



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:40 pm BST

PDB ID : 5O4V
Title : P.vivax NMT with aminomethylindazole and quinoline inhibitors bound
Authors : Brannigan, J.A.; Wilkinson, A.J.
Deposited on : 2017-05-31
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

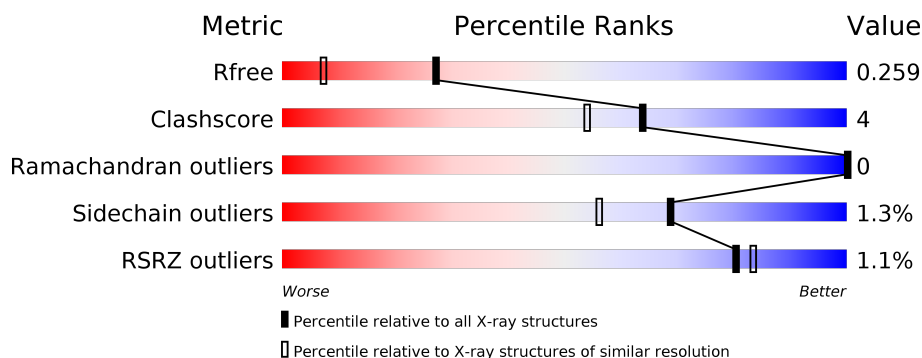
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	385	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
1	B	385	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	385	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

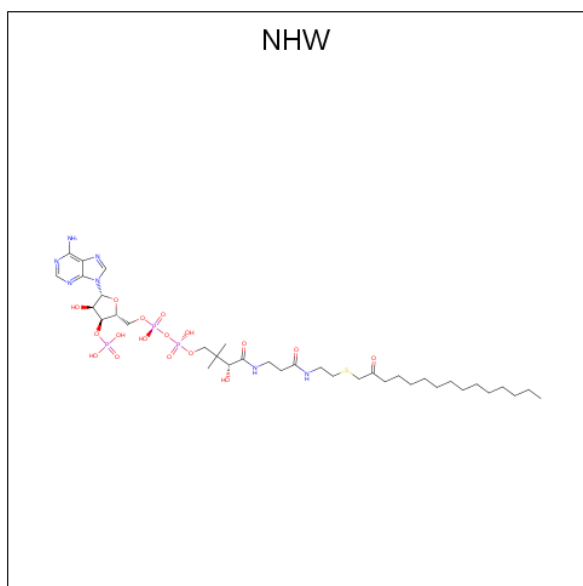
There are 9 unique types of molecules in this entry. The entry contains 11374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycylpeptide N-tetradecanoyltransferase.

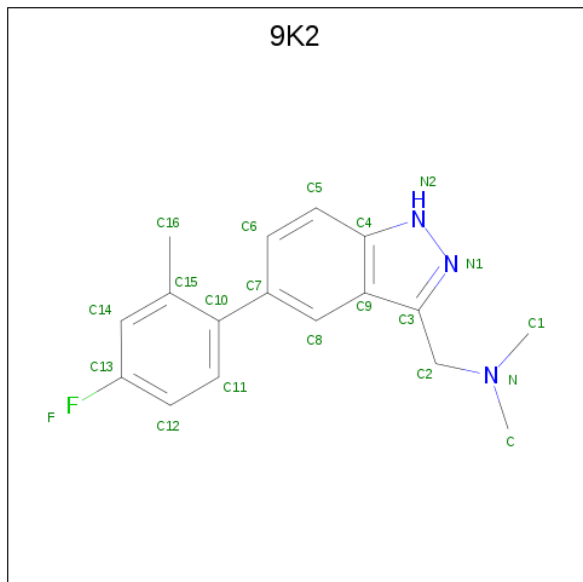
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	23	0
			3319	2160	542	605	12			
1	B	385	Total	C	N	O	S	0	26	0
			3333	2180	538	603	12			
1	C	368	Total	C	N	O	S	0	29	0
			3208	2099	509	589	11			

- Molecule 2 is 2-oxopentadecyl-CoA (three-letter code: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



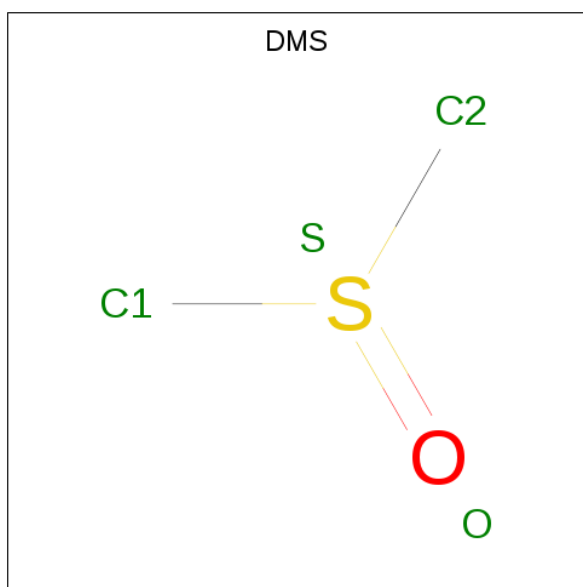
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

- Molecule 3 is 1-[5-(4-fluoranyl-2-methyl-phenyl)-1 {H}-indazol-3-yl]- {N}, {N}-dimethyl-methanamine (three-letter code: 9K2) (formula: $C_{17}H_{18}FN_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			21	17	1	3		
3	B	1	Total	C	F	N	0	0
			21	17	1	3		
3	C	1	Total	C	F	N	0	0
			21	17	1	3		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

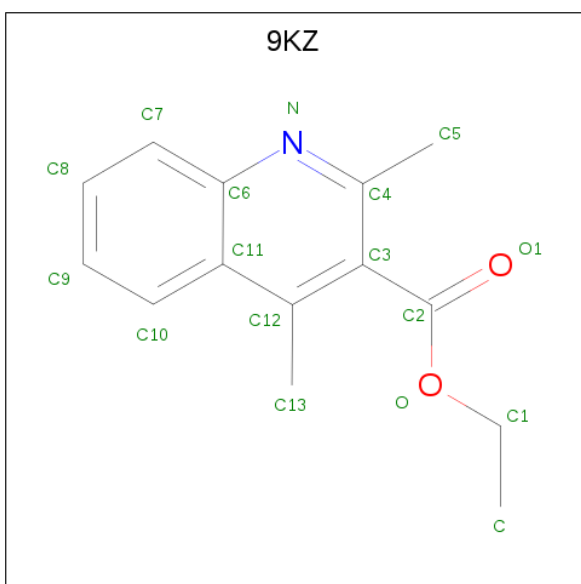
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is ethyl 2,4-dimethylquinoline-3-carboxylate (three-letter code: 9KZ) (formula: $C_{14}H_{15}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			17	14	1	2		
8	B	1	Total	C	N	O	0	0
			17	14	1	2		
8	C	1	Total	C	N	O	0	0
			17	14	1	2		

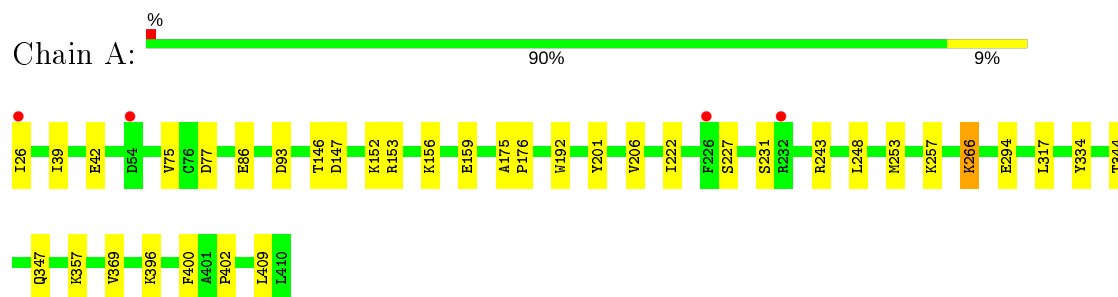
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	409	Total	O	0	0
			409	409		
9	B	411	Total	O	0	0
			411	411		
9	C	350	Total	O	0	0
			350	350		

