



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 12:56 PM EDT

PDB ID : 7JXP
Title : EGFR kinase (T790M/V948R) in complex with osimertinib and JBJ-04-125-02
Authors : Beyett, T.S.; Eck, M.J.
Deposited on : 2020-08-27
Resolution : 2.16 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 : 2.23.1
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) : 2.23.1

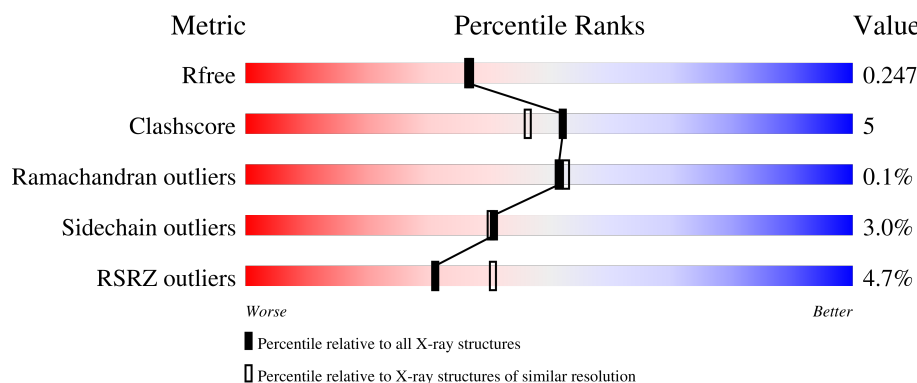
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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.



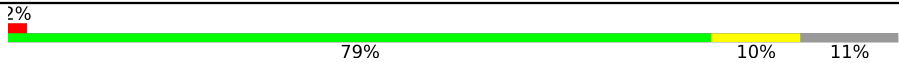
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	B	331	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	C	331	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>12%</div> </div> </div>
1	D	331	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>11%</div> </div> </div>
1	E	331	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>• 13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	331	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '79%', a yellow segment labeled '10%', and a grey segment at the end labeled '11%'.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15137 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	D	294	Total	C	N	O	S	0	1	0
			2377	1528	404	425	20			
1	A	308	Total	C	N	O	S	0	1	0
			2483	1593	422	448	20			
1	C	292	Total	C	N	O	S	0	2	0
			2368	1521	402	424	21			
1	F	294	Total	C	N	O	S	0	1	0
			2377	1528	404	425	20			
1	B	308	Total	C	N	O	S	0	1	0
			2483	1593	422	448	20			
1	E	287	Total	C	N	O	S	0	1	0
			2314	1488	391	416	19			

There are 30 discrepancies between the modelled and reference sequences:

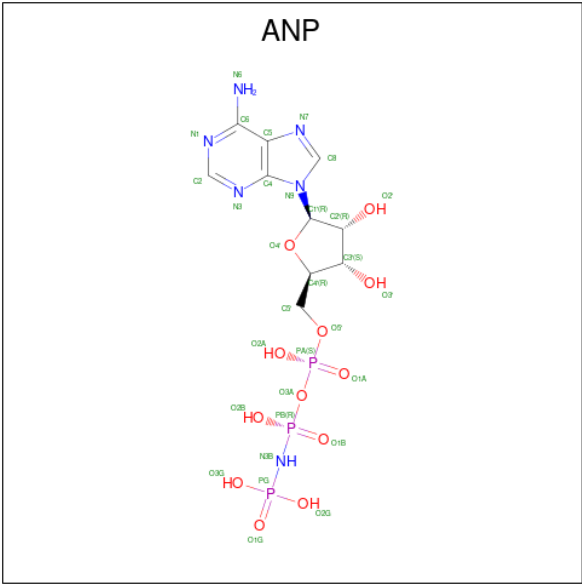
Chain	Residue	Modelled	Actual	Comment	Reference
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	694	THR	-	expression tag	UNP P00533
F	790	MET	THR	engineered mutation	UNP P00533
F	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
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

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

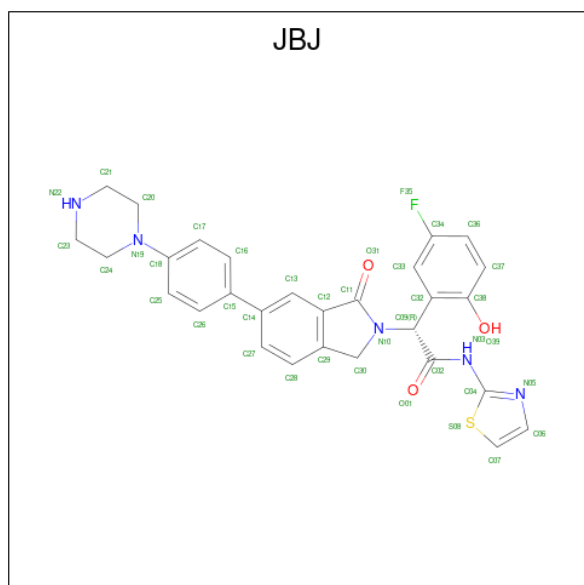


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

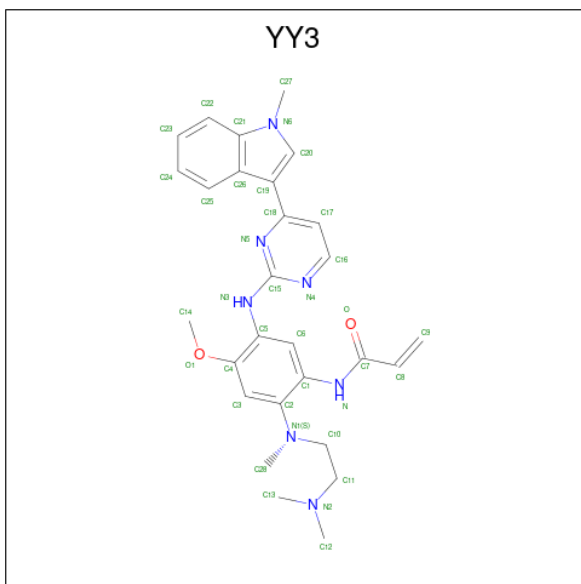
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- 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) (labeled as "Ligand of Interest" by depositor).



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

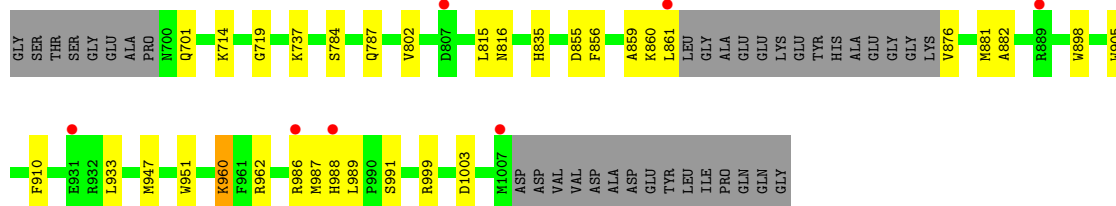
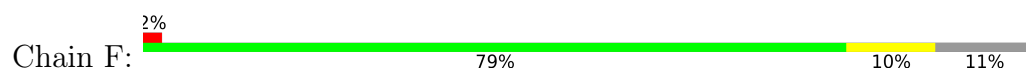
- Molecule 5 is N-(2-{[2-(dimethylamino)ethyl](methyl)amino}-4-methoxy-5-{[4-(1-methyl-1H-indol-3-yl)pyrimidin-2-yl]amino}phenyl)prop-2-enamide (three-letter code: YY3) (formula: C₂₈H₃₃N₇O₂) (labeled as "Ligand of Interest" by depositor).



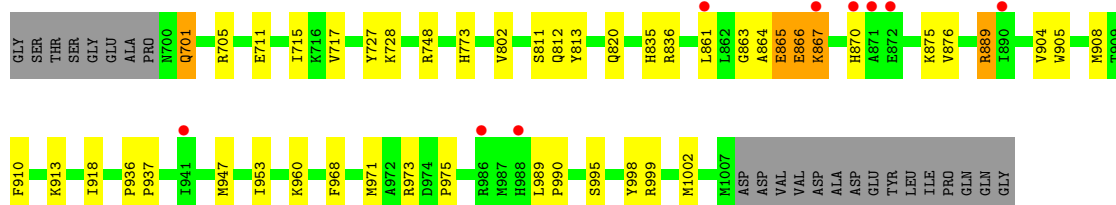
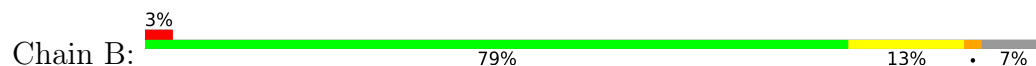
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			37	28	7	2		
5	E	1	Total	C	N	O	0	0
			37	28	7	2		

- Molecule 6 is water.

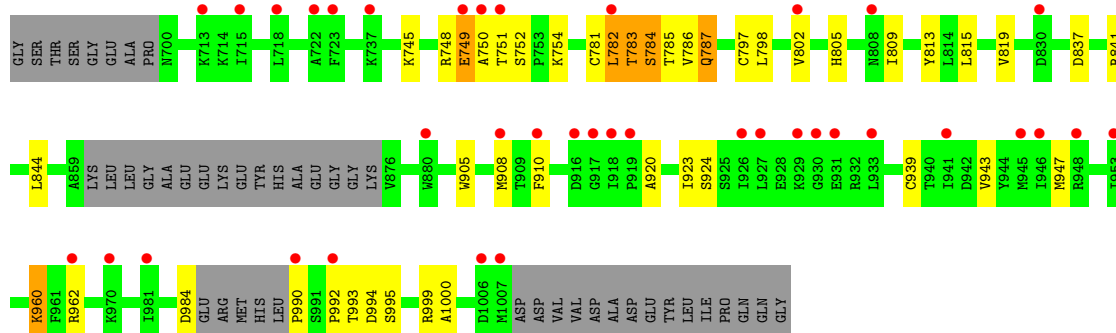
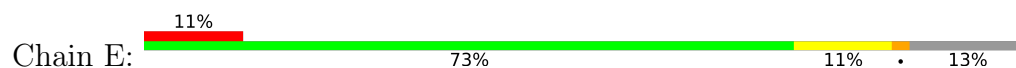
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	68	Total	O	0	0
			68	68		
6	A	91	Total	O	0	0
			91	91		
6	C	43	Total	O	0	0
			43	43		
6	F	40	Total	O	0	0
			40	40		
6	B	41	Total	O	0	0
			41	41		
6	E	16	Total	O	0	0
			16	16		



- 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	57.11Å 94.74Å 95.57Å 70.56° 78.40° 79.18°	Depositor
Resolution (Å)	89.11 – 2.16 89.11 – 2.16	Depositor EDS
% Data completeness (in resolution range)	83.1 (89.11-2.16) 83.1 (89.11-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.212 , 0.247 0.214 , 0.247	Depositor DCC
R_{free} test set	4040 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.169 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15137	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 41.15 % 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 2.4646e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, YY3, 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	0.48	0/2541	0.65	0/3433
1	B	0.50	0/2541	0.66	0/3433
1	C	0.44	0/2423	0.62	0/3275
1	D	0.49	0/2432	0.65	1/3287 (0.0%)
1	E	0.43	0/2367	0.65	0/3199
1	F	0.46	0/2432	0.62	0/3287
All	All	0.47	0/14736	0.64	1/19914 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	802	VAL	CG1-CB-CG2	-5.78	101.64	110.90

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	2483	0	2527	37	0
1	B	2483	0	2527	30	0
1	C	2368	0	2413	28	0
1	D	2377	0	2430	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2314	0	2359	27	0
1	F	2377	0	2430	17	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
2	D	31	0	13	1	0
2	F	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	A	39	0	0	1	0
4	B	39	0	0	0	0
4	C	39	0	0	0	0
4	D	39	0	0	0	0
4	E	39	0	0	0	0
4	F	39	0	0	2	0
5	C	37	0	32	2	0
5	E	37	0	32	0	0
6	A	91	0	0	6	0
6	B	41	0	0	2	0
6	C	43	0	0	4	0
6	D	68	0	0	6	0
6	E	16	0	0	0	0
6	F	40	0	0	2	0
All	All	15137	0	14802	162	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 5.

