



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 09:01 AM UTC

PDB ID : 7JXK / pdb_00007jxk
Title : EGFR kinase (T790M/V948R) in complex with PF-06747775 and JBJ-04-125-02
Authors : Beyett, T.S.; Eck, M.J.
Deposited on : 2020-08-27
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

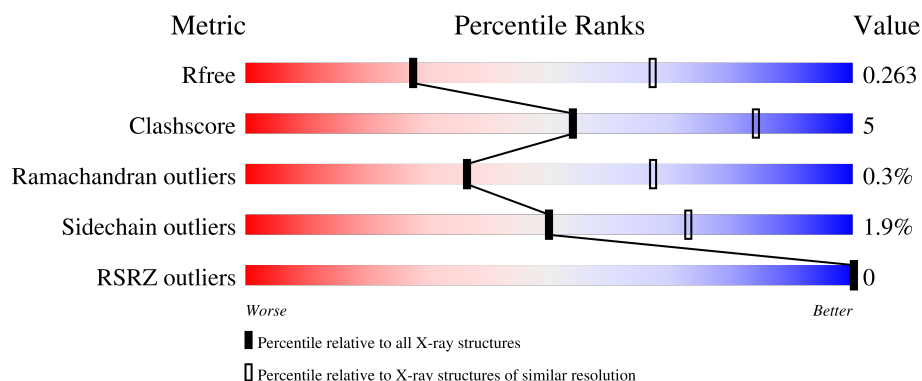
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	
1	B	331	
1	C	331	
1	D	331	
1	E	331	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	331	77% 10% • 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14507 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	293	Total	C	N	O	S	0	1	0
			2369	1522	403	424	20			
1	C	292	Total	C	N	O	S	0	1	0
			2361	1518	401	422	20			
1	F	292	Total	C	N	O	S	0	1	0
			2360	1516	401	423	20			
1	E	287	Total	C	N	O	S	0	1	0
			2314	1488	391	416	19			
1	B	290	Total	C	N	O	S	0	1	0
			2347	1507	399	421	20			

There are 30 discrepancies between the modelled and reference sequences:

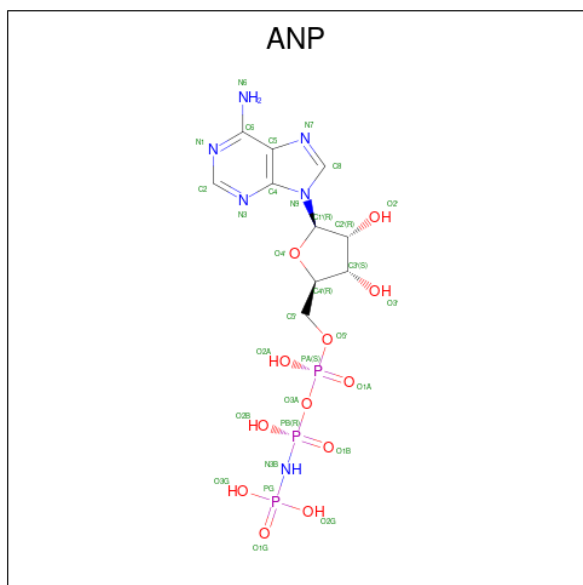
Chain	Residue	Modelled	Actual	Comment	Reference
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-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

Continued on next page...

Continued from previous page...

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
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
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

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

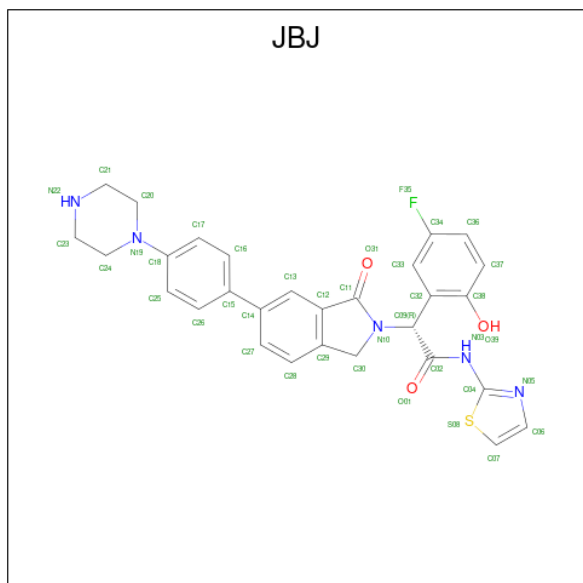


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

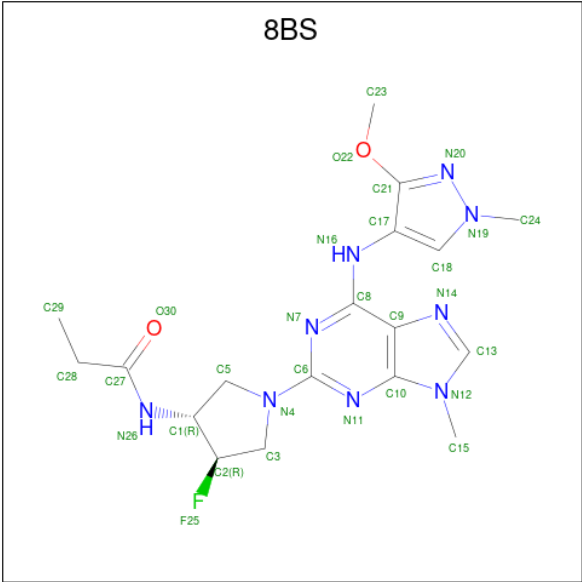
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- 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 (CCD ID: JBJ) (formula: $C_{29}H_{26}FN_5O_3S$) (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	E	1	Total	C	F	N	O	S	0	0
			39	29	1	5	3	1		

- Molecule 5 is N-[(3R,4R)-4-fluoro-1-{6-[(3-methoxy-1-methyl-1H-pyrazol-4-yl)amino]-9-methyl-9H-purin-2-yl}pyrrolidin-3-yl]propanamide (CCD ID: 8BS) (formula: $C_{18}H_{24}FN_9O_2$) (labeled as "Ligand of Interest" by depositor).

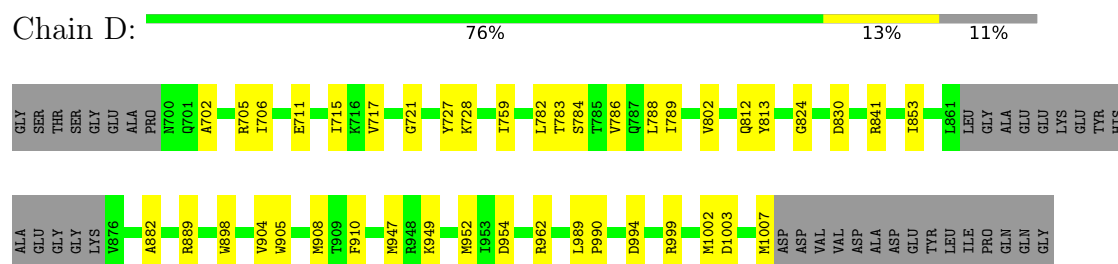


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			30	18	1	9	2		
5	C	1	Total	C	F	N	O	0	0
			30	18	1	9	2		
5	F	1	Total	C	F	N	O	0	0
			30	18	1	9	2		
5	E	1	Total	C	F	N	O	0	0
			30	18	1	9	2		

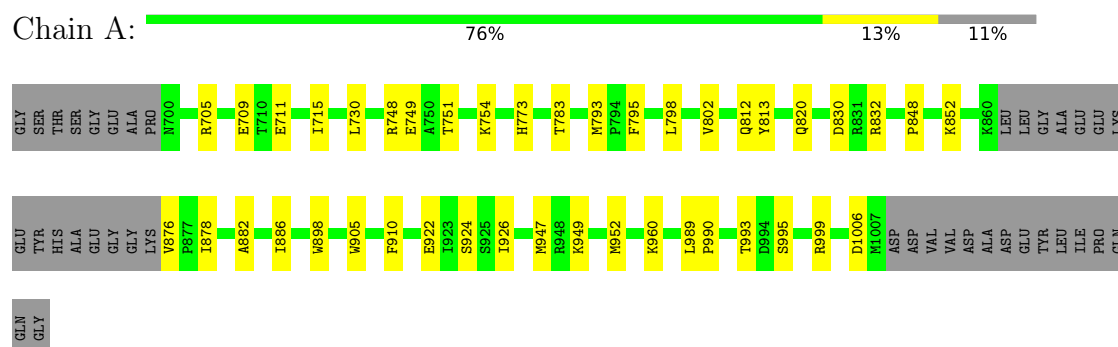
3 Residue-property plots

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

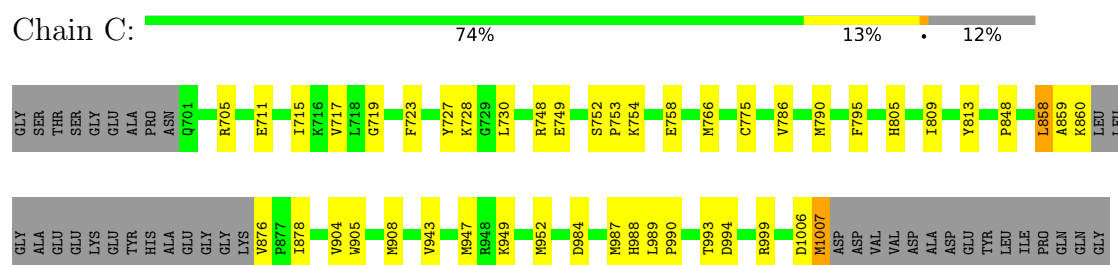
• Molecule 1: Epidermal growth factor receptor



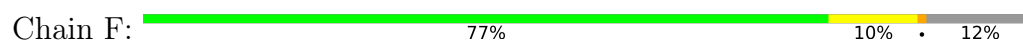
• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor

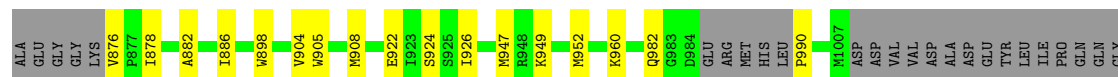


• Molecule 1: Epidermal growth factor receptor





Chain E: 76% 11% 13%



Chain B: 74% 13% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.85Å 87.37Å 91.31Å 62.06° 85.58° 73.33°	Depositor
Resolution (Å)	80.48 – 3.10 80.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.8 (80.48-3.10) 90.8 (80.48-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.222 , 0.261 0.222 , 0.263	Depositor DCC
R_{free} test set	1460 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14507	wwPDB-VP
Average B, all atoms (Å ²)	76.0	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 27.78 % 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 2.0690e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 8BS, 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	0.21	0/2424	0.49	0/3276
1	B	0.18	0/2402	0.45	0/3247
1	C	0.21	0/2416	0.47	0/3265
1	D	0.19	0/2432	0.47	2/3287 (0.1%)
1	E	0.15	0/2367	0.42	0/3199
1	F	0.20	0/2415	0.50	1/3265 (0.0%)
All	All	0.19	0/14456	0.47	3/19539 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	748	ARG	CA-CB-CG	5.08	124.26	114.10
1	D	784	SER	CA-C-N	5.06	130.19	122.65
1	D	784	SER	C-N-CA	5.06	130.19	122.65

