



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:00 PM UTC

PDB ID : 7JXM / pdb_00007jxm
Title : EGFR kinase (T790M/V948R) in complex with osimertinib and EAI045
Authors : Beyett, T.S.; Eck, M.J.
Deposited on : 2020-08-27
Resolution : 2.19 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

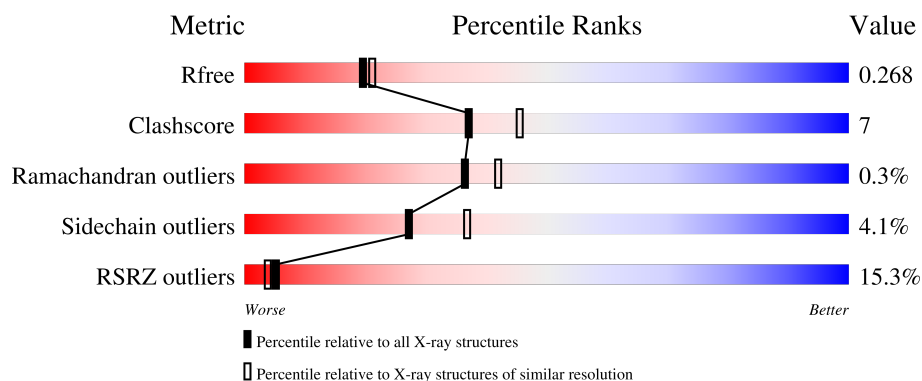
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	15% 75% 11% 13%
1	B	331	12% 53% 30% 6% 11%
1	C	331	14% 71% 15% 14%
1	D	331	12% 77% 11% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9753 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.

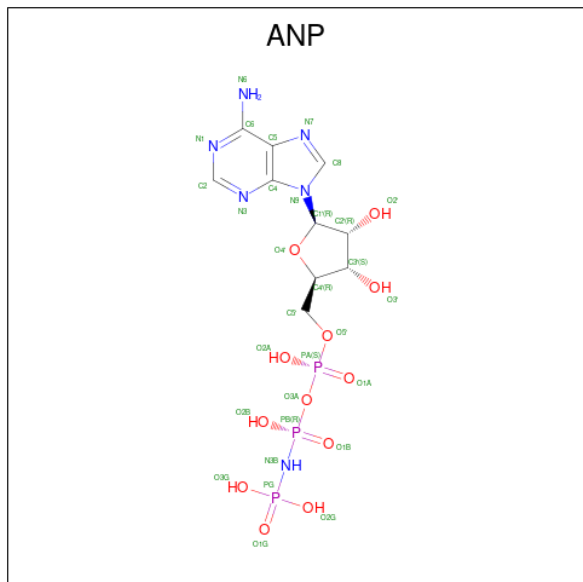
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	291	Total	C	N	O	S	0	0	0
			2350	1509	400	422	19			
1	A	287	Total	C	N	O	S	0	0	0
			2319	1492	395	414	18			
1	C	285	Total	C	N	O	S	0	0	0
			2305	1483	392	412	18			
1	B	296	Total	C	N	O	S	0	0	0
			2385	1530	404	432	19			

There are 20 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
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: $C_{10}H_{17}N_6O_{12}P_3$).

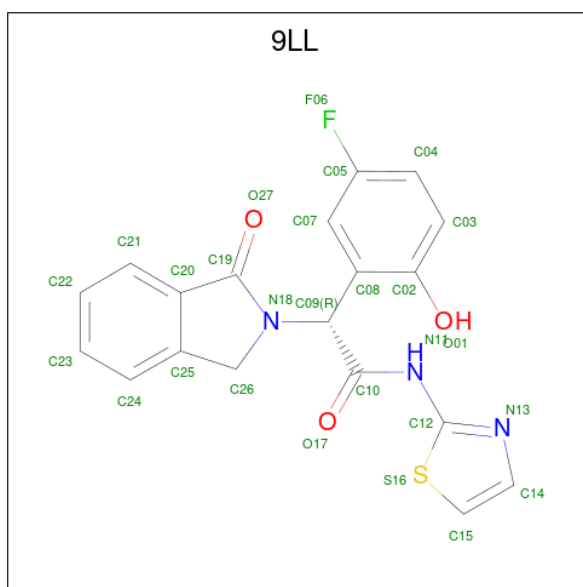


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

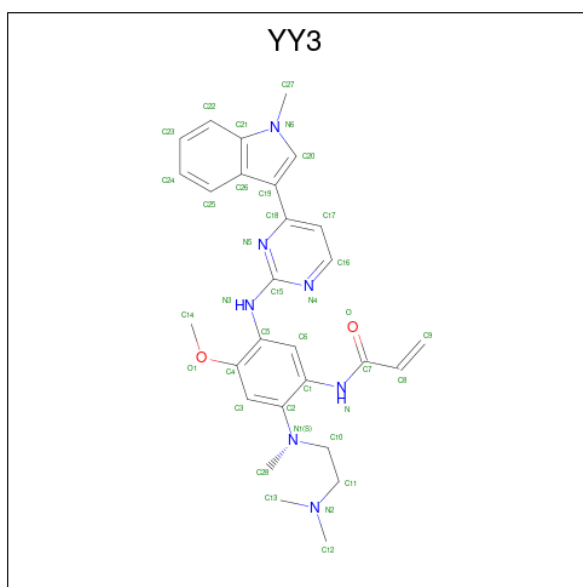
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (2R)-2-(5-fluoro-2-hydroxyphenyl)-2-(1-oxo-1,3-dihydro-2H-isoindol-2-yl)-N-(1,3-thiazol-2-yl)acetamide (CCD ID: 9LL) (formula: $C_{19}H_{14}FN_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	F	N	O	S	0	0
			27	19	1	3	3	1		
4	B	1	Total	C	F	N	O	S	0	0
			27	19	1	3	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 (CCD ID: YY3) (formula: C₂₈H₃₃N₇O₂) (labeled as "Ligand of Interest" by depositor).



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

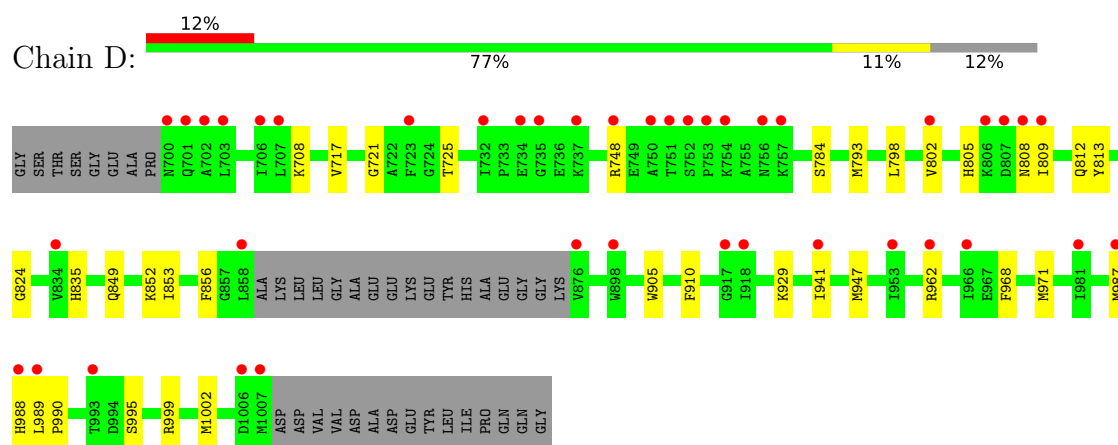
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	53	Total 53	O 53	0	0
6	A	55	Total 55	O 55	0	0
6	C	43	Total 43	O 43	0	0
6	B	56	Total 56	O 56	0	0

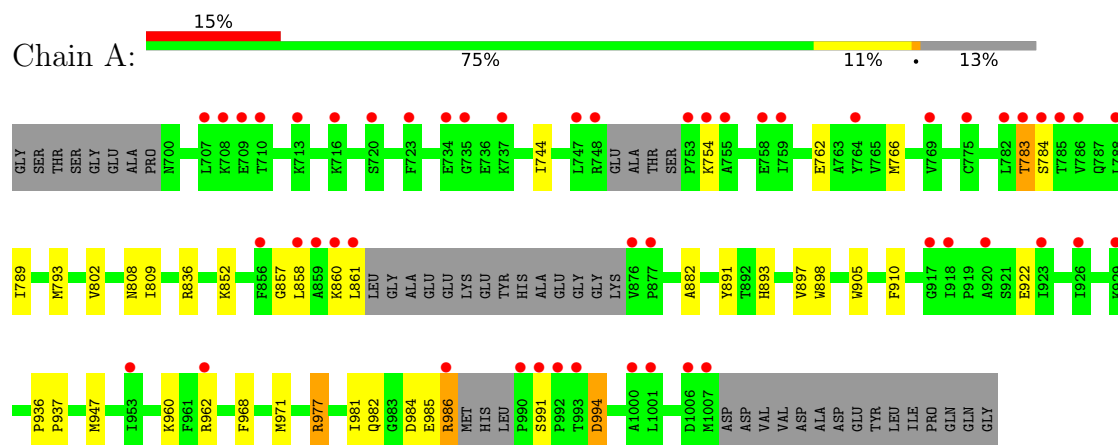
3 Residue-property plots [i](#)

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

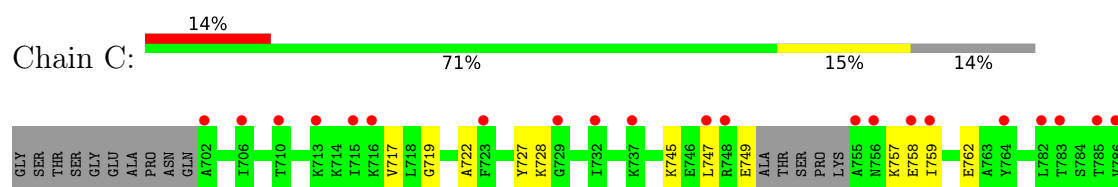
- Molecule 1: Epidermal growth factor receptor