All (162) 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:D:832:ARG:HD3	1:B:748:ARG:HH22	1.22	1.00
1:D:717:VAL:HG22	1:D:727:TYR:CE2	2.17	0.79
1:D:1007:MET:SD	6:D:1265:HOH:O	2.40	0.79
1:F:905:TRP:HD1	1:F:947:MET:HE1	1.52	0.75
1:C:802:VAL:HG12	1:C:910:PHE:HA	1.68	0.74
1:C:812:GLN:HG2	1:C:989:LEU:HG	1.68	0.74
1:C:990:PRO:HB2	1:C:994:ASP:HB2	1.67	0.74
1:D:812:GLN:HG2	1:D:989:LEU:HG	1.71	0.72
1:D:832:ARG:CD	1:B:748:ARG:HH22	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:LYS:NZ	6:C:1205:HOH:O	2.27	0.67
1:B:867:LYS:HB2	1:B:889:ARG:NH1	2.09	0.66
1:E:990:PRO:HB2	1:E:994:ASP:HB2	1.78	0.66
1:A:812:GLN:HG2	1:A:989:LEU:HG	1.78	0.65
1:E:802:VAL:HG12	1:E:910:PHE:HA	1.79	0.65
1:C:802:VAL:CG1	1:C:910:PHE:HA	2.28	0.63
1:D:802:VAL:HG12	1:D:910:PHE:HA	1.81	0.62
1:A:702:ALA:O	1:E:993:THR:HA	2.00	0.62
1:B:812:GLN:HG2	1:B:989:LEU:HG	1.83	0.61
1:D:802:VAL:CG1	1:D:910:PHE:HA	2.31	0.60
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.66	0.60
1:B:705:ARG:NH2	1:B:711:GLU:OE2	2.33	0.60
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.01	0.59
1:E:908[B]:MET:SD	1:E:939:CYS:SG	3.00	0.59
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.68	0.58
1:A:988:HIS:CD2	6:A:1208:HOH:O	2.56	0.58
1:C:723:PHE:HB2	1:C:747:LEU:HD22	1.84	0.58
1:A:813:TYR:OH	1:A:990:PRO:HD3	2.04	0.58
1:D:821:ILE:HG23	1:D:853:ILE:HD11	1.86	0.58
1:F:905:TRP:CD1	1:F:947:MET:HE1	2.37	0.57
1:F:876:VAL:HG12	1:F:881:MET:SD	2.45	0.57
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.69	0.56
1:A:1007:MET:SD	6:A:1288:HOH:O	2.58	0.56
1:D:804:GLU:HG3	6:D:1206:HOH:O	2.06	0.56
1:D:829:GLU:OE2	1:D:960:LYS:NZ	2.39	0.56
1:C:708:LYS:O	1:C:711:GLU:HG2	2.04	0.56
1:D:990:PRO:HB2	1:D:994:ASP:HB2	1.87	0.56
1:C:717:VAL:HG22	1:C:727:TYR:CE2	2.41	0.56
1:F:802:VAL:HG12	1:F:910:PHE:HA	1.88	0.56
1:B:867:LYS:HB2	1:B:889:ARG:HH11	1.70	0.56
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.05	0.55
1:A:702:ALA:HB1	1:E:992:PRO:HB2	1.87	0.55
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.41	0.55
1:E:920:ALA:HA	1:E:923:ILE:HG12	1.90	0.54
1:A:960:LYS:NZ	1:A:962:ARG:HH12	2.06	0.54
1:D:719:GLY:HA3	2:D:1101:ANP:H4'	1.88	0.54
1:A:905:TRP:CD1	1:A:947:MET:HE1	2.43	0.54
2:B:1101:ANP:O2G	2:B:1101:ANP:O1B	2.27	0.53
1:C:732:ILE:HG13	1:C:739:LYS:HG2	1.91	0.53
1:D:963:GLU:OE2	1:B:913:LYS:HD2	2.09	0.52
1:B:836:ARG:O	1:B:836:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.73	0.52
1:C:812:GLN:CG	1:C:989:LEU:HG	2.38	0.52
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.43	0.52
1:E:990:PRO:HG2	1:E:995:SER:OG	2.10	0.51
1:F:835:HIS:CD2	1:F:856:PHE:HB3	2.45	0.51
1:A:802:VAL:CG1	1:A:910:PHE:HA	2.40	0.51
1:C:988:HIS:O	6:C:1201:HOH:O	2.20	0.51
1:A:862:LEU:HD11	4:A:1103:JBJ:C24	2.42	0.50
1:E:802:VAL:CG1	1:E:910:PHE:HA	2.41	0.50
1:E:995:SER:O	1:E:999:ARG:HG3	2.11	0.50
1:A:995:SER:O	1:A:999:ARG:HG3	2.12	0.50
1:F:802:VAL:CG1	1:F:910:PHE:HA	2.42	0.50
1:E:837:ASP:OD1	1:E:841:ARG:NH1	2.44	0.50
1:D:995:SER:O	1:D:999:ARG:HG3	2.12	0.50
1:D:812:GLN:CG	1:D:989:LEU:HG	2.41	0.49
1:F:960:LYS:NZ	1:F:962:ARG:HH12	2.10	0.49
1:B:995:SER:O	1:B:999:ARG:HG3	2.12	0.49
1:E:960:LYS:NZ	1:E:962:ARG:HH12	2.10	0.49
1:B:973:ARG:NH2	6:B:1203:HOH:O	2.25	0.49
1:B:968:PHE:HA	1:B:971:MET:HE3	1.94	0.49
1:D:960:LYS:HE3	1:D:962:ARG:HH12	1.78	0.49
1:D:905:TRP:CD1	1:D:947:MET:HE1	2.47	0.49
1:E:797:CYS:HA	1:E:844:LEU:HA	1.95	0.49
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.48	0.49
1:C:989:LEU:HB3	1:C:990:PRO:HD2	1.94	0.48
1:A:717:VAL:HG22	1:A:727:TYR:CE2	2.48	0.48
1:B:835:HIS:O	1:B:836:ARG:HB3	2.14	0.48
1:D:988:HIS:N	6:D:1201:HOH:O	2.46	0.47
1:F:816:ASN:ND2	6:F:1201:HOH:O	2.22	0.47
1:D:890:ILE:HD11	1:A:865:GLU:CD	2.34	0.47
1:A:960:LYS:HZ1	1:A:962:ARG:HH12	1.62	0.47
1:E:813:TYR:OH	1:E:990:PRO:HD3	2.14	0.47
1:A:890:ILE:HG22	1:A:892:THR:HG23	1.97	0.47
1:A:922:GLU:O	1:A:926:ILE:HG23	2.14	0.47
1:C:876:VAL:HG12	1:C:881:MET:SD	2.54	0.47
1:A:736:GLU:OE1	6:A:1201:HOH:O	2.20	0.47
1:B:876:VAL:HG23	1:B:876:VAL:O	2.15	0.47
1:C:748:ARG:HG3	1:C:749:GLU:HG3	1.96	0.46
1:B:715:ILE:HG12	1:B:728:LYS:O	2.15	0.46
1:A:802:VAL:HG12	1:A:910:PHE:HA	1.97	0.46
1:E:815:LEU:O	1:E:819:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:783:THR:HG21	1:E:787:GLN:HE21	1.81	0.46
1:C:796:GLY:HA2	5:C:1102:YY3:C6	2.45	0.46
1:E:990:PRO:CB	1:E:994:ASP:HB2	2.44	0.46
1:D:812:GLN:NE2	6:D:1208:HOH:O	2.49	0.46
1:C:705:ARG:NH2	1:C:711:GLU:OE2	2.48	0.46
1:C:990:PRO:CB	1:C:994:ASP:HB2	2.40	0.46
1:C:816:ASN:ND2	6:C:1210:HOH:O	2.43	0.45
1:E:782:LEU:HA	1:E:786:VAL:HG22	1.97	0.45
1:E:960:LYS:HZ1	1:E:962:ARG:HH12	1.64	0.45
1:F:714:LYS:NZ	1:F:787:GLN:OE1	2.34	0.45
1:B:811:SER:OG	1:B:975:PRO:HB2	2.16	0.45
1:B:905:TRP:CD1	1:B:947:MET:HE1	2.50	0.45
1:F:882:ALA:HA	1:F:898:TRP:CD2	2.52	0.45
1:C:808:ASN:ND2	6:C:1211:HOH:O	2.49	0.45
4:F:1103:JBJ:S08	4:F:1103:JBJ:O01	2.75	0.45
1:B:863:GLY:O	1:B:864:ALA:HB3	2.17	0.45
1:F:933:LEU:HB2	1:F:951:TRP:CH2	2.52	0.44
1:A:869:TYR:HB3	1:A:876:VAL:HG22	2.00	0.44
1:A:835:HIS:O	1:A:836:ARG:HB3	2.17	0.44
1:B:802:VAL:CG1	1:B:910:PHE:HA	2.47	0.44
1:A:860:LYS:HB3	1:A:860:LYS:HE2	1.60	0.44
1:B:866:GLU:O	1:B:889:ARG:NH1	2.51	0.44
1:B:865:GLU:H	1:B:865:GLU:HG2	1.49	0.43
1:A:867:LYS:HA	1:A:889:ARG:NH1	2.34	0.43
1:D:916:ASP:HA	6:D:1202:HOH:O	2.17	0.43
1:B:701:GLN:H	1:B:701:GLN:HG2	1.53	0.43
1:F:737:LYS:HG2	1:F:737:LYS:O	2.18	0.43
1:A:702:ALA:CB	1:E:992:PRO:HB2	2.49	0.43
1:A:776:ARG:HH21	1:E:1000:ALA:HB2	1.83	0.43
1:E:805:HIS:O	1:E:809:ILE:HG13	2.19	0.43
1:D:989:LEU:HB3	1:D:990:PRO:HD2	2.00	0.43
1:A:703:LEU:HD13	1:A:768:SER:HA	1.99	0.43
1:A:867:LYS:HA	1:A:889:ARG:CZ	2.48	0.43
1:A:946:ILE:HD11	1:A:967:GLU:HG2	2.00	0.43
1:C:721:GLY:HA3	5:C:1102:YY3:H32	2.01	0.43
1:B:918:ILE:N	1:B:918:ILE:HD13	2.33	0.43
1:B:953:ILE:HG22	6:B:1232:HOH:O	2.19	0.43
1:D:973:ARG:NH2	6:D:1209:HOH:O	2.49	0.43
1:E:749:GLU:HB3	1:E:750:ALA:H	1.53	0.42
1:E:783:THR:O	1:E:784:SER:C	2.57	0.42
1:E:781:CYS:SG	1:E:783:THR:HG22	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:835:HIS:O	1:C:836:ARG:HB2	2.18	0.42
1:C:703:LEU:HD13	1:C:768:SER:HA	2.00	0.42
1:A:988:HIS:O	6:A:1202:HOH:O	2.21	0.42
1:F:999:ARG:HA	1:F:1003:ASP:HB3	2.00	0.42
1:C:879:LYS:HE2	1:C:923:ILE:HD11	2.01	0.42
1:B:773:HIS:CD2	1:B:820:GLN:HB3	2.55	0.42
1:A:877:PRO:O	1:A:881:MET:HG3	2.20	0.41
1:E:751:THR:CG2	1:E:784:SER:HA	2.50	0.41
1:A:1001:LEU:HD23	1:A:1001:LEU:HA	1.92	0.41
1:E:905:TRP:HD1	1:E:947:MET:HE1	1.84	0.41
1:C:933:LEU:HB2	1:C:951:TRP:CH2	2.55	0.41
1:B:936:PRO:HA	1:B:937:PRO:HD3	1.98	0.41
1:A:988:HIS:N	6:A:1202:HOH:O	2.53	0.41
1:C:805:HIS:O	1:C:809:ILE:HG13	2.21	0.41
1:F:815:LEU:HA	1:F:815:LEU:HD23	1.79	0.41
1:D:949:LYS:HG2	1:D:952:MET:CE	2.51	0.41
1:D:968:PHE:CD1	1:D:971:MET:HE3	2.56	0.41
1:F:719:GLY:HA3	2:F:1101:ANP:H4'	2.02	0.41
1:F:876:VAL:N	6:F:1210:HOH:O	2.54	0.41
1:A:868:GLU:C	1:A:870:HIS:H	2.24	0.41
1:B:904:VAL:O	1:B:908[B]:MET:HG3	2.22	0.40
1:A:937:PRO:HD2	6:A:1232:HOH:O	2.21	0.40
1:D:802:VAL:HG11	1:D:910:PHE:HA	2.04	0.40
1:D:944:TYR:CZ	1:D:948:ARG:HD3	2.56	0.40
1:A:760:LEU:HD23	1:A:760:LEU:HA	1.88	0.40
1:F:855:ASP:OD1	4:F:1103:JBJ:N03	2.54	0.40
1:A:812:GLN:CG	1:A:989:LEU:HG	2.48	0.40
1:B:866:GLU:O	1:B:867:LYS:HB2	2.22	0.40
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.22	0.40
1:E:798:LEU:O	1:E:802:VAL:HG23	2.21	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	307/331 (93%)	294 (96%)	13 (4%)	0	100	100
1	B	307/331 (93%)	300 (98%)	6 (2%)	1 (0%)	41	37
1	C	290/331 (88%)	283 (98%)	7 (2%)	0	100	100
1	D	291/331 (88%)	283 (97%)	8 (3%)	0	100	100
1	E	282/331 (85%)	271 (96%)	11 (4%)	0	100	100
1	F	291/331 (88%)	284 (98%)	6 (2%)	1 (0%)	41	37
All	All	1768/1986 (89%)	1715 (97%)	51 (3%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	859	ALA
1	B	867	LYS

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	273/290 (94%)	268 (98%)	5 (2%)	59	63
1	B	273/290 (94%)	263 (96%)	10 (4%)	34	32
1	C	263/290 (91%)	257 (98%)	6 (2%)	50	53
1	D	264/290 (91%)	261 (99%)	3 (1%)	73	78
1	E	257/290 (89%)	243 (95%)	14 (5%)	22	18
1	F	264/290 (91%)	254 (96%)	10 (4%)	33	31
All	All	1594/1740 (92%)	1546 (97%)	48 (3%)	41	40

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	860	LYS
1	D	861	LEU
1	D	987	MET
1	A	862	LEU
1	A	866	GLU
1	A	876	VAL
1	A	960	LYS
1	A	977	ARG
1	C	720	SER
1	C	757	LYS
1	C	783	THR
1	C	784	SER
1	C	960	LYS
1	C	987	MET
1	F	701	GLN
1	F	784	SER
1	F	860	LYS
1	F	861	LEU
1	F	960	LYS
1	F	986	ARG
1	F	987	MET
1	F	988	HIS
1	F	989	LEU
1	F	991	SER
1	B	701	GLN
1	B	861	LEU
1	B	865	GLU
1	B	866	GLU
1	B	870	HIS
1	B	875	LYS
1	B	889	ARG
1	B	960	LYS
1	B	998	TYR
1	B	1002	MET
1	E	745	LYS
1	E	748	ARG
1	E	749	GLU
1	E	752	SER
1	E	754	LYS
1	E	782	LEU
1	E	783	THR
1	E	784	SER
1	E	785	THR

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Mol	Chain	Res	Type
1	E	787	GLN
1	E	924	SER
1	E	943	VAL
1	E	960	LYS
1	E	984	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	888	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 16 ligands modelled in this entry, 4 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
5	YY3	E	1102	1	38,40,40	2.29	12 (31%)	50,56,56	2.22	13 (26%)
4	JBj	D	1103	-	42,44,44	1.85	11 (26%)	52,63,63	3.72	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	JBJ	C	1101	-	42,44,44	2.55	18 (42%)	52,63,63	4.42	21 (40%)
2	ANP	B	1101	3	29,33,33	1.04	3 (10%)	31,52,52	1.27	5 (16%)
2	ANP	A	1101	3	29,33,33	1.24	4 (13%)	31,52,52	1.30	5 (16%)
4	JBJ	B	1103	-	42,44,44	2.06	11 (26%)	52,63,63	3.60	18 (34%)
4	JBJ	A	1103	-	42,44,44	1.90	12 (28%)	52,63,63	3.50	16 (30%)
2	ANP	D	1101	3	29,33,33	1.09	3 (10%)	31,52,52	1.26	4 (12%)
5	YY3	C	1102	1	38,40,40	2.13	12 (31%)	50,56,56	2.10	11 (22%)
4	JBJ	F	1103	-	42,44,44	2.27	16 (38%)	52,63,63	4.24	17 (32%)
4	JBJ	E	1101	-	42,44,44	2.69	16 (38%)	52,63,63	4.12	15 (28%)
2	ANP	F	1101	3	29,33,33	1.16	4 (13%)	31,52,52	1.28	5 (16%)

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
5	YY3	E	1102	1	-	10/21/25/25	0/4/4/4
4	JBJ	D	1103	-	-	6/22/44/44	0/6/6/6
4	JBJ	C	1101	-	-	6/22/44/44	0/6/6/6
2	ANP	B	1101	3	-	3/14/38/38	0/3/3/3
2	ANP	A	1101	3	-	1/14/38/38	0/3/3/3
4	JBJ	B	1103	-	-	4/22/44/44	0/6/6/6
4	JBJ	A	1103	-	-	4/22/44/44	0/6/6/6
2	ANP	D	1101	3	-	6/14/38/38	0/3/3/3
5	YY3	C	1102	1	-	5/21/25/25	0/4/4/4
4	JBJ	F	1103	-	-	5/22/44/44	0/6/6/6
4	JBJ	E	1101	-	-	3/22/44/44	0/6/6/6
2	ANP	F	1101	3	-	4/14/38/38	0/3/3/3