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	2369	0	2418	23	0
1	B	2347	0	2390	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2361	0	2412	30	0
1	D	2377	0	2430	28	0
1	E	2314	0	2359	25	0
1	F	2360	0	2405	24	0
2	B	31	0	13	1	0
2	D	31	0	13	1	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	39	0	0	0	0
4	C	39	0	0	1	0
4	D	39	0	0	0	0
4	E	39	0	0	2	0
4	F	39	0	0	3	0
5	A	30	0	0	0	0
5	C	30	0	0	0	0
5	E	30	0	0	1	0
5	F	30	0	0	0	0
All	All	14507	0	14440	142	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 (142) 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:F:755:ALA:HB1	4:F:1102:JBJ:N22	2.03	0.73
1:E:723:PHE:HB3	1:E:747:LEU:HD22	1.78	0.65
1:A:832:ARG:HH22	1:B:724:GLY:C	2.04	0.64
1:D:830:ASP:HB3	1:C:717:VAL:HG11	1.81	0.62
1:B:705:ARG:NH2	1:B:711:GLU:OE2	2.33	0.60
1:D:812:GLN:HG2	1:D:989:LEU:HG	1.84	0.60
1:D:705:ARG:NH2	1:D:711:GLU:OE2	2.35	0.59
1:B:760:LEU:HD11	1:B:782:LEU:HD11	1.85	0.59
1:A:705:ARG:NH2	1:A:711:GLU:OE2	2.37	0.58
1:C:1007:MET:N	1:C:1007:MET:SD	2.76	0.58
1:F:813:TYR:OH	1:F:990:PRO:HD3	2.03	0.57
1:D:706:ILE:HG21	1:E:982:GLN:HG2	1.87	0.57
1:B:812:GLN:HG2	1:B:989:LEU:HG	1.86	0.57
1:A:812:GLN:HG2	1:A:989:LEU:HG	1.86	0.57
1:A:813:TYR:OH	1:A:990:PRO:HD3	2.05	0.57
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:962:ARG:HH22	1:C:719:GLY:HA2	1.71	0.56
1:C:723:PHE:HA	1:C:748:ARG:HE	1.69	0.56
1:F:905:TRP:HD1	1:F:947:MET:HE1	1.71	0.56
1:E:793:MET:O	5:E:1101:8BS:N16	2.39	0.55
1:B:748:ARG:HG3	1:B:749:GLU:H	1.71	0.55
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.06	0.55
1:E:775:CYS:HB3	1:E:790:MET:HE1	1.88	0.55
1:D:702:ALA:O	1:A:993:THR:HA	2.07	0.55
1:F:705:ARG:NH2	1:F:711:GLU:OE2	2.38	0.55
1:D:954:ASP:OD2	1:F:754:LYS:HD3	2.07	0.54
1:F:745:LYS:HB2	4:F:1102:JBJ:C06	2.37	0.54
1:F:990:PRO:HB2	1:F:994:ASP:HB2	1.89	0.54
1:E:783:THR:OG1	1:E:785:THR:O	2.20	0.54
1:D:706:ILE:HG21	1:E:982:GLN:CG	2.36	0.54
1:E:705:ARG:NH2	1:E:711:GLU:OE2	2.39	0.54
1:D:962:ARG:HH22	1:C:719:GLY:CA	2.21	0.53
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.73	0.53
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.09	0.53
1:F:812:GLN:HG2	1:F:989:LEU:HG	1.91	0.53
1:D:782:LEU:HD12	1:E:982:GLN:NE2	2.25	0.52
1:C:717:VAL:HG22	1:C:727:TYR:CE2	2.44	0.52
1:D:949:LYS:HG2	1:D:952:MET:HE3	1.92	0.52
1:A:793:MET:HE1	1:A:852:LYS:HD3	1.92	0.52
1:C:858:LEU:HD21	4:C:1102:JBJ:C11	2.40	0.52
1:E:905:TRP:HD1	1:E:947:MET:HE1	1.75	0.51
1:D:717:VAL:HG22	1:D:727:TYR:CE2	2.46	0.51
1:B:746:GLU:O	1:B:746:GLU:HG3	2.10	0.51
1:A:830:ASP:HA	1:B:720:SER:OG	2.12	0.50
1:C:858:LEU:O	1:C:860:LYS:N	2.45	0.50
1:F:759:ILE:HA	4:F:1102:JBJ:C16	2.42	0.50
1:B:949:LYS:HG2	1:B:952:MET:HE3	1.94	0.50
1:E:813:TYR:OH	1:E:990:PRO:HD3	2.11	0.50
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.46	0.50
1:F:717:VAL:HG22	1:F:727:TYR:CE2	2.47	0.50
1:C:949:LYS:HG2	1:C:952:MET:HE3	1.94	0.49
1:E:949:LYS:HG2	1:E:952:MET:HE3	1.93	0.49
1:D:706:ILE:HG21	1:E:982:GLN:CD	2.38	0.49
1:C:715:ILE:HG12	1:C:728:LYS:O	2.12	0.49
1:C:993:THR:HA	1:B:702:ALA:O	2.11	0.49
1:A:798:LEU:O	1:A:802:VAL:HG23	2.13	0.48
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:LYS:HG2	1:A:952:MET:HE3	1.95	0.48
1:E:715:ILE:HG12	1:E:728:LYS:O	2.14	0.48
1:C:705:ARG:NH2	1:C:711:GLU:OE2	2.47	0.47
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.79	0.47
1:F:715:ILE:HG12	1:F:728:LYS:O	2.14	0.47
1:A:886:ILE:HG21	1:A:924:SER:HB3	1.96	0.47
1:A:773:HIS:CD2	1:A:820:GLN:HB3	2.50	0.47
1:C:775:CYS:HB3	1:C:790:MET:HE1	1.96	0.47
1:B:715:ILE:HG12	1:B:728:LYS:O	2.14	0.47
1:C:989:LEU:HD22	1:C:990:PRO:HD2	1.96	0.47
1:F:949:LYS:HG2	1:F:952:MET:HE3	1.96	0.47
1:D:759:ILE:HD13	1:D:786:VAL:HG21	1.97	0.46
1:F:782:LEU:HD23	1:F:786:VAL:CG2	2.45	0.46
1:F:823:LYS:HA	1:F:965:ILE:HD11	1.96	0.46
1:D:788:LEU:C	1:D:789:ILE:HD12	2.40	0.46
1:E:759:ILE:HG12	4:E:1102:JBJ:C16	2.46	0.46
1:F:876:VAL:HG23	1:F:878:ILE:HG12	1.98	0.46
1:A:709:GLU:CG	1:A:783:THR:HG21	2.45	0.46
1:C:748:ARG:HH21	1:C:748:ARG:HG2	1.81	0.46
1:C:813:TYR:CE2	1:C:989:LEU:HD23	2.51	0.46
1:F:1002:MET:HE2	1:F:1002:MET:HB3	1.76	0.45
1:B:908[B]:MET:SD	1:B:943:VAL:HG11	2.56	0.45
1:E:717:VAL:HG22	1:E:727:TYR:CE2	2.52	0.45
1:D:715:ILE:HG12	1:D:728:LYS:O	2.16	0.44
1:F:798:LEU:O	1:F:802:VAL:HG23	2.18	0.44
1:A:802:VAL:HG12	1:A:910:PHE:HA	1.99	0.44
1:E:793:MET:HE1	1:E:852:LYS:HD3	1.98	0.44
1:C:858:LEU:HD23	1:C:858:LEU:HA	1.77	0.44
1:C:908[B]:MET:SD	1:C:943:VAL:HG11	2.58	0.44
1:F:748:ARG:HG2	1:F:748:ARG:O	2.18	0.44
1:A:709:GLU:HG3	1:A:783:THR:HG21	2.00	0.44
1:A:876:VAL:HG23	1:A:878:ILE:HG12	2.00	0.44
1:C:876:VAL:HG23	1:C:878:ILE:HG12	2.00	0.44
1:B:723:PHE:O	1:B:748:ARG:N	2.51	0.44
1:B:765:VAL:HG11	1:B:833:LEU:HD21	2.00	0.44
1:A:832:ARG:NH2	1:B:725:THR:OG1	2.51	0.43
1:B:726:VAL:HB	2:B:1101:ANP:H5'1	1.99	0.43
1:D:782:LEU:HD12	1:E:982:GLN:HE22	1.84	0.43
1:E:759:ILE:HG23	4:E:1102:JBJ:C27	2.49	0.43
1:E:886:ILE:HG21	1:E:924:SER:HB3	2.00	0.43
1:F:748:ARG:HH11	1:F:749:GLU:HG3	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:PHE:CZ	1:C:848:PRO:HD3	2.54	0.43
1:D:759:ILE:CD1	1:D:786:VAL:HG21	2.49	0.43
1:A:802:VAL:CG1	1:A:910:PHE:HA	2.48	0.43
1:F:751:THR:HB	1:F:752:SER:H	1.44	0.43
1:E:876:VAL:HG23	1:E:878:ILE:HG12	2.01	0.43
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.54	0.43
1:F:715:ILE:HD11	1:F:728:LYS:HG2	2.01	0.42
1:E:798:LEU:O	1:E:802:VAL:HG23	2.19	0.42
1:E:882:ALA:HA	1:E:898:TRP:CD2	2.53	0.42
1:B:1002:MET:HE2	1:B:1002:MET:HB3	1.80	0.42
1:E:904:VAL:O	1:E:908[B]:MET:HG3	2.19	0.42
1:B:887:LEU:HB3	1:B:888:HIS:CE1	2.55	0.42
1:A:795:PHE:CZ	1:A:848:PRO:HD3	2.55	0.42
1:C:904:VAL:O	1:C:908[B]:MET:HG3	2.20	0.42
1:C:999:ARG:NH2	1:C:1006:ASP:O	2.51	0.42
1:D:904:VAL:O	1:D:908[B]:MET:HG3	2.20	0.42
1:B:748:ARG:HG3	1:B:749:GLU:N	2.34	0.42
1:D:841:ARG:NE	2:D:1101:ANP:O3G	2.25	0.41
1:A:995:SER:O	1:A:999:ARG:HG3	2.20	0.41
1:C:805:HIS:O	1:C:809:ILE:HG13	2.19	0.41
1:B:715:ILE:HD11	1:B:728:LYS:HG2	2.02	0.41
1:A:922:GLU:O	1:A:926:ILE:HG23	2.21	0.41
1:F:1007:MET:HE3	1:F:1007:MET:HB3	1.79	0.41
1:B:823:LYS:HA	1:B:965:ILE:HD11	2.01	0.41
1:C:990:PRO:HB2	1:C:994:ASP:HB2	2.02	0.41
1:F:802:VAL:HG12	1:F:910:PHE:HA	2.01	0.41
1:A:715:ILE:HD13	1:A:730:LEU:HG	2.03	0.41
1:C:905:TRP:HB2	1:C:947:MET:HE3	2.01	0.41
1:E:720:SER:OG	1:E:748:ARG:NH1	2.51	0.41
1:D:999:ARG:HA	1:D:1003:ASP:HB3	2.02	0.41
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.86	0.41
1:D:802:VAL:HG12	1:D:910:PHE:HA	2.02	0.41
1:C:715:ILE:HD13	1:C:730:LEU:HG	2.03	0.41
1:C:989:LEU:HD23	1:C:989:LEU:HA	1.75	0.41
1:B:805:HIS:O	1:B:809:ILE:HG13	2.21	0.41
1:E:922:GLU:O	1:E:926:ILE:HG23	2.20	0.41
1:B:790:MET:HE3	1:B:790:MET:HB2	1.75	0.41
1:D:990:PRO:HB2	1:D:994:ASP:HB2	2.03	0.40
1:F:709:GLU:OE2	1:F:783:THR:HG21	2.21	0.40
1:D:824:GLY:HA3	1:D:853:ILE:HD12	2.04	0.40
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:984:ASP:HA	1:C:987:MET:HE3	2.03	0.40
1:D:1002:MET:HE2	1:D:1002:MET:HB3	1.81	0.40
1:C:715:ILE:HD11	1:C:728:LYS:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/331 (88%)	282 (97%)	7 (2%)	1 (0%)	36	67
1	B	287/331 (87%)	277 (96%)	9 (3%)	1 (0%)	36	67
1	C	289/331 (87%)	277 (96%)	10 (4%)	2 (1%)	18	49
1	D	291/331 (88%)	282 (97%)	7 (2%)	2 (1%)	18	49
1	E	282/331 (85%)	275 (98%)	7 (2%)	0	100	100
1	F	289/331 (87%)	278 (96%)	11 (4%)	0	100	100
All	All	1728/1986 (87%)	1671 (97%)	51 (3%)	6 (0%)	36	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	859	ALA
1	D	721	GLY
1	C	753	PRO
1	D	783	THR
1	A	1006	ASP
1	B	747	LEU

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	263/290 (91%)	258 (98%)	5 (2%)	50	73
1	B	261/290 (90%)	256 (98%)	5 (2%)	50	73
1	C	262/290 (90%)	253 (97%)	9 (3%)	32	63
1	D	264/290 (91%)	262 (99%)	2 (1%)	73	81
1	E	257/290 (89%)	256 (100%)	1 (0%)	84	86
1	F	262/290 (90%)	255 (97%)	7 (3%)	39	67
All	All	1569/1740 (90%)	1540 (98%)	29 (2%)	50	73

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	889	ARG
1	D	1007	MET
1	A	748	ARG
1	A	749	GLU
1	A	751	THR
1	A	754	LYS
1	A	960	LYS
1	C	749	GLU
1	C	752	SER
1	C	754	LYS
1	C	758	GLU
1	C	766	MET
1	C	786	VAL
1	C	858	LEU
1	C	988	HIS
1	C	1007	MET
1	F	723	PHE
1	F	748	ARG
1	F	749	GLU
1	F	751	THR
1	F	758	GLU
1	F	786	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1007	MET
1	E	960	LYS
1	B	746	GLU
1	B	762	GLU
1	B	783	THR
1	B	960	LYS
1	B	1007	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	849	GLN
1	D	888	HIS
1	A	701	GLN
1	A	849	GLN
1	C	701	GLN
1	C	849	GLN
1	F	849	GLN
1	E	812	GLN
1	E	816	ASN
1	E	982	GLN
1	B	791	GLN
1	B	849	GLN
1	B	888	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	B	1101	3	33,33,33	0.93	4 (12%)	45,52,52	0.58	0
2	ANP	D	1101	3	33,33,33	0.96	4 (12%)	45,52,52	0.64	1 (2%)
4	JBj	C	1102	-	44,44,44	2.64	17 (38%)	59,63,63	3.58	20 (33%)
5	8BS	A	1101	1	32,33,33	2.32	14 (43%)	37,48,48	2.20	9 (24%)
5	8BS	C	1101	1	32,33,33	2.32	13 (40%)	37,48,48	2.24	9 (24%)
5	8BS	E	1101	1	32,33,33	2.70	14 (43%)	37,48,48	2.25	10 (27%)
4	JBj	F	1102	-	44,44,44	2.54	18 (40%)	59,63,63	3.53	21 (35%)
4	JBj	A	1102	-	44,44,44	2.74	17 (38%)	59,63,63	3.55	19 (32%)
4	JBj	D	1103	-	44,44,44	1.81	12 (27%)	59,63,63	3.87	20 (33%)
4	JBj	E	1102	-	44,44,44	2.67	19 (43%)	59,63,63	3.45	17 (28%)
5	8BS	F	1101	1	32,33,33	2.59	15 (46%)	37,48,48	2.39	12 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	B	1101	3	-	3/18/38/38	0/3/3/3
2	ANP	D	1101	3	-	4/18/38/38	0/3/3/3
4	JBj	C	1102	-	-	3/24/44/44	0/6/6/6
5	8BS	A	1101	1	-	8/16/28/28	0/4/4/4
5	8BS	C	1101	1	-	6/16/28/28	0/4/4/4
5	8BS	E	1101	1	-	6/16/28/28	0/4/4/4
4	JBj	F	1102	-	-	2/24/44/44	0/6/6/6
4	JBj	A	1102	-	-	4/24/44/44	0/6/6/6
4	JBj	D	1103	-	-	4/24/44/44	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	JBJ	E	1102	-	-	1/24/44/44	0/6/6/6
5	8BS	F	1101	1	-	7/16/28/28	0/4/4/4

