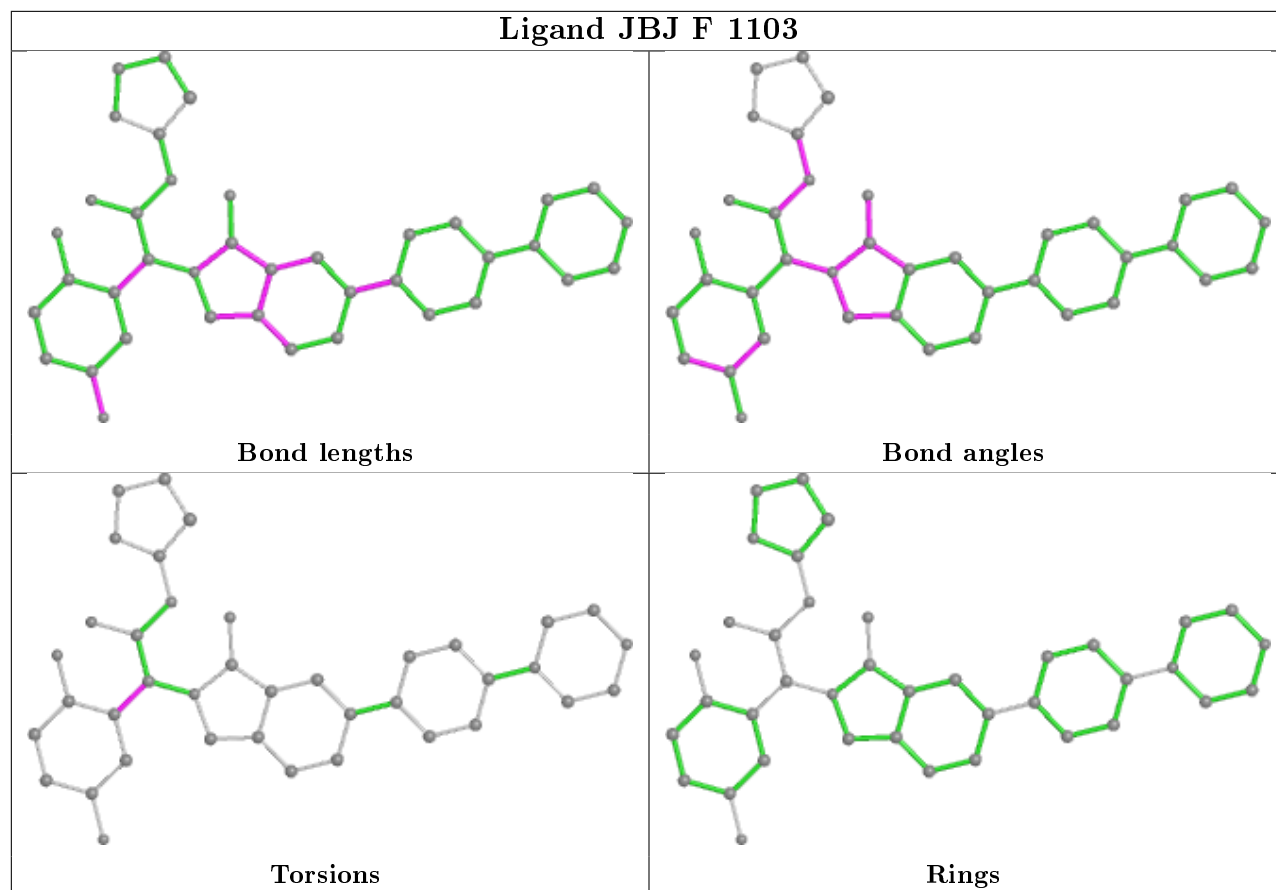
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	JBj	1	0
4	B	1103	JBj	1	0
4	E	1103	JBj	3	0
4	C	1103	JBj	1	0

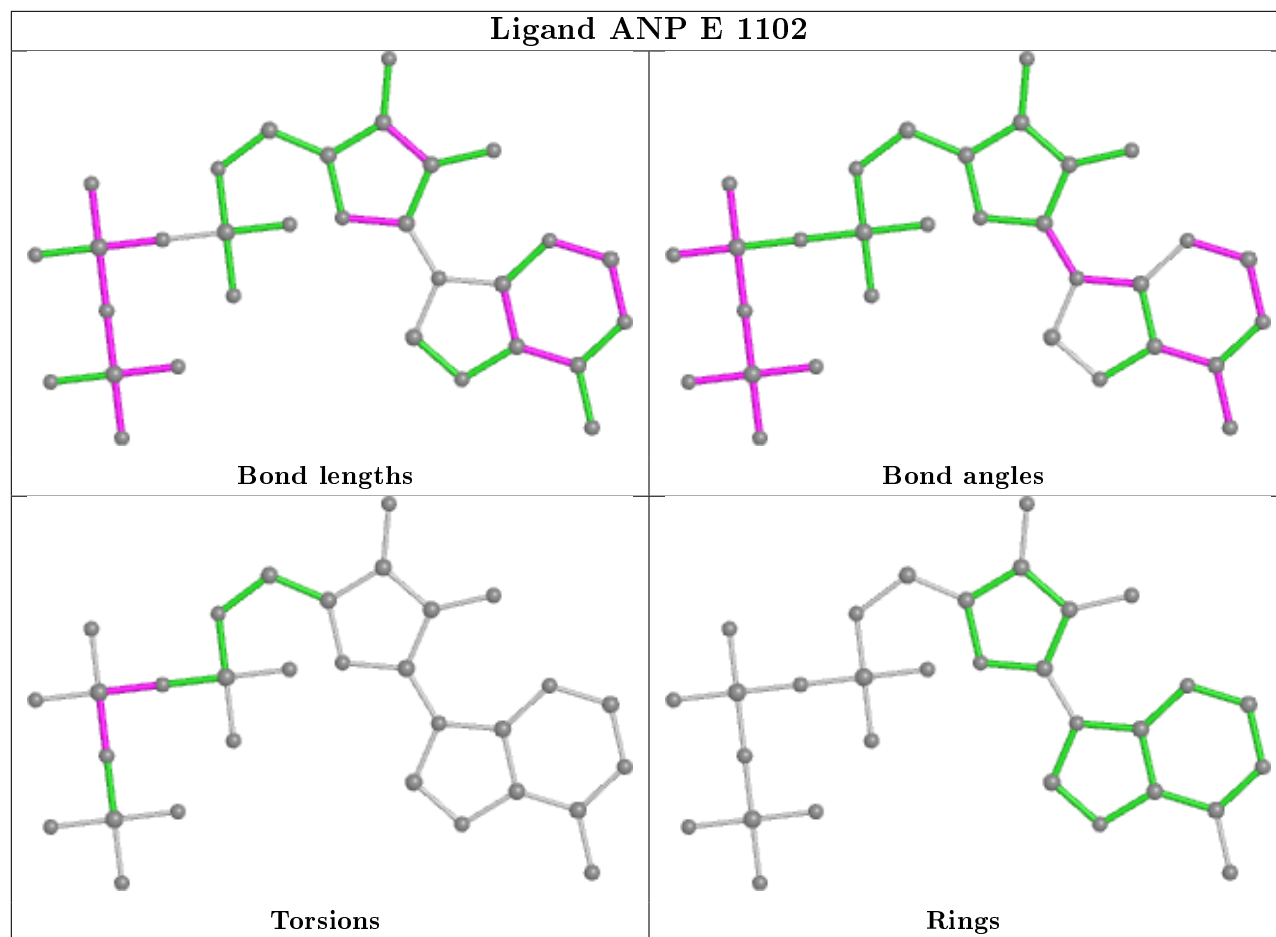
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