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1101	JBJ	C11-N10	7.53	1.43	1.36
5	E	1102	YY3	C7-N	7.13	1.47	1.35
4	B	1103	JBJ	C30-N10	7.10	1.52	1.46
4	F	1103	JBJ	C11-N10	6.72	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1101	JBj	C30-C29	6.50	1.59	1.50
4	F	1103	JBj	C18-N19	6.02	1.55	1.38
4	E	1101	JBj	C09-C02	5.77	1.60	1.54
4	C	1101	JBj	C30-N10	5.73	1.51	1.46
4	E	1101	JBj	C30-N10	5.60	1.51	1.46
4	E	1101	JBj	C09-N10	5.57	1.52	1.46
5	C	1102	YY3	C8-C7	5.50	1.57	1.48
5	C	1102	YY3	C7-N	5.10	1.44	1.35
4	A	1103	JBj	C18-N19	4.96	1.52	1.38
4	C	1101	JBj	C09-N10	4.78	1.51	1.46
4	A	1103	JBj	C11-N10	4.77	1.40	1.36
4	C	1101	JBj	C17-C18	4.70	1.48	1.39
4	D	1103	JBj	C30-N10	4.52	1.50	1.46
4	E	1101	JBj	C12-C11	4.51	1.56	1.48
4	D	1103	JBj	C18-N19	4.45	1.51	1.38
4	A	1103	JBj	C20-N19	4.45	1.53	1.46
4	C	1101	JBj	C16-C15	4.42	1.48	1.39
4	C	1101	JBj	C11-N10	4.35	1.40	1.36
4	E	1101	JBj	C18-N19	4.33	1.50	1.38
4	D	1103	JBj	C24-N19	4.30	1.53	1.46
4	B	1103	JBj	C24-N19	4.18	1.53	1.46
4	F	1103	JBj	C12-C11	4.13	1.55	1.48
5	E	1102	YY3	C1-C2	4.04	1.45	1.40
4	F	1103	JBj	C30-C29	4.02	1.55	1.50
4	B	1103	JBj	C30-C29	4.00	1.55	1.50
4	B	1103	JBj	C18-N19	3.89	1.49	1.38
4	E	1101	JBj	C20-N19	3.89	1.52	1.46
5	C	1102	YY3	C19-C18	-3.88	1.44	1.49
5	E	1102	YY3	C15-N3	3.85	1.44	1.36
4	F	1103	JBj	C02-N03	3.80	1.44	1.35
4	E	1101	JBj	C02-N03	3.75	1.44	1.35
4	A	1103	JBj	C30-N10	3.65	1.49	1.46
4	B	1103	JBj	C11-N10	3.65	1.39	1.36
5	E	1102	YY3	C5-N3	3.63	1.49	1.39
4	B	1103	JBj	C20-N19	3.61	1.52	1.46
4	C	1101	JBj	C15-C14	3.60	1.58	1.49
5	C	1102	YY3	C5-N3	3.57	1.49	1.39
4	D	1103	JBj	C12-C11	3.49	1.54	1.48
5	E	1102	YY3	C2-N1	3.49	1.49	1.41
4	D	1103	JBj	C02-N03	3.31	1.43	1.35
4	A	1103	JBj	C02-N03	3.30	1.43	1.35
4	C	1101	JBj	C18-N19	3.26	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1102	YY3	O1-C4	3.22	1.42	1.37
2	A	1101	ANP	PG-O3G	-3.22	1.48	1.56
4	C	1101	JBj	C25-C18	3.19	1.45	1.39
4	C	1101	JBj	C12-C11	3.11	1.53	1.48
5	E	1102	YY3	C6-C1	3.05	1.44	1.39
4	E	1101	JBj	C24-N19	3.03	1.51	1.46
2	F	1101	ANP	PG-O3G	-3.03	1.48	1.56
4	E	1101	JBj	C30-C29	3.01	1.54	1.50
4	F	1103	JBj	C24-N19	2.99	1.51	1.46
4	D	1103	JBj	C04-N03	2.94	1.41	1.36
4	C	1101	JBj	C20-N19	2.92	1.51	1.46
5	E	1102	YY3	O1-C4	2.89	1.41	1.37
4	C	1101	JBj	C28-C27	2.84	1.43	1.38
4	F	1103	JBj	C13-C12	2.83	1.44	1.39
5	E	1102	YY3	C15-N4	2.79	1.38	1.34
2	A	1101	ANP	PG-O2G	-2.74	1.49	1.56
2	D	1101	ANP	PG-N3B	2.71	1.70	1.63
4	F	1103	JBj	C17-C18	2.67	1.44	1.39
4	E	1101	JBj	C04-N03	2.64	1.41	1.36
4	C	1101	JBj	C28-C29	2.56	1.44	1.39
2	A	1101	ANP	PB-O2B	-2.54	1.49	1.56
4	C	1101	JBj	C17-C16	2.53	1.43	1.38
5	C	1102	YY3	C1-N	2.53	1.46	1.41
4	F	1103	JBj	C17-C16	2.51	1.43	1.38
2	F	1101	ANP	PB-O1B	2.51	1.50	1.46
5	E	1102	YY3	C15-N5	2.50	1.42	1.34
4	B	1103	JBj	C02-N03	2.49	1.41	1.35
4	B	1103	JBj	F35-C34	2.47	1.42	1.36
2	F	1101	ANP	PB-O2B	-2.47	1.50	1.56
4	A	1103	JBj	C38-C32	2.47	1.43	1.40
4	F	1103	JBj	C15-C14	2.47	1.55	1.49
4	A	1103	JBj	C26-C25	2.47	1.43	1.38
4	A	1103	JBj	C17-C18	2.45	1.44	1.39
5	C	1102	YY3	C15-N3	2.45	1.41	1.36
4	F	1103	JBj	F35-C34	2.44	1.42	1.36
2	B	1101	ANP	PB-O1B	2.42	1.50	1.46
4	E	1101	JBj	C17-C18	2.38	1.44	1.39
4	F	1103	JBj	C20-N19	2.38	1.50	1.46
4	C	1101	JBj	C02-N03	2.37	1.41	1.35
4	A	1103	JBj	F35-C34	2.36	1.42	1.36
4	E	1101	JBj	F35-C34	2.34	1.42	1.36
4	D	1103	JBj	C24-C23	2.34	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1101	JBj	C20-C21	2.34	1.57	1.51
4	C	1101	JBj	F35-C34	2.31	1.42	1.36
5	E	1102	YY3	C17-C16	2.30	1.43	1.38
4	A	1103	JBj	C24-C23	2.30	1.56	1.51
4	F	1103	JBj	C13-C14	2.26	1.43	1.39
5	E	1102	YY3	C10-C11	2.25	1.60	1.51
2	D	1101	ANP	PB-O3A	-2.25	1.56	1.59
4	D	1103	JBj	C17-C18	2.24	1.43	1.39
5	C	1102	YY3	C10-N1	2.23	1.53	1.46
4	D	1103	JBj	F35-C34	2.23	1.41	1.36
2	B	1101	ANP	PB-O3A	-2.23	1.56	1.59
4	A	1103	JBj	C24-N19	2.22	1.50	1.46
2	F	1101	ANP	PG-O2G	-2.20	1.50	1.56
5	C	1102	YY3	C13-N2	2.20	1.52	1.46
4	C	1101	JBj	C32-C09	-2.19	1.49	1.52
4	B	1103	JBj	C16-C15	2.19	1.44	1.39
4	F	1103	JBj	C24-C23	2.16	1.56	1.51
5	C	1102	YY3	C10-C11	2.15	1.59	1.51
4	B	1103	JBj	C28-C27	2.13	1.42	1.38
4	C	1101	JBj	C13-C14	2.13	1.43	1.39
4	F	1103	JBj	C16-C15	2.12	1.43	1.39
2	A	1101	ANP	PB-O1B	2.12	1.49	1.46
4	E	1101	JBj	C13-C14	2.11	1.43	1.39
4	B	1103	JBj	C17-C18	2.10	1.43	1.39
2	B	1101	ANP	PG-N3B	2.10	1.68	1.63
4	D	1103	JBj	C20-N19	2.09	1.50	1.46
5	E	1102	YY3	C11-N2	2.08	1.53	1.46
4	A	1103	JBj	C09-C02	-2.06	1.52	1.54
2	D	1101	ANP	PG-O1G	2.05	1.49	1.46
4	F	1103	JBj	C38-C32	2.05	1.42	1.40
5	C	1102	YY3	C2-N1	2.04	1.46	1.41
4	E	1101	JBj	C15-C14	2.04	1.54	1.49
5	C	1102	YY3	C12-N2	2.01	1.52	1.46
4	D	1103	JBj	C38-C32	2.01	1.42	1.40

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1101	JBj	C30-N10-C11	-18.52	105.50	113.12
4	E	1101	JBj	C30-N10-C11	-17.81	105.79	113.12
4	E	1101	JBj	C29-C30-N10	16.52	107.69	102.18
4	F	1103	JBj	C30-N10-C11	-16.52	106.32	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1103	JBj	C29-C30-N10	15.72	107.42	102.18
4	B	1103	JBj	C30-N10-C11	-15.64	106.69	113.12
4	C	1101	JBj	C29-C30-N10	15.55	107.36	102.18
4	A	1103	JBj	C30-N10-C11	-15.54	106.72	113.12
4	D	1103	JBj	C30-N10-C11	-13.46	107.58	113.12
4	D	1103	JBj	C29-C30-N10	11.91	106.15	102.18
4	C	1101	JBj	C12-C11-N10	11.13	113.01	106.44
4	A	1103	JBj	C29-C30-N10	10.76	105.76	102.18
4	B	1103	JBj	C12-C11-N10	10.51	112.65	106.44
4	D	1103	JBj	O31-C11-N10	-10.20	117.59	125.24
5	E	1102	YY3	C8-C7-N	9.98	120.42	113.84
5	C	1102	YY3	C8-C7-N	9.71	120.24	113.84
4	F	1103	JBj	C12-C11-N10	9.54	112.07	106.44
4	F	1103	JBj	O31-C11-N10	-9.06	118.45	125.24
4	A	1103	JBj	C12-C11-N10	8.86	111.67	106.44
4	B	1103	JBj	C29-C30-N10	8.74	105.09	102.18
4	D	1103	JBj	C12-C11-N10	8.43	111.42	106.44
4	F	1103	JBj	C29-C12-C11	-8.42	104.43	108.94
4	C	1101	JBj	O31-C11-N10	-7.99	119.25	125.24
4	E	1101	JBj	C12-C11-N10	7.89	111.10	106.44
4	B	1103	JBj	O31-C11-N10	-7.28	119.78	125.24
4	D	1103	JBj	O01-C02-C09	-7.26	111.25	120.97
4	A	1103	JBj	O31-C11-N10	-6.74	120.18	125.24
4	B	1103	JBj	O01-C02-C09	-6.56	112.18	120.97
4	D	1103	JBj	C29-C12-C11	-6.53	105.44	108.94
4	C	1101	JBj	C16-C17-C18	-6.36	111.95	120.32
4	E	1101	JBj	O01-C02-C09	-6.02	112.90	120.97
4	E	1101	JBj	O31-C11-N10	-5.99	120.75	125.24
4	F	1103	JBj	O01-C02-C09	-5.65	113.40	120.97
4	C	1101	JBj	O01-C02-C09	-5.52	113.58	120.97
4	E	1101	JBj	C29-C12-C11	-5.47	106.01	108.94
4	A	1103	JBj	O01-C02-C09	-5.14	114.08	120.97
4	A	1103	JBj	C29-C12-C11	-4.67	106.44	108.94
4	C	1101	JBj	C30-C29-C12	-4.31	107.06	109.75
4	E	1101	JBj	C21-C20-N19	4.29	119.77	110.48
5	E	1102	YY3	C6-C5-C4	-4.26	113.76	118.91
4	B	1103	JBj	C23-C24-N19	4.12	119.40	110.48
5	E	1102	YY3	O1-C4-C5	4.09	119.82	114.80
2	A	1101	ANP	O2B-PB-O1B	4.07	118.46	109.92
2	F	1101	ANP	O2B-PB-O1B	4.06	118.43	109.92
4	F	1103	JBj	C13-C12-C11	4.01	136.06	129.36
4	C	1101	JBj	C17-C16-C15	3.87	126.70	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	JBj	C30-N10-C09	3.81	127.42	123.86
5	C	1102	YY3	C16-N4-C15	3.79	118.81	115.45
4	B	1103	JBj	C21-C20-N19	3.79	118.69	110.48
5	E	1102	YY3	O1-C4-C3	-3.76	117.65	124.12
5	C	1102	YY3	C6-C5-C4	-3.75	114.38	118.91
5	E	1102	YY3	C3-C2-C1	-3.68	114.61	120.04
5	E	1102	YY3	N4-C15-N5	-3.62	123.12	126.55
4	C	1101	JBj	C25-C18-N19	-3.62	116.39	121.38
4	B	1103	JBj	C29-C12-C11	-3.61	107.01	108.94
4	A	1103	JBj	C30-N10-C09	3.58	127.21	123.86
4	D	1103	JBj	C13-C12-C11	3.57	135.34	129.36
4	C	1101	JBj	C29-C12-C11	-3.50	107.06	108.94
4	D	1103	JBj	C23-C24-N19	3.50	118.06	110.48
4	D	1103	JBj	C36-C34-C33	3.48	127.82	123.29
4	F	1103	JBj	C37-C36-C34	-3.40	114.85	118.36
4	E	1101	JBj	C13-C12-C11	3.36	134.98	129.36
4	C	1101	JBj	C21-C20-N19	3.36	117.76	110.48
4	F	1103	JBj	C36-C34-C33	3.31	127.59	123.29
4	C	1101	JBj	C30-C29-C28	3.24	135.23	128.85
4	E	1101	JBj	C36-C34-C33	3.20	127.45	123.29
2	D	1101	ANP	O1G-PG-N3B	-3.19	107.07	111.77
4	E	1101	JBj	C02-C09-N10	3.18	114.73	110.16
2	B	1101	ANP	O2G-PG-O1G	-3.15	105.54	113.45
5	C	1102	YY3	C3-C2-C1	-3.11	115.45	120.04
5	E	1102	YY3	C2-C3-C4	3.09	124.49	117.91
4	C	1101	JBj	C37-C36-C34	-3.06	115.20	118.36
4	D	1103	JBj	C26-C15-C14	3.05	126.64	121.36
4	E	1101	JBj	C37-C36-C34	-3.03	115.24	118.36
5	E	1102	YY3	O-C7-C8	-2.96	118.00	122.72
4	C	1101	JBj	O01-C02-N03	-2.92	117.64	123.93
4	A	1103	JBj	C36-C34-C33	2.90	127.06	123.29
4	C	1101	JBj	C28-C29-C12	-2.87	117.71	120.31
4	A	1103	JBj	C37-C36-C34	-2.83	115.44	118.36
5	C	1102	YY3	N4-C15-N5	-2.83	123.86	126.55
4	E	1101	JBj	O01-C02-N03	-2.83	117.84	123.93
4	B	1103	JBj	O01-C02-N03	-2.80	117.90	123.93
4	A	1103	JBj	C26-C15-C14	2.78	126.18	121.36
4	C	1101	JBj	C36-C34-C33	2.78	126.91	123.29
4	F	1103	JBj	C26-C25-C18	2.77	123.97	120.32
4	B	1103	JBj	C36-C34-C33	2.72	126.83	123.29
4	E	1101	JBj	C20-C21-N22	2.72	118.16	111.12
4	D	1103	JBj	C37-C36-C34	-2.71	115.57	118.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	JBj	C37-C36-C34	-2.67	115.61	118.36
4	F	1103	JBj	C38-C32-C09	2.67	124.45	120.58
2	D	1101	ANP	O1B-PB-N3B	-2.65	107.87	111.77
4	F	1103	JBj	C02-C09-N10	2.64	113.95	110.16
4	C	1101	JBj	C30-N10-C09	2.59	126.28	123.86
4	B	1103	JBj	C26-C25-C18	2.56	123.70	120.32
5	C	1102	YY3	C18-C19-C26	2.56	128.91	123.90
4	A	1103	JBj	C25-C18-C17	-2.54	113.99	119.16
5	C	1102	YY3	O-C7-N	-2.54	120.14	123.05
5	E	1102	YY3	C4-C5-N3	2.54	123.10	117.78
2	A	1101	ANP	O2G-PG-O1G	-2.53	107.08	113.45
4	D	1103	JBj	C24-C23-N22	2.52	117.66	111.12
4	F	1103	JBj	O01-C02-N03	-2.50	118.55	123.93
2	A	1101	ANP	O3G-PG-O1G	-2.48	107.21	113.45
2	B	1101	ANP	O3'-C3'-C2'	-2.48	103.81	111.82
4	F	1103	JBj	C25-C18-C17	-2.44	114.19	119.16
4	A	1103	JBj	C38-C32-C09	2.43	124.10	120.58
5	C	1102	YY3	C9-C8-C7	2.40	125.01	122.27
5	E	1102	YY3	C18-C19-C26	2.38	128.55	123.90
4	F	1103	JBj	C13-C14-C15	2.36	124.77	120.86
4	C	1101	JBj	C02-C09-N10	2.36	113.55	110.16
4	A	1103	JBj	C13-C12-C11	2.35	133.30	129.36
5	C	1102	YY3	C2-C3-C4	2.34	122.90	117.91
2	B	1101	ANP	PA-O3A-PB	-2.34	124.38	132.62
2	D	1101	ANP	C5-C6-N6	2.29	123.83	120.35
2	F	1101	ANP	O2G-PG-O1G	-2.29	107.71	113.45
4	A	1103	JBj	C25-C18-N19	2.27	124.51	121.38
2	B	1101	ANP	C5-C6-N6	2.26	123.79	120.35
4	B	1103	JBj	C02-C09-N10	2.25	113.38	110.16
4	D	1103	JBj	O01-C02-N03	-2.22	119.15	123.93
5	E	1102	YY3	C25-C26-C19	-2.22	132.46	135.63
2	D	1101	ANP	O2G-PG-O1G	-2.20	107.92	113.45
4	A	1103	JBj	O01-C02-N03	-2.20	119.19	123.93
4	B	1103	JBj	C38-C32-C09	2.19	123.75	120.58
2	F	1101	ANP	O3A-PB-N3B	-2.18	100.53	106.59
4	E	1101	JBj	F35-C34-C33	-2.18	115.14	118.25
2	F	1101	ANP	C5-C6-N6	2.17	123.66	120.35
4	B	1103	JBj	C27-C14-C15	2.17	125.12	121.36
2	A	1101	ANP	C5-C6-N6	2.16	123.64	120.35
4	C	1101	JBj	C27-C14-C13	-2.16	115.11	118.16
4	C	1101	JBj	C23-C24-N19	2.15	115.15	110.48
4	F	1103	JBj	C23-C24-N19	2.15	115.13	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1101	ANP	O3G-PG-O1G	-2.14	108.08	113.45
4	B	1103	JBj	C28-C29-C12	-2.14	118.37	120.31
5	E	1102	YY3	C11-C10-N1	2.13	115.72	112.31
4	B	1103	JBj	C30-C29-C28	2.13	133.05	128.85
4	F	1103	JBj	C26-C15-C14	2.12	125.03	121.36
2	A	1101	ANP	O3A-PB-N3B	-2.10	100.76	106.59
4	D	1103	JBj	C37-C38-C32	2.10	122.32	120.41
4	E	1101	JBj	C38-C32-C09	2.09	123.61	120.58
5	C	1102	YY3	C11-C10-N1	2.07	115.61	112.31
2	B	1101	ANP	O1B-PB-N3B	-2.06	108.73	111.77
5	C	1102	YY3	C25-C26-C19	-2.05	132.71	135.63
4	D	1103	JBj	C16-C15-C14	-2.04	117.83	121.36
5	E	1102	YY3	C10-N1-C2	2.03	125.40	117.16
4	D	1103	JBj	F35-C34-C33	-2.02	115.37	118.25
4	A	1103	JBj	C26-C25-C18	2.02	122.98	120.32
4	C	1101	JBj	O39-C38-C32	-2.01	114.45	119.52