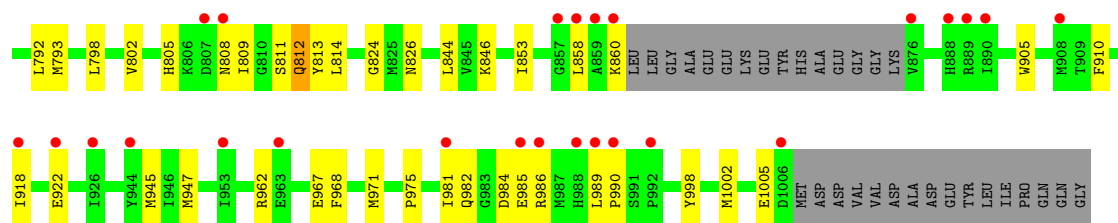


- Molecule 1: Epidermal growth factor receptor

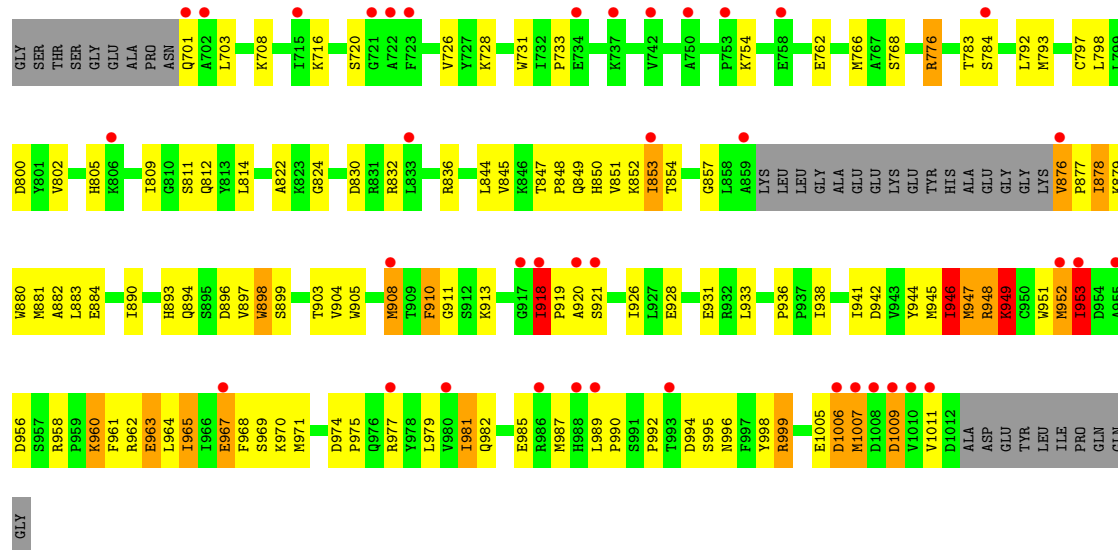


- Molecule 1: Epidermal growth factor receptor





• Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.55Å 103.22Å 87.04Å 90.00° 101.55° 90.00°	Depositor
Resolution (Å)	49.91 – 2.19 49.91 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.9 (49.91-2.19) 84.8 (49.91-2.19)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.227 , 0.271 0.229 , 0.268	Depositor DCC
R_{free} test set	1992 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9753	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, YY3, 9LL, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2368	0.63	0/3196
1	B	1.63	63/2437 (2.6%)	1.02	5/3297 (0.2%)
1	C	0.40	0/2355	0.65	0/3182
1	D	0.40	0/2402	0.62	0/3248
All	All	0.90	63/9562 (0.7%)	0.75	5/12923 (0.0%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	996	ASN	C-O	-7.77	1.15	1.24
1	B	847	THR	C-O	-7.18	1.18	1.24
1	B	844	LEU	C-O	-6.96	1.15	1.23
1	B	946	ILE	C-O	-6.82	1.16	1.24
1	B	999	ARG	C-O	-6.77	1.16	1.24
1	B	853	ILE	C-O	-6.64	1.17	1.24
1	B	848	PRO	C-O	-6.46	1.16	1.24
1	B	931	GLU	C-O	-6.44	1.16	1.23
1	B	995	SER	C-O	-6.44	1.16	1.24
1	B	918	ILE	CA-C	-6.42	1.48	1.53
1	B	897	VAL	C-O	-6.39	1.16	1.24
1	B	941	ILE	C-O	-6.39	1.16	1.24
1	B	965	ILE	C-O	-6.31	1.17	1.24
1	B	992	PRO	C-O	-6.24	1.16	1.24
1	B	944	TYR	C-O	-6.22	1.16	1.24
1	B	953	ILE	C-O	-6.19	1.17	1.24
1	B	981	ILE	C-O	-6.15	1.17	1.24
1	B	845	VAL	C-O	-6.10	1.17	1.24
1	B	850	HIS	C-O	-6.07	1.16	1.23
1	B	878	ILE	C-O	-6.01	1.17	1.24
1	B	998	TYR	C-O	-5.97	1.17	1.24
1	B	956	ASP	C-O	-5.97	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	964	LEU	C-O	-5.96	1.17	1.24
1	B	904	VAL	C-O	-5.89	1.17	1.24
1	B	942	ASP	C-O	-5.86	1.17	1.24
1	B	949	LYS	C-O	-5.85	1.17	1.24
1	B	910	PHE	C-O	-5.84	1.16	1.23
1	B	958	ARG	C-O	-5.80	1.16	1.23
1	B	896	ASP	C-O	-5.76	1.17	1.24
1	B	884	GLU	C-O	-5.76	1.16	1.24
1	B	877	PRO	CA-C	-5.73	1.48	1.53
1	B	936	PRO	C-O	-5.68	1.18	1.24
1	B	960	LYS	C-O	-5.62	1.16	1.23
1	B	898	TRP	C-O	-5.61	1.17	1.24
1	B	994	ASP	C-O	-5.59	1.17	1.24
1	B	913	LYS	C-O	-5.55	1.16	1.24
1	B	918	ILE	C-O	-5.53	1.16	1.24
1	B	854	THR	C-O	-5.51	1.16	1.23
1	B	933	LEU	C-O	-5.47	1.17	1.23
1	B	894	GLN	C-O	-5.42	1.17	1.24
1	B	963	GLU	C-O	-5.41	1.17	1.24
1	B	882	ALA	C-O	-5.36	1.17	1.23
1	B	928	GLU	C-O	-5.34	1.17	1.24
1	B	851	VAL	C-O	-5.34	1.17	1.23
1	B	893	HIS	C-O	-5.33	1.17	1.24
1	B	970	LYS	C-O	-5.32	1.17	1.24
1	B	911	GLY	C-O	-5.31	1.17	1.24
1	B	880	TRP	C-O	-5.30	1.17	1.24
1	B	968	PHE	C-O	-5.29	1.17	1.24
1	B	969	SER	C-O	-5.28	1.18	1.24
1	B	948	ARG	C-O	-5.20	1.17	1.24
1	B	947	MET	C-O	-5.19	1.18	1.24
1	B	919	PRO	CA-C	-5.17	1.45	1.52
1	B	899	SER	C-O	-5.14	1.17	1.24
1	B	920	ALA	C-O	-5.14	1.17	1.24
1	B	961	PHE	C-O	-5.10	1.18	1.24
1	B	952	MET	C-O	-5.07	1.17	1.23
1	B	903	THR	C-O	-5.05	1.18	1.24
1	B	938	ILE	C-O	-5.04	1.17	1.24
1	B	879	LYS	C-O	-5.03	1.17	1.24
1	B	1011	VAL	C-O	-5.03	1.18	1.24
1	B	921	SER	C-O	-5.02	1.17	1.24
1	B	881	MET	C-O	-5.00	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	974	ASP	CA-C-N	5.86	127.16	119.84
1	B	974	ASP	C-N-CA	5.86	127.16	119.84
1	B	1005	GLU	CB-CA-C	5.56	118.95	109.72
1	B	1007	MET	N-CA-C	5.54	122.59	110.80
1	B	890	ILE	CB-CA-C	-5.10	103.99	110.98