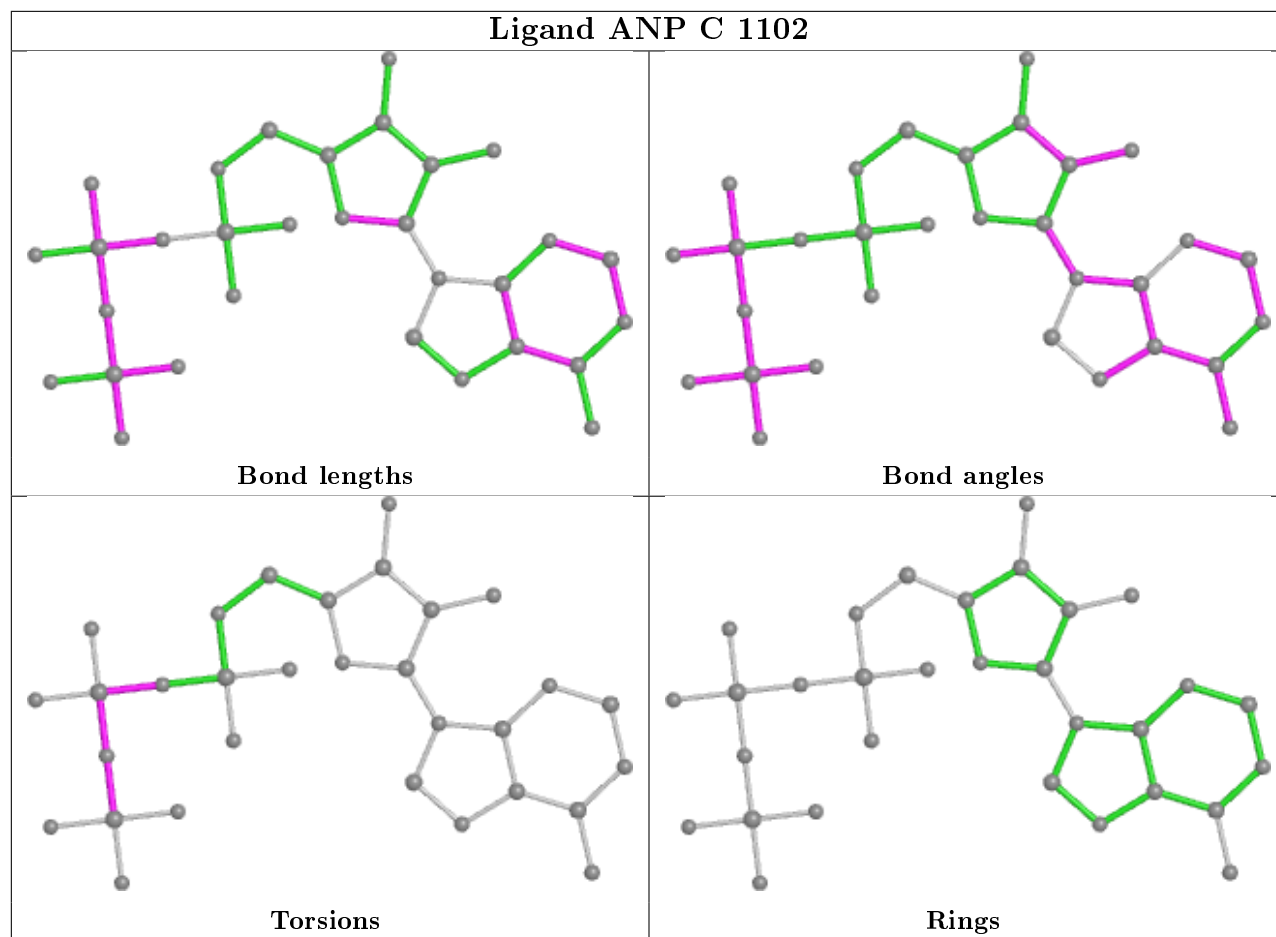
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