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1101	ANP	PB-N3B-PG-O1G
2	D	1101	ANP	PA-O3A-PB-O1B
2	D	1101	ANP	PA-O3A-PB-O2B
2	A	1101	ANP	PG-N3B-PB-O3A
2	F	1101	ANP	PB-N3B-PG-O1G
2	F	1101	ANP	PA-O3A-PB-O1B
2	F	1101	ANP	PA-O3A-PB-O2B
2	B	1101	ANP	PB-N3B-PG-O1G
2	B	1101	ANP	PG-N3B-PB-O1B
4	A	1103	JBj	C02-C09-C32-C38
5	C	1102	YY3	N-C7-C8-C9
5	C	1102	YY3	O-C7-C8-C9
5	E	1102	YY3	C10-C11-N2-C12
5	E	1102	YY3	C11-C10-N1-C28
5	E	1102	YY3	C11-C10-N1-C2
5	E	1102	YY3	N-C7-C8-C9
5	E	1102	YY3	O-C7-C8-C9
4	D	1103	JBj	C17-C18-N19-C20
4	D	1103	JBj	C25-C18-N19-C20
5	E	1102	YY3	N1-C10-C11-N2
5	E	1102	YY3	C1-C2-N1-C10

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Mol	Chain	Res	Type	Atoms
4	C	1101	JBj	C25-C18-N19-C20
4	C	1101	JBj	C25-C18-N19-C24
4	C	1101	JBj	C17-C18-N19-C24
5	C	1102	YY3	C1-C2-N1-C28
5	E	1102	YY3	C10-C11-N2-C13
4	C	1101	JBj	C17-C18-N19-C20
4	A	1103	JBj	N10-C09-C32-C33
4	B	1103	JBj	N10-C09-C32-C33
5	C	1102	YY3	N1-C10-C11-N2
2	D	1101	ANP	PG-N3B-PB-O3A
2	B	1101	ANP	PG-N3B-PB-O3A
5	C	1102	YY3	C3-C2-N1-C28
4	D	1103	JBj	C02-C09-C32-C38
4	B	1103	JBj	C02-C09-C32-C38
5	E	1102	YY3	C5-C4-O1-C14
4	D	1103	JBj	C02-C09-N10-C30
4	C	1101	JBj	C02-C09-N10-C30
2	D	1101	ANP	PG-N3B-PB-O1B
2	D	1101	ANP	PB-O3A-PA-O1A
4	F	1103	JBj	C17-C18-N19-C24
4	D	1103	JBj	C32-C09-N10-C30
4	C	1101	JBj	C32-C09-N10-C30
4	F	1103	JBj	C32-C09-N10-C30
4	E	1101	JBj	C13-C14-C15-C26
5	E	1102	YY3	C3-C4-O1-C14
4	A	1103	JBj	N10-C09-C32-C38
4	B	1103	JBj	N10-C09-C32-C38
2	F	1101	ANP	PG-N3B-PB-O3A
4	D	1103	JBj	C02-C09-C32-C33
4	A	1103	JBj	C02-C09-C32-C33
4	F	1103	JBj	C02-C09-C32-C33
4	B	1103	JBj	C02-C09-C32-C33
4	E	1101	JBj	C13-C14-C15-C16
4	F	1103	JBj	C02-C09-C32-C38
4	F	1103	JBj	C25-C18-N19-C24
4	E	1101	JBj	C27-C14-C15-C26

There are no ring outliers.

6 monomers are involved in 8 short contacts:

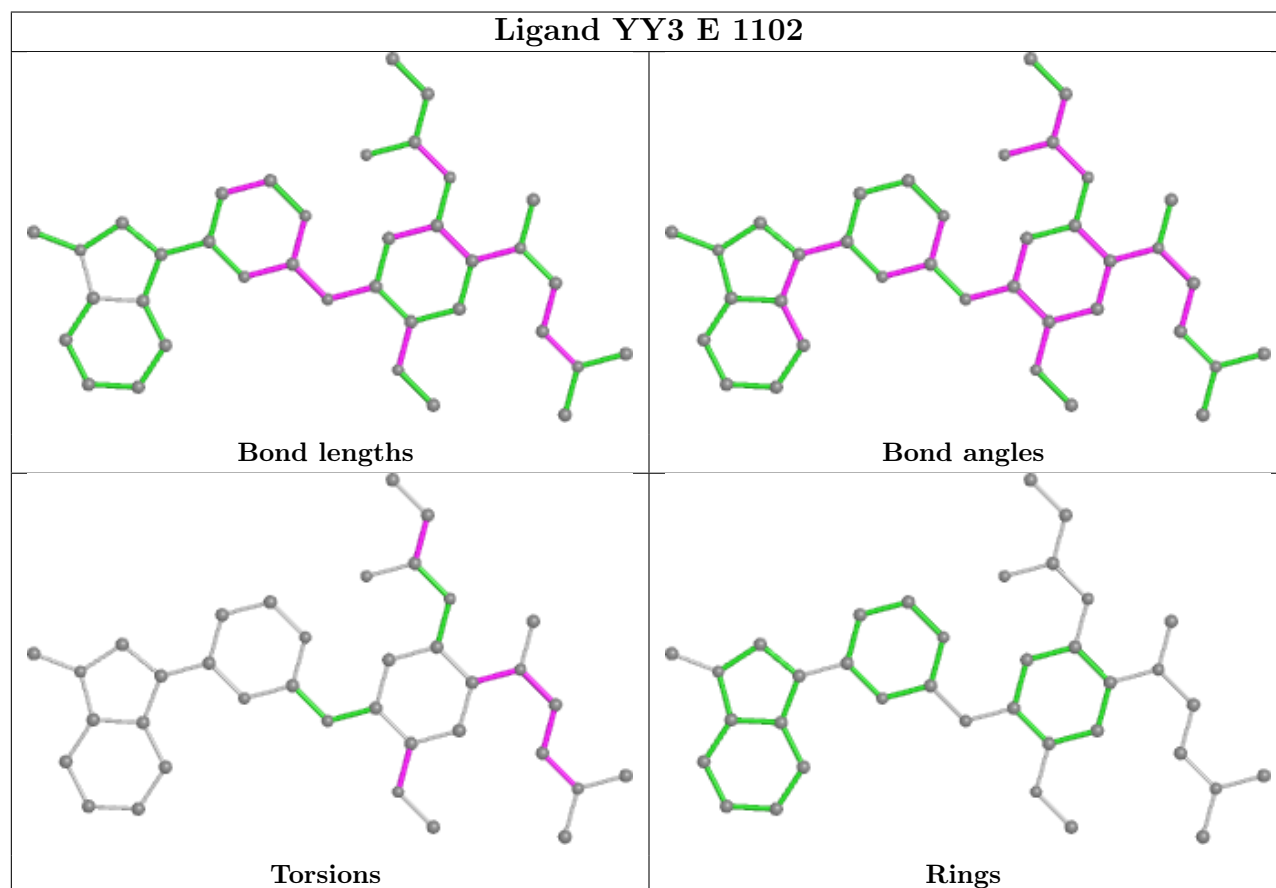
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	ANP	1	0