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1102	JBJ	C09-C02	8.35	1.63	1.54
4	E	1102	JBJ	C09-C02	7.94	1.62	1.54
4	A	1102	JBJ	C09-C02	7.82	1.62	1.54
4	A	1102	JBJ	C11-N10	7.03	1.43	1.36
5	E	1101	8BS	C6-N4	6.53	1.49	1.35
4	C	1102	JBJ	C11-N10	5.74	1.41	1.36
4	F	1102	JBJ	C09-N10	5.55	1.53	1.46
4	E	1102	JBJ	C11-N10	5.53	1.41	1.36
4	F	1102	JBJ	C30-C29	5.53	1.57	1.50
4	F	1102	JBJ	C09-C02	5.39	1.60	1.54
4	F	1102	JBJ	C11-N10	5.25	1.41	1.36
4	F	1102	JBJ	C04-S08	5.19	1.80	1.74
4	F	1102	JBJ	C30-N10	4.95	1.52	1.47
5	E	1101	8BS	C21-N20	4.89	1.38	1.31
5	F	1101	8BS	C21-N20	4.79	1.38	1.31
5	A	1101	8BS	C21-N20	4.74	1.38	1.31
5	F	1101	8BS	C6-N4	4.73	1.45	1.35
5	E	1101	8BS	C18-N19	4.66	1.39	1.34
5	C	1101	8BS	C21-N20	4.62	1.38	1.31
5	C	1101	8BS	C18-N19	4.62	1.39	1.34
4	A	1102	JBJ	C04-S08	4.58	1.80	1.74
4	E	1102	JBJ	C04-S08	4.58	1.80	1.74
4	E	1102	JBJ	C30-C29	4.56	1.56	1.50
4	C	1102	JBJ	C30-C29	4.52	1.56	1.50
5	E	1101	8BS	C3-C2	4.52	1.60	1.51
4	A	1102	JBJ	C09-N10	4.44	1.51	1.46
4	C	1102	JBJ	C09-N10	4.40	1.51	1.46
5	F	1101	8BS	C18-C17	4.29	1.42	1.36
5	A	1101	8BS	C18-C17	4.28	1.42	1.36
5	C	1101	8BS	C18-C17	4.27	1.42	1.36
5	F	1101	8BS	C18-N19	4.25	1.38	1.34
4	E	1102	JBJ	C09-N10	4.24	1.51	1.46
4	E	1102	JBJ	C30-N10	4.20	1.51	1.47
4	A	1102	JBJ	C30-C29	4.18	1.55	1.50
4	C	1102	JBJ	C04-S08	4.12	1.79	1.74
5	A	1101	8BS	C24-N19	4.11	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1101	8BS	C27-N26	4.03	1.42	1.34
4	A	1102	JBj	C18-N19	4.02	1.49	1.38
5	F	1101	8BS	C27-N26	4.00	1.42	1.34
5	A	1101	8BS	C18-N19	3.98	1.38	1.34
5	F	1101	8BS	C24-N19	3.89	1.50	1.46
4	C	1102	JBj	C12-C11	3.83	1.55	1.48
4	A	1102	JBj	C30-N10	3.81	1.51	1.47
4	A	1102	JBj	C12-C11	3.80	1.54	1.48
5	E	1101	8BS	C5-C1	3.78	1.59	1.52
4	D	1103	JBj	C11-N10	3.74	1.39	1.36
5	E	1101	8BS	C6-N7	3.71	1.41	1.34
5	F	1101	8BS	C1-N26	3.69	1.52	1.46
5	C	1101	8BS	C24-N19	3.68	1.50	1.46
4	E	1102	JBj	C02-N03	3.65	1.43	1.36
4	C	1102	JBj	C02-N03	3.64	1.43	1.36
4	D	1103	JBj	C18-N19	3.61	1.48	1.38
4	C	1102	JBj	C18-N19	3.60	1.48	1.38
4	E	1102	JBj	C24-N19	3.56	1.52	1.46
4	E	1102	JBj	C18-N19	3.56	1.48	1.38
5	E	1101	8BS	C18-C17	3.53	1.41	1.36
4	A	1102	JBj	C02-N03	3.53	1.43	1.36
4	D	1103	JBj	C04-S08	3.52	1.78	1.74
4	D	1103	JBj	C09-N10	3.48	1.50	1.46
5	C	1101	8BS	C3-C2	3.47	1.58	1.51
5	A	1101	8BS	C13-N12	3.43	1.43	1.36
5	F	1101	8BS	C5-N4	3.41	1.51	1.46
4	D	1103	JBj	C12-C11	3.39	1.54	1.48
4	E	1102	JBj	C20-N19	3.30	1.52	1.46
5	C	1101	8BS	C6-N4	3.26	1.42	1.35
4	D	1103	JBj	C30-N10	3.25	1.50	1.47
5	E	1101	8BS	C15-N12	-3.24	1.40	1.46
5	F	1101	8BS	C13-N12	3.24	1.43	1.36
5	E	1101	8BS	C17-N16	3.22	1.43	1.37
4	A	1102	JBj	C20-N19	3.19	1.52	1.46
4	F	1102	JBj	C18-N19	3.18	1.47	1.38
4	A	1102	JBj	C24-N19	3.17	1.52	1.46
4	C	1102	JBj	C24-N19	3.16	1.52	1.46
4	C	1102	JBj	C30-N10	3.13	1.50	1.47
4	E	1102	JBj	C06-N05	3.06	1.43	1.38
4	F	1102	JBj	C12-C11	2.96	1.53	1.48
4	A	1102	JBj	C38-C32	2.94	1.43	1.40
4	C	1102	JBj	C38-C32	2.94	1.43	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1102	JBj	C12-C11	2.93	1.53	1.48
5	F	1101	8BS	C6-N7	2.93	1.40	1.34
4	C	1102	JBj	C06-N05	2.90	1.43	1.38
4	F	1102	JBj	C38-C32	2.90	1.43	1.40
5	C	1101	8BS	C13-N12	2.89	1.42	1.36
4	F	1102	JBj	C06-N05	2.86	1.43	1.38
5	E	1101	8BS	C24-N19	2.86	1.49	1.46
5	A	1101	8BS	C10-N11	2.85	1.37	1.34
4	E	1102	JBj	C38-C32	2.83	1.43	1.40
4	A	1102	JBj	C06-N05	2.82	1.43	1.38
5	C	1101	8BS	C27-N26	2.81	1.40	1.34
5	A	1101	8BS	C10-N12	2.81	1.41	1.37
4	D	1103	JBj	C09-C02	2.80	1.57	1.54
5	C	1101	8BS	C6-N7	2.76	1.39	1.34
4	A	1102	JBj	C04-N03	2.74	1.42	1.38
4	E	1102	JBj	C04-N03	2.74	1.42	1.38
5	E	1101	8BS	C8-N7	2.72	1.39	1.34
4	D	1103	JBj	C02-N03	2.71	1.41	1.36
5	F	1101	8BS	C5-C1	2.71	1.57	1.52
4	F	1102	JBj	C02-N03	2.71	1.41	1.36
5	E	1101	8BS	C5-N4	2.70	1.50	1.46
5	A	1101	8BS	C1-N26	-2.69	1.41	1.46
4	E	1102	JBj	F35-C34	2.66	1.42	1.36
2	B	1101	ANP	PG-O1G	2.65	1.50	1.46
4	A	1102	JBj	F35-C34	2.64	1.42	1.36
2	D	1101	ANP	PG-N3B	2.62	1.70	1.63
5	A	1101	8BS	C9-C10	2.62	1.43	1.39
4	F	1102	JBj	F35-C34	2.62	1.42	1.36
5	A	1101	8BS	C3-C2	2.61	1.56	1.51
5	F	1101	8BS	C10-N11	2.61	1.37	1.34
4	C	1102	JBj	F35-C34	2.61	1.42	1.36
4	F	1102	JBj	C28-C27	2.58	1.43	1.38
4	D	1103	JBj	C30-C29	2.54	1.53	1.50
2	D	1101	ANP	PG-O1G	2.53	1.50	1.46
4	F	1102	JBj	C24-N19	2.52	1.51	1.46
5	A	1101	8BS	F25-C2	-2.51	1.34	1.40
2	D	1101	ANP	PB-O3A	-2.50	1.56	1.59
4	D	1103	JBj	C38-C32	2.50	1.43	1.40
5	C	1101	8BS	C10-N11	2.48	1.37	1.34
5	A	1101	8BS	C6-N4	2.48	1.40	1.35
4	D	1103	JBj	F35-C34	2.48	1.42	1.36
4	F	1102	JBj	C32-C09	2.47	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	ANP	PG-N3B	2.47	1.69	1.63
5	F	1101	8BS	C8-N7	2.47	1.39	1.34
5	A	1101	8BS	C5-N4	2.45	1.50	1.46
4	A	1102	JBj	C32-C09	2.41	1.55	1.52
2	B	1101	ANP	PB-O1B	2.40	1.49	1.46
2	D	1101	ANP	PB-O1B	2.33	1.49	1.46
4	C	1102	JBj	C24-C23	2.32	1.57	1.51
5	F	1101	8BS	C17-N16	2.32	1.41	1.37
5	C	1101	8BS	C8-N7	2.31	1.38	1.34
5	F	1101	8BS	C9-C10	2.30	1.43	1.39
4	E	1102	JBj	C17-C18	2.30	1.43	1.39
4	F	1102	JBj	C17-C18	2.29	1.43	1.39
4	D	1103	JBj	C32-C09	2.28	1.55	1.52
4	F	1102	JBj	C04-N03	2.24	1.41	1.38
4	E	1102	JBj	C28-C27	2.23	1.42	1.38
4	C	1102	JBj	C20-N19	2.22	1.50	1.46
4	E	1102	JBj	C32-C09	2.21	1.55	1.52
4	E	1102	JBj	C17-C16	2.21	1.42	1.38
5	A	1101	8BS	C17-N16	2.18	1.41	1.37
4	A	1102	JBj	C26-C25	2.14	1.42	1.38
4	C	1102	JBj	C04-N03	2.11	1.41	1.38
5	E	1101	8BS	C17-C21	2.05	1.46	1.42
2	B	1101	ANP	PB-O3A	-2.04	1.56	1.59
5	C	1101	8BS	C5-N4	2.04	1.49	1.46
4	F	1102	JBj	C28-C29	2.03	1.42	1.39
4	C	1102	JBj	C20-C21	2.02	1.56	1.51
5	C	1101	8BS	C1-N26	2.01	1.49	1.46