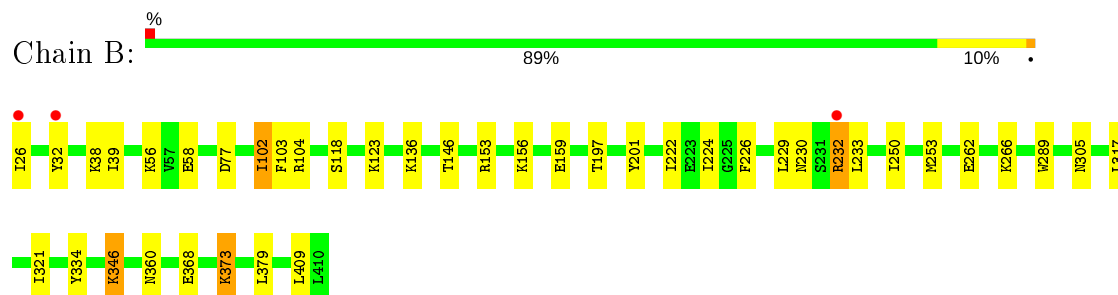
3 Residue-property plots [i](#)

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

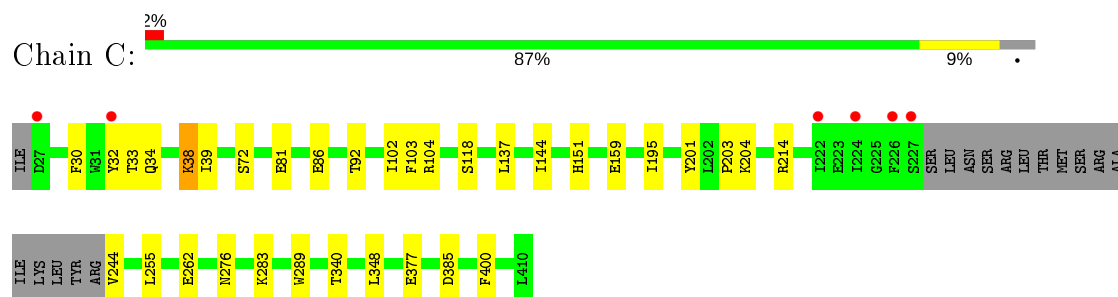
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.56Å 121.88Å 179.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.53 – 1.70 60.94 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (89.53-1.70) 98.6 (60.94-1.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.207 , 0.258 0.210 , 0.259	Depositor DCC
R_{free} test set	6874 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11374	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, 9K2, NHW, DMS, SO4, 9KZ

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	0.92	1/3453 (0.0%)	0.91	5/4671 (0.1%)
1	B	0.94	0/3491	0.93	4/4716 (0.1%)
1	C	0.92	0/3361	0.87	1/4546 (0.0%)
All	All	0.93	1/10305 (0.0%)	0.90	10/13933 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	TRP	CE3-CZ3	5.25	1.47	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	104	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	153	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	77	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	77	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	396	LYS	N-CA-CB	-5.61	100.51	110.60
1	A	77	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	A	153	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	93	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	255	LEU	CB-CG-CD1	-5.09	102.35	111.00

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	3319	0	3357	26	0
1	B	3333	0	3413	32	0
1	C	3208	0	3250	26	0
2	A	64	0	60	0	0
2	B	64	0	60	0	0
2	C	64	0	60	0	0
3	A	21	0	0	0	0
3	B	21	0	0	0	0
3	C	21	0	0	0	0
4	A	4	0	6	2	0
4	B	4	0	6	0	0
4	C	4	0	6	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	A	17	0	0	1	0
8	B	17	0	0	2	0
8	C	17	0	0	0	0
9	A	409	0	0	9	0
9	B	411	0	0	1	0
9	C	350	0	0	3	0
All	All	11374	0	10218	85	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 4.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81[A]:GLU:OE2	9:C:602:HOH:O	1.68	1.10
1:B:123[B]:LYS:H	1:B:123[B]:LYS:HD3	1.21	0.99
1:C:151:HIS:CE1	1:C:276[A]:ASN:HD21	1.93	0.86
1:C:30:PHE:O	1:C:33[A]:THR:HG22	1.78	0.84
1:C:32[A]:TYR:CD1	1:C:38[A]:LYS:HE2	2.19	0.77
1:A:86[A]:GLU:OE1	9:A:603:HOH:O	2.05	0.74
1:A:294[B]:GLU:OE1	9:A:604:HOH:O	2.05	0.74
1:A:86[B]:GLU:OE2	9:A:602:HOH:O	2.04	0.73
1:B:197:THR:HG23	1:B:409[B]:LEU:HD12	1.70	0.72
1:A:344:THR:H	1:A:347:GLN:HE21	1.37	0.72
1:A:146:THR:HG21	1:A:159[A]:GLU:CG	2.21	0.70
1:B:368:GLU:OE1	1:B:373[A]:LYS:HE3	1.91	0.70
1:B:123[B]:LYS:H	1:B:123[B]:LYS:CD	1.95	0.69
4:A:503:DMS:H13	9:A:645:HOH:O	1.93	0.68
1:A:222[A]:ILE:HD13	1:A:227:SER:HB2	1.76	0.67
1:A:146:THR:CG2	1:A:159[A]:GLU:HG3	2.27	0.64
1:C:262[A]:GLU:HG3	1:C:283:LYS:HZ2	1.64	0.63
1:A:146:THR:HG21	1:A:159[A]:GLU:HG3	1.80	0.62
1:A:147[A]:ASP:OD2	1:A:156[A]:LYS:HE2	1.99	0.62
1:B:222[A]:ILE:HD12	1:B:229:LEU:HG	1.82	0.62
1:B:226:PHE:CE2	8:B:507:9KZ:C1	2.83	0.62
1:B:346[A]:LYS:HD3	1:B:379:LEU:HD21	1.83	0.61
1:B:230[B]:ASN:ND2	1:B:233:LEU:H	1.99	0.61
1:C:262[A]:GLU:HG3	1:C:283:LYS:NZ	2.18	0.58
1:A:152[B]:LYS:HD2	9:A:608:HOH:O	2.04	0.57
1:B:146:THR:C	1:B:156[A]:LYS:HE3	2.24	0.57
1:C:102[A]:ILE:HD11	9:C:868:HOH:O	2.05	0.56
1:B:56:LYS:HB3	1:B:58:GLU:HG2	1.89	0.55
1:B:39:ILE:HD12	1:B:201:TYR:HE2	1.72	0.54
1:A:39:ILE:HD12	1:A:201:TYR:HE2	1.72	0.54
1:C:151:HIS:CE1	1:C:276[A]:ASN:ND2	2.71	0.54
1:A:248:LEU:HD13	1:A:253[B]:MET:HB2	1.88	0.53
1:A:257:LYS:HE3	9:A:707:HOH:O	2.08	0.53
1:C:92:THR:O	1:C:104:ARG:HD2	2.08	0.52
1:C:262[A]:GLU:CG	1:C:283:LYS:NZ	2.73	0.52
1:B:222[B]:ILE:HD13	1:B:229:LEU:HD21	1.91	0.52
1:C:32[A]:TYR:CE1	1:C:38[A]:LYS:HE2	2.45	0.51
1:C:86[B]:GLU:HG3	1:C:137:LEU:HD22	1.93	0.50
1:B:102:ILE:HG12	1:B:103:PHE:CD2	2.46	0.50
1:B:230[B]:ASN:HD22	1:B:232:ARG:H	1.59	0.50
1:B:159[A]:GLU:HG3	1:B:409[A]:LEU:HD21	1.94	0.50
1:C:102[A]:ILE:HG23	1:C:103:PHE:CD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HB3	1:A:334:TYR:CE1	2.47	0.50
1:B:360:ASN:ND2	9:B:610:HOH:O	2.45	0.49
1:B:230[A]:ASN:HD22	1:B:232:ARG:HD2	1.76	0.49
1:A:344:THR:H	1:A:347:GLN:NE2	2.09	0.48
1:A:357:LYS:HE2	9:A:872:HOH:O	2.13	0.48
1:A:42:GLU:OE2	1:B:346[B]:LYS:HD3	2.14	0.48
1:C:159[A]:GLU:OE2	4:C:503:DMS:C1	2.62	0.48
1:A:206[B]:VAL:HG22	1:A:400:PHE:CE2	2.48	0.47
1:B:146:THR:CA	1:B:156[A]:LYS:HE3	2.44	0.47
1:B:102:ILE:HD11	1:B:103:PHE:CZ	2.50	0.47
1:A:75:VAL:HG23	9:A:912:HOH:O	2.15	0.46
1:C:276[A]:ASN:ND2	1:C:400:PHE:CE1	2.84	0.46
1:B:317:LEU:HB3	1:B:334:TYR:CE1	2.51	0.46
1:B:32[B]:TYR:CD1	1:B:38[B]:LYS:HE3	2.50	0.46
1:C:159[A]:GLU:HG3	1:C:195:ILE:HG23	1.98	0.46
1:C:159[A]:GLU:OE2	4:C:503:DMS:H13	2.16	0.45
1:B:262:GLU:OE2	1:B:266[A]:LYS:NZ	2.44	0.45
1:A:266[A]:LYS:HE3	1:A:266[A]:LYS:HB3	1.46	0.45
1:B:262:GLU:HG3	1:B:266[A]:LYS:HE3	1.98	0.45
1:A:159[A]:GLU:OE1	4:A:503:DMS:H11	2.17	0.44
8:A:508:9KZ:C5	8:A:508:9KZ:C1	2.95	0.44
1:C:39:ILE:HD11	1:C:201:TYR:CE2	2.52	0.44
1:B:39:ILE:CD1	1:B:201:TYR:HE2	2.31	0.44
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.52	0.43
1:A:159[B]:GLU:OE2	1:A:409:LEU:HD13	2.18	0.43
1:A:243[B]:ARG:HG3	9:A:814:HOH:O	2.19	0.42
1:A:175:ALA:HB3	1:A:176:PRO:HD3	2.01	0.42
1:B:226:PHE:CZ	8:B:507:9KZ:C1	3.03	0.42
1:C:340:THR:HB	1:C:348:LEU:HD22	2.01	0.42
1:C:377[A]:GLU:OE1	1:C:377[A]:GLU:HA	2.20	0.42
1:B:224:ILE:HG21	1:B:321:ILE:HD13	2.02	0.41
1:C:244:VAL:N	9:C:610:HOH:O	2.53	0.41
1:B:39:ILE:HA	1:B:39:ILE:HD13	1.89	0.41
1:C:203:PRO:HA	1:C:204:LYS:HA	1.91	0.41
1:A:369:VAL:HA	1:A:402:PRO:O	2.21	0.41
1:B:118:SER:HB3	1:B:289:TRP:CZ2	2.56	0.41
1:B:250:ILE:HB	1:B:253[B]:MET:HG2	2.03	0.40
1:C:33[A]:THR:HG23	1:C:34:GLN:OE1	2.22	0.40
1:C:144:ILE:HD11	4:C:503:DMS:H11	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	406/385 (106%)	396 (98%)	10 (2%)	0	100	100
1	B	409/385 (106%)	399 (98%)	10 (2%)	0	100	100
1	C	393/385 (102%)	380 (97%)	13 (3%)	0	100	100
All	All	1208/1155 (105%)	1175 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/351 (107%)	370 (99%)	4 (1%)	73	63
1	B	377/351 (107%)	369 (98%)	8 (2%)	53	36
1	C	364/351 (104%)	357 (98%)	7 (2%)	57	41
All	All	1115/1053 (106%)	1096 (98%)	19 (2%)	69	46