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	2319	0	2371	21	0
1	B	2385	0	2421	58	0
1	C	2305	0	2349	33	0
1	D	2350	0	2392	30	0
2	A	31	0	13	0	0
2	C	31	0	13	2	0
2	D	31	0	13	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	27	0	0	0	0
4	D	27	0	0	1	0
5	B	37	0	33	8	0
6	A	55	0	0	1	0
6	B	56	0	0	4	0
6	C	43	0	0	2	0
6	D	53	0	0	3	0
All	All	9753	0	9605	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:CYS:SG	5:B:1101:YY3:H22	1.38	1.62
1:B:797:CYS:SG	5:B:1101:YY3:C9	2.10	1.39
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.43	0.79
1:B:960:LYS:HB2	1:B:963:GLU:HG3	1.65	0.79
1:D:941:ILE:HD11	1:A:922:GLU:HG2	1.68	0.76
1:B:797:CYS:CB	5:B:1101:YY3:H22	2.14	0.76
1:D:721:GLY:O	1:D:748:ARG:NH1	2.23	0.72
1:A:991:SER:HB2	1:A:994:ASP:HB2	1.73	0.70
1:B:918:ILE:HD13	1:B:918:ILE:N	2.07	0.69
1:C:945:MET:HE2	1:C:945:MET:HA	1.73	0.68
1:C:802:VAL:HG12	1:C:910:PHE:HA	1.76	0.68
1:C:918:ILE:HD12	1:B:945:MET:HE1	1.76	0.67
1:B:797:CYS:SG	5:B:1101:YY3:H23	2.31	0.66
5:B:1101:YY3:H25	5:B:1101:YY3:N5	2.09	0.65
1:C:846:LYS:NZ	1:C:1005:GLU:OE2	2.29	0.64
1:A:968:PHE:HA	1:A:971:MET:HE3	1.79	0.63
1:C:905:TRP:CD1	1:C:947:MET:HE1	2.30	0.62
1:A:762:GLU:OE2	1:A:860:LYS:HB3	2.00	0.62
1:C:798:LEU:O	1:C:802:VAL:HG23	2.01	0.60
1:D:802:VAL:HG12	1:D:910:PHE:HA	1.84	0.60
1:B:762:GLU:O	1:B:766:MET:HG2	2.02	0.59
1:B:949:LYS:HG3	1:B:952:MET:HE3	1.83	0.59
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.69	0.57
1:B:908:MET:HE2	1:B:979:LEU:HD11	1.87	0.57
1:C:812:GLN:HG2	1:C:975:PRO:HG3	1.87	0.56
1:C:802:VAL:CG1	1:C:910:PHE:HA	2.36	0.56
1:B:949:LYS:HA	1:B:952:MET:HE3	1.87	0.56
1:D:748:ARG:HH22	1:B:832:ARG:CD	2.19	0.56
1:B:802:VAL:HG12	1:B:910:PHE:HA	1.86	0.56
1:D:748:ARG:HH22	1:B:832:ARG:HD3	1.71	0.56
1:B:703:LEU:HD22	1:B:776:ARG:HH12	1.70	0.55
1:D:813:TYR:OH	1:D:990:PRO:HD3	2.07	0.55
1:B:798:LEU:O	1:B:802:VAL:HG23	2.07	0.55
1:A:962:ARG:HD3	6:A:1247:HOH:O	2.06	0.54
1:A:793:MET:HE1	1:A:852:LYS:HD3	1.89	0.54
1:D:812:GLN:HG2	1:D:989:LEU:HG	1.90	0.54
1:B:805:HIS:O	1:B:809:ILE:HG13	2.07	0.53
1:B:814:LEU:HB3	1:B:908:MET:HE3	1.89	0.53
1:C:824:GLY:HA3	1:C:853:ILE:HD12	1.91	0.53
1:A:802:VAL:HG13	1:A:809:ILE:HD12	1.91	0.52
1:B:726:VAL:HG21	5:B:1101:YY3:C21	2.39	0.52
1:B:918:ILE:N	1:B:918:ILE:CD1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:802:VAL:CG1	1:D:910:PHE:HA	2.40	0.52
1:C:968:PHE:HA	1:C:971:MET:HE3	1.91	0.52
1:B:802:VAL:CG1	1:B:910:PHE:HA	2.39	0.52
1:D:824:GLY:HA3	1:D:853:ILE:HD12	1.92	0.52
1:C:808:ASN:O	1:C:808:ASN:ND2	2.42	0.51
1:B:967:GLU:HG3	1:B:971:MET:HE2	1.92	0.51
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.75	0.51
1:B:883:LEU:HD23	1:B:953:ILE:HD13	1.92	0.51
1:B:876:VAL:HG23	1:B:878:ILE:HG12	1.92	0.51
1:B:962:ARG:HG3	6:B:1229:HOH:O	2.10	0.50
1:A:766:MET:HE2	1:A:857:GLY:C	2.37	0.50
1:B:728:LYS:HD2	1:B:792:LEU:HD21	1.94	0.50
1:B:905:TRP:HB2	1:B:947:MET:HE1	1.93	0.50
1:B:731:TRP:CH2	1:B:733:PRO:HG3	2.47	0.50
1:A:802:VAL:CG1	1:A:910:PHE:HA	2.42	0.49
1:D:725:THR:OG1	1:B:832:ARG:NH2	2.45	0.49
1:C:728:LYS:HD2	1:C:792:LEU:HD21	1.94	0.49
1:A:802:VAL:HG12	1:A:910:PHE:HA	1.94	0.49
1:B:999:ARG:HD3	6:B:1209:HOH:O	2.13	0.49
1:B:946:ILE:HD13	1:B:971:MET:HE1	1.95	0.48
1:B:812:GLN:HG2	1:B:989:LEU:HG	1.95	0.48
1:B:1009:ASP:OD1	1:B:1009:ASP:N	2.39	0.48
1:B:849:GLN:NE2	1:B:990:PRO:HG3	2.29	0.48
1:D:798:LEU:O	1:D:802:VAL:HG23	2.14	0.47
1:B:836:ARG:NH2	6:B:1201:HOH:O	2.31	0.47
1:D:968:PHE:HA	1:D:971:MET:HE3	1.97	0.47
1:A:766:MET:HE2	1:A:857:GLY:HA3	1.95	0.47
1:B:703:LEU:HD22	1:B:776:ARG:NH1	2.28	0.47
1:B:716:LYS:HE2	6:B:1230:HOH:O	2.13	0.47
1:B:824:GLY:HA3	1:B:853:ILE:HD12	1.96	0.47
1:A:977:ARG:HD2	1:A:977:ARG:O	2.14	0.47
1:D:849:GLN:CD	1:D:990:PRO:HG3	2.40	0.47
1:A:893:HIS:O	1:A:897:VAL:HG23	2.13	0.46
1:D:849:GLN:NE2	1:D:990:PRO:HG3	2.30	0.46
1:D:988:HIS:N	6:D:1204:HOH:O	2.41	0.46
1:C:745:LYS:HD3	1:C:747:LEU:HD21	1.97	0.46
1:C:981:ILE:HB	1:C:984:ASP:HB2	1.97	0.46
1:C:811:SER:OG	1:C:975:PRO:HB2	2.16	0.45
1:B:948:ARG:HE	1:B:948:ARG:HB3	1.67	0.45
1:D:805:HIS:O	1:D:809:ILE:HG13	2.16	0.45
1:C:826:ASN:ND2	6:C:1209:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:748:ARG:NH2	1:B:832:ARG:HD3	2.32	0.45
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.52	0.45
1:B:977:ARG:O	1:B:977:ARG:HG2	2.17	0.44
1:A:808:ASN:HA	1:A:986:ARG:NH1	2.32	0.44
1:B:898:TRP:CE3	1:B:951:TRP:HA	2.52	0.44
1:C:809:ILE:HB	1:C:910:PHE:HE1	1.82	0.44
1:B:766:MET:HE1	1:B:857:GLY:HA3	2.00	0.44
1:C:805:HIS:O	1:C:809:ILE:HG13	2.17	0.44
1:B:703:LEU:HD13	1:B:768:SER:HA	2.00	0.44
4:D:1103:9LL:O17	4:D:1103:9LL:S16	2.76	0.44
1:C:918:ILE:HD12	1:B:945:MET:CE	2.46	0.44
1:D:708:LYS:HB3	1:D:708:LYS:HE2	1.70	0.43
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.18	0.43
1:C:918:ILE:HD12	1:B:945:MET:SD	2.59	0.43
1:D:717:VAL:HG11	1:B:830:ASP:HB3	2.00	0.43
1:A:744:ILE:HG12	1:A:789:ILE:HG13	2.00	0.43
1:D:812:GLN:CG	1:D:989:LEU:HG	2.49	0.42
1:B:883:LEU:HD23	1:B:953:ILE:CD1	2.48	0.42
5:B:1101:YY3:N5	5:B:1101:YY3:C6	2.71	0.42
1:C:717:VAL:HG22	1:C:727:TYR:CE2	2.54	0.42
1:A:905:TRP:CD1	1:A:947:MET:HE1	2.52	0.42
1:B:793:MET:HE1	1:B:852:LYS:HD3	2.02	0.42
1:A:836:ARG:HG2	1:A:891:TYR:CD1	2.54	0.42
1:C:858:LEU:HD12	1:C:858:LEU:HA	1.80	0.42
1:D:929:LYS:NZ	6:D:1210:HOH:O	2.51	0.42
1:B:811:SER:OG	1:B:975:PRO:HB2	2.19	0.42
1:B:989:LEU:HD22	1:B:990:PRO:HD3	2.02	0.41
1:C:962:ARG:HG3	6:C:1209:HOH:O	2.20	0.41
1:C:793:MET:HG3	1:C:844:LEU:HD13	2.01	0.41
1:D:793:MET:HE1	1:D:852:LYS:HD3	2.03	0.41
1:D:962:ARG:HG3	6:D:1218:HOH:O	2.19	0.41
1:B:822:ALA:HB1	1:B:965:ILE:HG13	2.03	0.41
1:D:748:ARG:NH2	1:B:832:ARG:CD	2.82	0.41
1:D:805:HIS:HB3	1:D:808:ASN:HB2	2.02	0.41
1:C:989:LEU:HB3	1:C:990:PRO:HD2	2.03	0.41
1:B:800:ASP:OD2	5:B:1101:YY3:H14	2.20	0.41
1:B:926:ILE:HD13	1:B:926:ILE:HG21	1.83	0.41
1:C:967:GLU:HG2	1:C:971:MET:HE2	2.03	0.41
1:C:984:ASP:C	1:C:986:ARG:H	2.27	0.41
1:C:1002:MET:HE2	1:C:1002:MET:HB3	1.96	0.41
1:B:812:GLN:CG	1:B:989:LEU:HG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:835:HIS:CD2	1:D:856:PHE:HB3	2.56	0.41
1:A:936:PRO:HA	1:A:937:PRO:HD3	1.99	0.41
1:D:1002:MET:HE2	1:D:1002:MET:HB3	1.93	0.40
1:B:708:LYS:HB3	1:B:708:LYS:HE2	1.67	0.40
1:D:941:ILE:HD12	1:D:941:ILE:HA	1.89	0.40
1:C:719:GLY:HA3	2:C:1101:ANP:H4'	2.03	0.40
1:D:995:SER:O	1:D:999:ARG:HG3	2.21	0.40
1:A:981:ILE:HB	1:A:984:ASP:HB2	2.03	0.40
1:C:722:ALA:N	2:C:1101:ANP:O1G	2.40	0.40
1:B:953:ILE:H	1:B:953:ILE:HG22	1.59	0.40
1:C:809:ILE:HG22	1:C:814:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/331 (84%)	272 (98%)	6 (2%)	1 (0%)	30	34
1	B	292/331 (88%)	281 (96%)	9 (3%)	2 (1%)	18	19
1	C	279/331 (84%)	269 (96%)	10 (4%)	0	100	100
1	D	287/331 (87%)	282 (98%)	5 (2%)	0	100	100
All	All	1137/1324 (86%)	1104 (97%)	30 (3%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1007	MET
1	B	1006	ASP
1	A	783	THR

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	257/290 (89%)	246 (96%)	11 (4%)	26	35
1	B	265/290 (91%)	246 (93%)	19 (7%)	13	15
1	C	255/290 (88%)	244 (96%)	11 (4%)	26	35
1	D	261/290 (90%)	259 (99%)	2 (1%)	73	85
All	All	1038/1160 (90%)	995 (96%)	43 (4%)	27	37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	784	SER
1	D	987	MET
1	A	754	LYS
1	A	783	THR
1	A	784	SER
1	A	858	LEU
1	A	861	LEU
1	A	960	LYS
1	A	977	ARG
1	A	982	GLN
1	A	985	GLU
1	A	986	ARG
1	A	994	ASP
1	C	749	GLU
1	C	757	LYS
1	C	758	GLU
1	C	759	ILE
1	C	762	GLU
1	C	812	GLN
1	C	860	LYS
1	C	922	GLU
1	C	982	GLN
1	C	985	GLU
1	C	998	TYR

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Mol	Chain	Res	Type
1	B	701	GLN
1	B	720	SER
1	B	754	LYS
1	B	776	ARG
1	B	783	THR
1	B	784	SER
1	B	876	VAL
1	B	908	MET
1	B	918	ILE
1	B	946	ILE
1	B	949	LYS
1	B	953	ILE
1	B	967	GLU
1	B	981	ILE
1	B	982	GLN
1	B	985	GLU
1	B	987	MET
1	B	1006	ASP
1	B	1009	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	791	GLN
1	A	826	ASN
1	A	849	GLN
1	C	805	HIS
1	C	808	ASN
1	C	888	HIS
1	B	701	GLN
1	B	849	GLN
1	B	893	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	9LL	B	1102	-	30,30,30	3.32	18 (60%)	39,43,43	3.80	16 (41%)
2	ANP	A	1101	3	33,33,33	1.28	4 (12%)	45,52,52	1.21	4 (8%)
2	ANP	C	1101	3	33,33,33	1.15	5 (15%)	45,52,52	0.89	1 (2%)
2	ANP	D	1101	3	33,33,33	1.23	5 (15%)	45,52,52	0.86	1 (2%)
5	YY3	B	1101	-	40,40,40	3.24	22 (55%)	56,56,56	3.49	22 (39%)
4	9LL	D	1103	-	30,30,30	3.24	17 (56%)	39,43,43	3.76	17 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	9LL	B	1102	-	-	1/16/28/28	0/4/4/4
2	ANP	A	1101	3	-	9/18/38/38	0/3/3/3
2	ANP	C	1101	3	-	4/18/38/38	0/3/3/3
2	ANP	D	1101	3	-	6/18/38/38	0/3/3/3
5	YY3	B	1101	-	-	4/25/25/25	0/4/4/4
4	9LL	D	1103	-	-	1/16/28/28	0/4/4/4