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1103	JBj	C30-N10-C11	-19.30	105.02	113.15
4	A	1102	JBj	C30-N10-C11	-18.11	105.51	113.15
4	F	1102	JBj	C30-N10-C11	-18.06	105.54	113.15
4	C	1102	JBj	C30-N10-C11	-17.82	105.64	113.15
4	E	1102	JBj	C30-N10-C11	-17.65	105.71	113.15
4	D	1103	JBj	C29-C30-N10	10.54	107.92	102.31
4	C	1102	JBj	C29-C30-N10	10.03	107.65	102.31
4	F	1102	JBj	C12-C11-N10	9.72	112.60	106.42
4	A	1102	JBj	C29-C30-N10	9.60	107.42	102.31
4	D	1103	JBj	C12-C11-N10	9.53	112.48	106.42
4	E	1102	JBj	C12-C11-N10	9.11	112.22	106.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1102	JB	C12-C11-N10	8.89	112.07	106.42
4	E	1102	JB	C29-C30-N10	8.70	106.94	102.31
4	A	1102	JB	C12-C11-N10	8.68	111.94	106.42
4	F	1102	JB	C29-C30-N10	8.30	106.72	102.31
5	A	1101	8BS	C5-C1-C2	-7.59	94.25	103.50
4	D	1103	JB	O31-C11-N10	-7.26	119.57	125.34
5	F	1101	8BS	C28-C27-N26	6.50	124.28	115.78
4	F	1102	JB	O31-C11-N10	-6.22	120.40	125.34
4	C	1102	JB	O31-C11-N10	-6.18	120.42	125.34
4	D	1103	JB	O01-C02-C09	-6.14	112.54	120.95
4	E	1102	JB	O31-C11-N10	-6.04	120.54	125.34
4	C	1102	JB	C02-N03-C04	5.72	131.51	124.54
4	A	1102	JB	O31-C11-N10	-5.64	120.86	125.34
5	E	1101	8BS	C28-C27-N26	5.64	123.15	115.78
5	E	1101	8BS	N7-C6-N4	5.63	125.13	117.12
4	D	1103	JB	C02-N03-C04	5.63	131.39	124.54
5	E	1101	8BS	C3-N4-C5	-5.56	103.56	111.64
4	D	1103	JB	C29-C12-C11	-5.52	105.94	108.94
4	E	1102	JB	O01-C02-C09	-5.46	113.47	120.95
4	E	1102	JB	C02-N03-C04	5.40	131.12	124.54
5	C	1101	8BS	C1-N26-C27	5.40	132.40	123.40
5	F	1101	8BS	C5-C1-C2	-5.37	96.94	103.50
4	A	1102	JB	C29-C12-C11	-5.24	106.10	108.94
5	C	1101	8BS	C5-C1-C2	-5.21	97.14	103.50
4	A	1102	JB	O01-C02-C09	-5.19	113.84	120.95
4	C	1102	JB	C29-C12-C11	-4.98	106.24	108.94
5	C	1101	8BS	N7-C6-N4	4.91	124.11	117.12
4	A	1102	JB	C02-N03-C04	4.82	130.41	124.54
5	F	1101	8BS	N7-C6-N4	4.74	123.87	117.12
4	F	1102	JB	C02-N03-C04	4.71	130.27	124.54
5	F	1101	8BS	C3-N4-C5	-4.55	105.03	111.64
4	F	1102	JB	O01-C02-C09	-4.32	115.03	120.95
5	A	1101	8BS	C3-N4-C5	-4.19	105.55	111.64
5	C	1101	8BS	N11-C6-N4	-4.19	111.15	117.12
4	E	1102	JB	C29-C12-C11	-4.15	106.69	108.94
4	C	1102	JB	O01-C02-C09	-4.10	115.32	120.95
5	F	1101	8BS	C1-N26-C27	4.10	130.24	123.40
5	E	1101	8BS	N11-C6-N4	-4.06	111.34	117.12
5	E	1101	8BS	C1-N26-C27	4.01	130.10	123.40
5	C	1101	8BS	C3-N4-C5	-3.90	105.98	111.64
4	C	1102	JB	C02-C09-N10	3.90	115.65	110.14
4	C	1102	JB	C21-C20-N19	3.88	118.82	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1101	8BS	C21-N20-N19	3.84	105.56	103.53
5	A	1101	8BS	C21-N20-N19	3.74	105.50	103.53
4	F	1102	JBj	C29-C12-C11	-3.70	106.93	108.94
5	C	1101	8BS	C28-C27-N26	3.69	120.59	115.78
5	F	1101	8BS	N11-C6-N4	-3.68	111.88	117.12
5	A	1101	8BS	N7-C6-N4	3.59	122.23	117.12
5	A	1101	8BS	C28-C27-N26	3.57	120.45	115.78
5	C	1101	8BS	C21-N20-N19	3.54	105.39	103.53
4	D	1103	JBj	C38-C32-C09	3.45	126.60	121.14
4	F	1102	JBj	C02-C09-N10	3.41	114.96	110.14
4	D	1103	JBj	C37-C36-C34	-3.41	114.87	118.38
5	A	1101	8BS	N11-C6-N4	-3.39	112.29	117.12
4	F	1102	JBj	C21-C20-N19	3.33	117.61	110.38
4	A	1102	JBj	O01-C02-N03	-3.23	117.31	122.61
4	D	1103	JBj	C13-C12-C11	3.20	134.88	129.39
4	E	1102	JBj	S08-C04-N05	-3.18	108.60	114.59
5	E	1101	8BS	C5-N4-C6	3.17	128.53	123.41
4	D	1103	JBj	C02-C09-N10	3.15	114.59	110.14
4	A	1102	JBj	S08-C04-N05	-3.14	108.66	114.59
4	C	1102	JBj	N03-C04-N05	3.13	127.13	121.19
4	F	1102	JBj	C37-C36-C34	-3.12	115.17	118.38
4	D	1103	JBj	S08-C04-N05	-3.09	108.76	114.59
4	C	1102	JBj	S08-C04-N05	-3.07	108.81	114.59
4	F	1102	JBj	S08-C04-N05	-3.07	108.81	114.59
4	D	1103	JBj	O01-C02-N03	-3.06	117.59	122.61
4	A	1102	JBj	N03-C04-N05	3.05	126.96	121.19
4	F	1102	JBj	O01-C02-N03	-3.03	117.64	122.61
4	E	1102	JBj	N03-C04-N05	3.01	126.90	121.19
4	E	1102	JBj	O01-C02-N03	-2.96	117.75	122.61
4	A	1102	JBj	C26-C15-C14	2.96	126.37	121.25
4	E	1102	JBj	C07-S08-C04	2.95	93.45	90.07
5	A	1101	8BS	C24-N19-N20	2.92	122.54	119.57
4	F	1102	JBj	N03-C04-N05	2.91	126.69	121.19
5	E	1101	8BS	C21-N20-N19	2.88	105.05	103.53
4	A	1102	JBj	C07-S08-C04	2.88	93.37	90.07
4	C	1102	JBj	C13-C12-C11	2.84	134.26	129.39
4	A	1102	JBj	C13-C12-C11	2.81	134.22	129.39
4	C	1102	JBj	C07-S08-C04	2.81	93.28	90.07
4	F	1102	JBj	C30-N10-C09	2.77	126.43	123.84
4	A	1102	JBj	C21-C20-N19	2.74	116.33	110.38
4	A	1102	JBj	C37-C36-C34	-2.72	115.59	118.38
5	F	1101	8BS	C24-N19-N20	2.71	122.33	119.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1101	8BS	N11-C10-N12	2.66	129.43	126.13
4	D	1103	JBj	C24-N19-C20	-2.64	105.62	111.57
5	E	1101	8BS	C24-N19-N20	2.63	122.25	119.57
4	C	1102	JBj	O01-C02-N03	-2.58	118.38	122.61
5	E	1101	8BS	C5-C1-C2	-2.58	100.36	103.50
4	D	1103	JBj	N03-C04-N05	2.56	126.04	121.19
5	C	1101	8BS	N11-C10-N12	2.56	129.29	126.13
4	E	1102	JBj	C37-C36-C34	-2.55	115.75	118.38
4	E	1102	JBj	C23-C24-N19	2.53	115.89	110.38
5	C	1101	8BS	C24-N19-N20	2.53	122.15	119.57
4	F	1102	JBj	C36-C34-C33	2.52	126.56	123.23
4	F	1102	JBj	C07-S08-C04	2.48	92.91	90.07
4	D	1103	JBj	C07-S08-C04	2.44	92.86	90.07
4	C	1102	JBj	C36-C34-C33	2.44	126.45	123.23
4	F	1102	JBj	C30-C29-C12	-2.43	108.20	109.73
4	A	1102	JBj	C36-C34-C33	2.41	126.41	123.23
4	E	1102	JBj	C21-C20-N19	2.34	115.48	110.38
4	E	1102	JBj	C36-C34-C33	2.33	126.30	123.23
5	F	1101	8BS	C5-N4-C6	2.32	127.16	123.41
5	E	1101	8BS	O30-C27-C28	-2.31	115.90	122.13
4	D	1103	JBj	C36-C34-C33	2.30	126.28	123.23
4	C	1102	JBj	C24-C23-N22	2.30	116.77	110.90
4	C	1102	JBj	C23-C24-N19	2.28	115.33	110.38
4	D	1103	JBj	C25-C18-N19	2.27	124.55	121.39
4	A	1102	JBj	C25-C18-N19	2.25	124.52	121.39
4	C	1102	JBj	C20-C21-N22	2.25	116.64	110.90
4	C	1102	JBj	C37-C36-C34	-2.24	116.08	118.38
4	E	1102	JBj	C13-C12-C11	2.22	133.20	129.39
4	F	1102	JBj	C27-C14-C15	2.20	125.05	121.25
4	A	1102	JBj	C23-C24-N19	2.19	115.15	110.38
4	F	1102	JBj	C13-C12-C11	2.18	133.13	129.39
4	F	1102	JBj	C30-C29-C28	2.18	133.37	128.70
5	F	1101	8BS	N11-C10-N12	2.15	128.78	126.13
5	F	1101	8BS	O30-C27-N26	-2.14	119.33	122.95
5	F	1101	8BS	O30-C27-C28	-2.12	116.39	122.13
4	F	1102	JBj	C28-C29-C12	-2.12	118.43	120.28
4	D	1103	JBj	C25-C18-C17	-2.11	115.15	119.18
4	C	1102	JBj	C30-C29-C12	-2.11	108.40	109.73
4	D	1103	JBj	C32-C09-C02	-2.10	107.69	112.87
2	D	1101	ANP	O3G-PG-O1G	-2.09	108.20	113.45
4	E	1102	JBj	C30-C29-C12	-2.04	108.45	109.73
4	A	1102	JBj	C24-N19-C20	-2.02	107.01	111.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1101	8BS	C5-N4-C6	2.01	126.66	123.41

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1101	ANP	PB-N3B-PG-O1G
2	D	1101	ANP	C5'-O5'-PA-O1A
2	B	1101	ANP	PB-N3B-PG-O1G
4	F	1102	JBj	N05-C04-N03-C02
5	A	1101	8BS	N7-C6-N4-C5
5	A	1101	8BS	N11-C6-N4-C5
5	A	1101	8BS	C21-C17-N16-C8
5	A	1101	8BS	C18-C17-N16-C8
5	A	1101	8BS	C17-C21-O22-C23
5	C	1101	8BS	N7-C6-N4-C5
5	C	1101	8BS	N11-C6-N4-C5
5	C	1101	8BS	C21-C17-N16-C8
5	C	1101	8BS	C18-C17-N16-C8
5	C	1101	8BS	C2-C1-N26-C27
5	F	1101	8BS	C21-C17-N16-C8
5	F	1101	8BS	C18-C17-N16-C8
5	F	1101	8BS	C2-C1-N26-C27
5	E	1101	8BS	N7-C6-N4-C5
5	E	1101	8BS	N11-C6-N4-C5
5	E	1101	8BS	C21-C17-N16-C8
5	E	1101	8BS	C18-C17-N16-C8
5	E	1101	8BS	C2-C1-N26-C27
4	F	1102	JBj	S08-C04-N03-C02
4	D	1103	JBj	C25-C18-N19-C20
4	D	1103	JBj	C17-C18-N19-C20
5	F	1101	8BS	N7-C6-N4-C3
5	F	1101	8BS	N11-C6-N4-C3
4	D	1103	JBj	N10-C09-C32-C33
4	A	1102	JBj	C13-C14-C15-C16
4	A	1102	JBj	C13-C14-C15-C26
5	A	1101	8BS	N20-C21-O22-C23
5	A	1101	8BS	C5-C1-N26-C27
5	F	1101	8BS	N26-C27-C28-C29
5	A	1101	8BS	C2-C1-N26-C27
5	F	1101	8BS	O30-C27-C28-C29
4	A	1102	JBj	C27-C14-C15-C16

Continued on next page...

Continued from previous page...

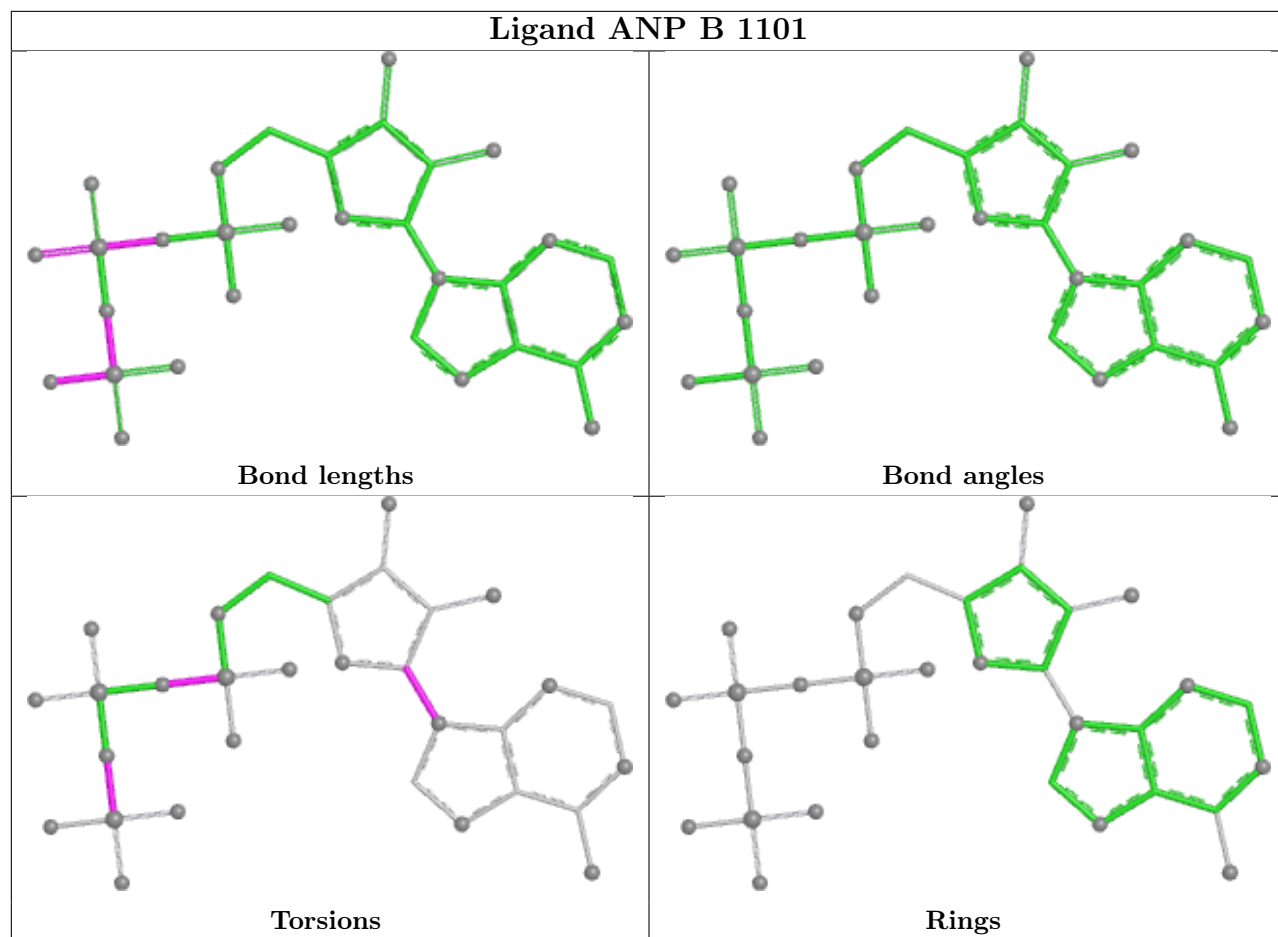
Mol	Chain	Res	Type	Atoms
2	D	1101	ANP	PB-O3A-PA-O2A
4	C	1102	JBj	C25-C18-N19-C24
4	A	1102	JBj	C27-C14-C15-C26
4	C	1102	JBj	C32-C09-N10-C30
4	E	1102	JBj	N10-C09-C32-C38
4	C	1102	JBj	C17-C18-N19-C24
2	B	1101	ANP	PB-O3A-PA-O1A
5	C	1101	8BS	C5-C1-N26-C27
5	E	1101	8BS	C5-C1-N26-C27
2	B	1101	ANP	C2'-C1'-N9-C8
4	D	1103	JBj	C02-C09-C32-C38
2	D	1101	ANP	PB-O3A-PA-O1A