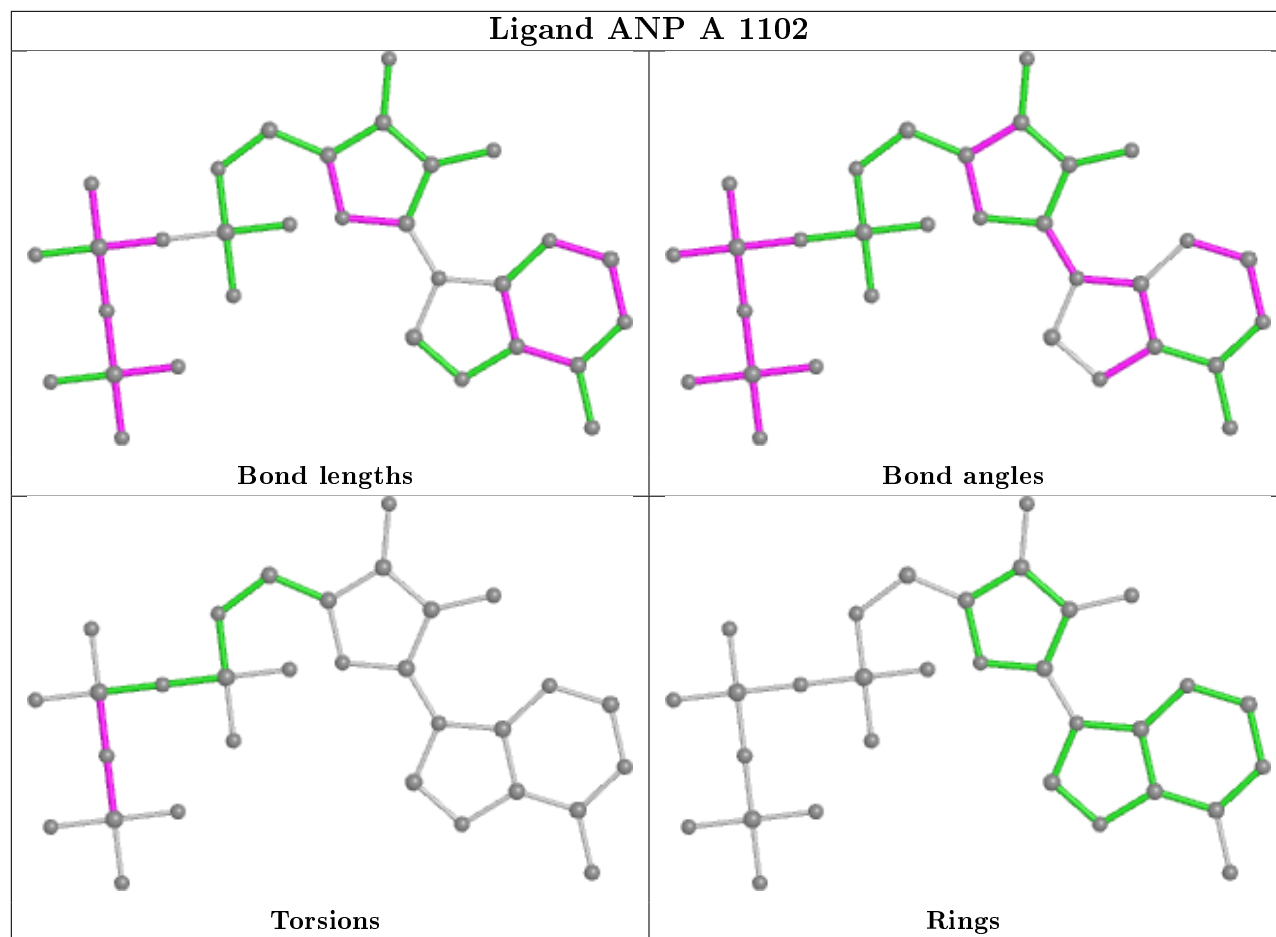


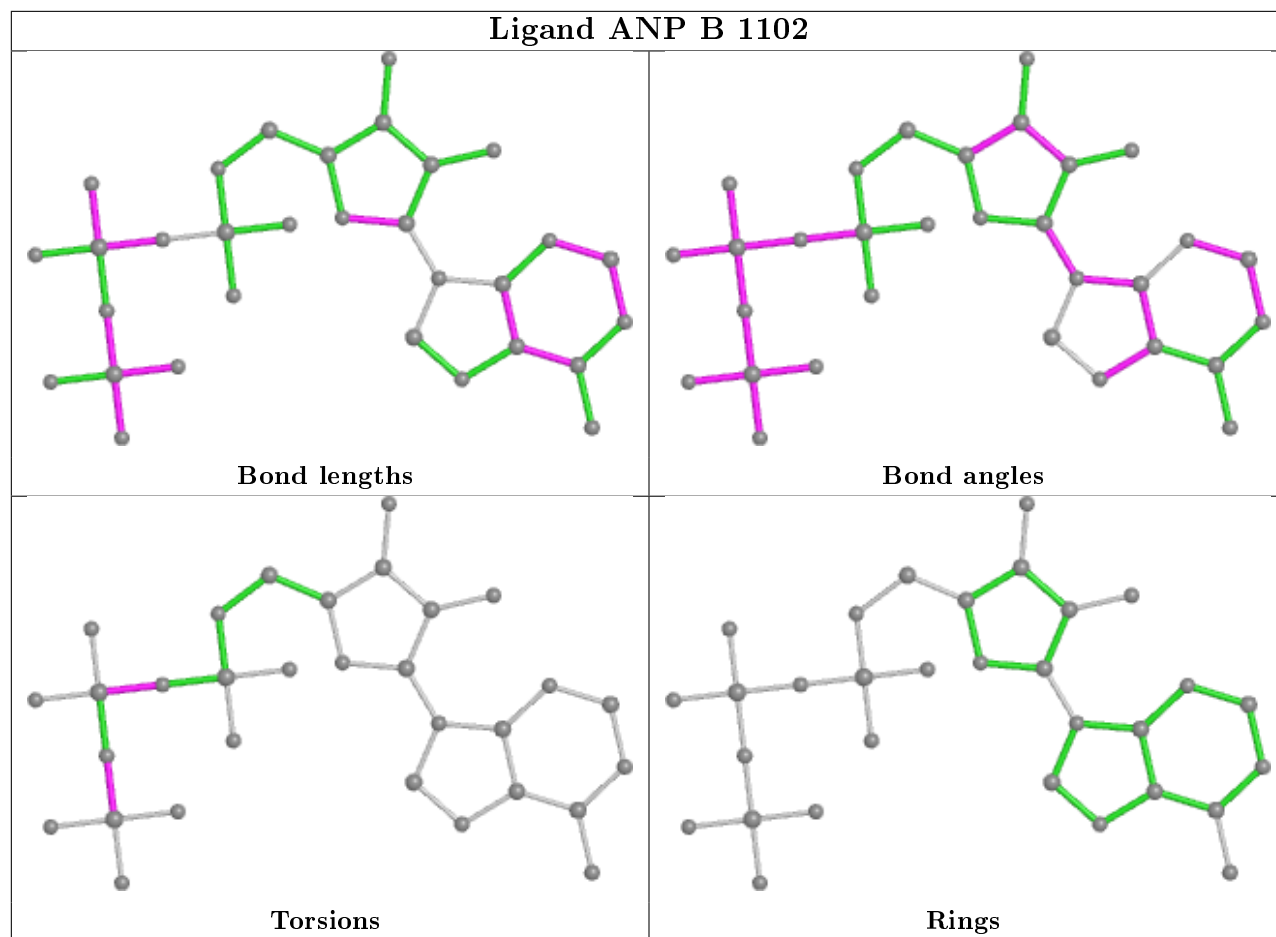


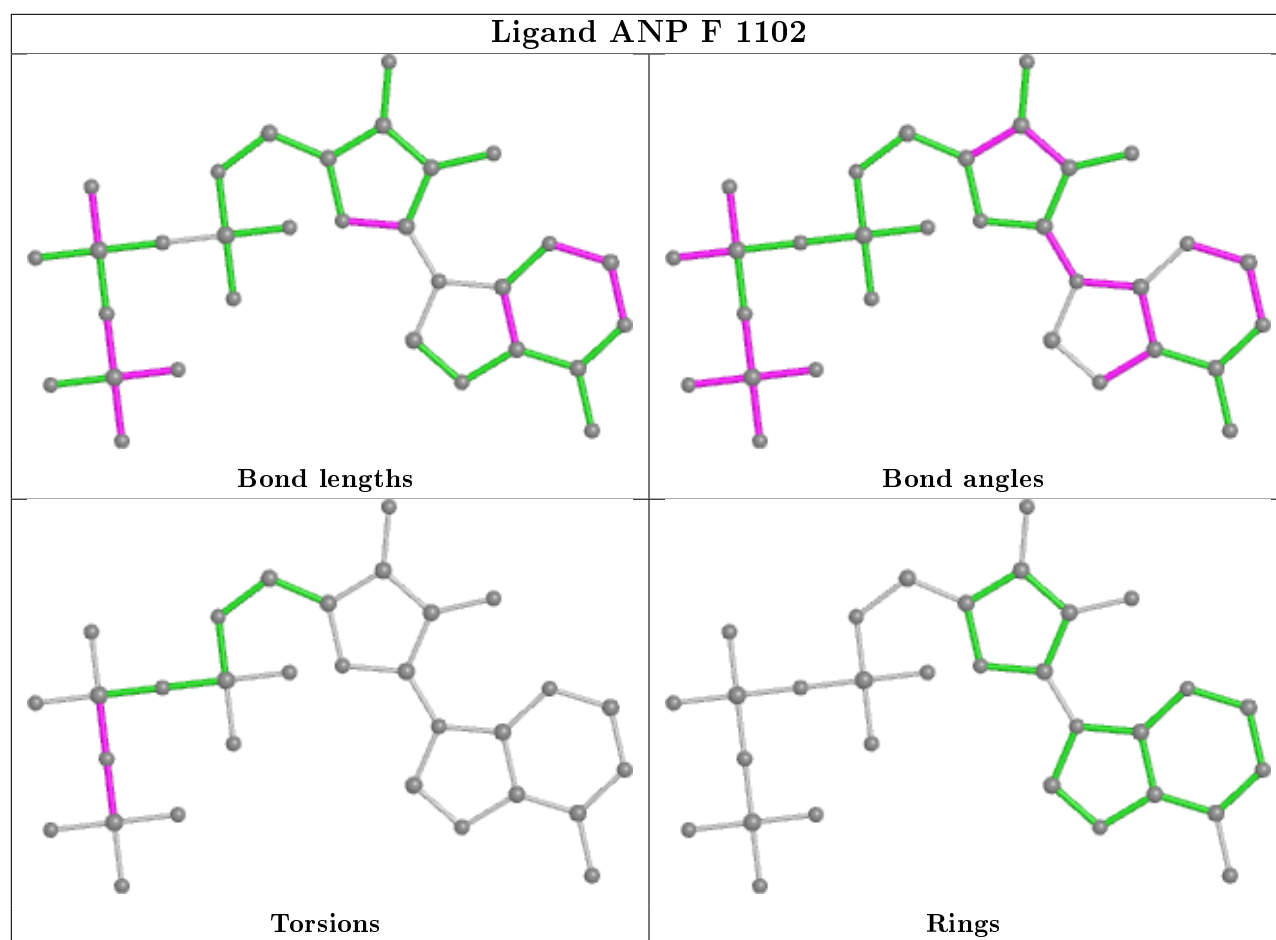