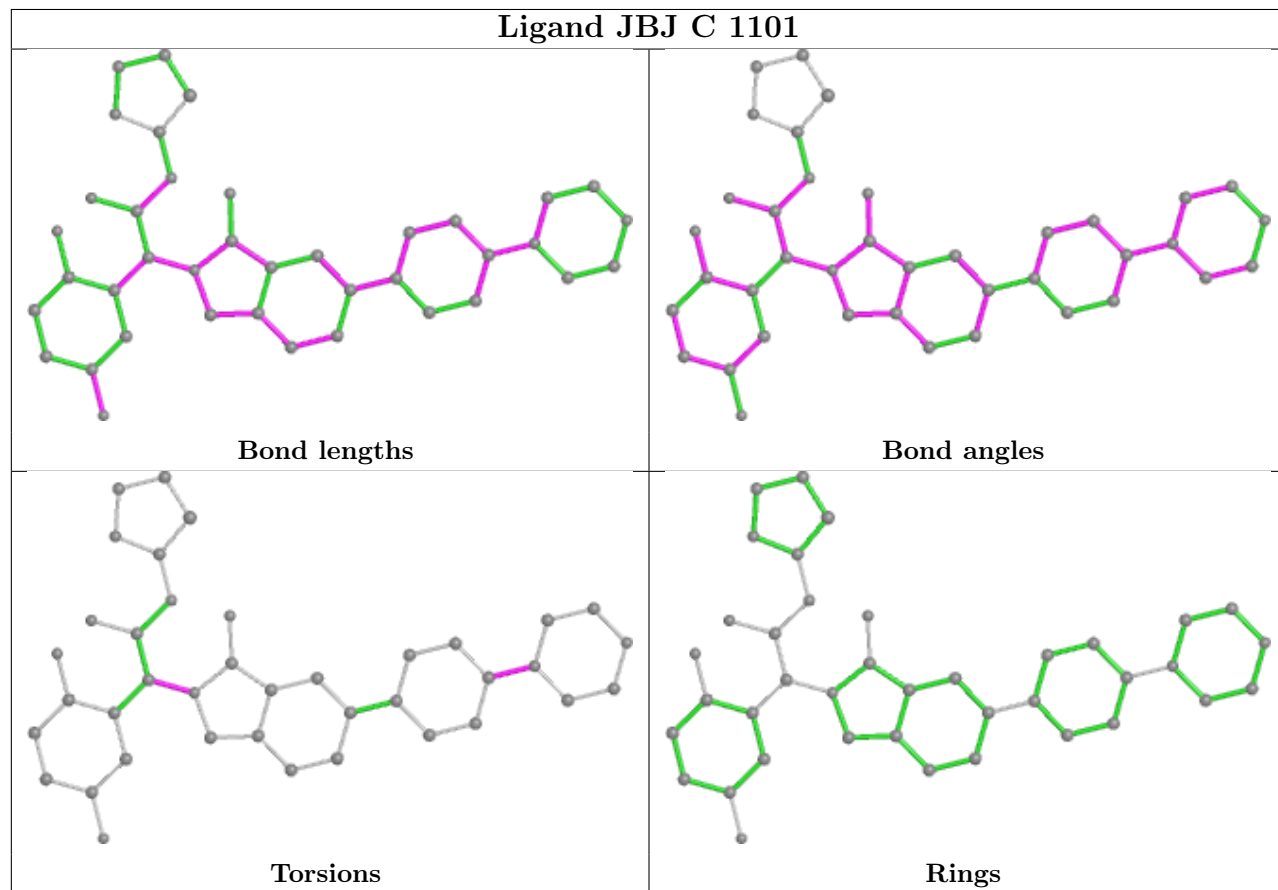
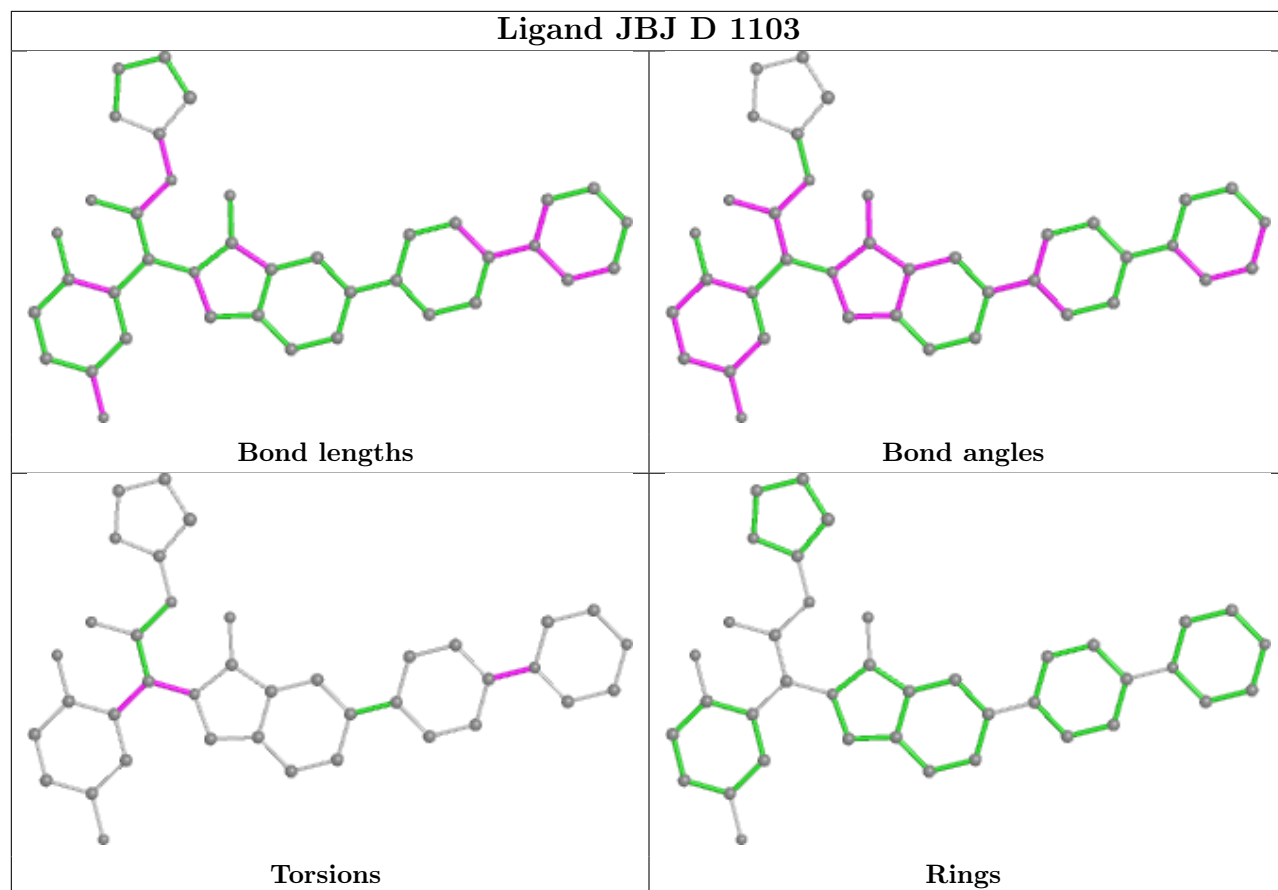
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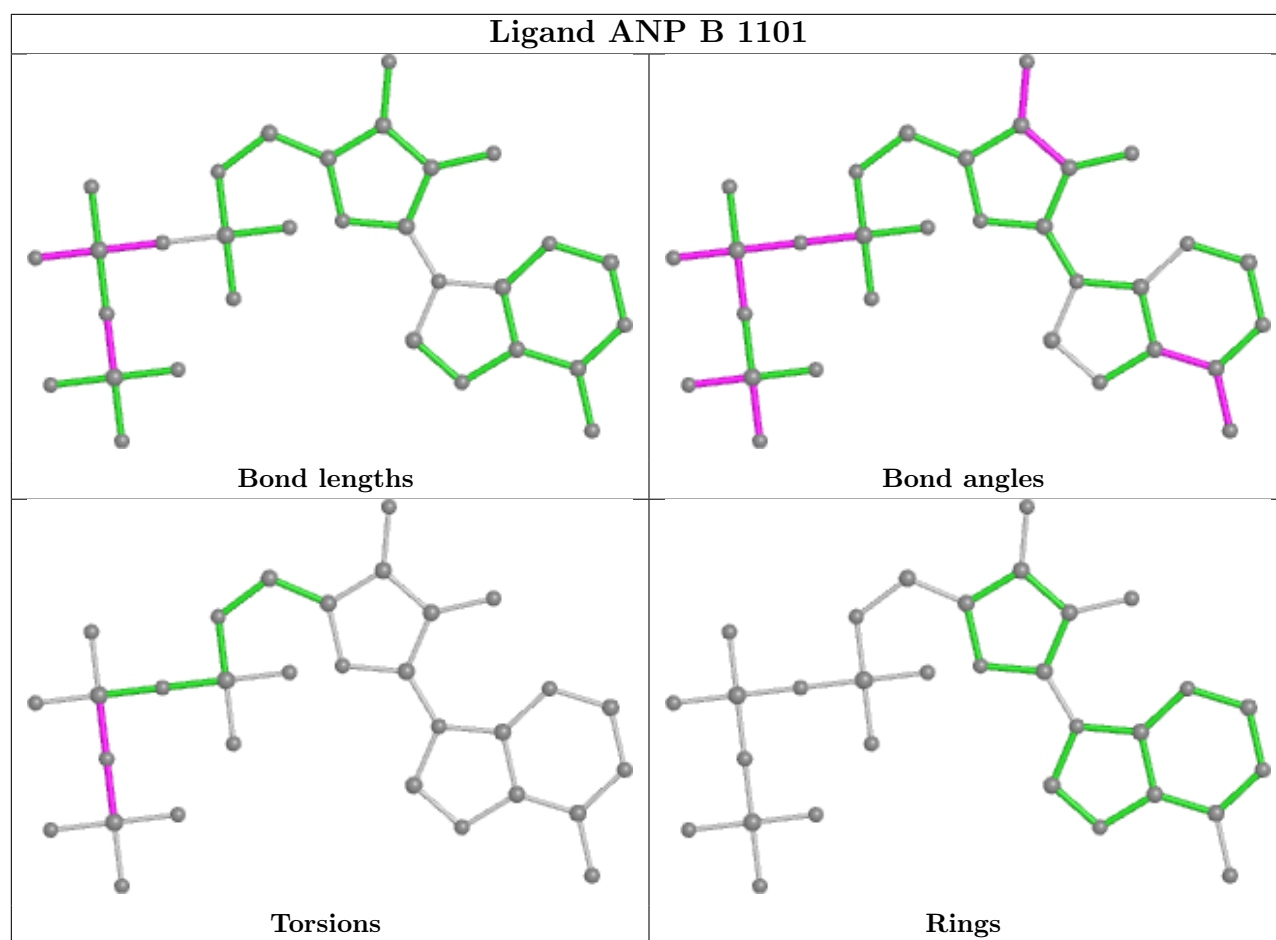
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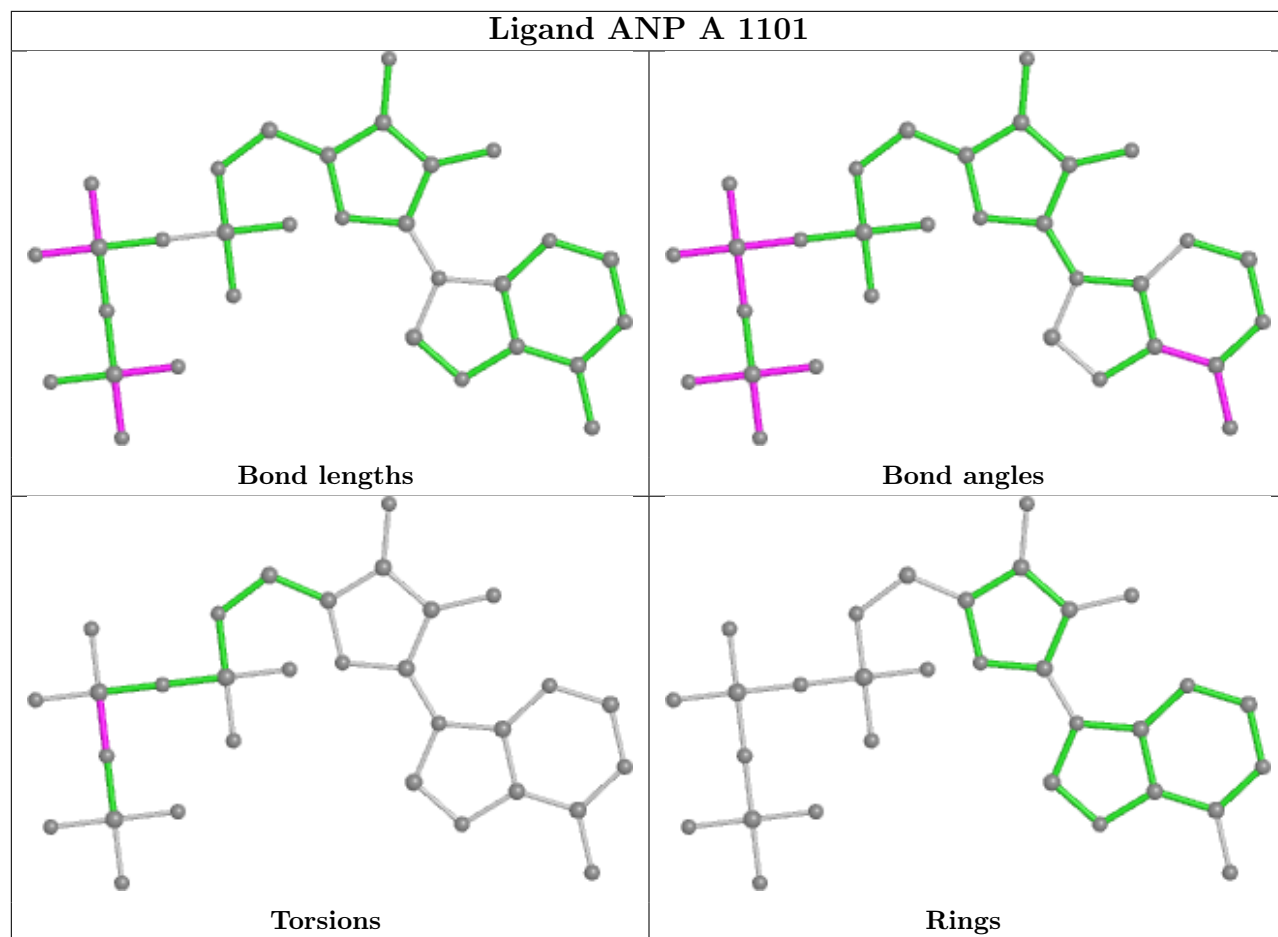
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	JBJ	1	0
2	D	1101	ANP	1	0
5	C	1102	YY3	2	0
4	F	1103	JBJ	2	0
2	F	1101	ANP	1	0

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.