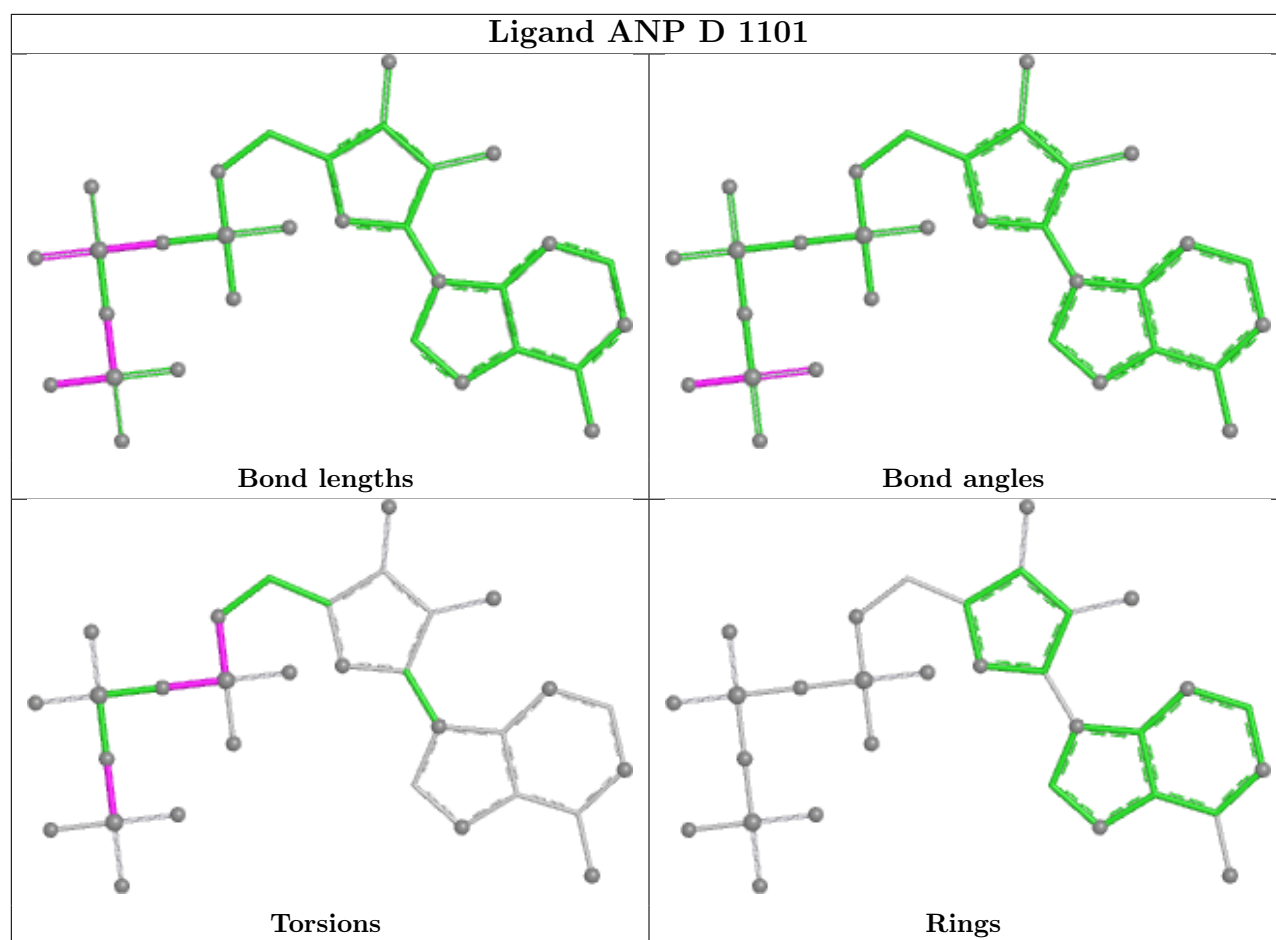
There are no ring outliers.

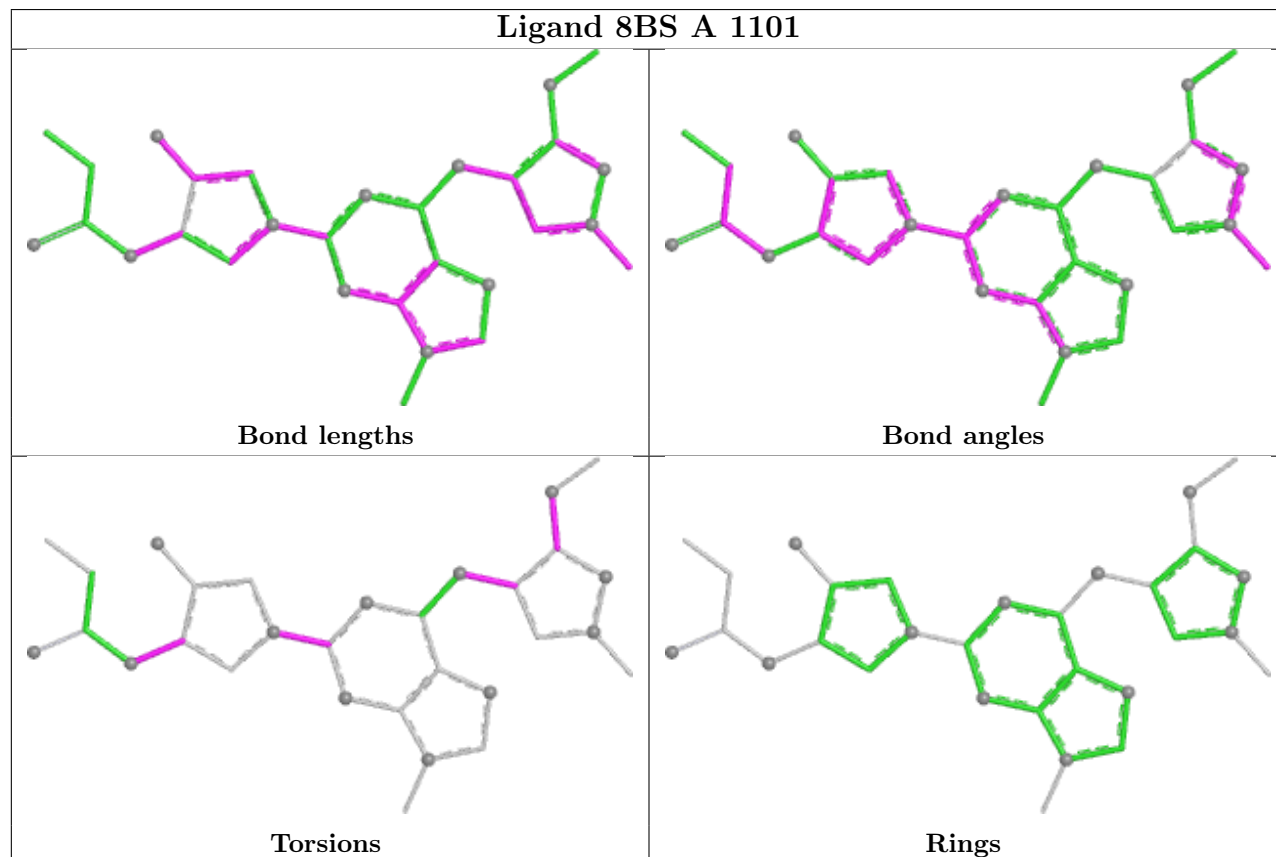
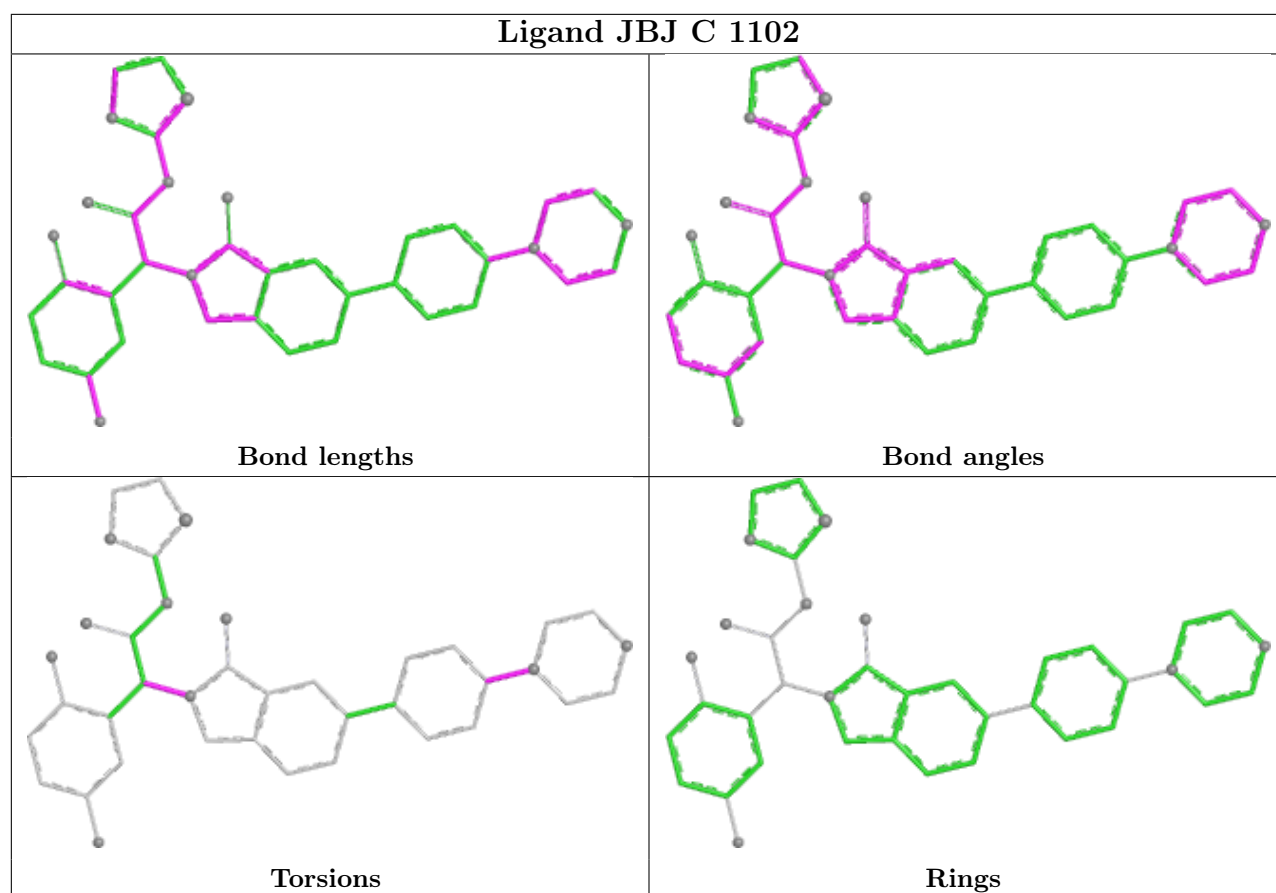
6 monomers are involved in 9 short contacts:

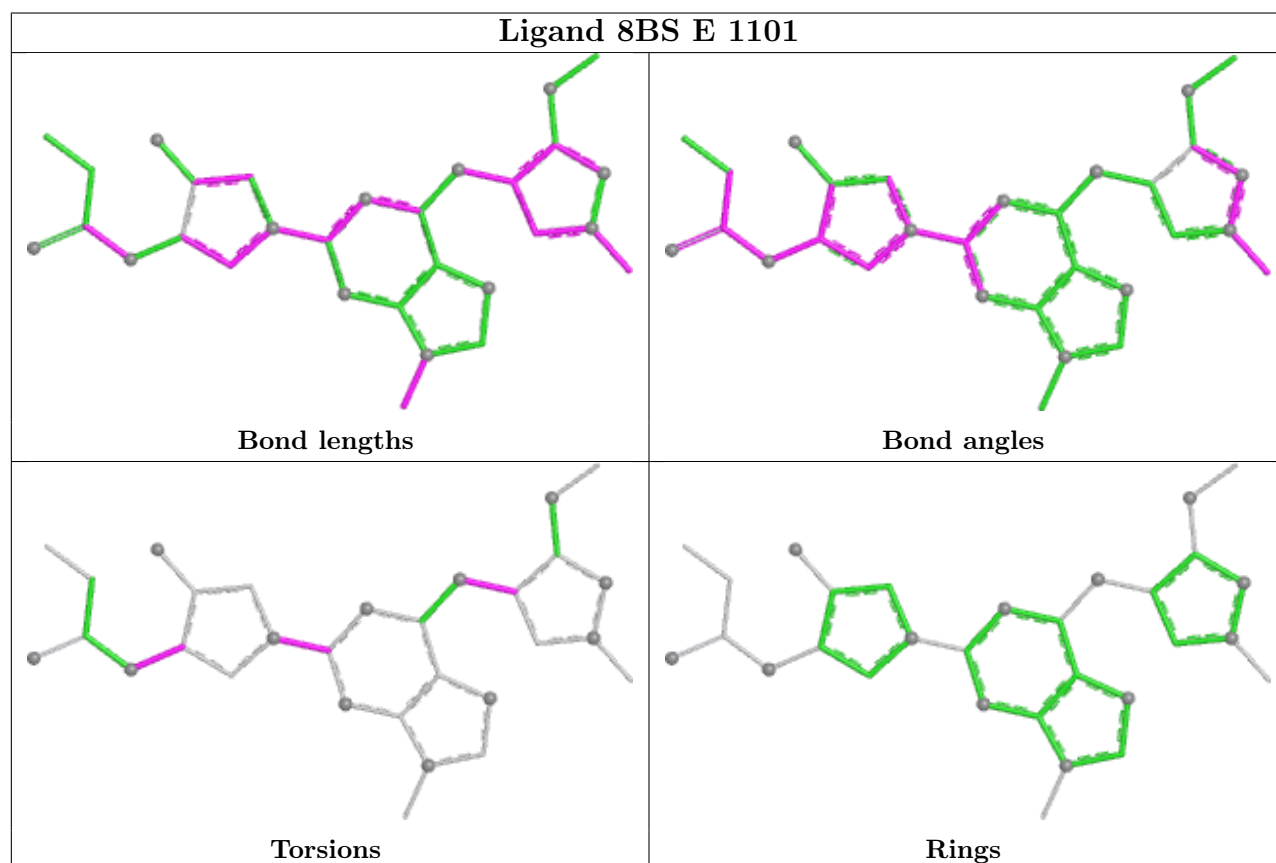
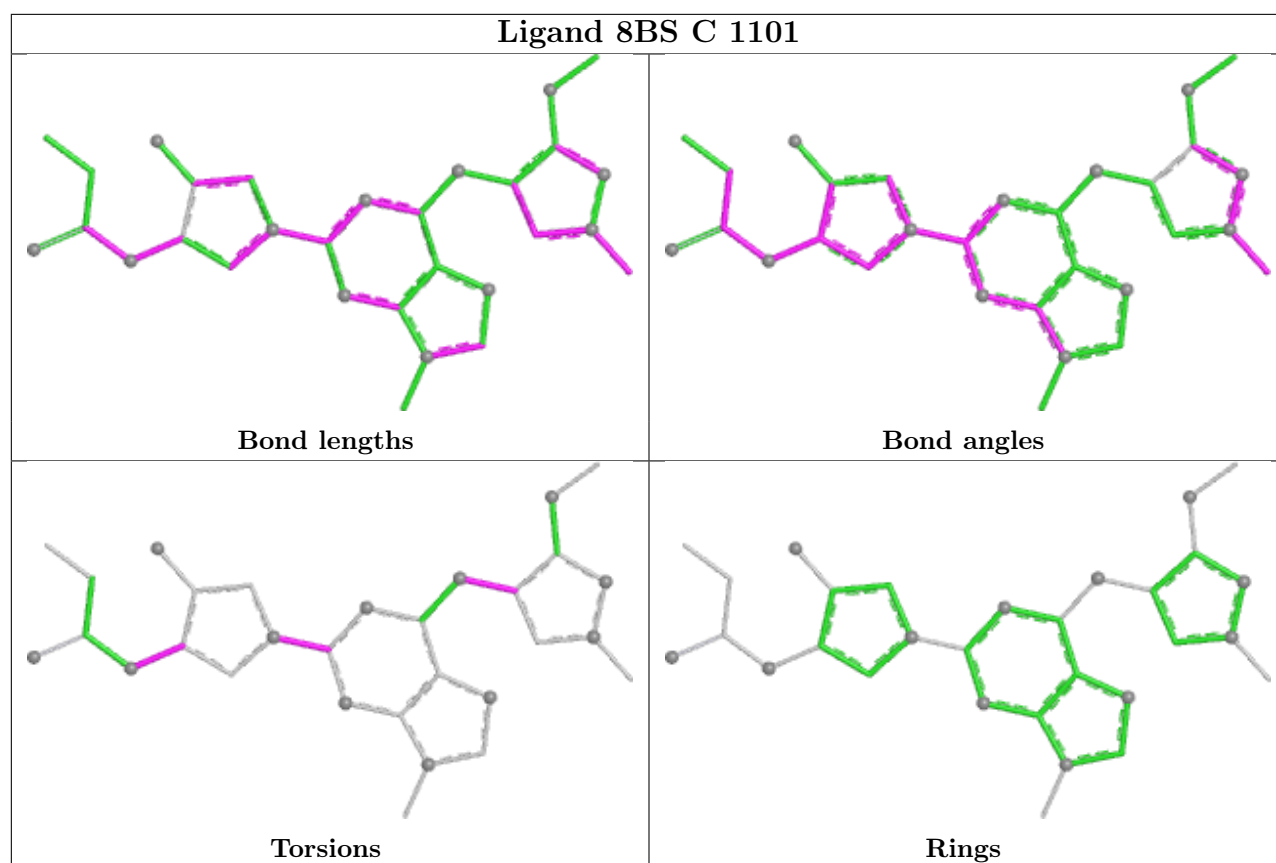
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	ANP	1	0
2	D	1101	ANP	1	0
4	C	1102	JBj	1	0
5	E	1101	8BS	1	0
4	F	1102	JBj	3	0
4	E	1102	JBj	2	0