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	231	SER
1	A	266[A]	LYS
1	A	266[B]	LYS
1	B	26	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	102	ILE
1	B	136	LYS
1	B	232	ARG
1	B	346[A]	LYS
1	B	346[B]	LYS
1	B	373[A]	LYS
1	B	373[B]	LYS
1	C	38[A]	LYS
1	C	38[B]	LYS
1	C	72[A]	SER
1	C	72[B]	SER
1	C	214[A]	ARG
1	C	214[B]	ARG
1	C	385	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	106	ASN
1	A	193	GLN
1	A	249	ASN
1	A	347	GLN
1	A	350	GLN
1	B	34	GLN
1	B	106	ASN
1	B	193	GLN
1	B	274	GLN
1	B	360	ASN
1	C	193	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	DMS	C	503	-	3,3,3	0.58	0	3,3,3	1.05	0
7	SO4	A	506	-	4,4,4	0.44	0	6,6,6	0.13	0
3	9K2	B	502	-	21,23,23	1.39	3 (14%)	26,33,33	2.43	10 (38%)
7	SO4	B	506	-	4,4,4	0.23	0	6,6,6	1.15	1 (16%)
8	9KZ	A	508	-	18,18,18	3.18	8 (44%)	24,25,25	2.26	8 (33%)
2	NHW	C	501	5	58,66,66	1.02	5 (8%)	70,92,92	1.40	7 (10%)
2	NHW	B	501	5	58,66,66	1.03	2 (3%)	70,92,92	1.29	6 (8%)
8	9KZ	B	507	-	18,18,18	2.52	7 (38%)	24,25,25	2.04	7 (29%)
7	SO4	A	507	-	4,4,4	0.45	0	6,6,6	0.88	0
7	SO4	C	506	-	4,4,4	0.36	0	6,6,6	0.15	0
3	9K2	C	502	-	21,23,23	2.16	5 (23%)	26,33,33	2.44	8 (30%)
2	NHW	A	501	5	58,66,66	1.25	8 (13%)	70,92,92	1.37	10 (14%)
8	9KZ	C	507	-	18,18,18	2.50	4 (22%)	24,25,25	2.20	8 (33%)
3	9K2	A	502	-	21,23,23	1.54	4 (19%)	26,33,33	2.35	9 (34%)
4	DMS	A	503	-	3,3,3	0.55	0	3,3,3	1.83	1 (33%)
4	DMS	B	503	-	3,3,3	0.47	0	3,3,3	1.13	0

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
3	9K2	B	502	-	-	0/7/8/8	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	9KZ	A	508	-	-	2/7/7/7	0/2/2/2
2	NHW	B	501	5	-	3/61/81/81	0/3/3/3
8	9KZ	B	507	-	-	1/7/7/7	0/2/2/2
2	NHW	A	501	5	-	4/61/81/81	0/3/3/3
2	NHW	C	501	5	-	2/61/81/81	0/3/3/3
3	9K2	C	502	-	-	0/7/8/8	0/3/3/3
8	9KZ	C	507	-	-	0/7/7/7	0/2/2/2
3	9K2	A	502	-	-	0/7/8/8	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	508	9KZ	C3-C12	10.73	1.47	1.38
8	C	507	9KZ	C3-C12	8.24	1.45	1.38
8	B	507	9KZ	C3-C12	7.00	1.44	1.38
3	C	502	9K2	C2-C3	6.65	1.54	1.51
2	A	501	NHW	C4A-N3A	4.16	1.41	1.35
2	B	501	NHW	O4X-C1X	3.92	1.46	1.41
8	A	508	9KZ	C3-C4	3.90	1.48	1.41
8	B	507	9KZ	C11-C6	3.86	1.48	1.42
8	B	507	9KZ	C3-C4	3.80	1.48	1.41
3	C	502	9K2	C10-C7	-3.73	1.42	1.49
3	B	502	9K2	C10-C7	-3.61	1.42	1.49
8	A	508	9KZ	O-C2	3.30	1.41	1.33
8	A	508	9KZ	C11-C6	3.29	1.47	1.42
3	C	502	9K2	C5-C6	3.25	1.43	1.36
8	B	507	9KZ	O1-C2	-3.14	1.14	1.22
8	C	507	9KZ	C6-N	-3.11	1.32	1.37
3	A	502	9K2	C14-C13	2.81	1.42	1.37
3	A	502	9K2	C5-C6	2.74	1.42	1.36
3	B	502	9K2	C5-C6	2.68	1.42	1.36
8	A	508	9KZ	C7-C6	-2.68	1.37	1.41
3	A	502	9K2	C12-C13	2.63	1.42	1.37
2	C	501	NHW	O4X-C4X	2.56	1.50	1.45
8	A	508	9KZ	C4-N	2.49	1.35	1.32
2	A	501	NHW	C14-C11	2.47	1.59	1.53
2	A	501	NHW	O4X-C1X	2.43	1.44	1.41
3	A	502	9K2	C8-C7	2.42	1.44	1.38
8	B	507	9KZ	O-C2	2.40	1.39	1.33
2	A	501	NHW	C6-C5	2.33	1.55	1.51
2	A	501	NHW	C7-C6	2.31	1.58	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NHW	C2-C3	2.29	1.60	1.51
8	C	507	9KZ	C3-C4	2.29	1.45	1.41
8	B	507	9KZ	C6-N	-2.27	1.33	1.37
3	C	502	9K2	C3-N1	2.25	1.36	1.34
2	A	501	NHW	C3M-C2M	2.20	1.60	1.52
3	C	502	9K2	N2-N1	2.20	1.42	1.37
8	A	508	9KZ	C9-C10	2.18	1.41	1.36
8	B	507	9KZ	C7-C6	-2.18	1.38	1.41
2	C	501	NHW	P3X-O3X	2.15	1.63	1.59
2	A	501	NHW	O10-C10	2.14	1.46	1.42
2	C	501	NHW	CP-C1M	2.10	1.54	1.51
2	C	501	NHW	P2A-O5A	-2.09	1.43	1.50
3	B	502	9K2	C2-C3	2.09	1.52	1.51
2	B	501	NHW	P3X-O3X	2.08	1.63	1.59
8	A	508	9KZ	C12-C11	2.07	1.48	1.42
2	A	501	NHW	C2A-N3A	2.01	1.35	1.32
8	C	507	9KZ	C10-C11	-2.00	1.38	1.42