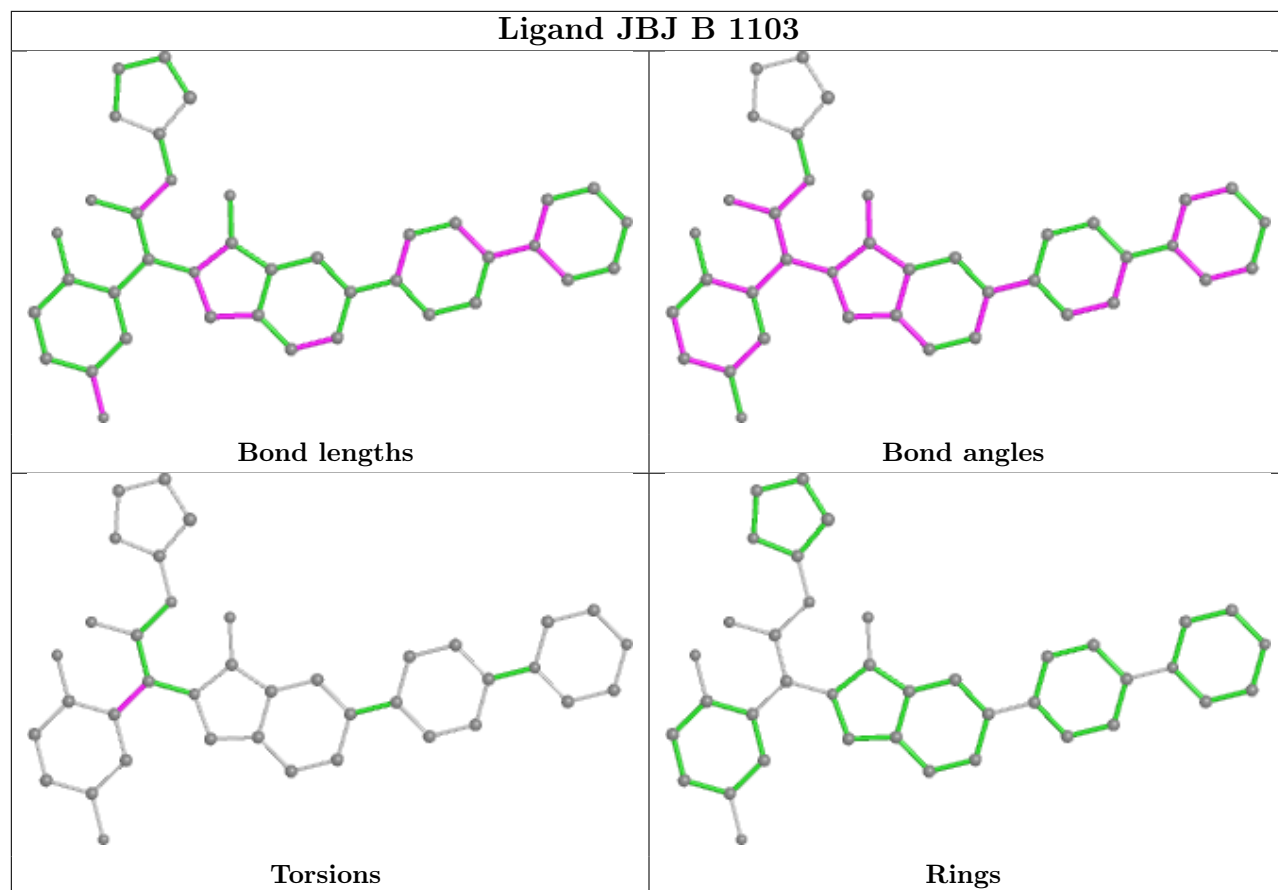




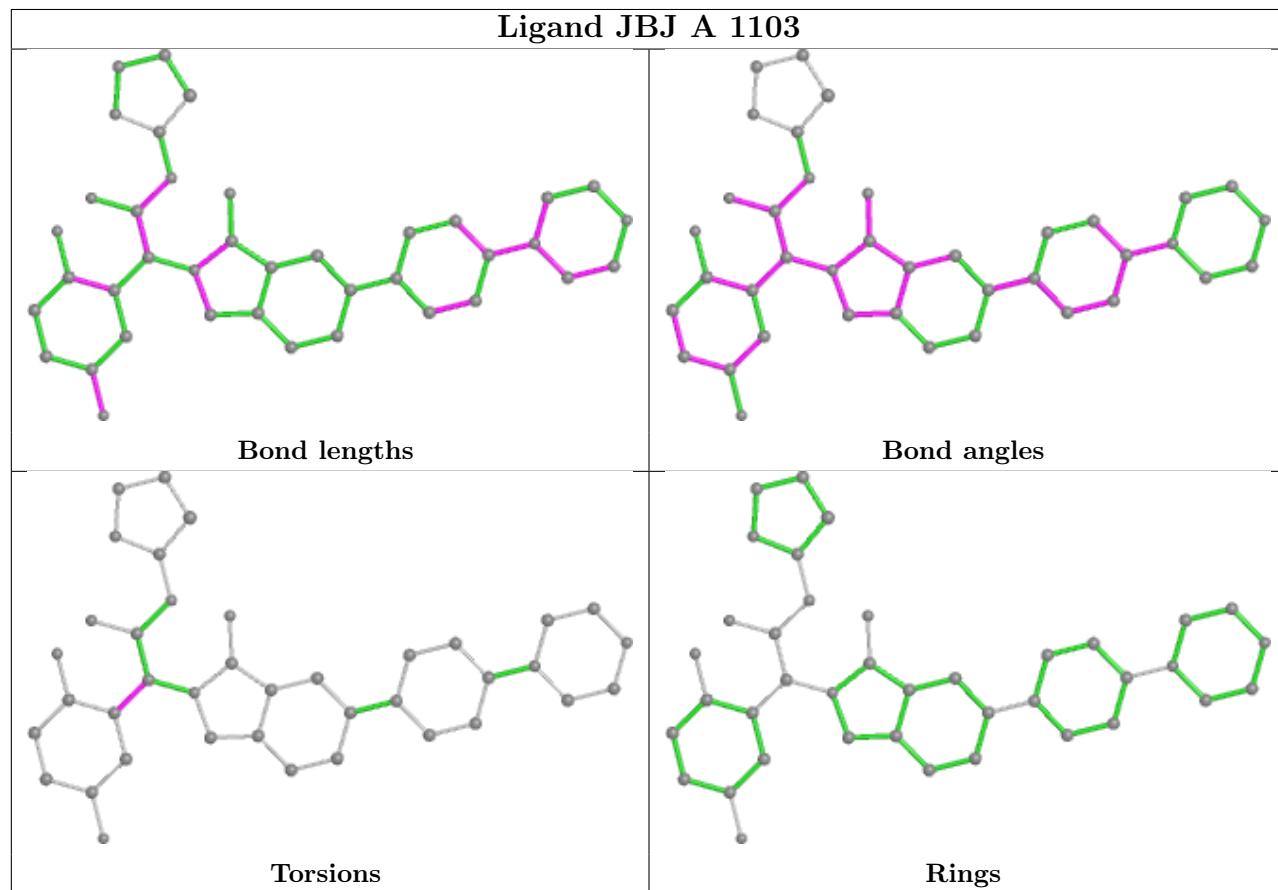


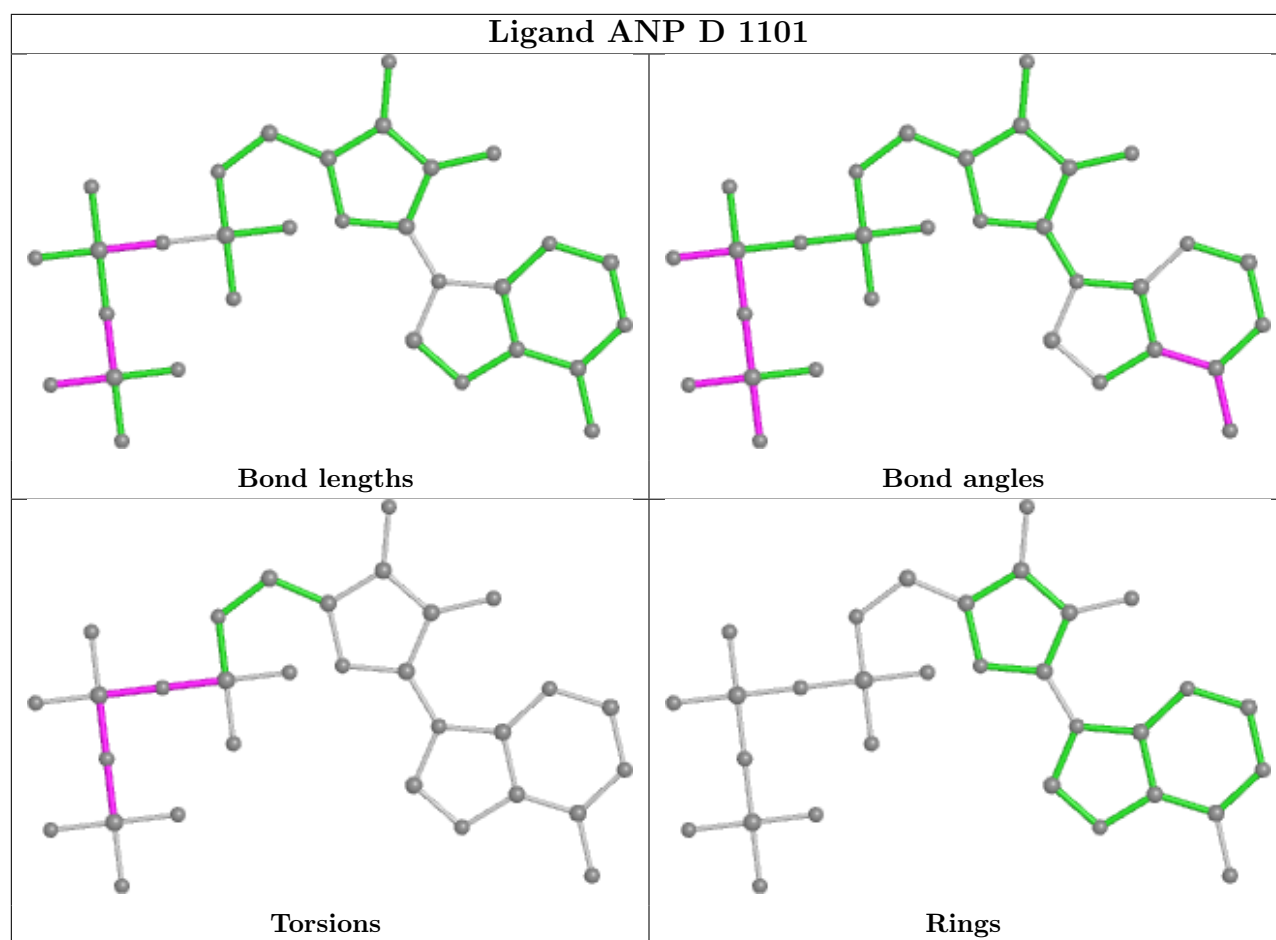


Ligand JBJ B 1103

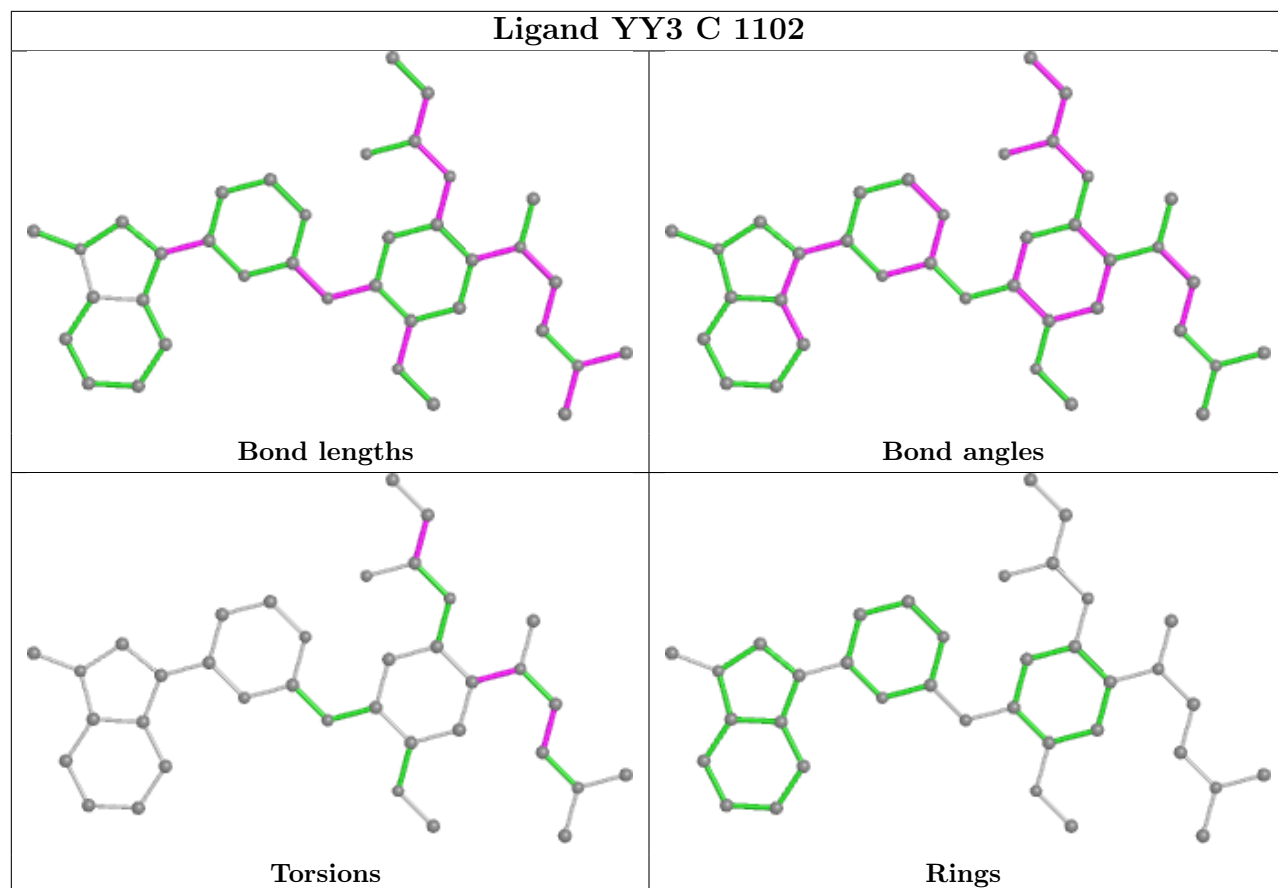


Ligand JBJ A 1103

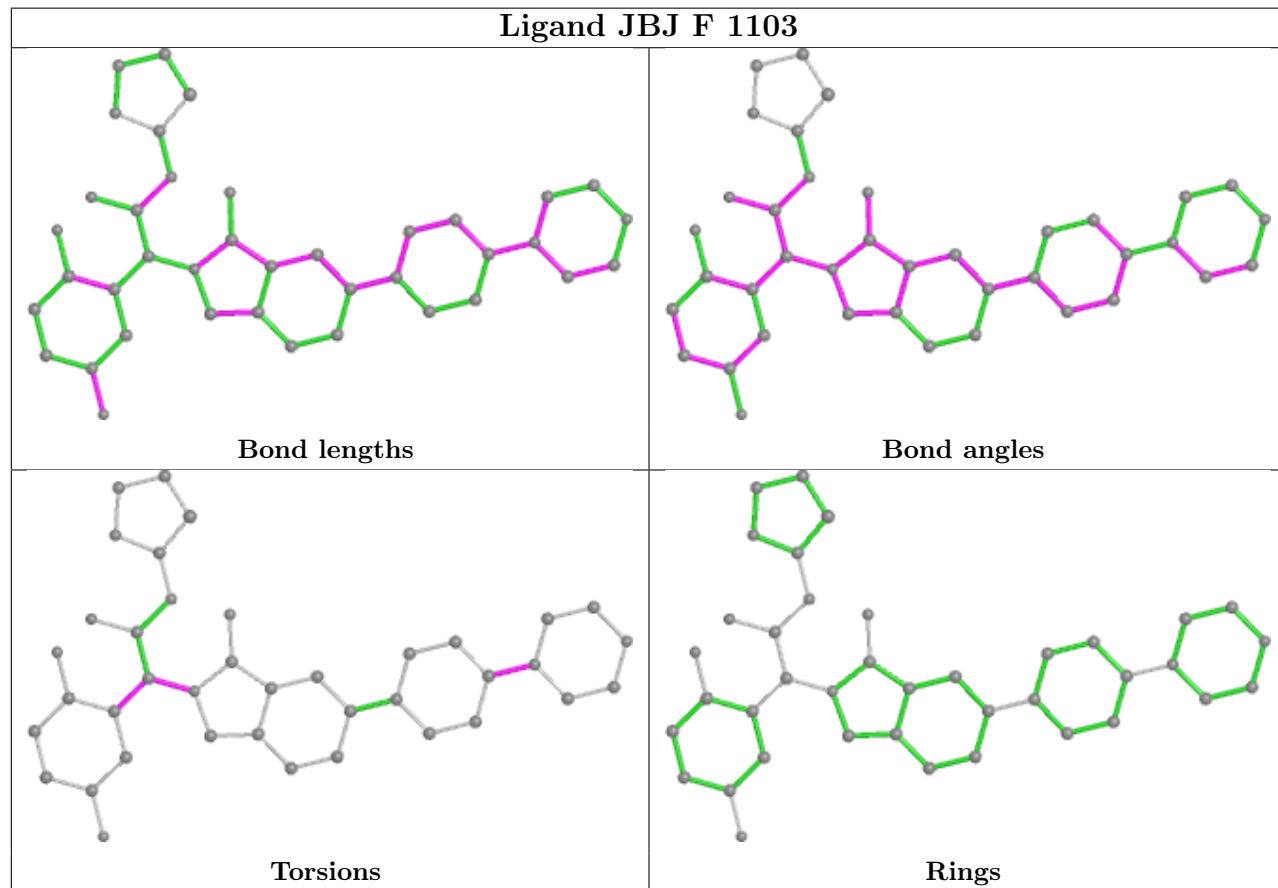


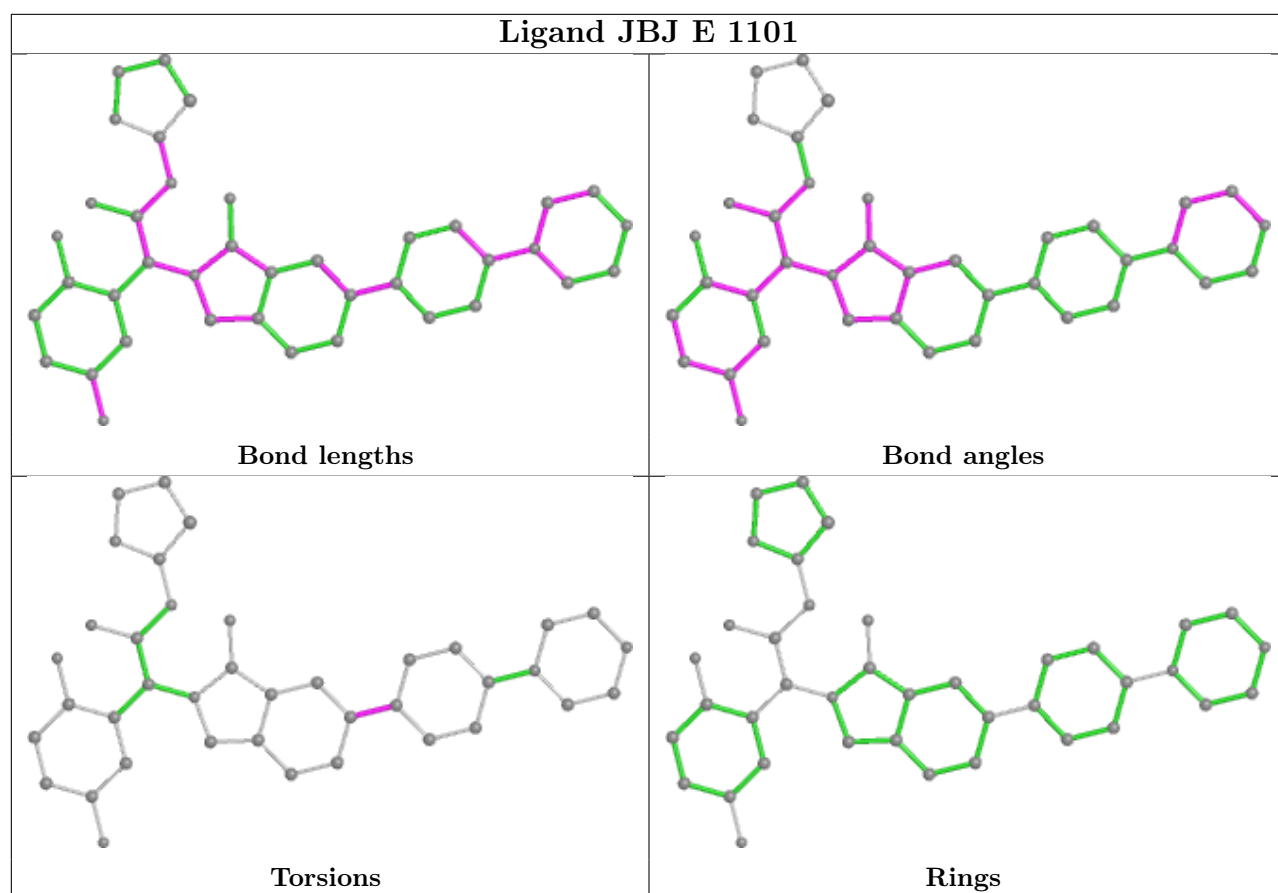


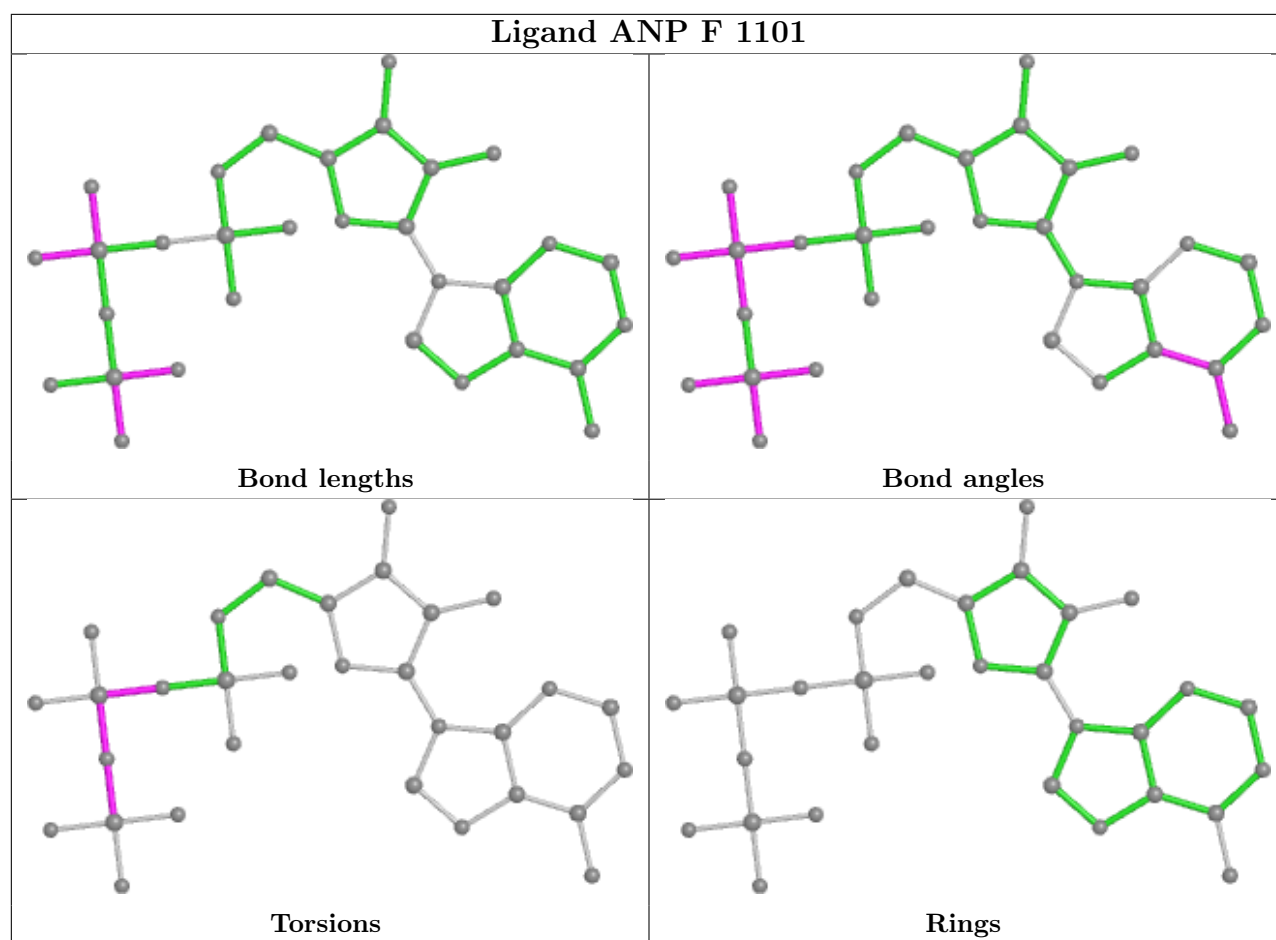
Ligand YY3 C 1102



Ligand JBJ F 1103







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	308/331 (93%)	0.07	8 (2%)	56	64	28, 47, 77, 106	0
1	B	308/331 (93%)	0.17	9 (2%)	51	61	32, 53, 85, 100	0
1	C	292/331 (88%)	0.24	13 (4%)	33	42	31, 57, 84, 105	0
1	D	294/331 (88%)	0.05	8 (2%)	54	63	28, 46, 72, 84	0
1	E	287/331 (86%)	0.81	38 (13%)	3	4	46, 79, 116, 139	0
1	F	294/331 (88%)	0.19	7 (2%)	59	67	35, 56, 82, 102	0
All	All	1783/1986 (89%)	0.25	83 (4%)	31	41	28, 55, 96, 139	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	870	HIS	5.2
1	A	890	ILE	4.9
1	C	988	HIS	4.3
1	E	917	GLY	4.3
1	E	751	THR	4.3
1	E	931	GLU	4.1
1	E	945	MET	4.1
1	C	1006	ASP	4.0
1	E	990	PRO	4.0
1	C	990	PRO	3.8
1	B	872	GLU	3.7
1	F	931	GLU	3.6
1	E	933	LEU	3.6
1	E	953	ILE	3.5
1	D	988	HIS	3.5
1	C	931	GLU	3.4
1	F	807	ASP	3.3
1	E	941	ILE	3.2
1	E	948	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	722	ALA	3.2
1	E	749	GLU	3.2
1	E	1007	MET	3.1
1	E	946	ILE	3.1
1	E	981	ILE	3.1
1	B	941	ILE	3.0
1	C	859	ALA	3.0
1	E	802	VAL	2.9
1	D	734	GLU	2.9
1	E	929	LYS	2.9
1	E	750	ALA	2.9
1	E	782	LEU	2.9
1	A	1007	MET	2.9
1	C	986	ARG	2.9
1	A	986	ARG	2.9
1	E	908[A]	MET	2.9
1	E	926	ILE	2.8
1	F	988	HIS	2.8
1	A	931	GLU	2.8
1	E	1006	ASP	2.7
1	E	919	PRO	2.7
1	F	986	ARG	2.7
1	E	723	PHE	2.7
1	A	870	HIS	2.6
1	C	1007	MET	2.6
1	D	990	PRO	2.6
1	C	715	ILE	2.6
1	E	927	LEU	2.6
1	B	890	ILE	2.5
1	A	1006	ASP	2.5