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.

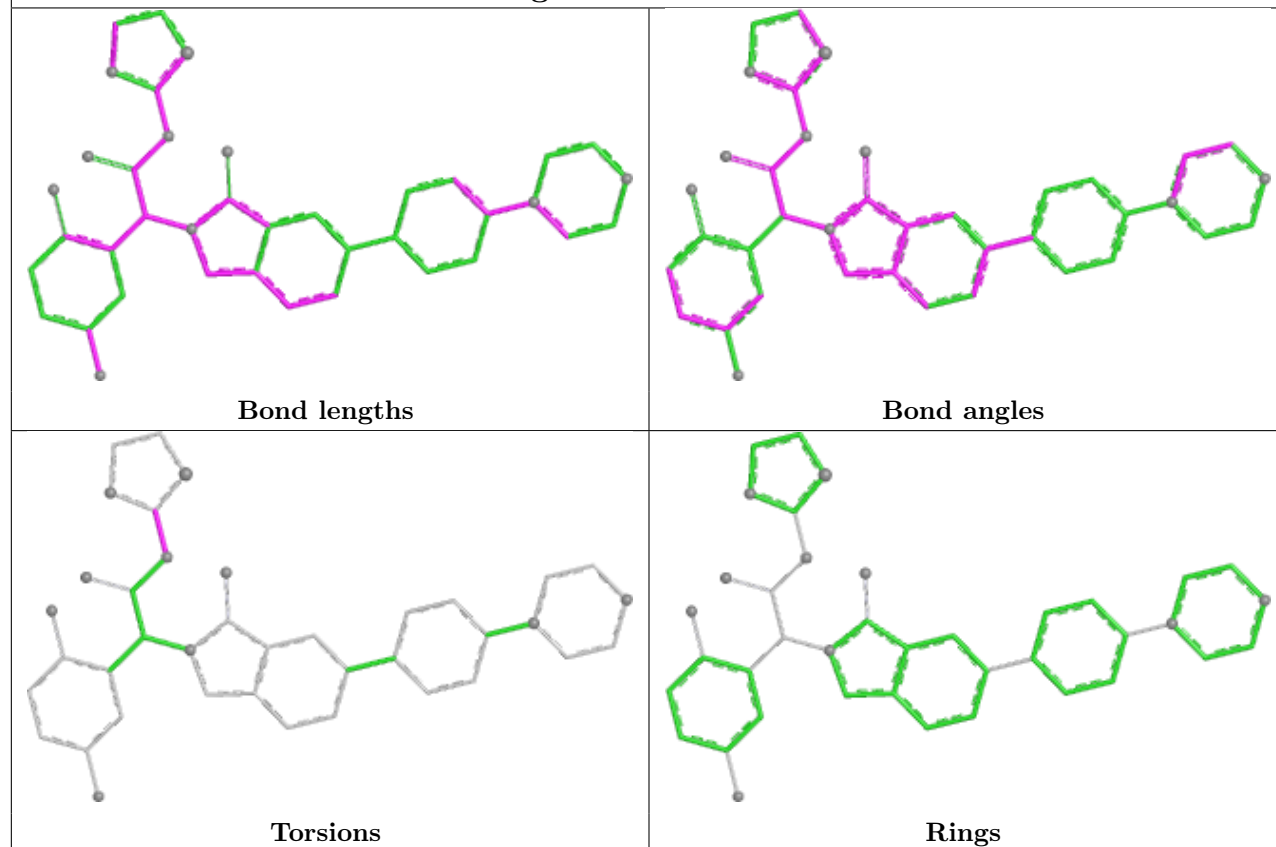




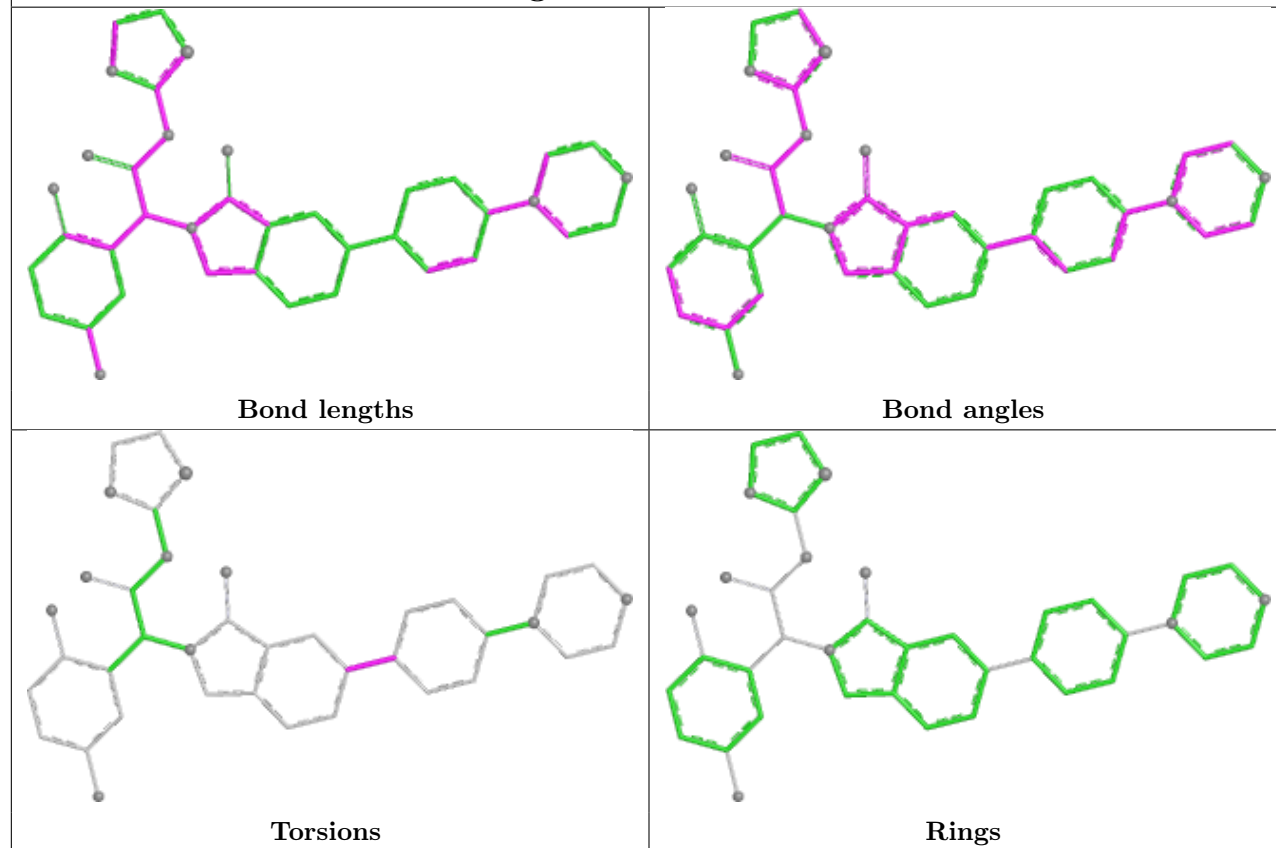


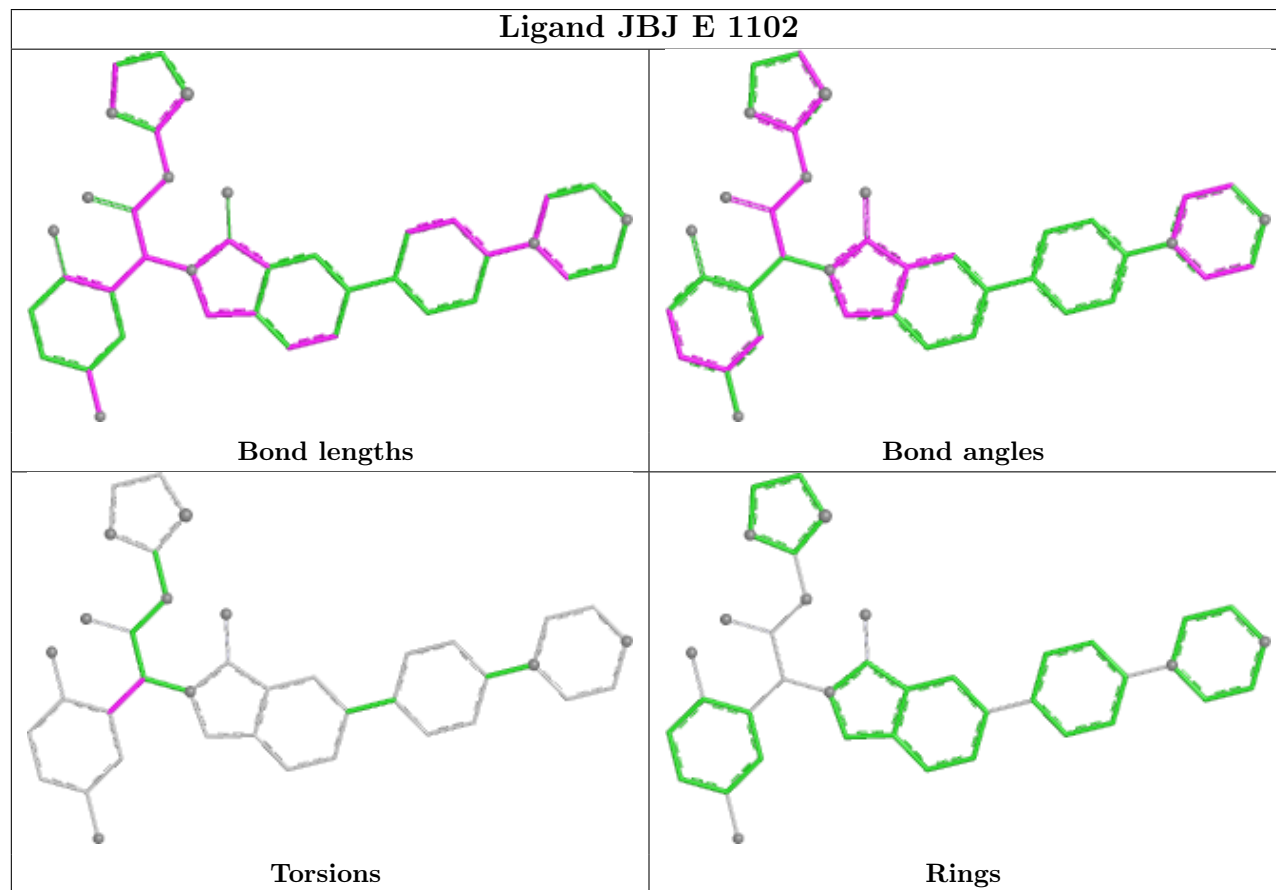
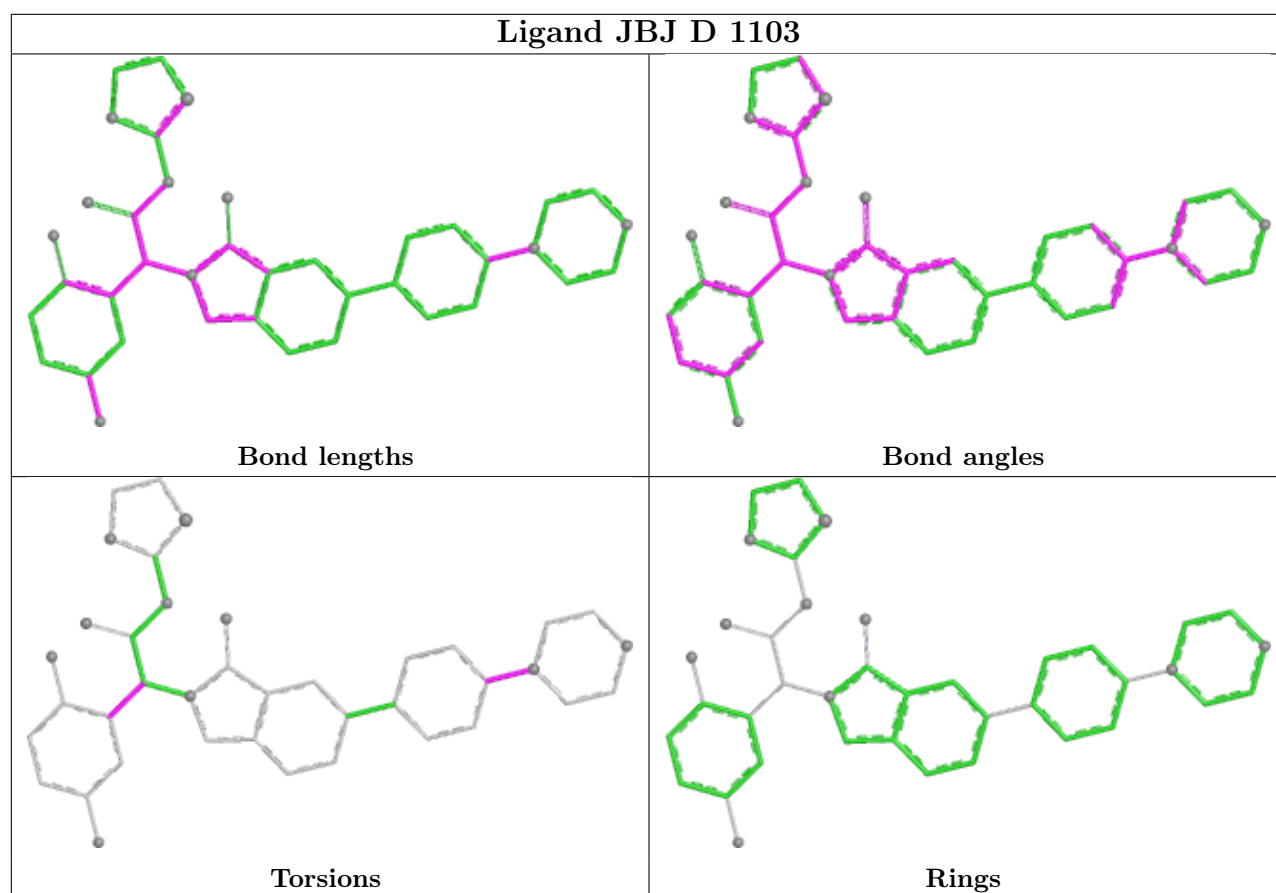