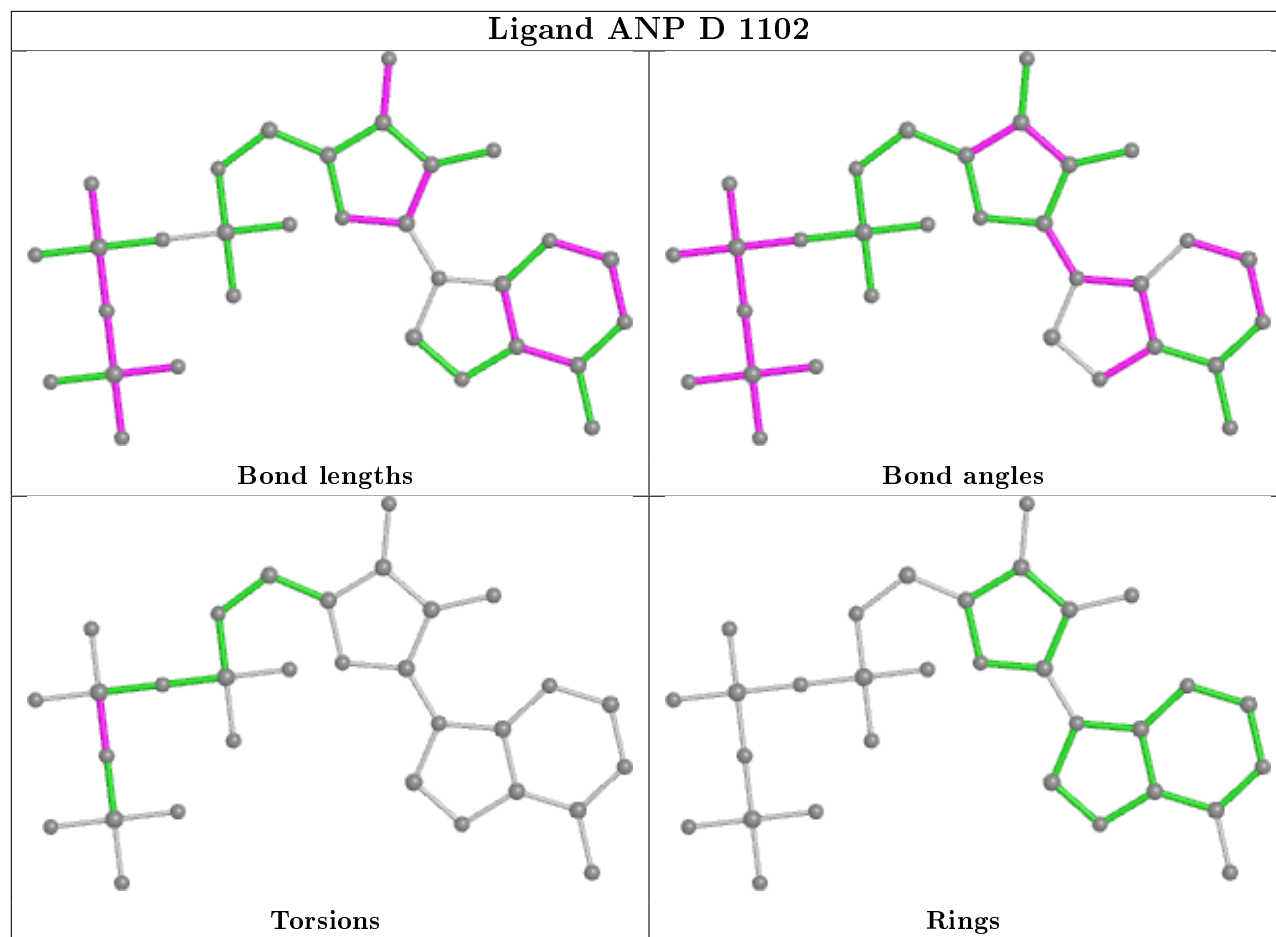


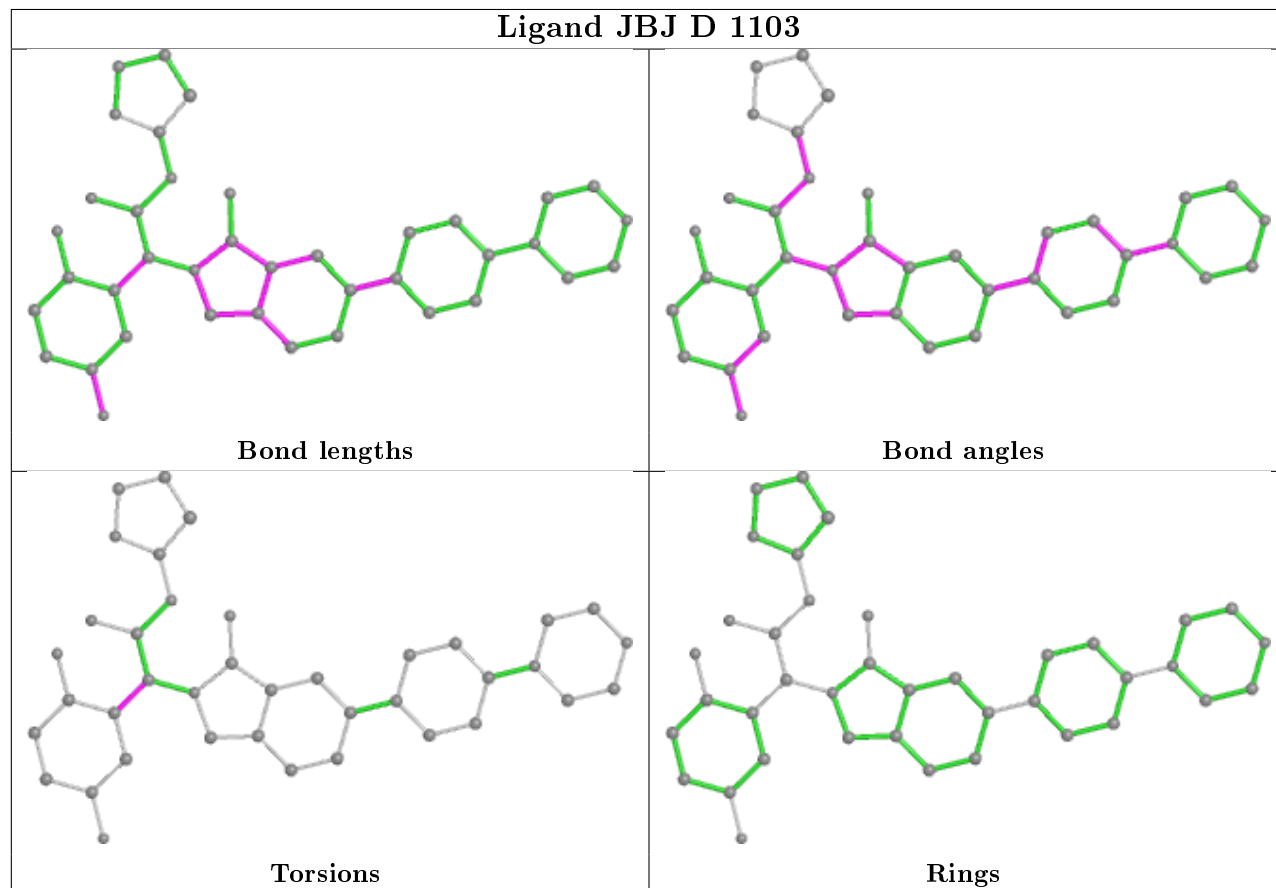
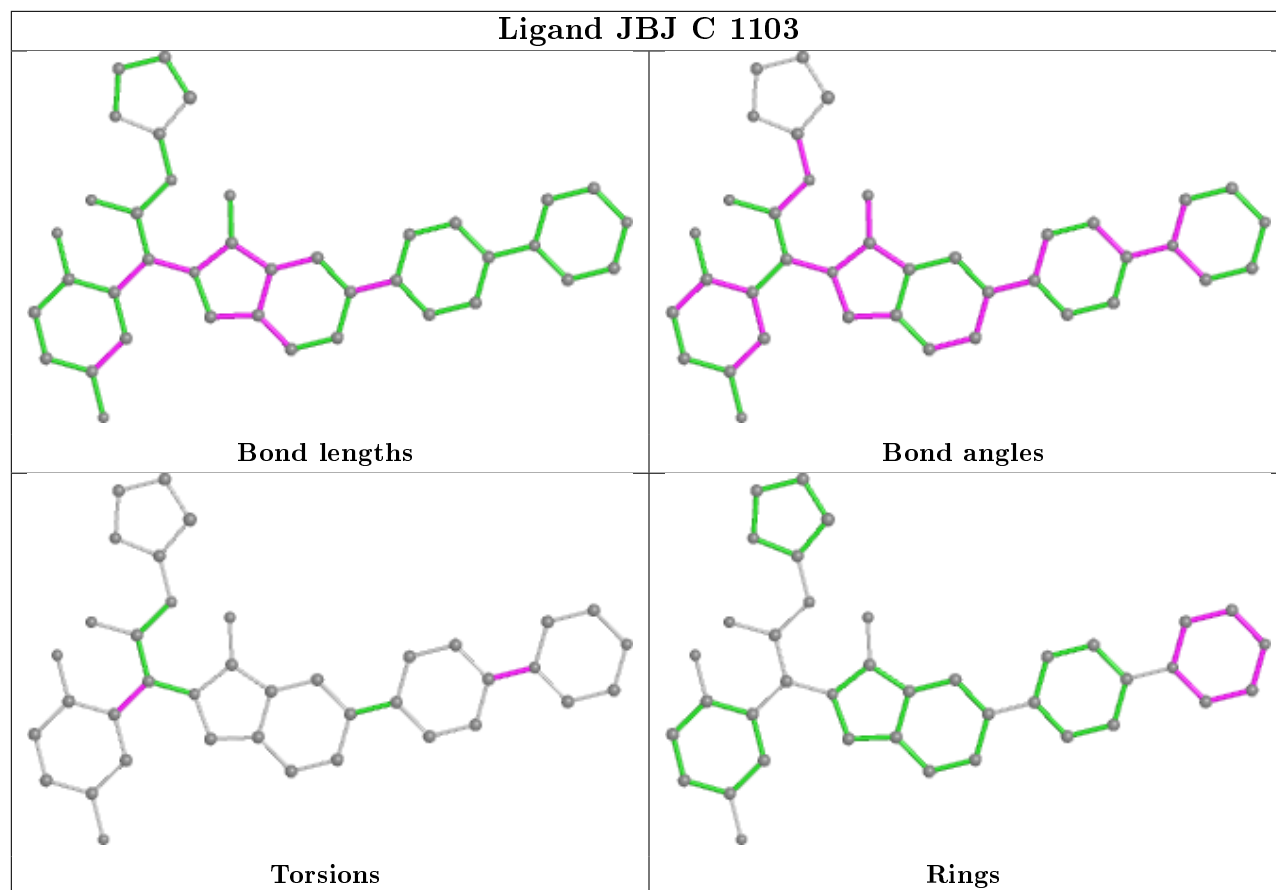