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1102	9LL	C19-N18	9.69	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1101	YY3	C21-N6	-7.41	1.27	1.38
5	B	1101	YY3	C8-C7	-7.08	1.37	1.48
4	D	1103	9LL	C19-N18	6.89	1.43	1.36
4	D	1103	9LL	C12-S16	6.53	1.82	1.74
5	B	1101	YY3	C26-C21	-5.99	1.33	1.41
5	B	1101	YY3	C20-N6	-5.97	1.28	1.37
4	D	1103	9LL	C09-C10	5.72	1.60	1.54
4	B	1102	9LL	C09-C10	5.65	1.60	1.54
4	D	1103	9LL	C07-C05	5.36	1.46	1.37
4	B	1102	9LL	C07-C05	5.24	1.46	1.37
5	B	1101	YY3	O-C7	-5.20	1.14	1.24
5	B	1101	YY3	C18-N5	-5.01	1.27	1.34
5	B	1101	YY3	C27-N6	-5.00	1.38	1.46
4	B	1102	9LL	C12-S16	4.67	1.80	1.74
5	B	1101	YY3	C18-C19	-4.64	1.38	1.48
4	B	1102	9LL	C08-C09	4.64	1.57	1.52
4	D	1103	9LL	C04-C05	4.56	1.46	1.37
4	B	1102	9LL	C12-N11	4.54	1.44	1.38
4	D	1103	9LL	C20-C19	4.48	1.56	1.48
5	B	1101	YY3	C25-C26	-4.15	1.33	1.39
4	D	1103	9LL	C26-N18	4.06	1.51	1.47
4	B	1102	9LL	C04-C05	4.05	1.45	1.37
4	B	1102	9LL	C10-N11	3.94	1.43	1.36
5	B	1101	YY3	O1-C14	-3.90	1.31	1.42
4	D	1103	9LL	C10-N11	3.87	1.43	1.36
5	B	1101	YY3	C20-C19	-3.84	1.33	1.37
2	D	1101	ANP	PA-O3A	3.76	1.63	1.59
2	A	1101	ANP	PA-O3A	3.76	1.63	1.59
4	D	1103	9LL	C12-N13	3.60	1.37	1.31
5	B	1101	YY3	C1-C2	-3.47	1.36	1.40
4	B	1102	9LL	C12-N13	3.40	1.36	1.31
5	B	1101	YY3	C22-C21	-3.37	1.34	1.39
4	D	1103	9LL	C08-C09	3.21	1.56	1.52
4	D	1103	9LL	C12-N11	3.17	1.42	1.38
4	B	1102	9LL	C20-C19	3.16	1.53	1.48
5	B	1101	YY3	C24-C25	-3.13	1.33	1.38
2	C	1101	ANP	PB-O1B	3.12	1.50	1.46
2	A	1101	ANP	PG-O1G	2.96	1.50	1.46
5	B	1101	YY3	C23-C22	-2.95	1.33	1.38
2	D	1101	ANP	PG-N3B	2.87	1.70	1.63
2	A	1101	ANP	PB-O1B	2.83	1.50	1.46
4	D	1103	9LL	O01-C02	2.78	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1102	9LL	C26-C25	2.76	1.53	1.50
5	B	1101	YY3	O1-C4	-2.74	1.32	1.37
4	B	1102	9LL	C23-C24	2.73	1.43	1.38
2	D	1101	ANP	PG-O1G	2.68	1.50	1.46
2	D	1101	ANP	PB-O1B	2.67	1.50	1.46
4	D	1103	9LL	C26-C25	2.65	1.53	1.50
2	C	1101	ANP	PG-N3B	2.58	1.70	1.63
4	D	1103	9LL	C14-C15	2.57	1.40	1.34
5	B	1101	YY3	C15-N4	-2.54	1.31	1.34
5	B	1101	YY3	C3-C4	-2.50	1.34	1.38
2	C	1101	ANP	PG-O1G	2.47	1.49	1.46
2	A	1101	ANP	PG-N3B	2.44	1.69	1.63
4	B	1102	9LL	C14-C15	2.42	1.39	1.34
4	B	1102	9LL	C02-C08	2.37	1.42	1.40
4	D	1103	9LL	C20-C25	2.36	1.42	1.39
2	C	1101	ANP	PA-O3A	2.30	1.62	1.59
2	D	1101	ANP	PB-N3B	2.26	1.69	1.63
4	B	1102	9LL	C22-C21	2.25	1.42	1.38
4	D	1103	9LL	C23-C24	2.22	1.42	1.38
4	B	1102	9LL	C26-N18	2.21	1.49	1.47
5	B	1101	YY3	C15-N3	-2.20	1.31	1.36
4	D	1103	9LL	C22-C21	2.16	1.42	1.38
5	B	1101	YY3	C9-C8	2.14	1.40	1.30
5	B	1101	YY3	C26-C19	-2.10	1.42	1.47
4	B	1102	9LL	C21-C20	2.07	1.43	1.39
5	B	1101	YY3	C16-N4	-2.06	1.30	1.34
2	C	1101	ANP	PB-O3A	-2.03	1.56	1.59
4	B	1102	9LL	C20-C25	2.01	1.42	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1102	9LL	C26-N18-C19	-14.55	107.02	113.15
5	B	1101	YY3	C9-C8-C7	-14.22	106.60	122.22
4	D	1103	9LL	C26-N18-C19	-12.92	107.70	113.15
5	B	1101	YY3	C8-C7-N	12.76	122.50	113.84
4	B	1102	9LL	C25-C26-N18	11.13	108.23	102.31
4	D	1103	9LL	C25-C26-N18	10.46	107.87	102.31
4	D	1103	9LL	O27-C19-N18	-7.70	119.22	125.34
5	B	1101	YY3	C21-N6-C20	6.83	113.49	108.54
5	B	1101	YY3	C26-C19-C20	-6.36	102.71	106.02
4	D	1103	9LL	C04-C05-C07	-6.26	114.96	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1102	9LL	C04-C05-C07	-6.08	115.20	123.23
4	B	1102	9LL	O27-C19-N18	-5.72	120.80	125.34
4	D	1103	9LL	C26-N18-C09	5.35	128.84	123.84
5	B	1101	YY3	O-C7-C8	-5.29	114.77	122.70
5	B	1101	YY3	C6-C5-C4	-5.11	112.96	118.95
5	B	1101	YY3	C16-C17-C18	-4.77	114.08	117.02
4	B	1102	9LL	C26-N18-C09	4.26	127.82	123.84
4	D	1103	9LL	C08-C07-C05	4.22	124.08	118.57
4	D	1103	9LL	C10-N11-C12	-4.03	119.63	124.54
4	B	1102	9LL	C08-C07-C05	4.03	123.83	118.57
4	B	1102	9LL	F06-C05-C07	4.00	123.97	118.28
4	D	1103	9LL	C26-C25-C20	-3.72	107.39	109.73
4	B	1102	9LL	C20-C19-N18	3.64	108.73	106.42
5	B	1101	YY3	O1-C4-C5	3.62	119.32	114.81
5	B	1101	YY3	C27-N6-C21	-3.59	122.36	125.69
5	B	1101	YY3	C26-C19-C18	3.51	131.26	126.36
4	D	1103	9LL	C20-C19-N18	3.50	108.64	106.42
5	B	1101	YY3	O1-C4-C3	-3.48	118.09	124.08
4	B	1102	9LL	C26-C25-C20	-3.46	107.56	109.73
4	B	1102	9LL	C03-C04-C05	3.35	121.82	118.38
2	A	1101	ANP	O1G-PG-N3B	-3.35	106.84	111.77
2	A	1101	ANP	C5-C4-N9	-3.29	102.23	105.81
5	B	1101	YY3	C26-C21-N6	-3.13	106.00	107.91
4	B	1102	9LL	S16-C12-N13	-3.12	108.72	114.59
4	D	1103	9LL	F06-C05-C07	3.11	122.71	118.28
4	B	1102	9LL	C14-C15-S16	-3.09	106.33	110.27
4	D	1103	9LL	S16-C12-N13	-2.96	109.02	114.59
4	D	1103	9LL	C03-C04-C05	2.95	121.41	118.38
2	A	1101	ANP	C4-C5-N7	2.87	113.86	110.58
4	B	1102	9LL	C15-S16-C12	2.85	93.33	90.07
5	B	1101	YY3	C18-N5-C15	2.84	119.02	116.87
5	B	1101	YY3	C4-C5-N3	2.82	124.39	118.10
4	D	1103	9LL	C14-C15-S16	-2.81	106.68	110.27
5	B	1101	YY3	C3-C2-C1	-2.68	116.22	119.95
4	D	1103	9LL	C15-S16-C12	2.62	93.07	90.07
5	B	1101	YY3	C2-C3-C4	2.61	123.54	118.01
5	B	1101	YY3	C11-C10-N1	2.54	116.57	112.41
4	B	1102	9LL	S16-C12-N11	2.53	127.81	123.29
4	D	1103	9LL	C08-C09-C10	-2.50	106.70	112.87
5	B	1101	YY3	C16-N4-C15	2.43	117.45	115.42
5	B	1101	YY3	C21-C26-C19	2.38	108.20	106.83
5	B	1101	YY3	N4-C15-N5	-2.37	124.13	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1103	9LL	F06-C05-C04	2.36	122.33	118.55
5	B	1101	YY3	C10-N1-C2	2.29	126.44	117.16
2	D	1101	ANP	O2B-PB-O1B	-2.27	105.00	109.87
2	A	1101	ANP	C6-C5-C4	-2.25	114.10	117.18
5	B	1101	YY3	C1-C2-N1	2.24	122.78	118.29
2	C	1101	ANP	O1B-PB-N3B	-2.23	108.49	111.77
4	B	1102	9LL	C08-C09-C10	-2.11	107.67	112.87
4	B	1102	9LL	C26-C25-C24	2.06	133.11	128.70
4	D	1103	9LL	O17-C10-C09	-2.03	118.17	120.95

There are no chirality outliers.