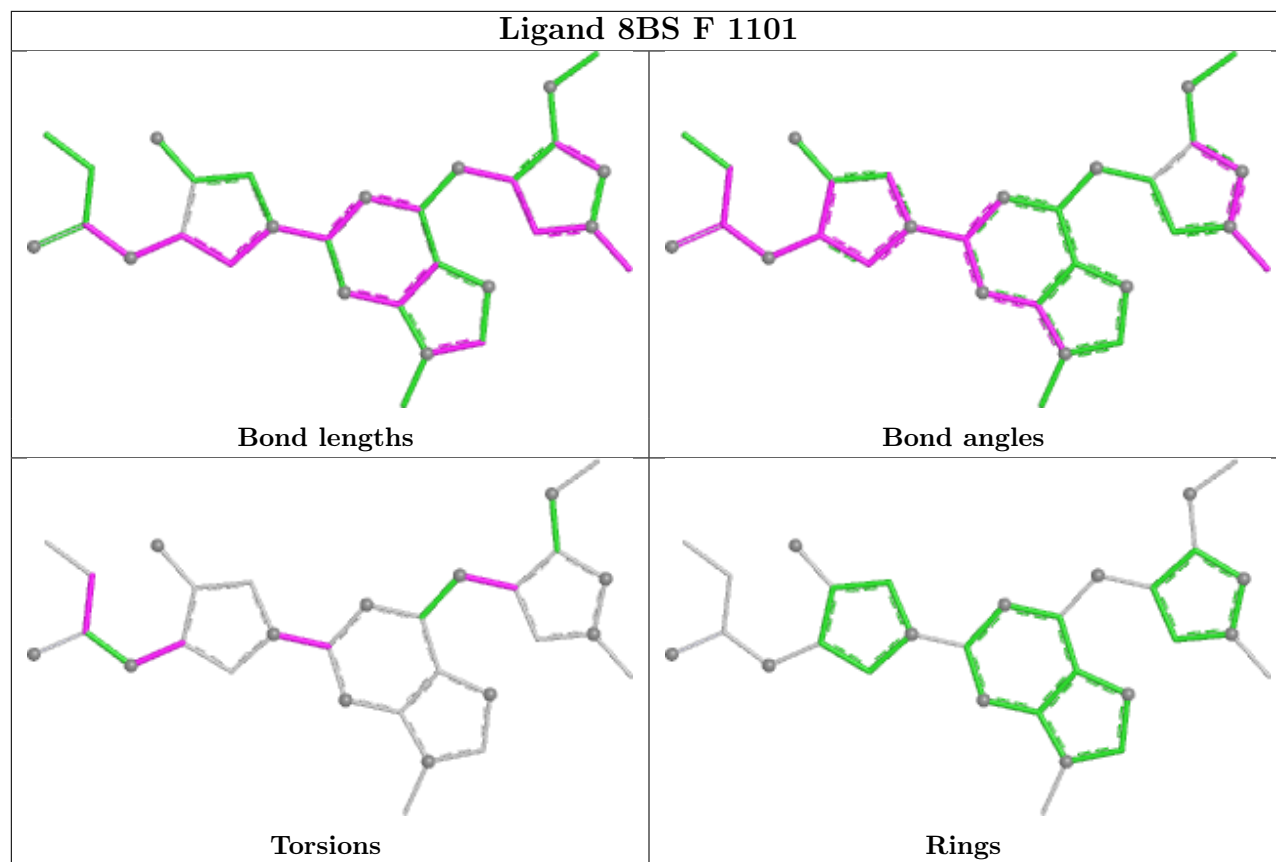
Ligand JBJ F 1102



Ligand JBJ A 1102







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	293/331 (88%)	-0.31	0 100 100	32, 62, 97, 113	1 (0%)
1	B	290/331 (87%)	-0.08	0 100 100	44, 93, 136, 188	1 (0%)
1	C	292/331 (88%)	-0.08	0 100 100	48, 83, 126, 148	1 (0%)
1	D	294/331 (88%)	-0.33	0 100 100	31, 63, 98, 120	1 (0%)
1	E	287/331 (86%)	-0.23	0 100 100	43, 80, 120, 138	1 (0%)
1	F	292/331 (88%)	-0.16	0 100 100	35, 65, 95, 108	1 (0%)
All	All	1748/1986 (88%)	-0.20	0 100 100	31, 72, 120, 188	6 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ANP	B	1101	31/31	0.72	0.11	49,75,110,130	0

Continued on next page...

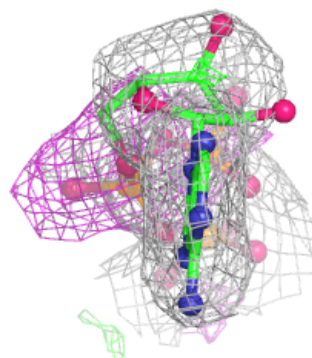
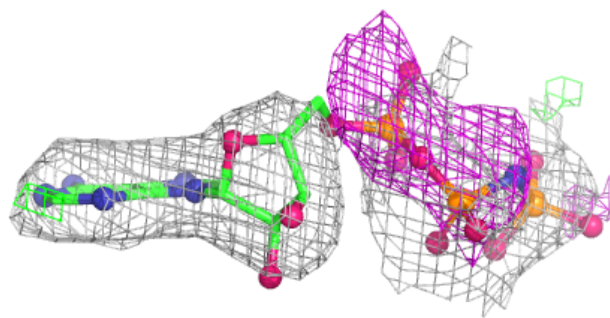
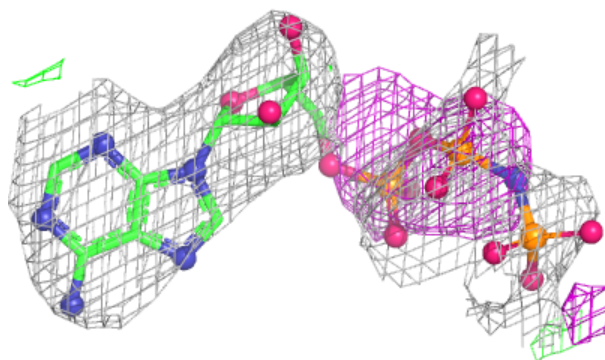
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	8BS	E	1101	30/30	0.82	0.16	84,98,106,107	0
2	ANP	D	1101	31/31	0.83	0.12	41,53,79,86	0
5	8BS	F	1101	30/30	0.87	0.14	85,97,109,116	0
4	JBj	C	1102	39/39	0.87	0.14	64,76,118,121	0
5	8BS	A	1101	30/30	0.88	0.17	59,71,81,87	0
5	8BS	C	1101	30/30	0.90	0.15	88,105,118,122	0
4	JBj	E	1102	39/39	0.90	0.13	59,71,117,124	0
4	JBj	F	1102	39/39	0.90	0.13	57,67,93,96	0
4	JBj	A	1102	39/39	0.91	0.11	55,65,106,111	0
3	MG	B	1102	1/1	0.93	0.10	83,83,83,83	0
4	JBj	D	1103	39/39	0.93	0.11	58,69,107,116	0
3	MG	D	1102	1/1	0.97	0.05	57,57,57,57	0

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

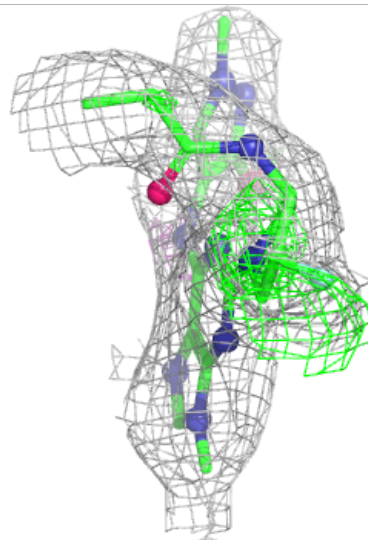
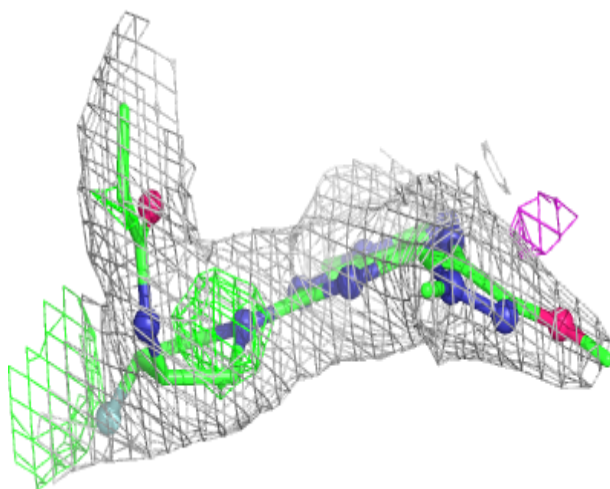
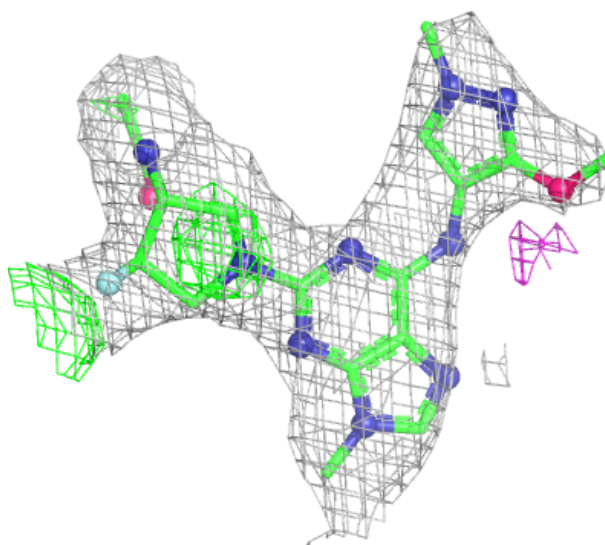
Electron density around ANP B 1101:

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



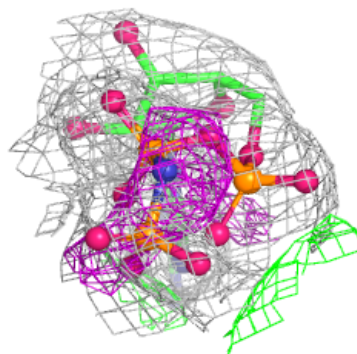
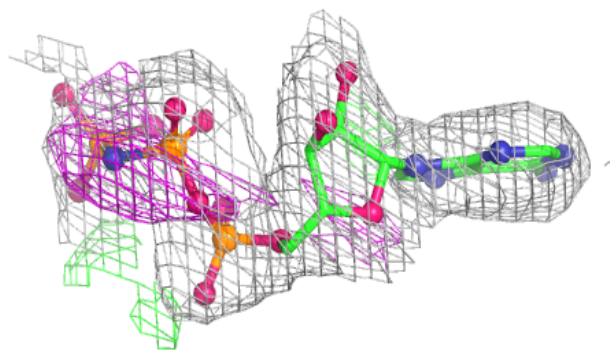
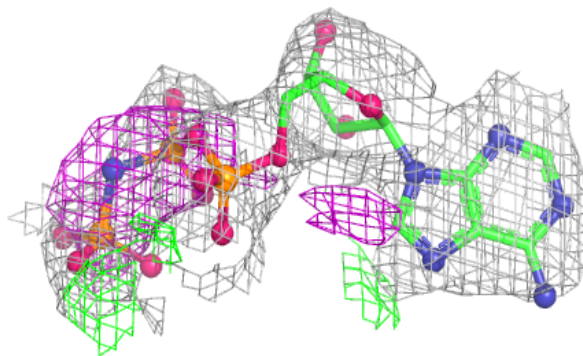
Electron density around 8BS E 1101:

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



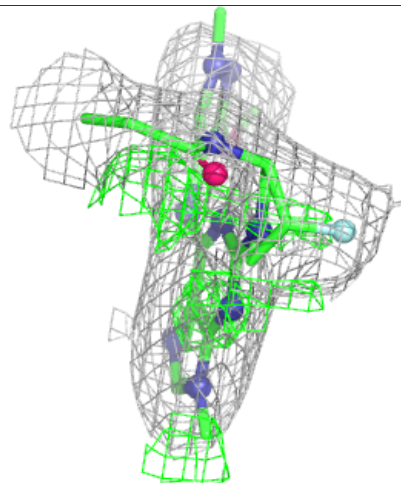
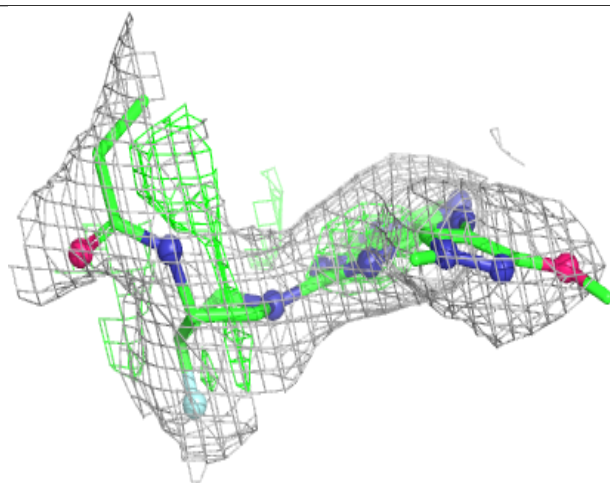
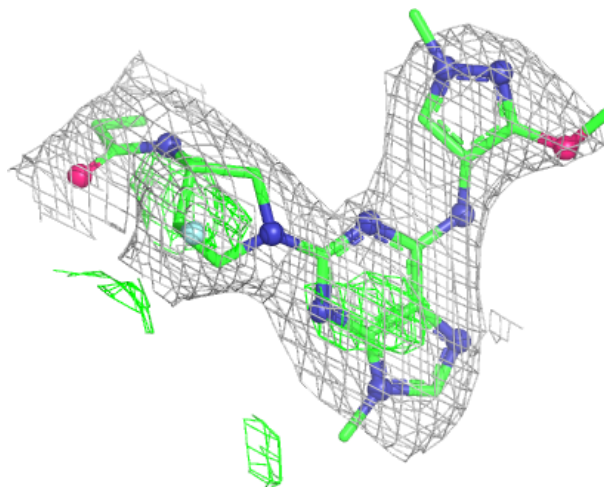
Electron density around ANP D 1101:

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



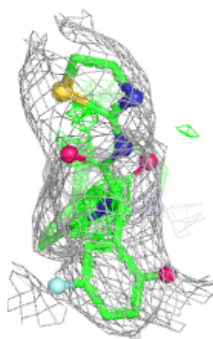
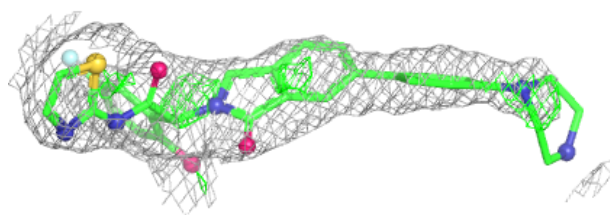
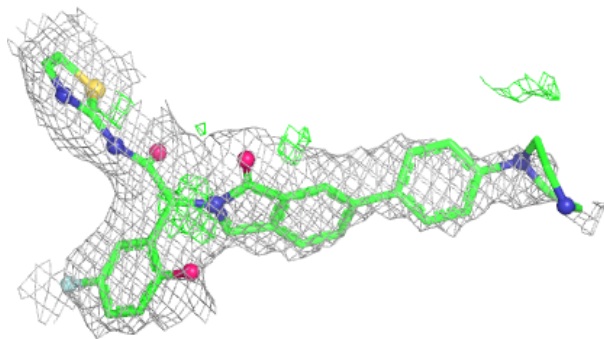
Electron density around 8BS F 1101:

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



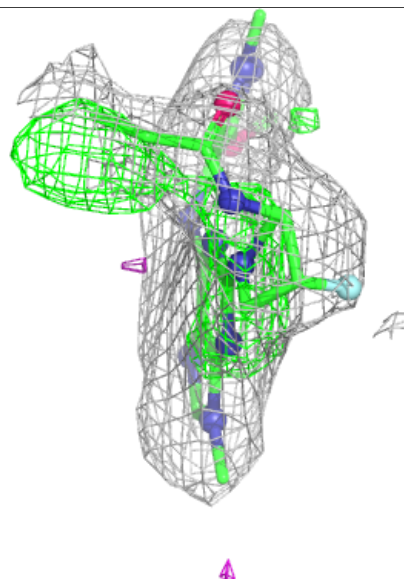
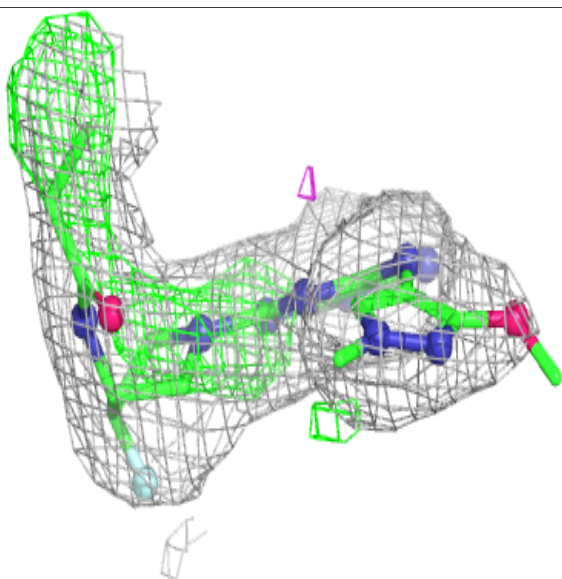
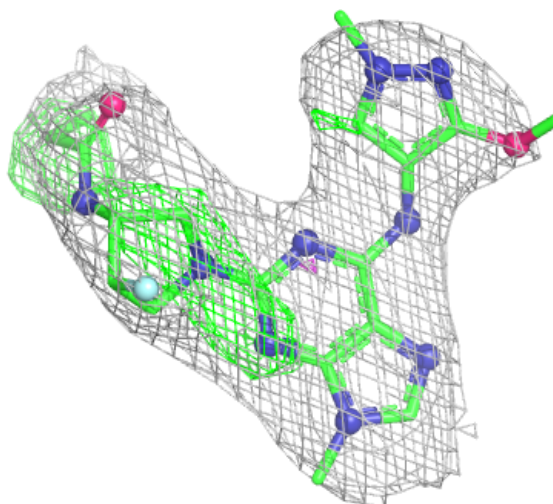
Electron density around JBJ C 1102:

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



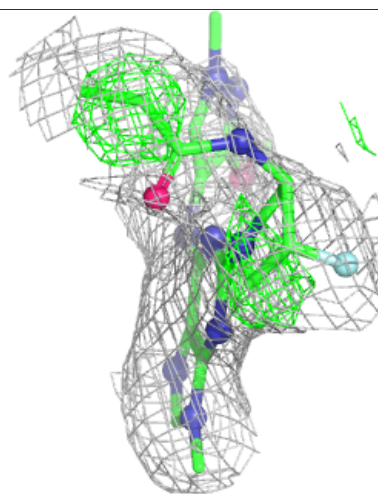
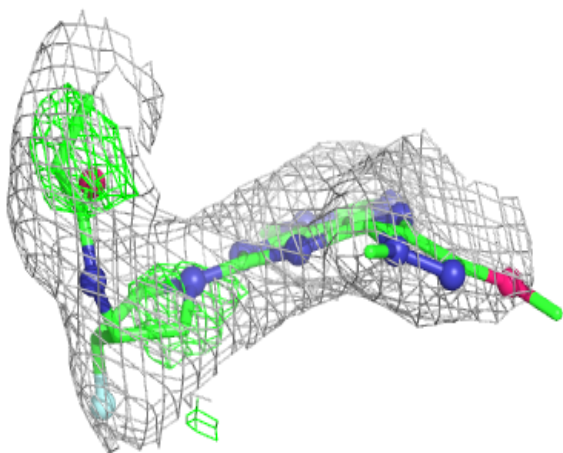
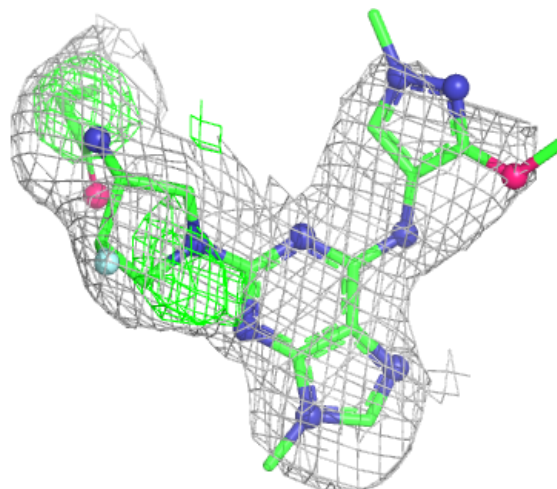
Electron density around 8BS A 1101:

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



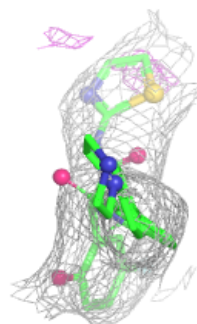
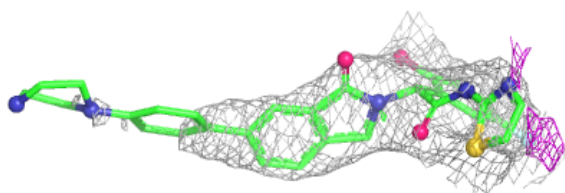
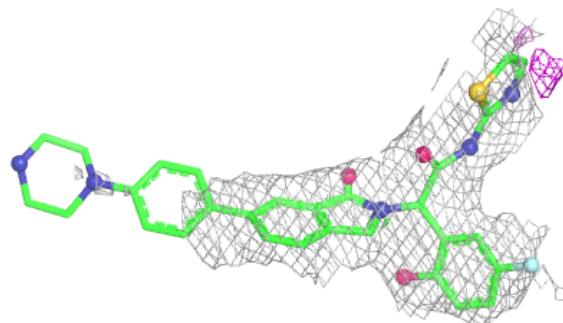
Electron density around 8BS C 1101:

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

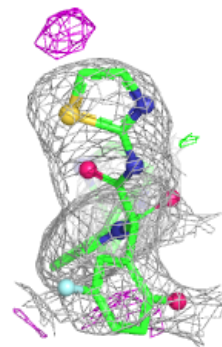
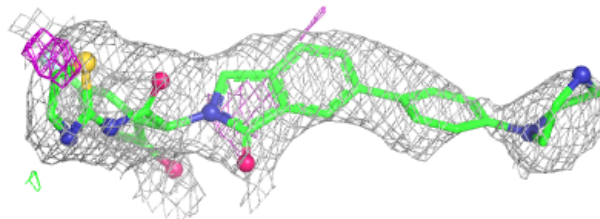
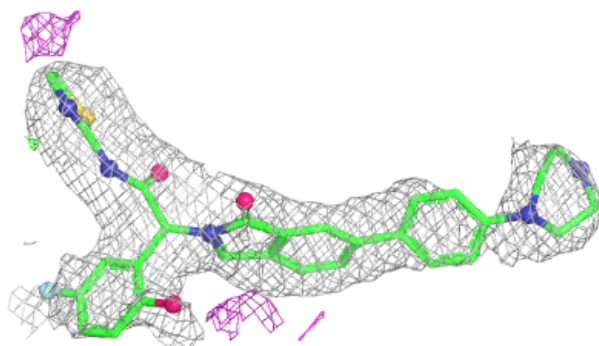


Electron density around JBJ E 1102:

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

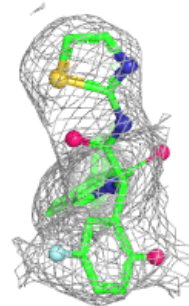
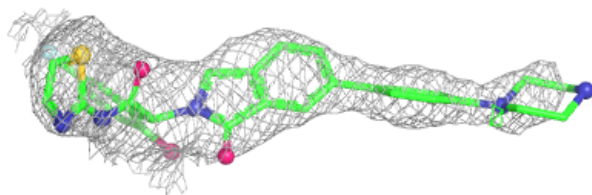
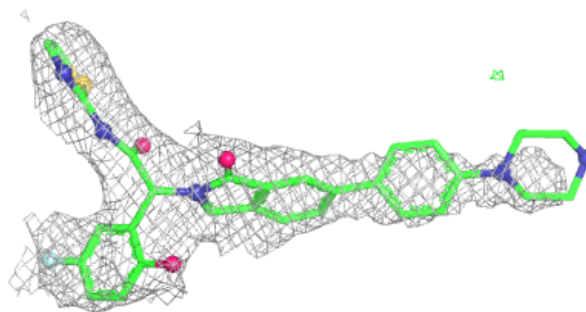
**Electron density around JBJ F 1102:**

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

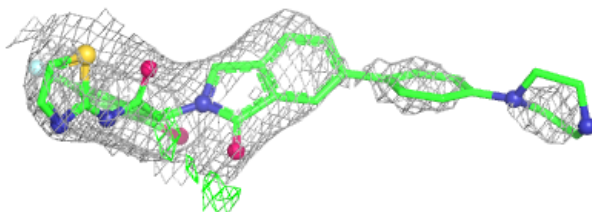
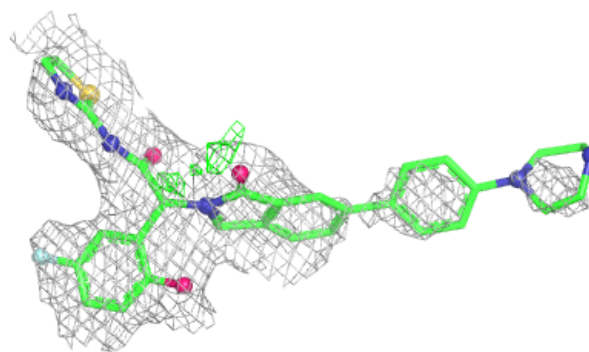


Electron density around JBJ A 1102:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.