5.7 Other polymers [i](#)

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	306/331 (92%)	-0.34	1 (0%) 94 93	20, 32, 50, 63	0
1	B	296/331 (89%)	-0.08	2 (0%) 87 86	28, 44, 71, 84	0
1	C	295/331 (89%)	0.01	6 (2%) 65 63	28, 48, 69, 75	0
1	D	307/331 (92%)	-0.26	5 (1%) 72 70	22, 35, 59, 84	0
1	E	298/331 (90%)	-0.25	3 (1%) 82 81	24, 40, 61, 76	0
1	F	298/331 (90%)	-0.01	11 (3%) 41 39	27, 47, 68, 91	0
All	All	1800/1986 (90%)	-0.16	28 (1%) 72 70	20, 40, 66, 91	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	988	HIS	4.2
1	F	988	HIS	3.4
1	D	872	GLU	3.4
1	F	989	LEU	3.2
1	B	988	HIS	3.1
1	E	698	ALA	3.1
1	F	986	ARG	3.0
1	F	987	MET	3.0
1	B	859	ALA	3.0
1	D	876	VAL	3.0
1	F	981	ILE	2.8
1	D	871	ALA	2.8
1	E	859	ALA	2.8
1	C	983	GLY	2.6
1	F	917	GLY	2.5
1	F	890	ILE	2.5
1	C	887	LEU	2.5
1	F	863	GLY	2.5
1	D	870	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	980	VAL	2.2
1	C	886	ILE	2.1
1	C	923	ILE	2.1
1	D	873	GLY	2.1
1	F	936	PRO	2.1
1	C	926	ILE	2.0
1	E	862	LEU	2.0
1	F	1009	ASP	2.0
1	F	943	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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.

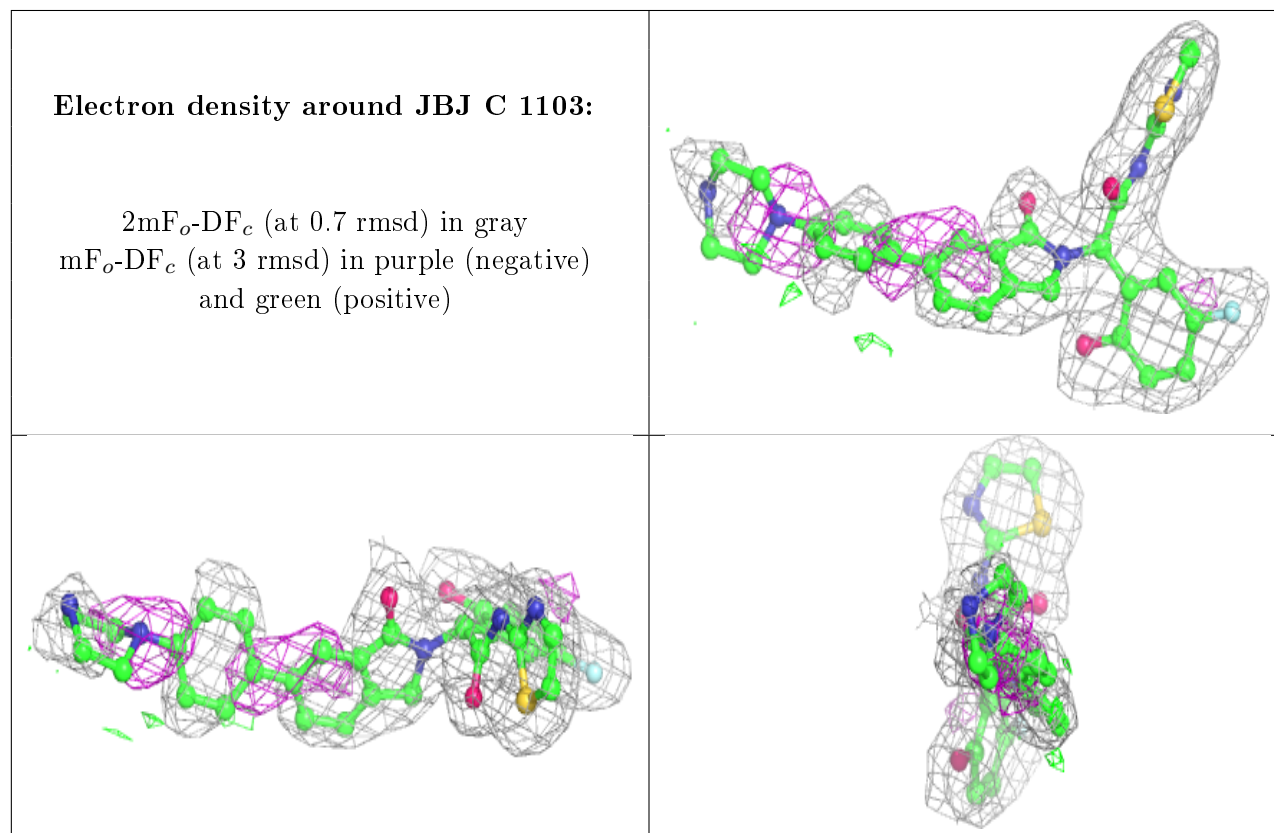
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	F	1101	1/1	0.83	0.13	39,39,39,39	0
2	MG	D	1101	1/1	0.83	0.21	26,26,26,26	0
2	MG	A	1101	1/1	0.84	0.10	24,24,24,24	0
2	MG	E	1101	1/1	0.85	0.13	30,30,30,30	0
4	JBj	C	1103	39/39	0.86	0.21	29,38,61,63	0
4	JBj	B	1103	39/39	0.88	0.22	35,42,70,74	0
4	JBj	E	1103	39/39	0.90	0.16	27,35,54,57	0
4	JBj	F	1103	39/39	0.93	0.14	29,37,66,69	0
2	MG	C	1101	1/1	0.93	0.12	40,40,40,40	0
2	MG	B	1101	1/1	0.96	0.14	39,39,39,39	0
3	ANP	F	1102	31/31	0.96	0.10	26,36,44,52	0
3	ANP	B	1102	31/31	0.96	0.11	32,39,44,48	0
4	JBj	D	1103	39/39	0.96	0.12	23,29,52,54	0
4	JBj	A	1103	39/39	0.97	0.10	20,25,34,37	0