All (25) torsion outliers are listed below:

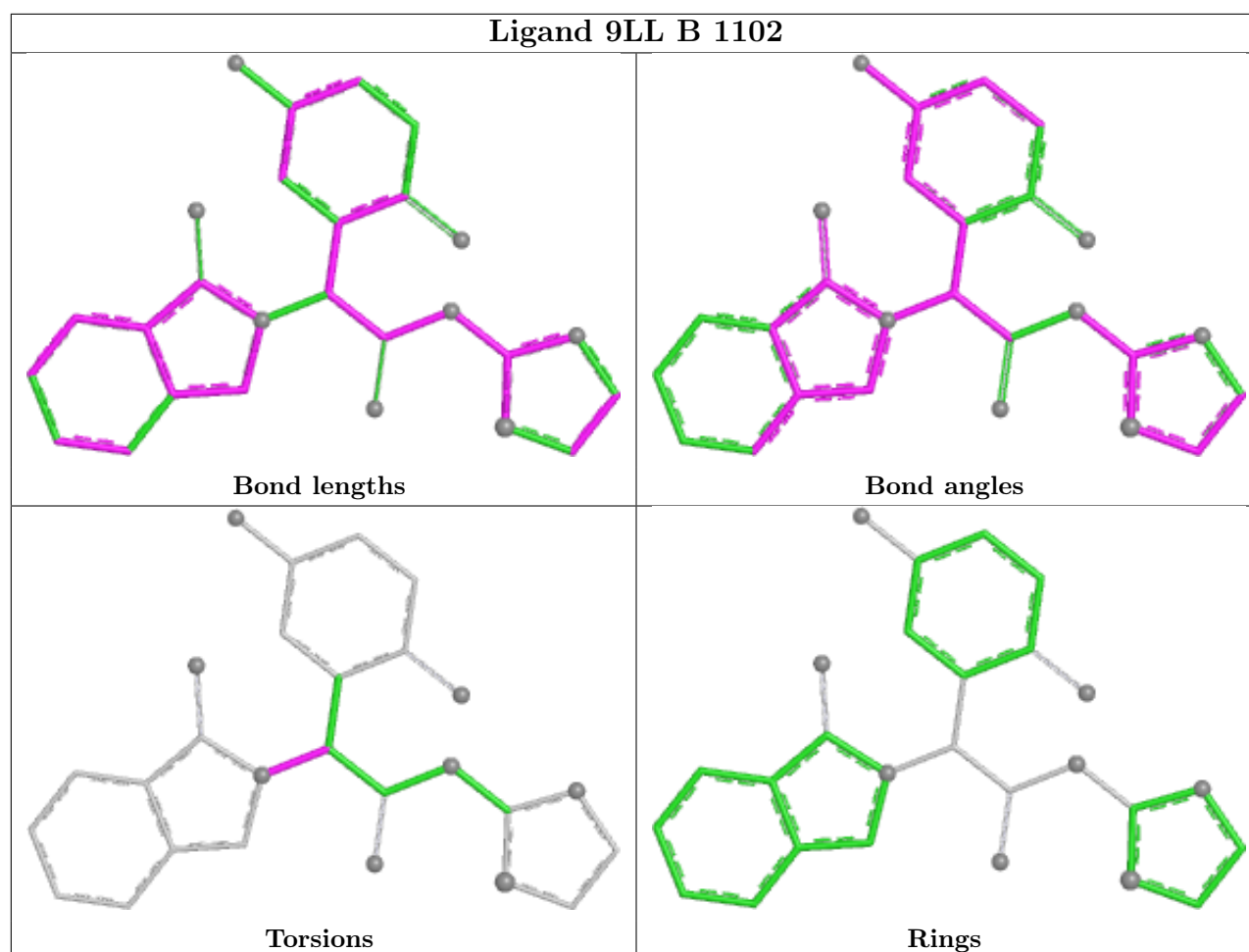
Mol	Chain	Res	Type	Atoms
2	D	1101	ANP	PB-N3B-PG-O1G
2	D	1101	ANP	PG-N3B-PB-O1B
2	D	1101	ANP	PA-O3A-PB-O2B
2	A	1101	ANP	PB-N3B-PG-O1G
2	A	1101	ANP	PG-N3B-PB-O1B
2	A	1101	ANP	PG-N3B-PB-O3A
2	A	1101	ANP	PA-O3A-PB-O1B
2	A	1101	ANP	PA-O3A-PB-O2B
2	A	1101	ANP	C5'-O5'-PA-O1A
2	A	1101	ANP	O4'-C4'-C5'-O5'
2	C	1101	ANP	PB-N3B-PG-O1G
2	C	1101	ANP	PG-N3B-PB-O1B
2	C	1101	ANP	PA-O3A-PB-O1B
4	D	1103	9LL	C08-C09-N18-C26
5	B	1101	YY3	C3-C2-N1-C10
5	B	1101	YY3	N-C7-C8-C9
5	B	1101	YY3	O-C7-C8-C9
2	A	1101	ANP	C3'-C4'-C5'-O5'
5	B	1101	YY3	C1-C2-N1-C10
4	B	1102	9LL	C08-C09-N18-C26
2	D	1101	ANP	C5'-O5'-PA-O1A
2	D	1101	ANP	C5'-O5'-PA-O3A
2	A	1101	ANP	C5'-O5'-PA-O3A
2	C	1101	ANP	PA-O3A-PB-O2B
2	D	1101	ANP	PA-O3A-PB-O1B

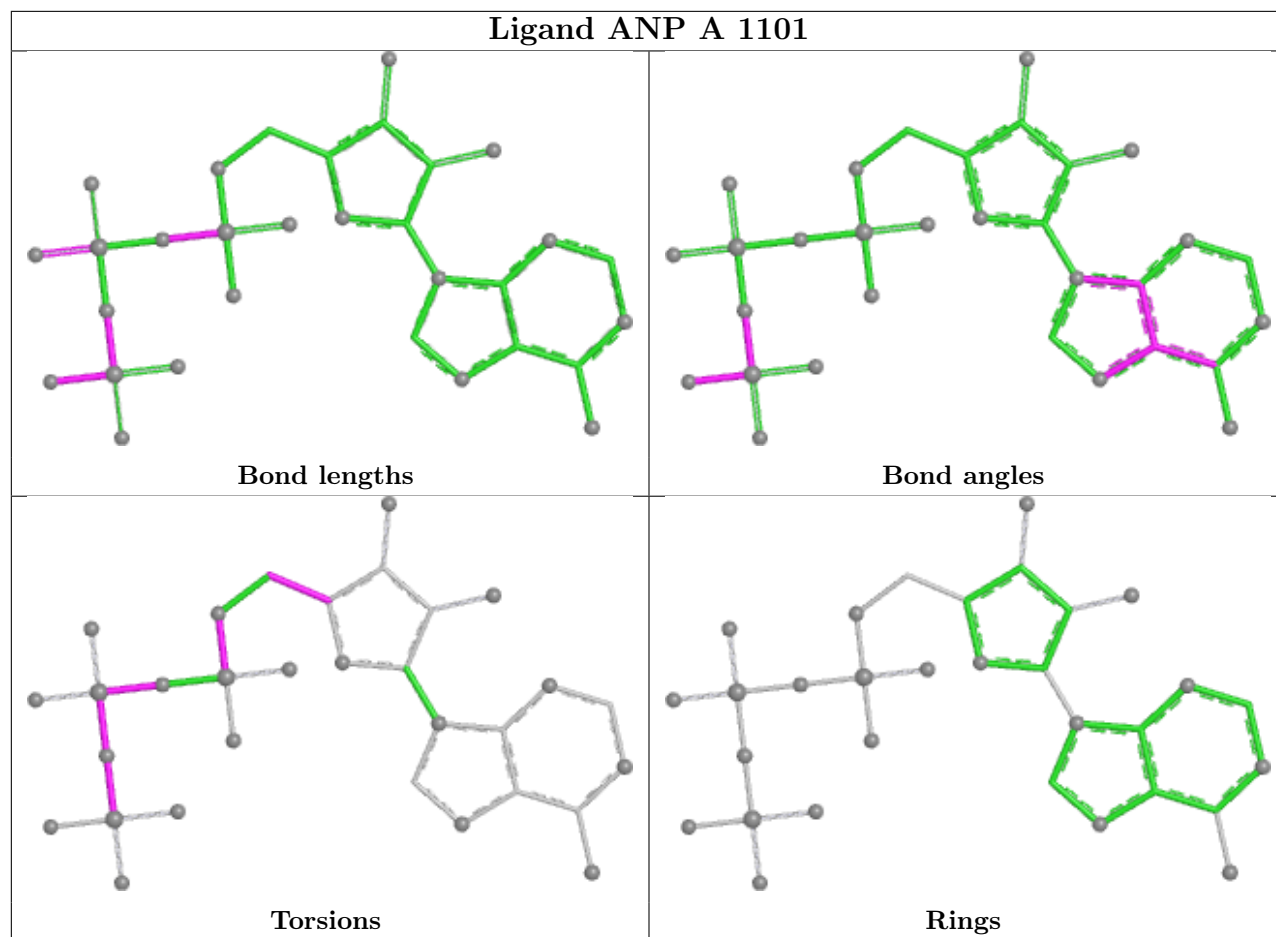
There are no ring outliers.

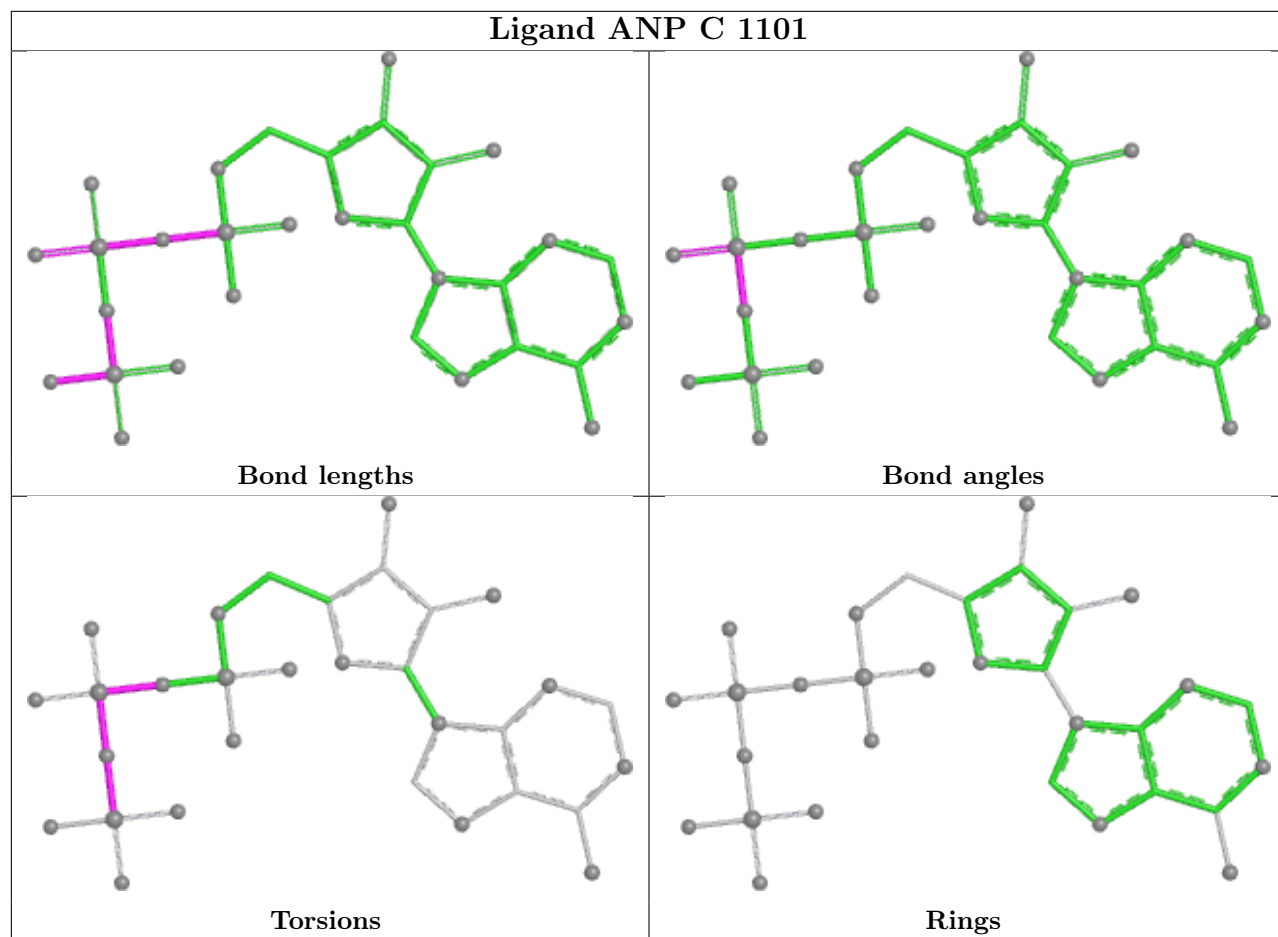
3 monomers are involved in 11 short contacts:

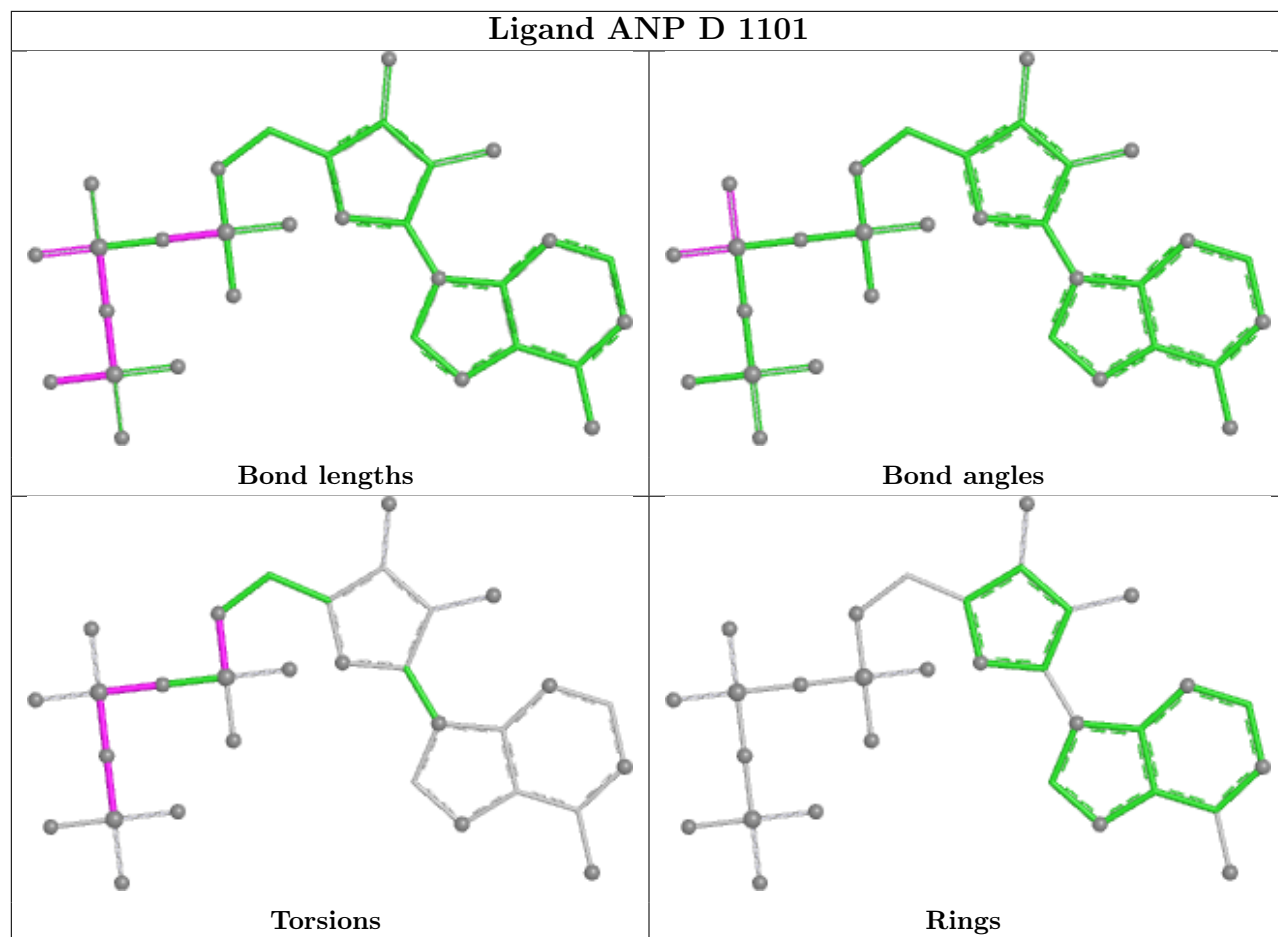
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	ANP	2	0
5	B	1101	YY3	8	0
4	D	1103	9LL	1	0

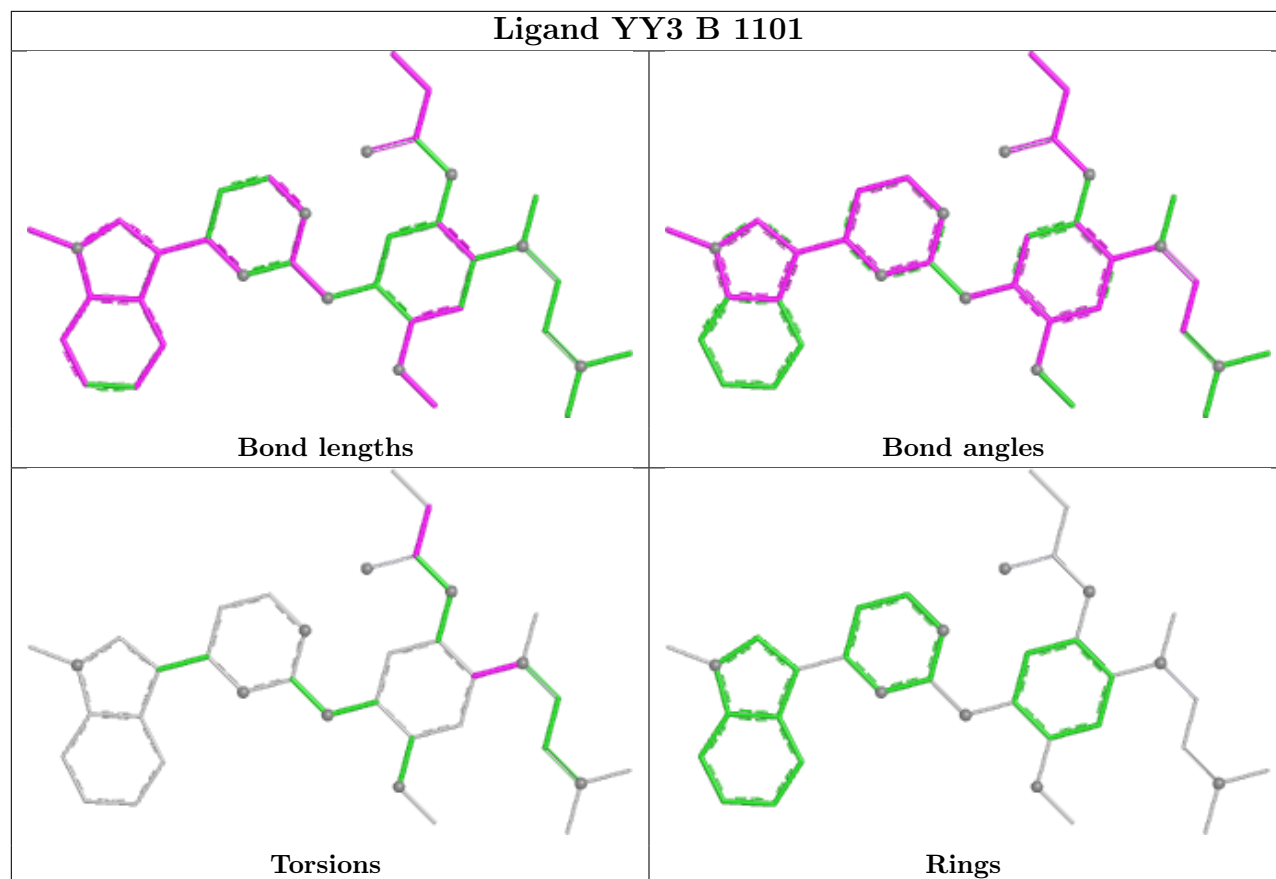
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