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	507	9KZ	C4-N-C6	6.93	125.12	118.38
3	C	502	9K2	C3-C2-N	-6.56	104.14	113.48
2	B	501	NHW	N3A-C2A-N1A	-5.89	119.47	128.68
8	A	508	9KZ	C3-C4-N	-5.84	118.92	122.50
3	B	502	9K2	C3-C2-N	-5.84	105.17	113.48
2	C	501	NHW	N3A-C2A-N1A	-5.33	120.34	128.68
2	A	501	NHW	N3A-C2A-N1A	-5.23	120.50	128.68
3	C	502	9K2	C-N-C2	5.16	121.35	110.69
3	A	502	9K2	C1-N-C2	5.13	121.30	110.69
3	A	502	9K2	C-N-C2	4.86	120.74	110.69
2	C	501	NHW	C2-S1-CP	-4.57	94.06	101.71
8	B	507	9KZ	C3-C4-N	-4.53	119.73	122.50
3	B	502	9K2	C-N-C1	4.49	121.33	109.73
3	B	502	9K2	C1-N-C2	4.27	119.51	110.69
8	A	508	9KZ	C4-N-C6	4.25	122.51	118.38
3	A	502	9K2	C3-C2-N	-4.13	107.60	113.48
3	A	502	9K2	C12-C13-C14	-4.13	117.93	123.29
8	B	507	9KZ	C4-N-C6	4.11	122.38	118.38
3	B	502	9K2	C-N-C2	3.99	118.94	110.69
3	A	502	9K2	C15-C14-C13	3.99	122.14	119.26
8	B	507	9KZ	O-C2-C3	3.95	121.23	112.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	9K2	C1-N-C2	3.83	118.61	110.69
3	C	502	9K2	C-N-C1	3.71	119.32	109.73
8	A	508	9KZ	O-C2-C3	3.62	120.48	112.33
8	C	507	9KZ	O-C2-C3	3.53	120.27	112.33
2	C	501	NHW	O1M-C1M-CP	-3.44	117.26	122.17
3	C	502	9K2	C15-C14-C13	3.26	121.62	119.26
8	C	507	9KZ	C5-C4-C3	-3.20	118.20	122.27
8	A	508	9KZ	C10-C11-C6	3.13	121.83	118.33
3	A	502	9K2	F-C13-C14	3.03	122.58	118.25
2	B	501	NHW	P2A-O3A-P1A	-3.01	122.50	132.83
3	B	502	9K2	C7-C10-C15	2.99	128.58	122.48
3	B	502	9K2	F-C13-C14	2.98	122.51	118.25
3	B	502	9K2	C12-C13-C14	-2.97	119.44	123.29
3	C	502	9K2	C8-C9-C4	2.96	122.30	118.26
8	B	507	9KZ	C5-C4-N	2.92	121.34	116.97
2	C	501	NHW	CP-C1M-C2M	2.91	121.77	115.52
3	A	502	9K2	C-N-C1	2.88	117.19	109.73
8	B	507	9KZ	C3-C12-C11	-2.84	114.34	117.50
8	C	507	9KZ	O-C2-O1	-2.82	117.95	123.67
2	C	501	NHW	C3-N4-C5	2.80	128.04	122.84
8	B	507	9KZ	C5-C4-C3	-2.77	118.75	122.27
8	A	508	9KZ	C12-C3-C2	-2.76	115.72	119.93
8	C	507	9KZ	C7-C6-N	2.75	122.88	118.69
8	C	507	9KZ	C11-C6-N	-2.70	119.95	122.81
3	C	502	9K2	C12-C13-C14	-2.67	119.82	123.29
8	A	508	9KZ	C12-C11-C6	-2.62	116.22	118.53
3	C	502	9K2	C6-C5-C4	-2.52	117.66	120.84
3	B	502	9K2	C16-C15-C14	-2.52	114.83	119.49
2	A	501	NHW	C14-C11-C10	2.49	113.14	108.82
2	A	501	NHW	C5X-C4X-C3X	-2.48	106.17	114.40
4	A	503	DMS	O-S-C1	2.48	119.20	106.54
3	B	502	9K2	C11-C10-C7	-2.47	113.80	118.68
2	A	501	NHW	C2A-N1A-C6A	2.44	122.93	118.75
2	A	501	NHW	C1X-N9A-C4A	-2.43	122.36	126.64
2	A	501	NHW	P2A-O3A-P1A	-2.41	124.55	132.83
8	A	508	9KZ	C7-C6-C11	-2.40	116.39	119.13
8	C	507	9KZ	C5-C4-N	2.38	120.54	116.97
2	A	501	NHW	C2-S1-CP	-2.35	97.77	101.71
2	B	501	NHW	O4X-C1X-C2X	-2.32	103.53	106.93
2	C	501	NHW	P2A-O3A-P1A	-2.32	124.88	132.83
2	A	501	NHW	O4X-C1X-C2X	-2.29	103.58	106.93
8	A	508	9KZ	O-C1-C	2.27	116.75	108.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	9K2	C7-C10-C15	2.25	127.08	122.48
2	C	501	NHW	C2-C3-N4	-2.25	107.69	112.42
3	A	502	9K2	C11-C10-C15	-2.20	116.60	119.35
2	A	501	NHW	C4A-C5A-N7A	-2.18	107.13	109.40
8	B	507	9KZ	C9-C8-C7	2.15	123.45	120.44
2	B	501	NHW	C13-C11-C10	2.12	112.50	108.82
2	A	501	NHW	C6-C7-N8	-2.09	107.67	111.90
7	B	506	SO4	O4-S-O1	2.07	120.13	109.31
3	B	502	9K2	C11-C12-C13	2.06	120.49	118.36
8	C	507	9KZ	C3-C4-N	-2.06	121.24	122.50
2	B	501	NHW	C2-C3-N4	-2.05	108.11	112.42
2	B	501	NHW	C4M-C3M-C2M	-2.02	105.95	113.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	508	9KZ	C3-C2-O-C1
8	A	508	9KZ	O1-C2-O-C1
8	B	507	9KZ	C-C1-O-C2
2	A	501	NHW	C7M-C8M-C9M-CAM
2	C	501	NHW	C6-C7-N8-C9
2	C	501	NHW	C4M-C5M-C6M-C7M
2	B	501	NHW	P2A-O3A-P1A-O2A
2	A	501	NHW	P2A-O3A-P1A-O1A
2	B	501	NHW	C11-C12-O6A-P2A
2	A	501	NHW	C11-C12-O6A-P2A
2	B	501	NHW	C4M-C5M-C6M-C7M
2	A	501	NHW	C4M-C5M-C6M-C7M