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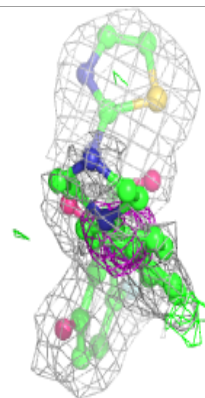
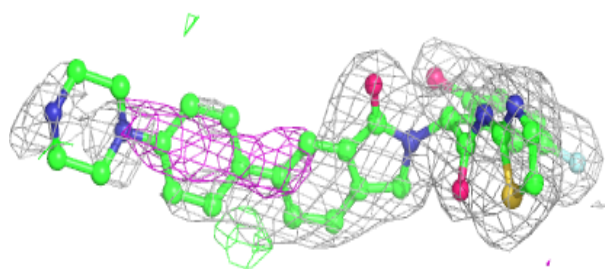
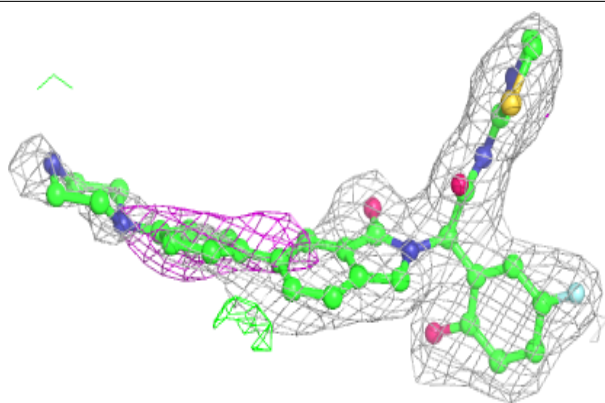
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ANP	C	1102	31/31	0.97	0.10	28,35,44,56	0
3	ANP	D	1102	31/31	0.98	0.13	22,27,31,33	0
3	ANP	E	1102	31/31	0.98	0.11	23,31,42,46	0
3	ANP	A	1102	31/31	0.98	0.12	20,24,26,33	0

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.

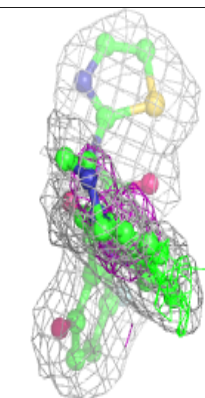
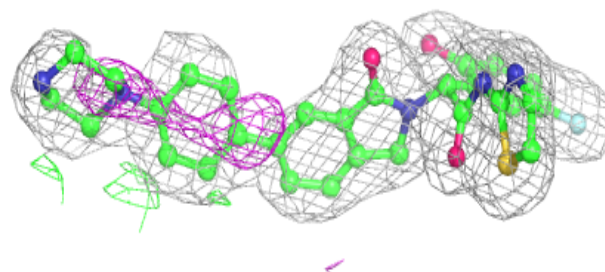
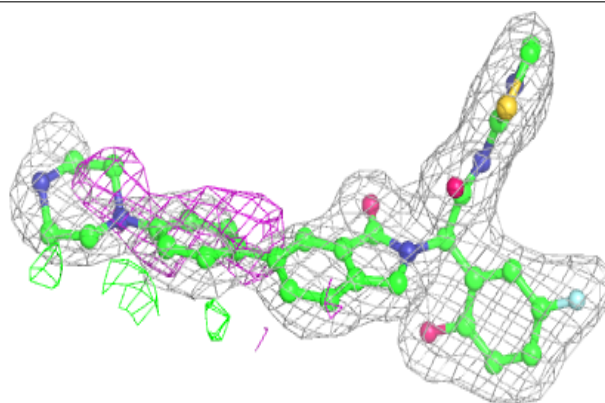


Electron density around JBJ B 1103:

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

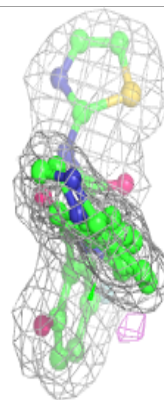
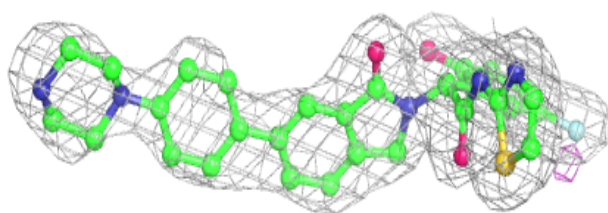
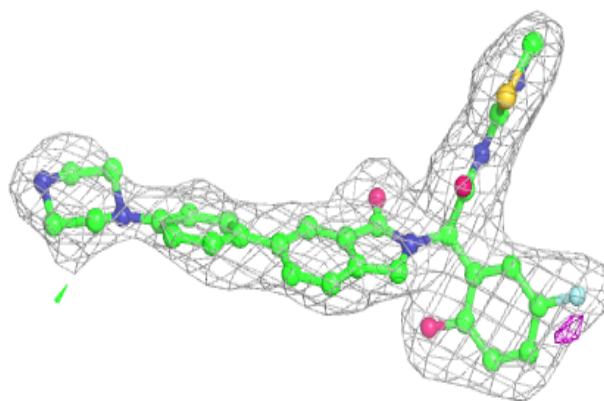
**Electron density around JBJ E 1103:**