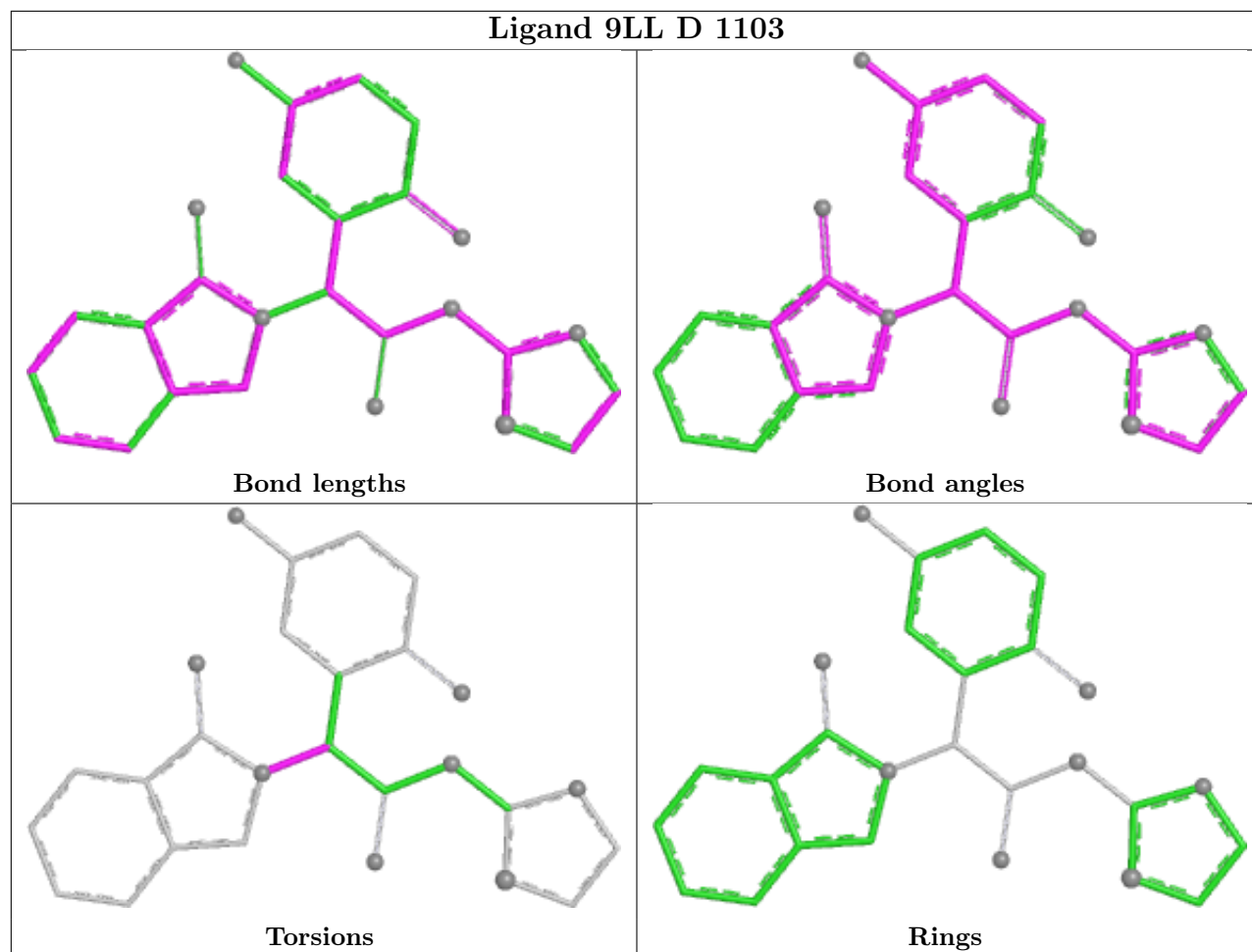












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	287/331 (86%)	1.23	51 (17%) 4 3	26, 48, 73, 92	0
1	B	296/331 (89%)	1.17	39 (13%) 7 5	33, 50, 75, 92	0
1	C	285/331 (86%)	1.27	46 (16%) 4 3	32, 52, 76, 88	0
1	D	291/331 (87%)	1.15	41 (14%) 6 4	30, 48, 75, 86	0
All	All	1159/1324 (87%)	1.21	177 (15%) 5 4	26, 50, 75, 92	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	722	ALA	5.3
1	B	1010	VAL	4.9
1	A	876	VAL	4.9
1	A	783	THR	4.9
1	A	990	PRO	4.7
1	A	992	PRO	4.7
1	C	755	ALA	4.5
1	C	859	ALA	4.4
1	D	1007	MET	4.4
1	C	953	ILE	4.3
1	A	859	ALA	4.3
1	C	1006	ASP	4.3
1	A	753	PRO	4.3
1	B	1011	VAL	4.2
1	B	859	ALA	4.2
1	D	723	PHE	4.2
1	A	986	ARG	4.1
1	A	861	LEU	4.1
1	C	764	TYR	4.0
1	C	808	ASN	4.0
1	B	723	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	734	GLU	3.9
1	A	775	CYS	3.9
1	A	755	ALA	3.9
1	C	876	VAL	3.8
1	A	723	PHE	3.8
1	D	988	HIS	3.8
1	D	808	ASN	3.7
1	C	988	HIS	3.7
1	D	754	LYS	3.7
1	C	758	GLU	3.6
1	A	1006	ASP	3.6
1	B	753	PRO	3.6
1	C	858	LEU	3.6
1	C	992	PRO	3.5
1	A	1001	LEU	3.5
1	C	783	THR	3.5
1	D	858	LEU	3.4
1	A	993	THR	3.4
1	B	988	HIS	3.4
1	A	785	THR	3.4
1	D	737	LYS	3.4
1	A	920	ALA	3.4
1	D	876	VAL	3.3
1	C	737	LYS	3.3
1	D	807	ASP	3.2
1	C	857	GLY	3.1
1	C	702	ALA	3.1
1	A	784	SER	3.1
1	C	747	LEU	3.1
1	C	715	ILE	3.1
1	D	700	ASN	3.1
1	D	917	GLY	3.0
1	D	734	GLU	3.0
1	C	985	GLU	3.0
1	A	754	LYS	3.0
1	D	702	ALA	3.0
1	B	758	GLU	3.0
1	B	806	LYS	3.0
1	B	701	GLN	3.0
1	A	1007	MET	3.0
1	A	737	LYS	2.9
1	A	858	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	713	LYS	2.9
1	A	926	ILE	2.9
1	D	962	ARG	2.9
1	A	991	SER	2.9
1	D	953	ILE	2.9
1	A	748	ARG	2.9
1	B	715	ILE	2.9
1	B	918	ILE	2.9
1	A	764	TYR	2.9
1	C	986	ARG	2.8
1	B	737	LYS	2.8
1	D	987	MET	2.8
1	D	802	VAL	2.8
1	A	769	VAL	2.8
1	A	929	LYS	2.8
1	C	748	ARG	2.8
1	B	986	ARG	2.7
1	C	782	LEU	2.7
1	B	908	MET	2.7
1	A	918	ILE	2.7
1	D	1006	ASP	2.7
1	C	729	GLY	2.7
1	B	702	ALA	2.7
1	D	707	LEU	2.6
1	D	751	THR	2.6
1	A	708	LYS	2.6
1	A	735	GLY	2.6
1	D	750	ALA	2.6
1	B	920	ALA	2.6
1	B	742	VAL	2.6
1	B	993	THR	2.6
1	A	953	ILE	2.5
1	D	993	THR	2.5
1	B	1007	MET	2.5
1	D	706	ILE	2.5
1	D	735	GLY	2.5
1	D	918	ILE	2.5
1	C	785	THR	2.5
1	B	955	ALA	2.5
1	C	989	LEU	2.5
1	A	860	LYS	2.5
1	B	721	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	918	ILE	2.5
1	D	756	ASN	2.5
1	C	710	THR	2.5
1	B	989	LEU	2.5
1	C	723	PHE	2.5
1	C	860	LYS	2.5
1	A	759	ILE	2.5
1	C	759	ILE	2.5
1	B	1006	ASP	2.4
1	B	1009	ASP	2.4
1	A	782	LEU	2.4
1	D	748	ARG	2.4
1	A	877	PRO	2.4
1	A	962	ARG	2.4
1	D	732	ILE	2.4
1	B	876	VAL	2.4
1	D	757	LYS	2.4
1	D	753	PRO	2.4
1	D	703	LEU	2.4
1	A	758	GLU	2.4
1	A	923	ILE	2.4
1	B	784	SER	2.4
1	A	747	LEU	2.3
1	D	981	ILE	2.3
1	C	890	ILE	2.3
1	A	713	LYS	2.3
1	C	732	ILE	2.3
1	A	707	LEU	2.3
1	A	788	LEU	2.3
1	B	952	MET	2.3
1	B	1008	ASP	2.3
1	B	980	VAL	2.2
1	A	709	GLU	2.2
1	A	856	PHE	2.2
1	D	809	ILE	2.2
1	C	756	ASN	2.2
1	A	786	VAL	2.2
1	D	941	ILE	2.2
1	C	981	ILE	2.2
1	A	716	LYS	2.2
1	B	967	GLU	2.1
1	C	786	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	921	SER	2.1
1	C	944	TYR	2.1
1	A	710	THR	2.1
1	D	898	TRP	2.1
1	C	706	ILE	2.1
1	A	917	GLY	2.1
1	A	1000	ALA	2.1
1	B	750	ALA	2.1
1	A	734	GLU	2.1
1	C	807	ASP	2.1
1	C	990	PRO	2.1
1	B	977	ARG	2.1
1	D	834	VAL	2.1
1	D	806	LYS	2.1
1	A	720	SER	2.1
1	C	908	MET	2.1
1	C	922	GLU	2.1
1	C	963	GLU	2.1
1	B	917	GLY	2.1
1	D	966	ILE	2.1
1	C	926	ILE	2.1
1	B	853	ILE	2.1
1	B	953	ILE	2.1
1	D	989	LEU	2.0
1	B	833	LEU	2.0
1	C	889	ARG	2.0
1	D	752	SER	2.0
1	D	701	GLN	2.0
1	C	888	HIS	2.0
1	C	716	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

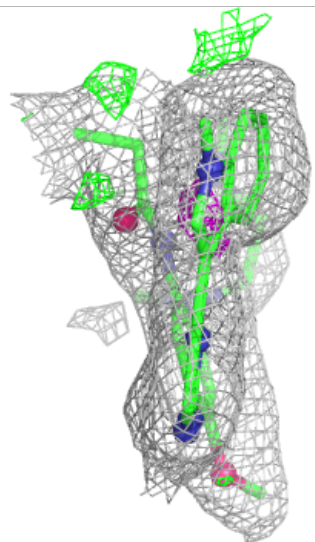
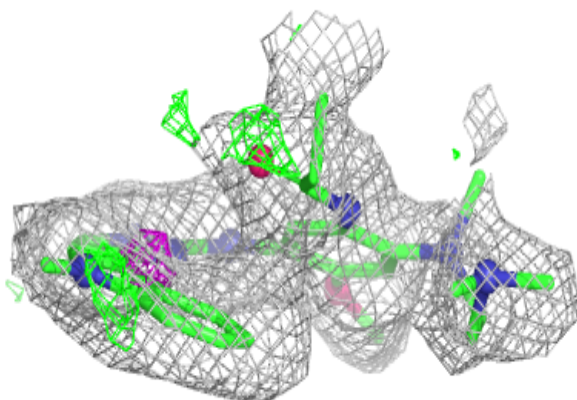
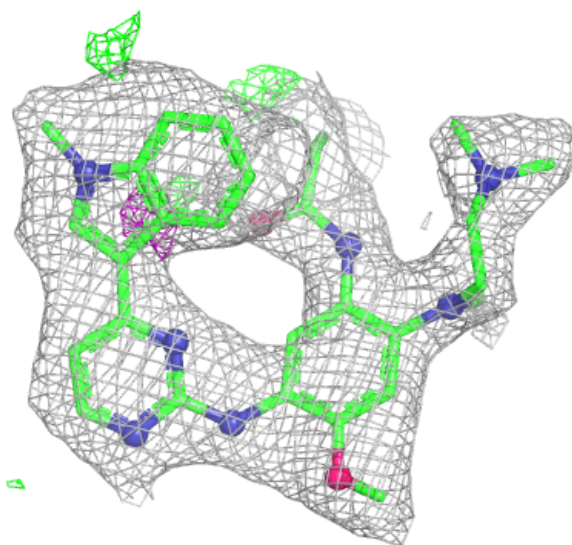
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	YY3	B	1101	37/37	0.82	0.16	40,53,65,68	0
2	ANP	D	1101	31/31	0.86	0.13	36,52,65,74	0
2	ANP	A	1101	31/31	0.88	0.12	42,51,60,65	0
2	ANP	C	1101	31/31	0.89	0.12	43,51,62,73	0
4	9LL	B	1102	27/27	0.91	0.11	42,47,57,59	0
3	MG	D	1102	1/1	0.92	0.10	56,56,56,56	0
3	MG	C	1102	1/1	0.93	0.07	51,51,51,51	0
4	9LL	D	1103	27/27	0.93	0.10	33,46,52,61	0
3	MG	A	1102	1/1	0.98	0.15	39,39,39,39	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.