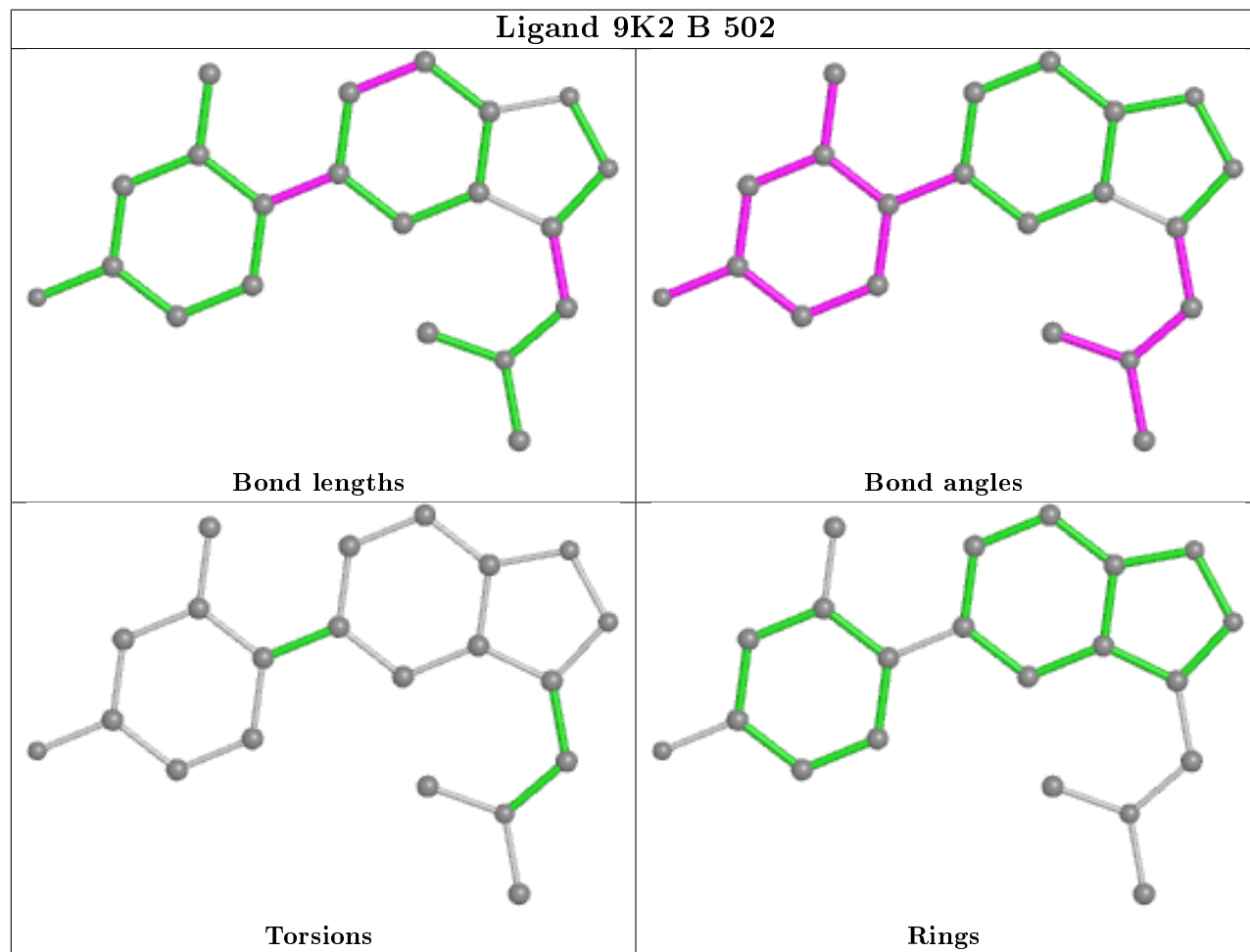
There are no ring outliers.

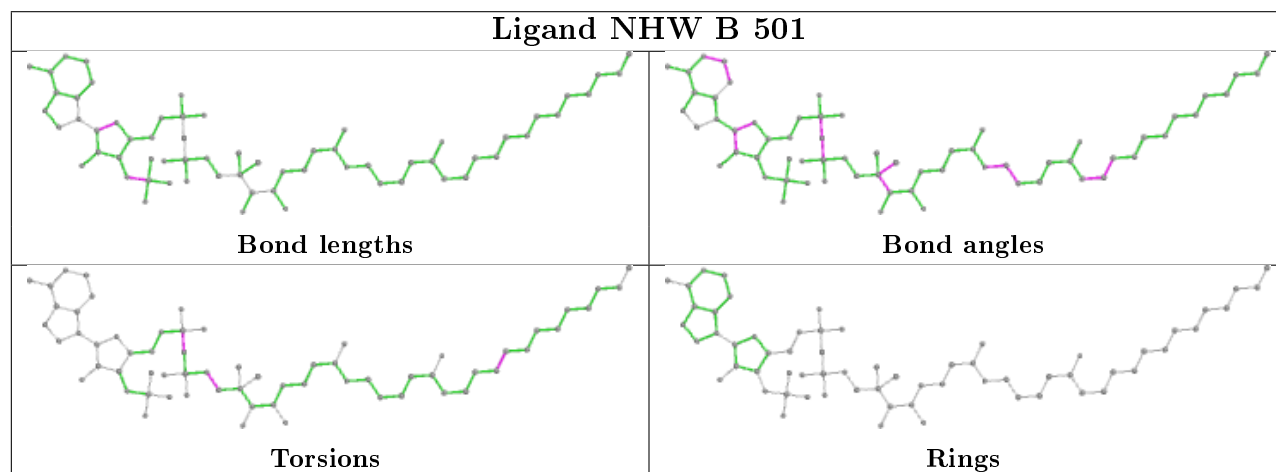
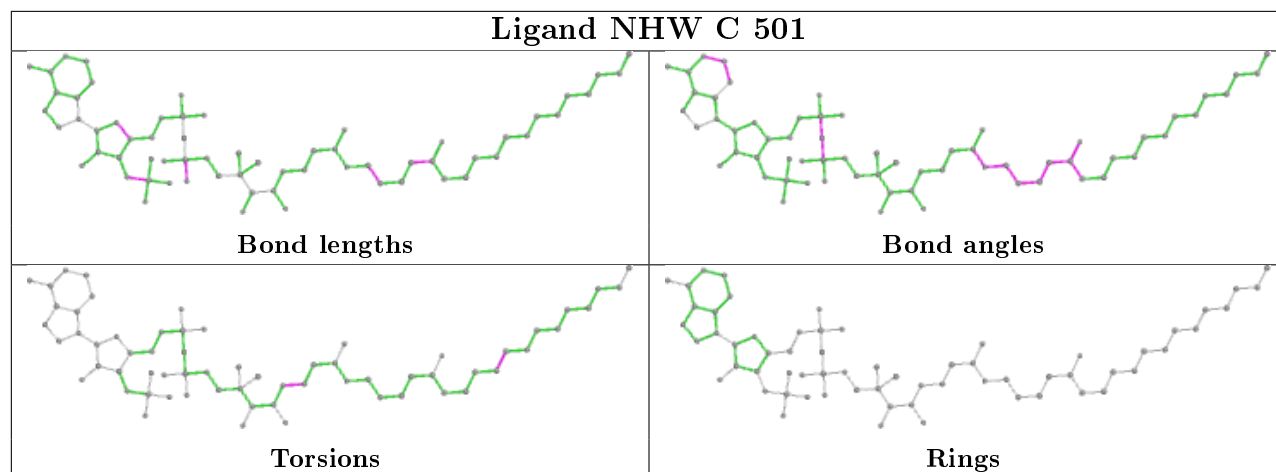
4 monomers are involved in 8 short contacts:

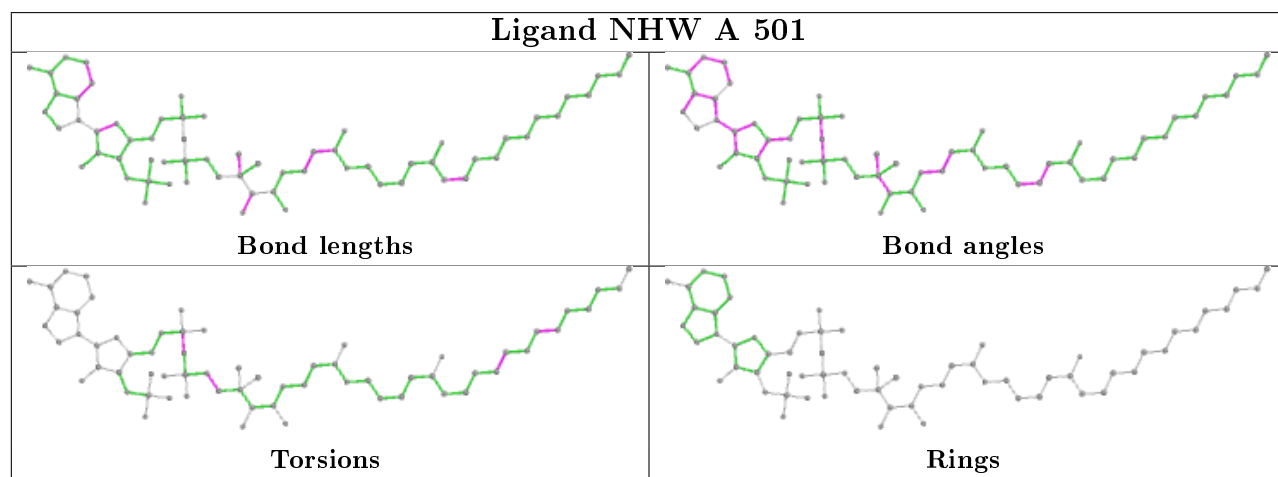
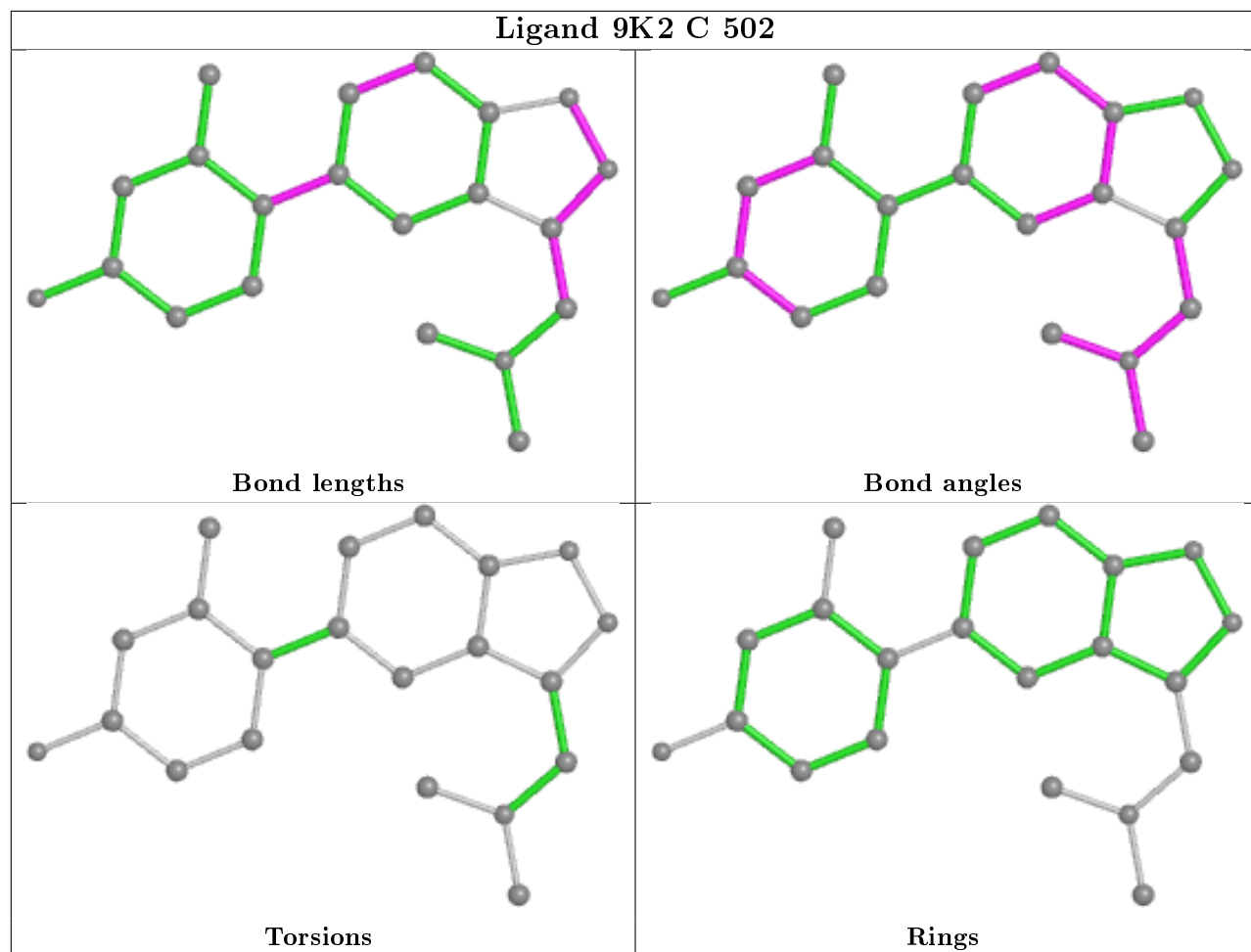
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	DMS	3	0
8	A	508	9KZ	1	0
8	B	507	9KZ	2	0
4	A	503	DMS	2	0

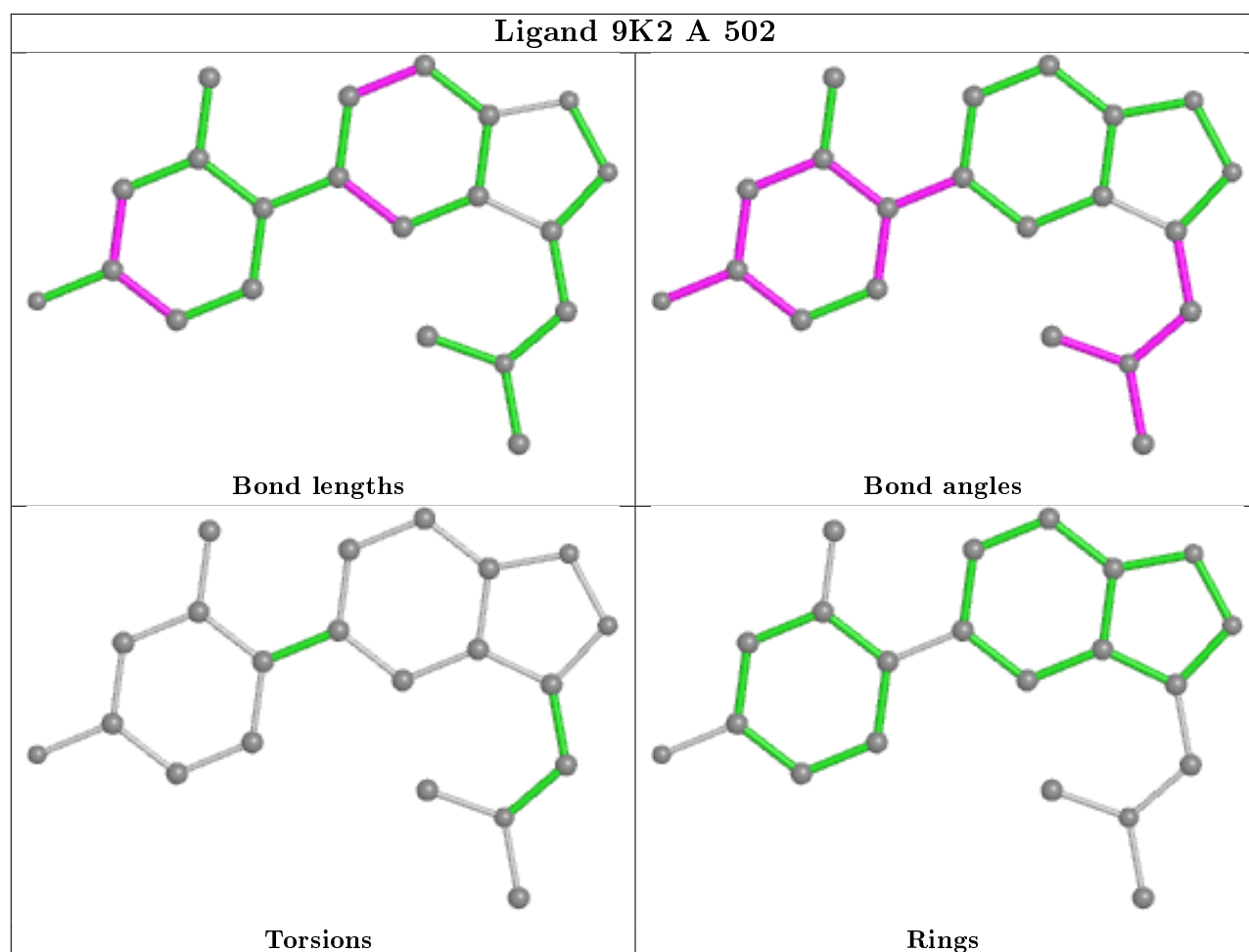
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.