1	C	717	VAL	2.5
1	B	988	HIS	2.5
1	E	830	ASP	2.5
1	B	871	ALA	2.5
1	E	916	ASP	2.4
1	F	1007	MET	2.4
1	E	880	TRP	2.4
1	B	986	ARG	2.4
1	B	861	LEU	2.4
1	D	754	LYS	2.4
1	C	876	VAL	2.4
1	D	1006	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	713	LYS	2.4
1	A	869	TYR	2.3
1	E	962	ARG	2.3
1	E	918	ILE	2.3
1	D	860	LYS	2.3
1	D	861	LEU	2.2
1	E	718	LEU	2.2
1	E	970	LYS	2.2
1	E	930	GLY	2.2
1	C	890	ILE	2.2
1	F	861	LEU	2.2
1	E	992	PRO	2.2
1	A	988	HIS	2.2
1	D	807	ASP	2.2
1	F	889	ARG	2.2
1	C	953	ILE	2.1
1	E	910	PHE	2.1
1	E	808	ASN	2.1
1	C	713	LYS	2.1
1	B	867	LYS	2.1
1	E	737	LYS	2.1
1	E	715	ILE	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.

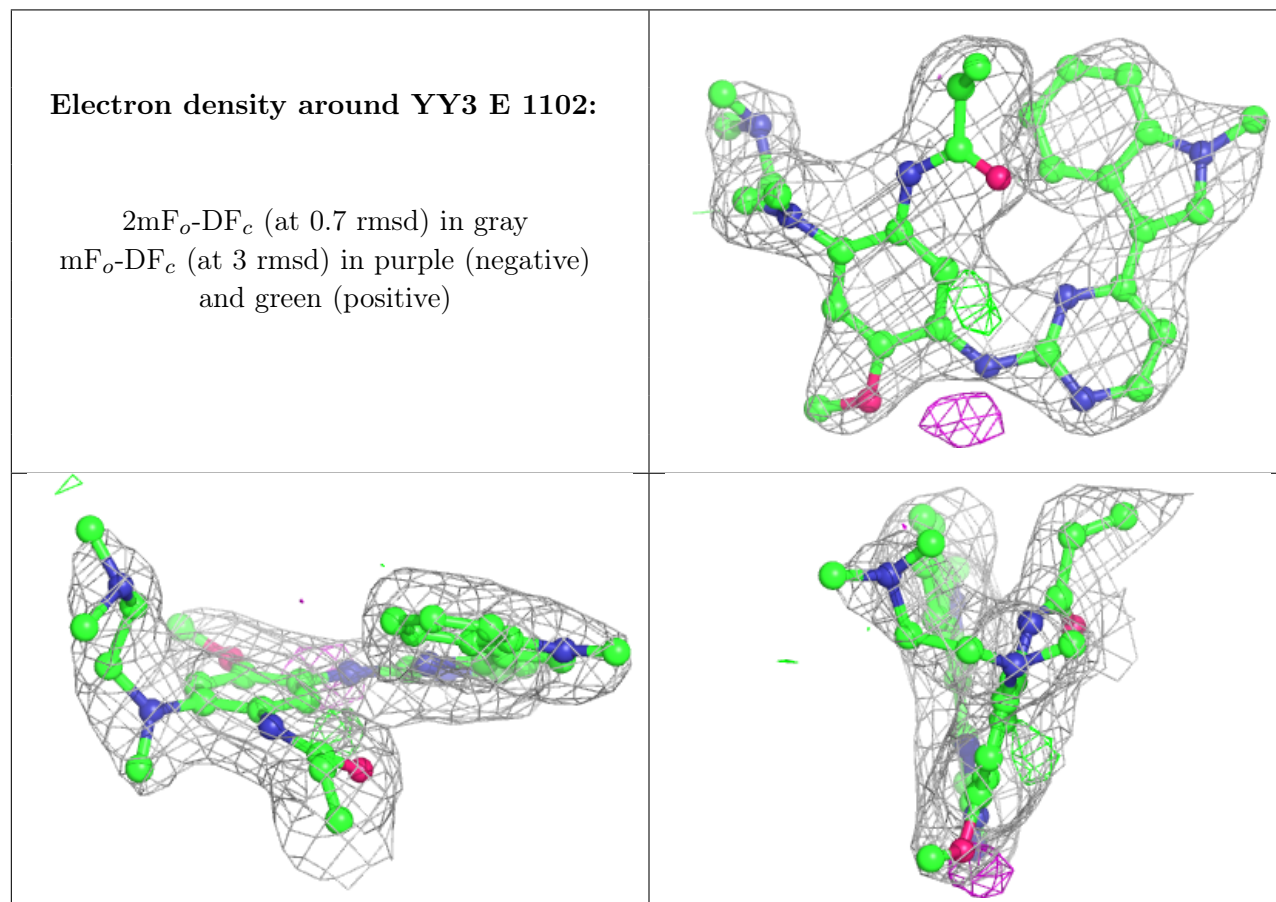
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	YY3	E	1102	37/37	0.89	0.15	57,65,73,75	0

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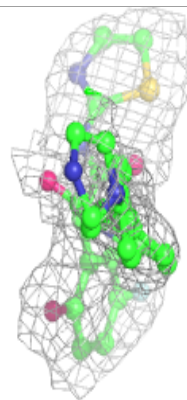
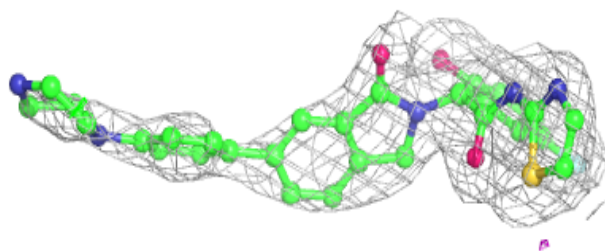
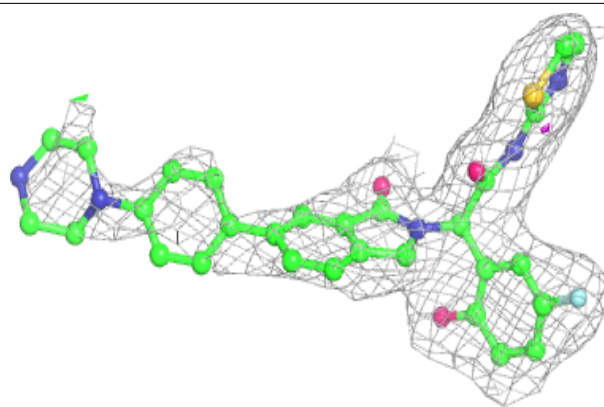
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	F	1102	1/1	0.90	0.14	48,48,48,48	0
4	JBj	E	1101	39/39	0.91	0.20	46,65,92,93	0
4	JBj	F	1103	39/39	0.95	0.17	30,44,73,74	0
2	ANP	F	1101	31/31	0.95	0.10	35,48,58,61	0
5	YY3	C	1102	37/37	0.95	0.14	35,47,62,67	0
4	JBj	D	1103	39/39	0.95	0.17	31,38,72,78	0
4	JBj	B	1103	39/39	0.96	0.14	29,39,69,72	0
3	MG	A	1102	1/1	0.96	0.13	36,36,36,36	0
4	JBj	C	1101	39/39	0.96	0.14	37,50,76,78	0
2	ANP	D	1101	31/31	0.96	0.11	32,41,49,57	0
3	MG	B	1102	1/1	0.97	0.12	42,42,42,42	0
2	ANP	B	1101	31/31	0.97	0.09	38,43,51,54	0
4	JBj	A	1103	39/39	0.97	0.14	30,39,63,74	0
3	MG	D	1102	1/1	0.98	0.03	43,43,43,43	0
2	ANP	A	1101	31/31	0.98	0.11	31,37,55,56	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.