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

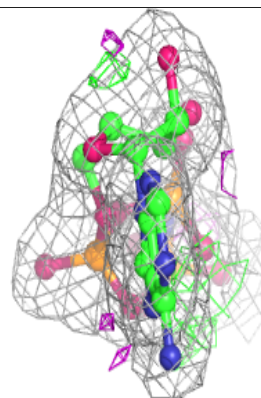
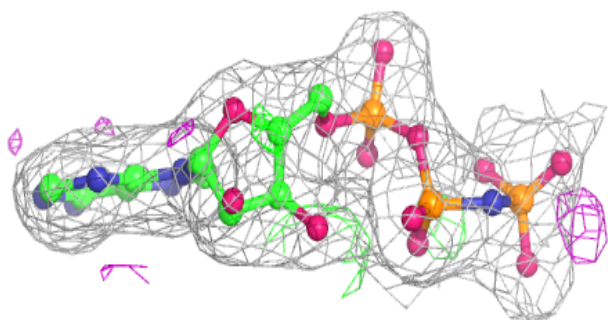
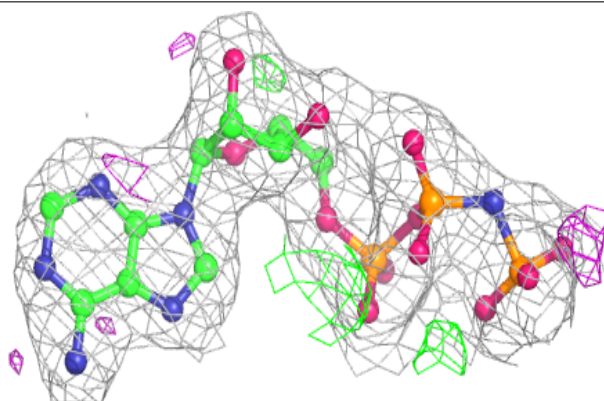


Electron density around JBJ F 1103:

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

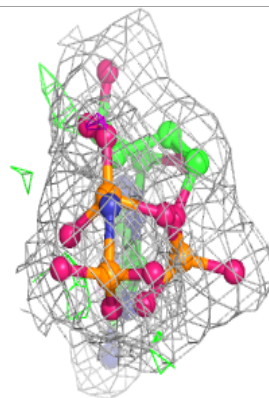
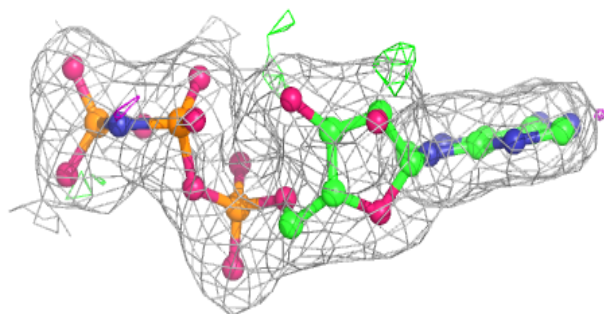
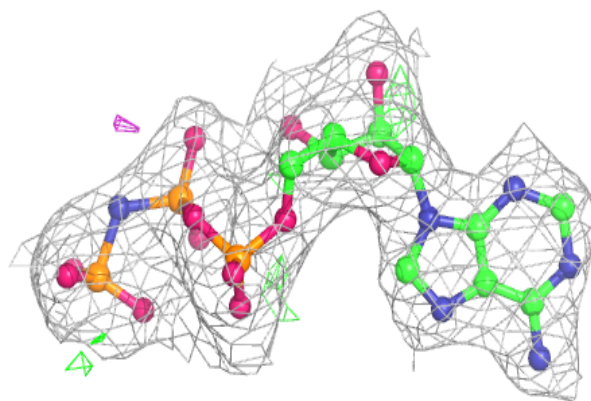
**Electron density around ANP F 1102:**

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

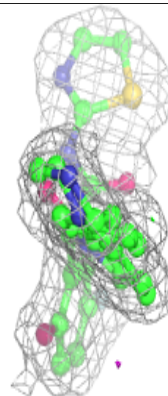
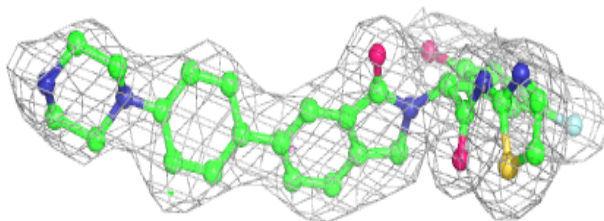
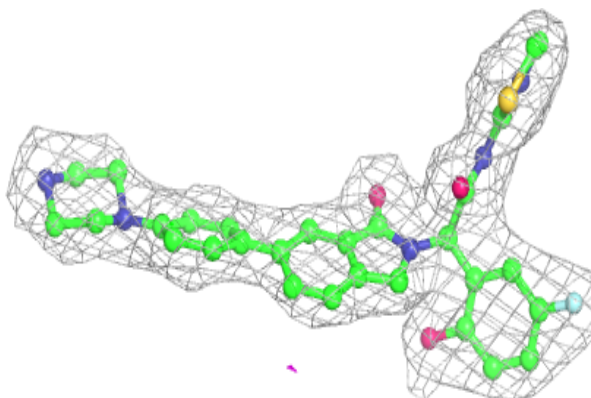


Electron density around ANP B 1102:

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

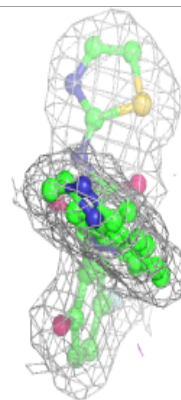
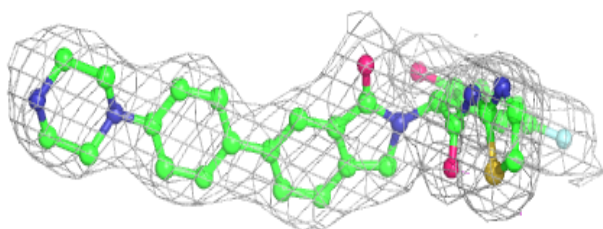
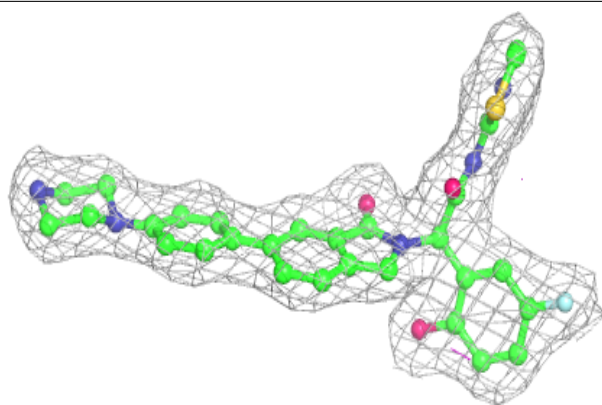
**Electron density around JBJ D 1103:**

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

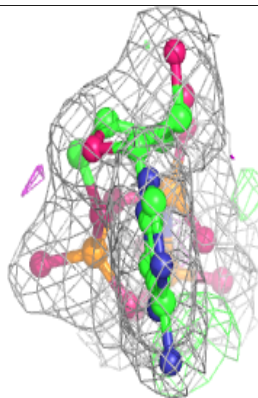
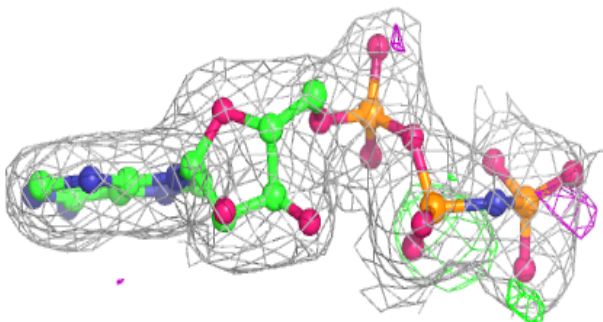
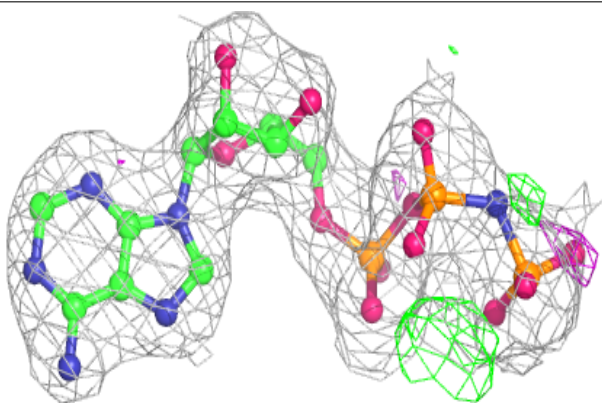