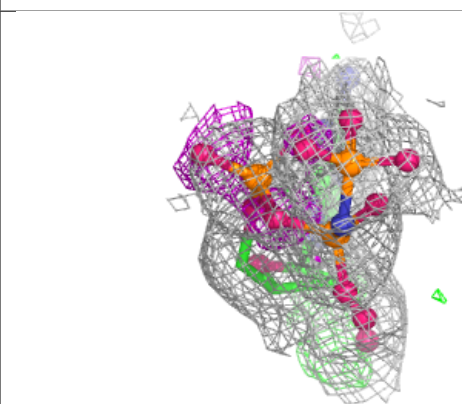
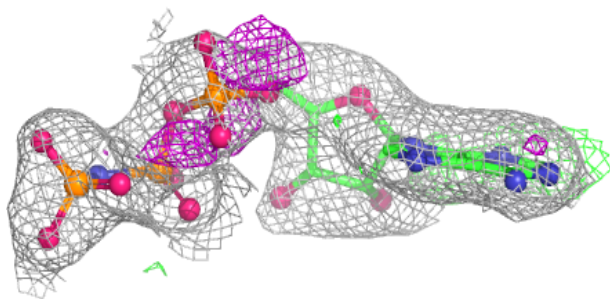
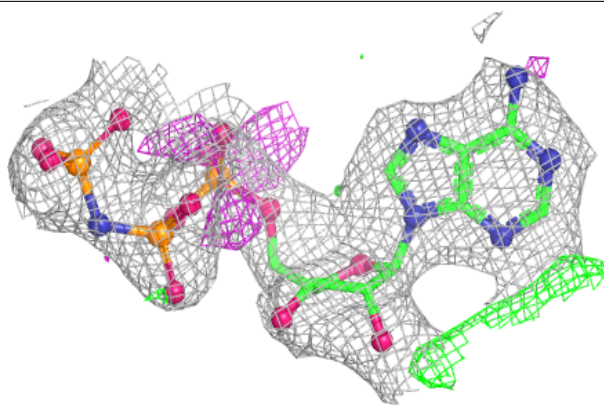
Electron density around YY3 B 1101:

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

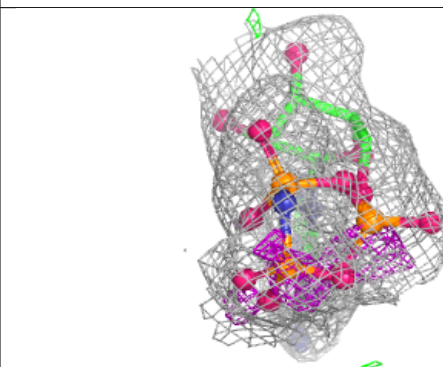
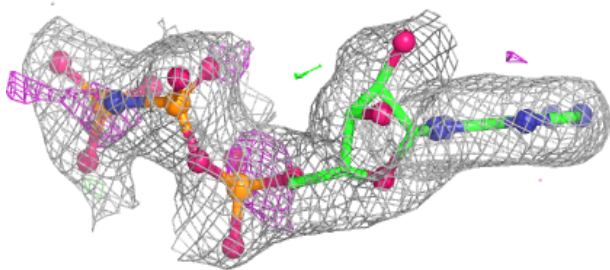
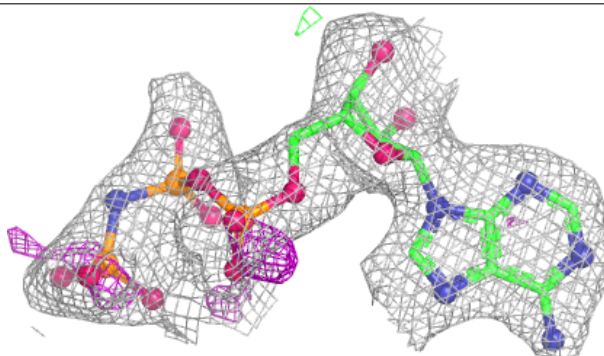


Electron density around ANP D 1101:

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

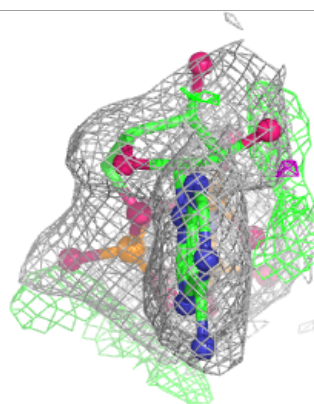
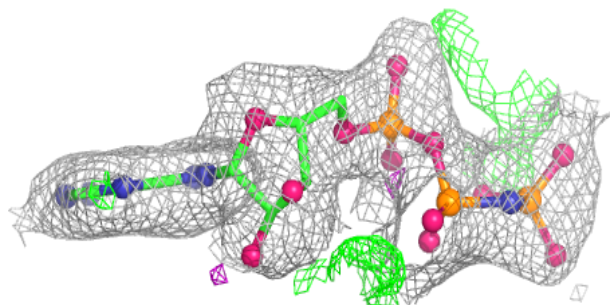
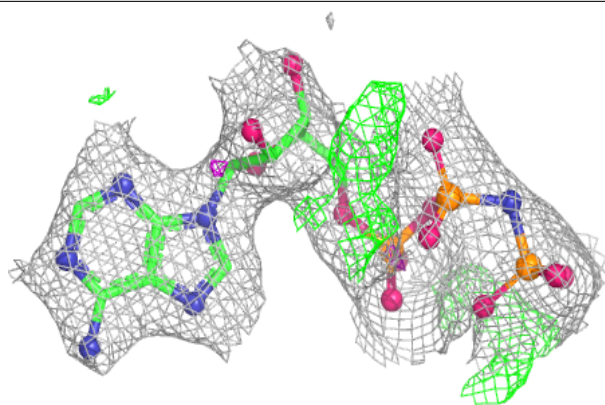
**Electron density around ANP A 1101:**

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



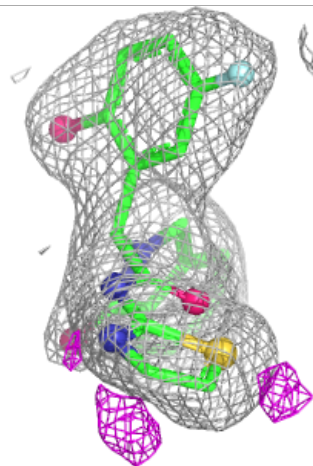
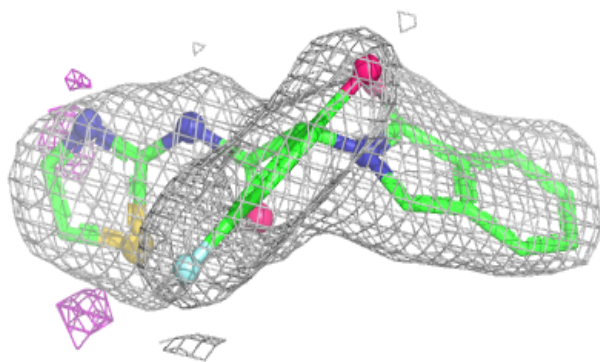
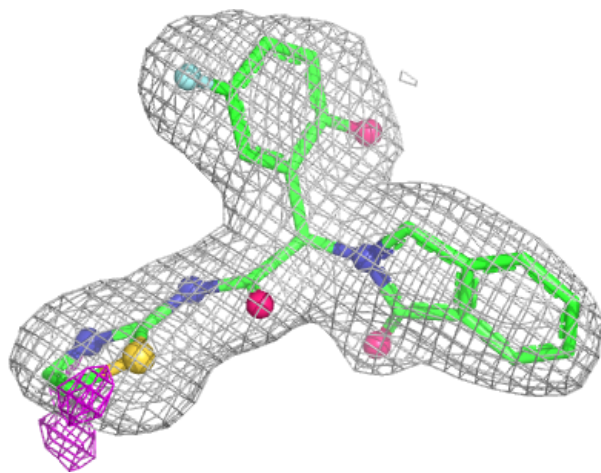
Electron density around ANP C 1101:

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



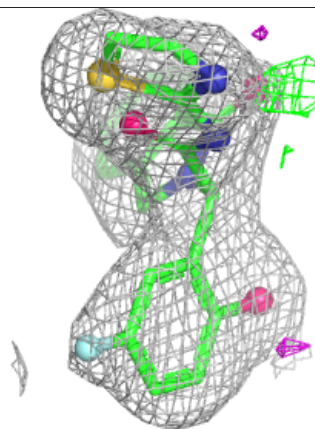
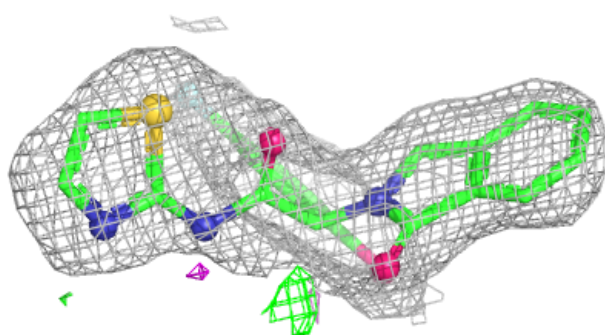
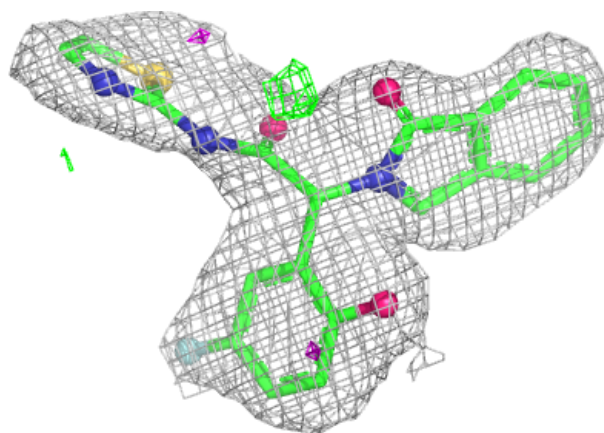
Electron density around 9LL B 1102:

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



Electron density around 9LL 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 ⓘ

There are no such residues in this entry.