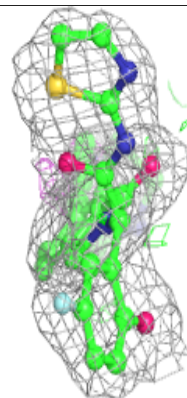
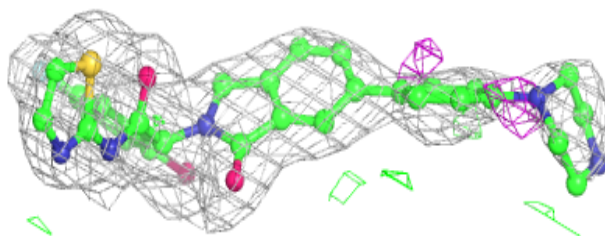
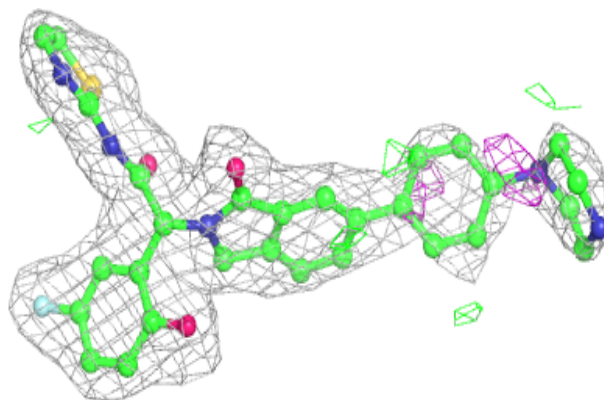


Electron density around JBJ E 1101:

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

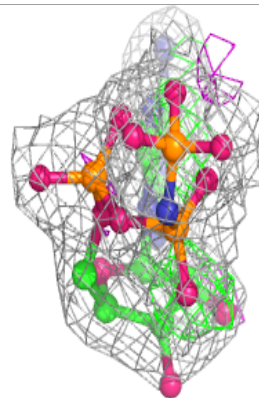
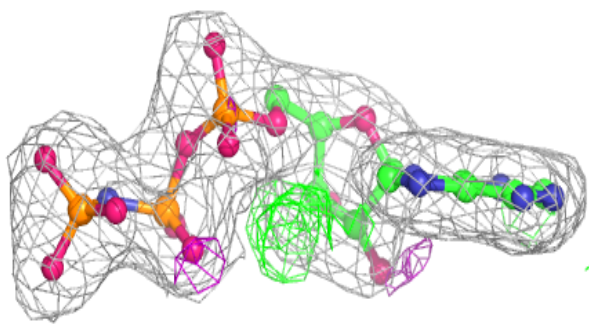
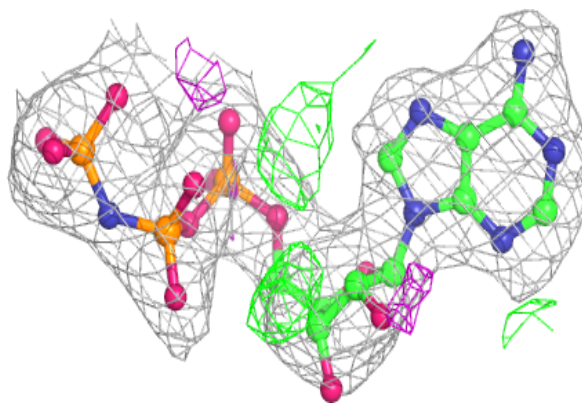
**Electron density around JBJ F 1103:**

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

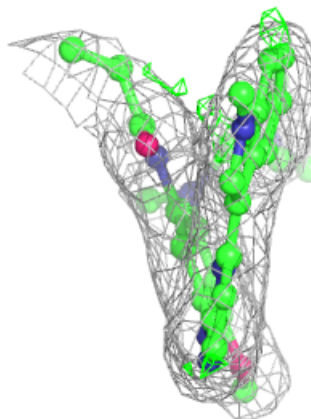
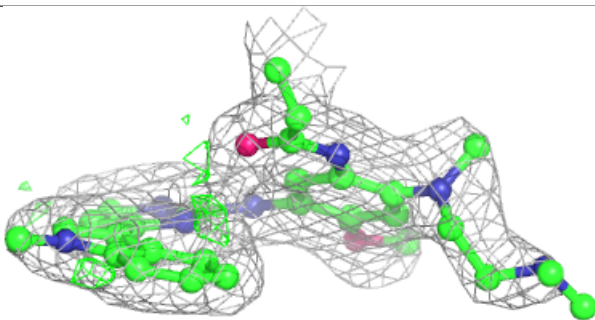
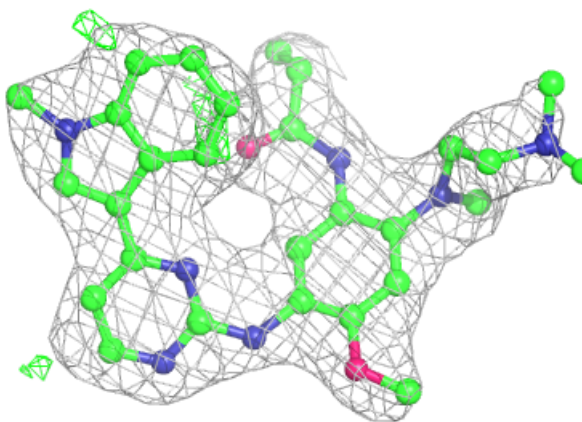


Electron density around ANP F 1101:

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

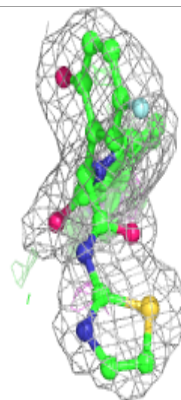
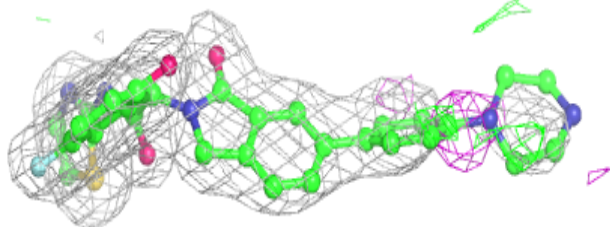
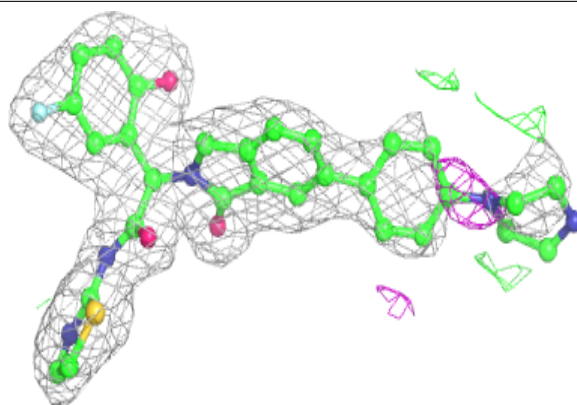
**Electron density around YY3 C 1102:**

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

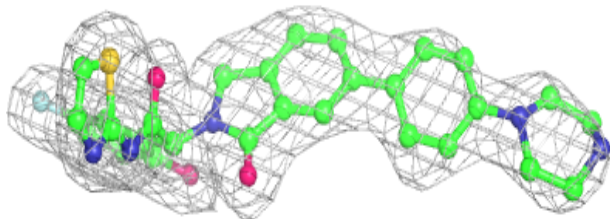
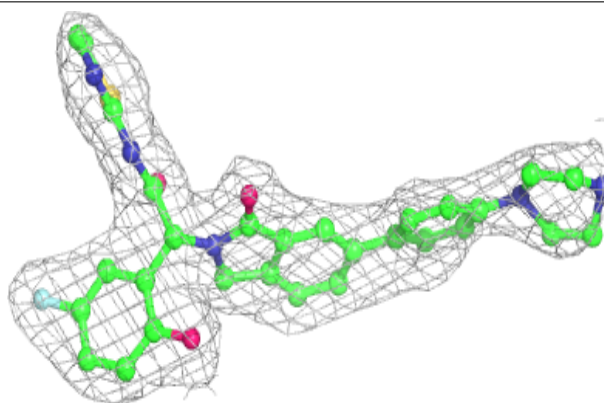


Electron density around JBJ D 1103:

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

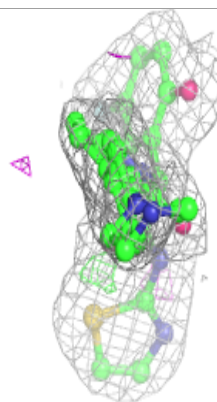
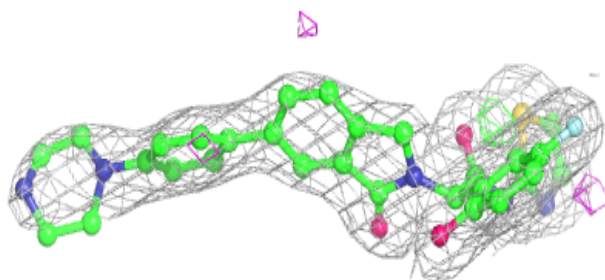
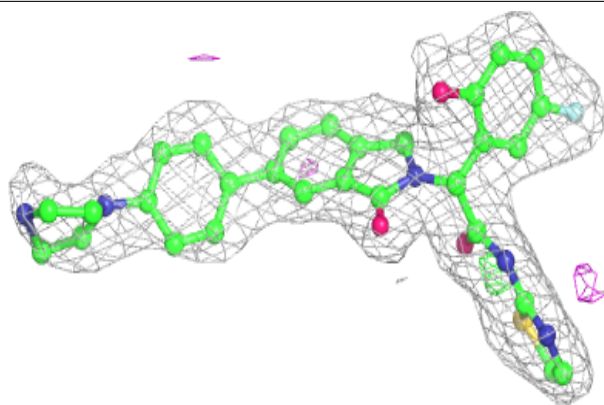
**Electron density around JBJ B 1103:**

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

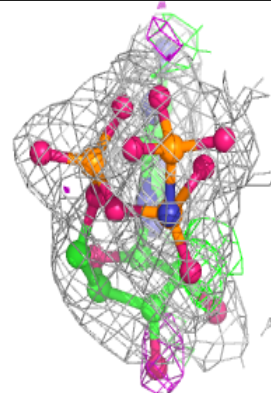
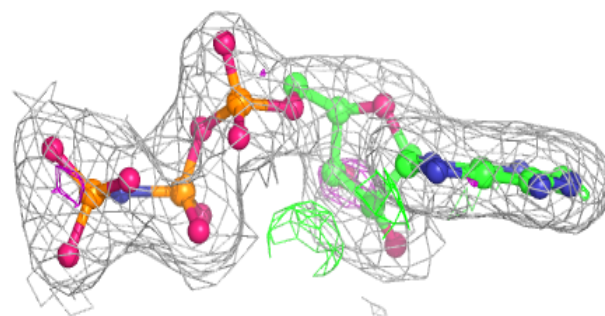
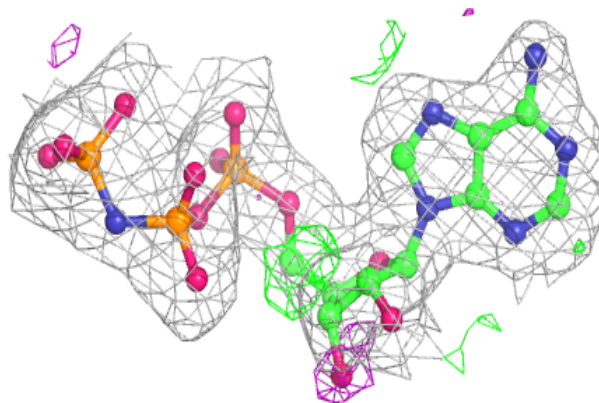


Electron density around JBJ C 1101:

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

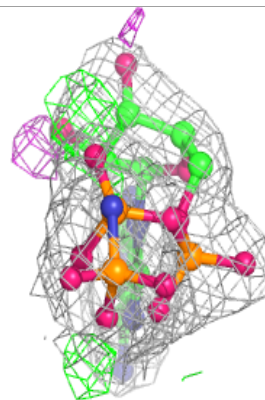
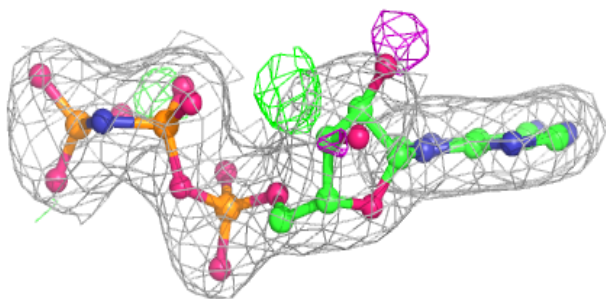
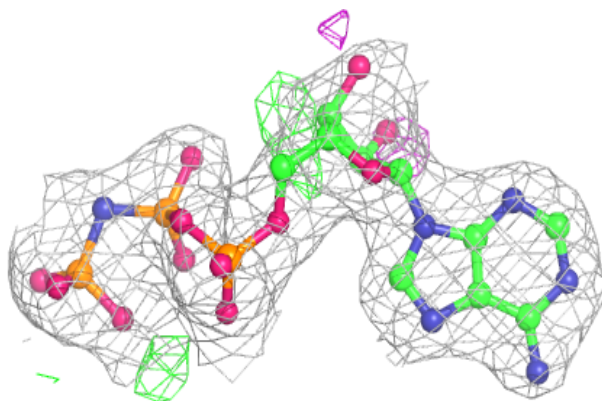
**Electron density around ANP D 1101:**

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

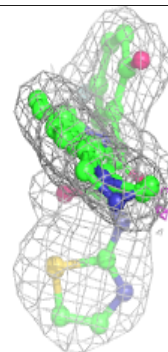
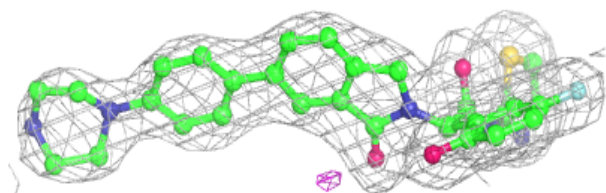
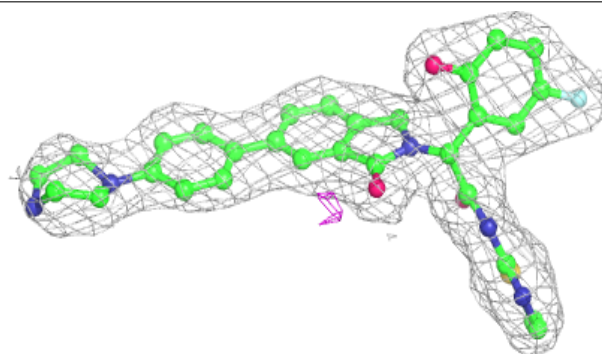


Electron density around ANP B 1101:

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

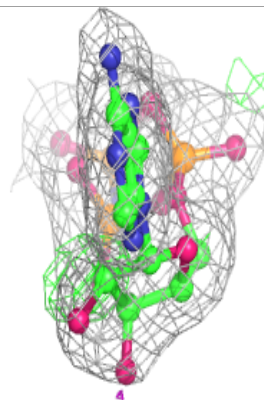
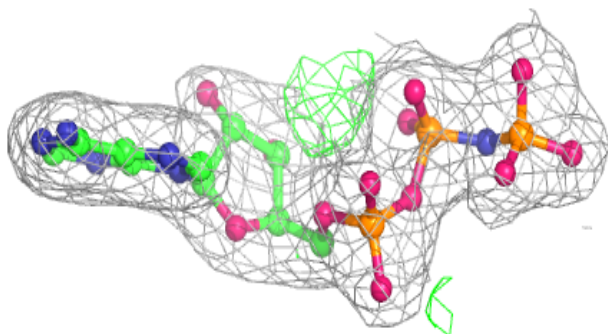
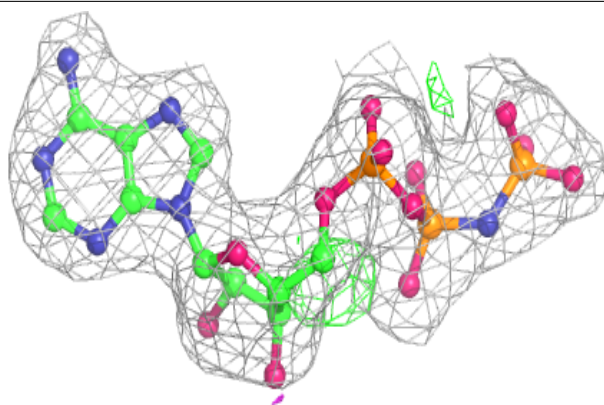
**Electron density around JBJ A 1103:**

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



Electron density around ANP A 1101:

$2mF_o-DF_c$ (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.