Electron density around JBJ A 1103:

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

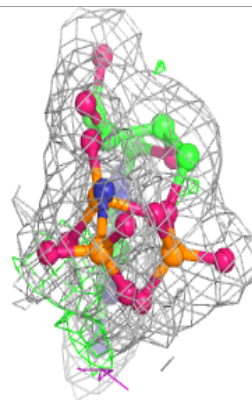
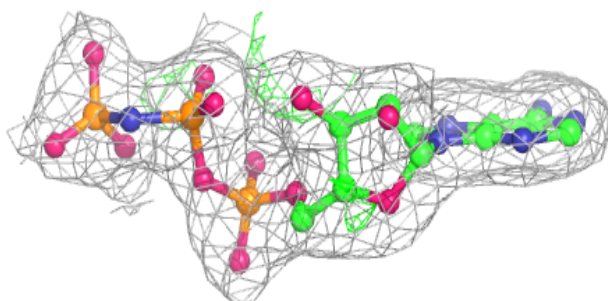
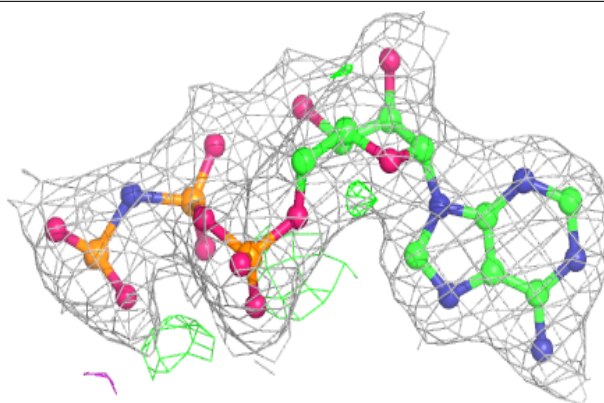
**Electron density around ANP C 1102:**

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

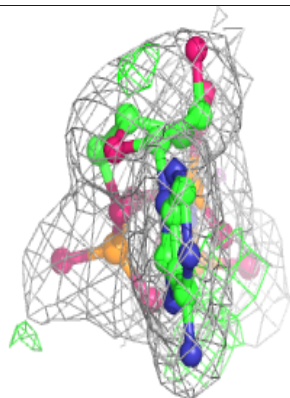
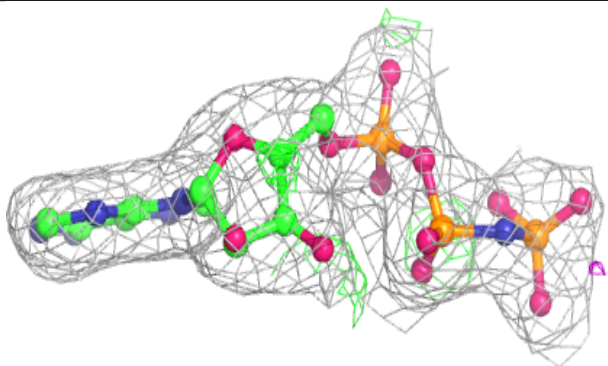
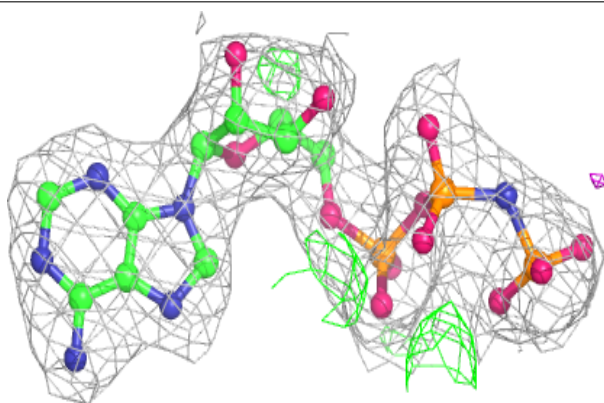


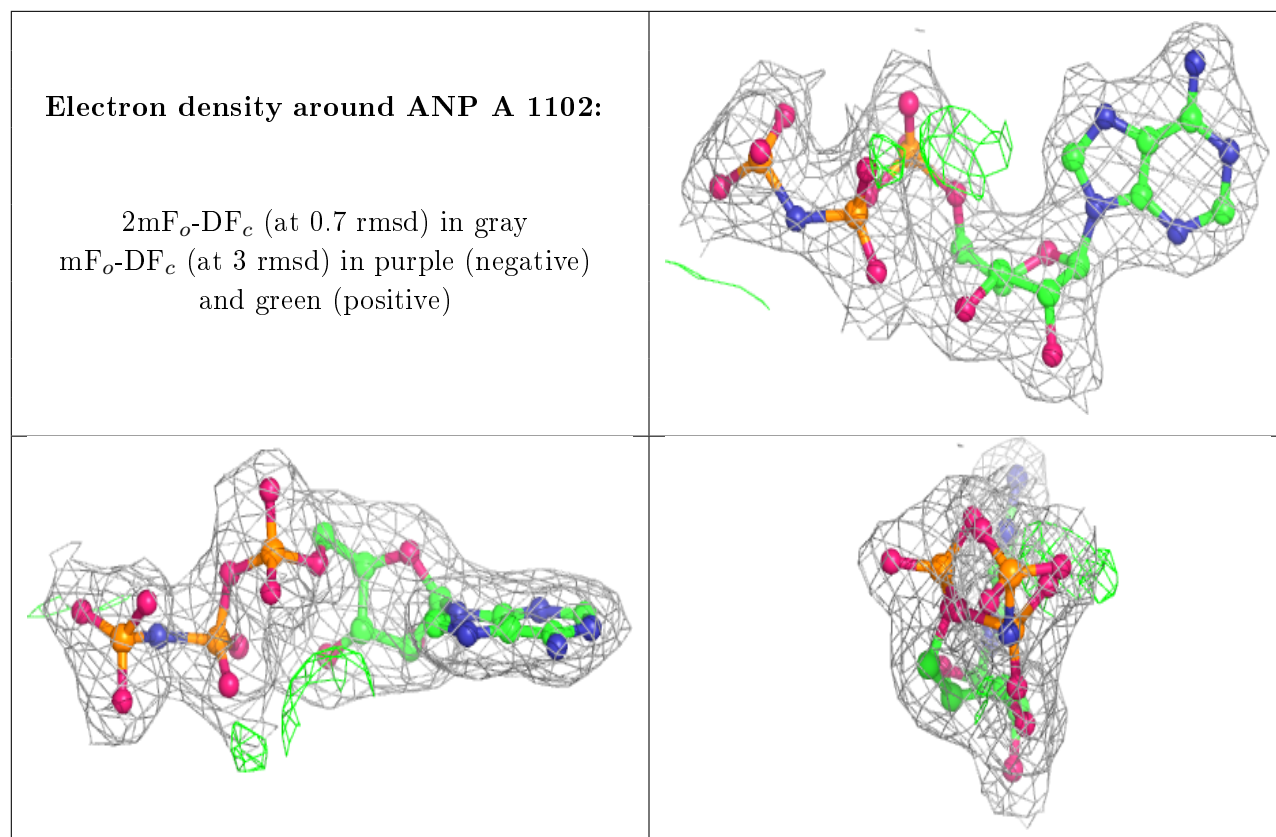
Electron density around ANP D 1102:

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

**Electron density around ANP E 1102:**

$2mF_o-DF_c$ (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.