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	385/385 (100%)	-0.12	4 (1%) 82 85	12, 18, 32, 59	13 (3%)
1	B	385/385 (100%)	-0.15	3 (0%) 86 88	11, 17, 32, 64	7 (1%)
1	C	368/385 (95%)	-0.07	6 (1%) 72 76	11, 18, 34, 107	11 (2%)
All	All	1138/1155 (98%)	-0.11	13 (1%) 80 83	11, 18, 34, 107	31 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	SER	7.2
1	B	232	ARG	4.6
1	B	26	ILE	4.4
1	C	226	PHE	4.0
1	A	232	ARG	3.6
1	A	26	ILE	3.5
1	C	222[A]	ILE	3.3
1	C	32[A]	TYR	3.0
1	B	32[A]	TYR	2.4
1	A	54	ASP	2.3
1	C	224	ILE	2.2
1	A	226	PHE	2.1
1	C	27	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

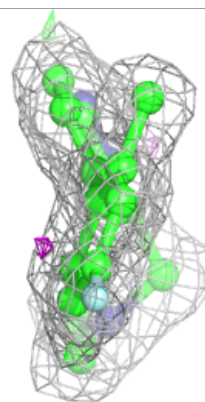
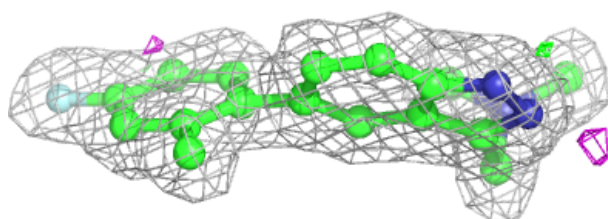
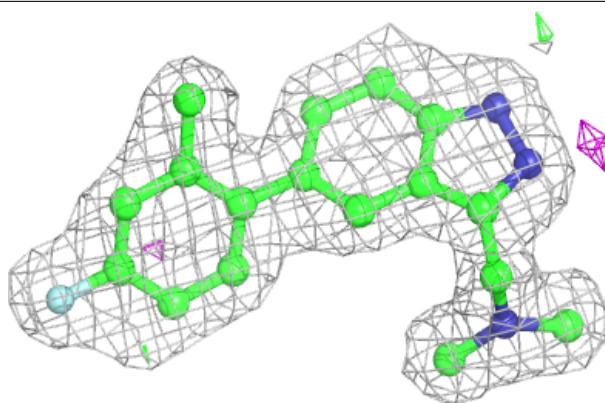
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	A	506	5/5	0.49	0.36	84,91,95,96	0
4	DMS	A	503	4/4	0.52	0.24	39,44,54,66	0
4	DMS	C	503	4/4	0.54	0.31	65,78,83,88	0
7	SO4	C	506	5/5	0.63	0.32	108,117,122,126	0
4	DMS	B	503	4/4	0.74	0.17	50,54,56,66	0
7	SO4	A	507	5/5	0.81	0.21	54,54,62,66	0
8	9KZ	B	507	17/17	0.84	0.14	16,19,28,33	0
7	SO4	B	506	5/5	0.91	0.14	40,50,52,52	0
3	9K2	C	502	21/21	0.91	0.09	20,22,26,31	0
3	9K2	B	502	21/21	0.91	0.09	18,20,22,24	0
8	9KZ	C	507	17/17	0.92	0.10	19,20,31,31	0
8	9KZ	A	508	17/17	0.92	0.10	16,17,26,30	0
3	9K2	A	502	21/21	0.93	0.10	17,19,22,22	0
2	NHW	B	501	64/64	0.96	0.08	11,14,17,18	0
2	NHW	A	501	64/64	0.96	0.08	11,15,19,22	0
2	NHW	C	501	64/64	0.97	0.08	11,16,20,24	0
5	MG	B	504	1/1	0.98	0.06	29,29,29,29	0
5	MG	C	504	1/1	0.98	0.11	27,27,27,27	0
5	MG	A	504	1/1	0.98	0.07	27,27,27,27	0
6	CL	A	505	1/1	0.99	0.06	17,17,17,17	0
6	CL	B	505	1/1	1.00	0.09	16,16,16,16	0
6	CL	C	505	1/1	1.00	0.06	17,17,17,17	0

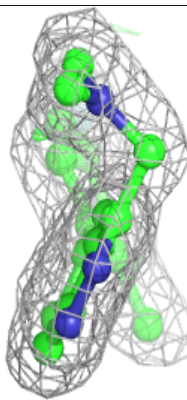
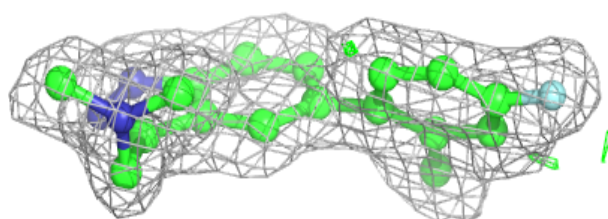
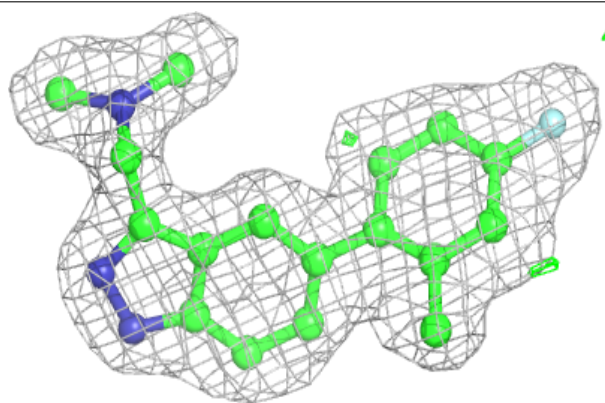
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9K2 C 502:

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

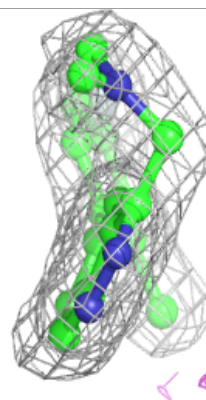
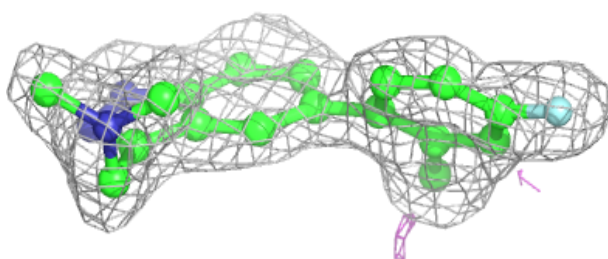
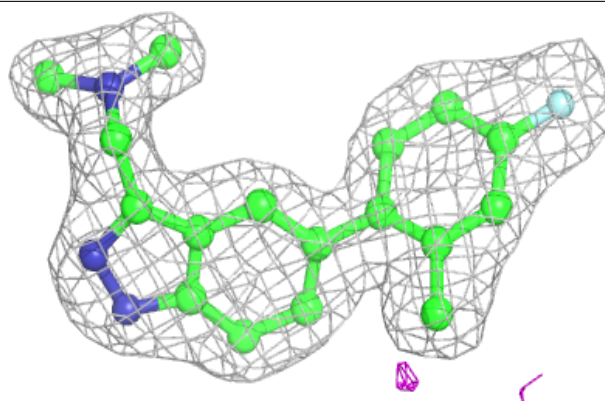
**Electron density around 9K2 B 502:**

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

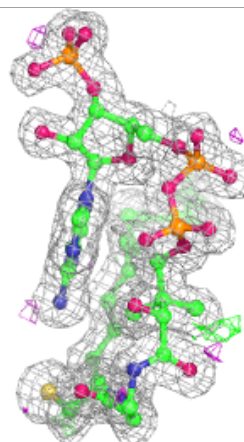
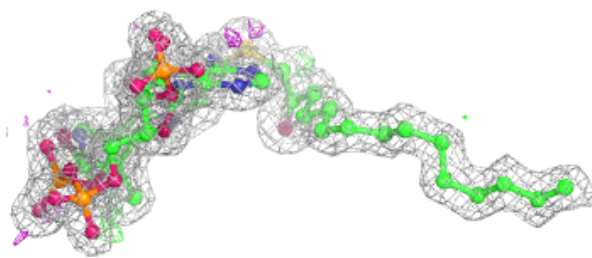
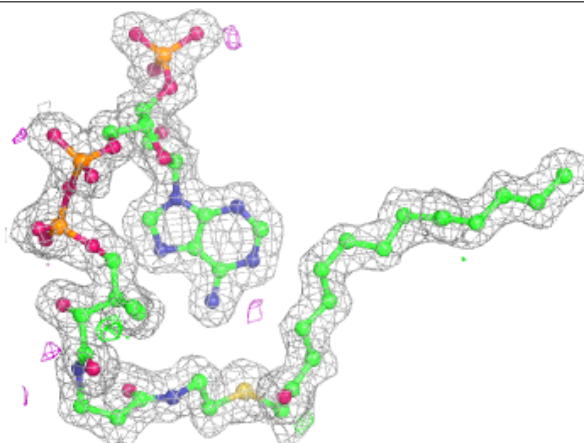


Electron density around 9K2 A 502:

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

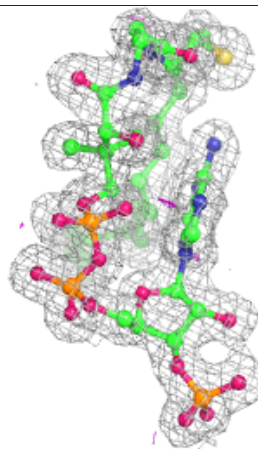
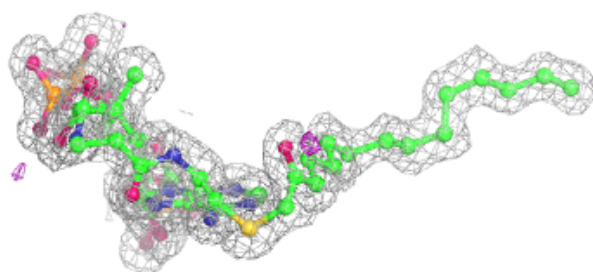
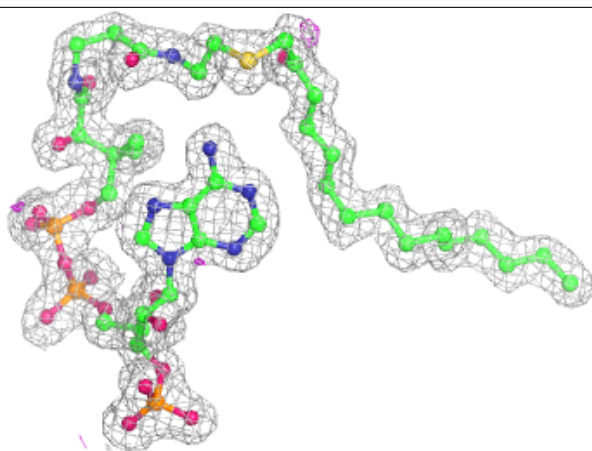
**Electron density around NHW B 501:**

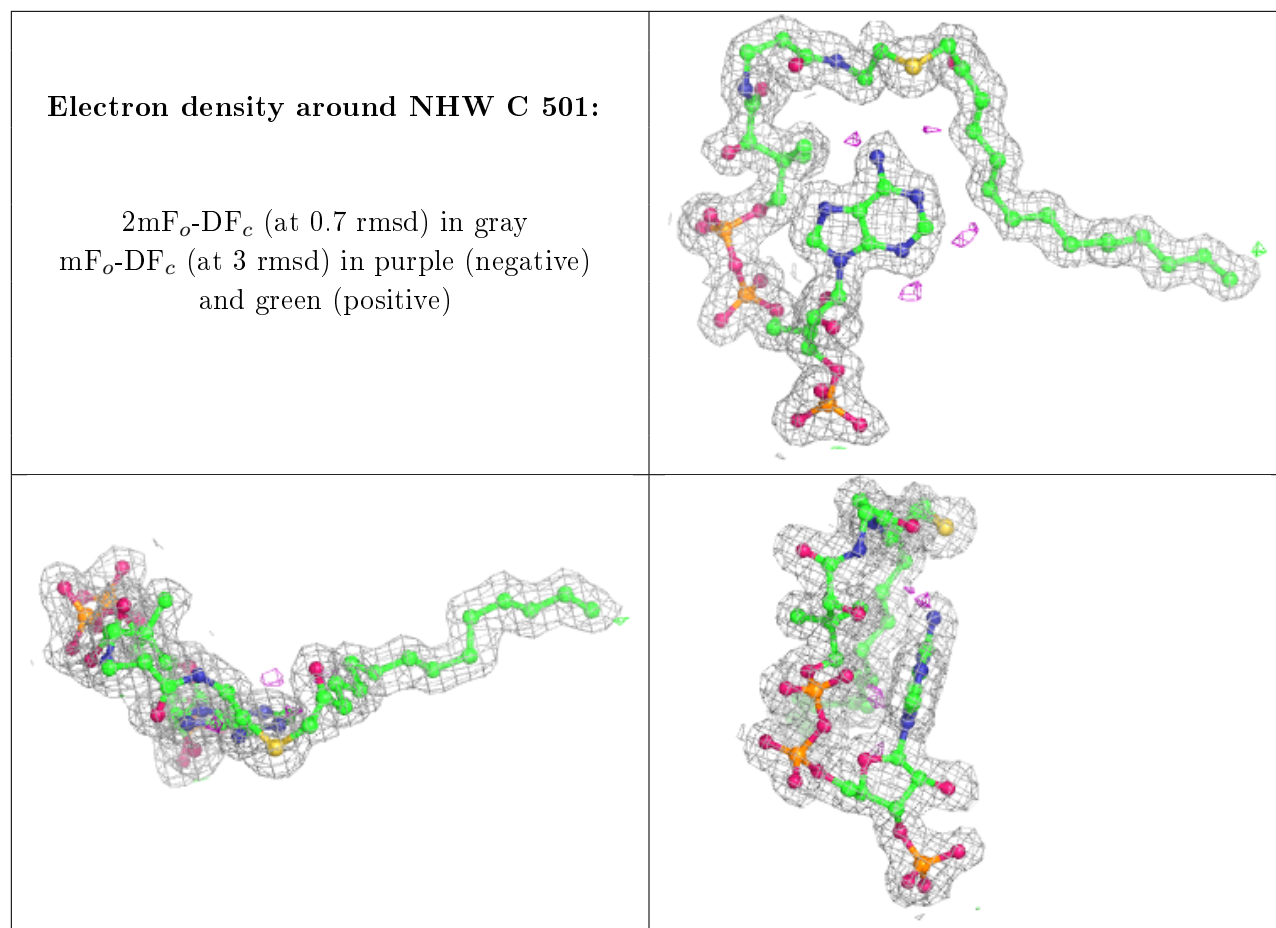
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NHW A 501:

$2mF_o-DF_c$ (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.