



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:34 PM UTC

PDB ID : 5O48 / pdb_00005o48
Title : P.vivax NMT with an aminomethylindazole inhibitor bound
Authors : Brannigan, J.A.; Wilkinson, A.J.
Deposited on : 2017-05-26
Resolution : 1.69 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

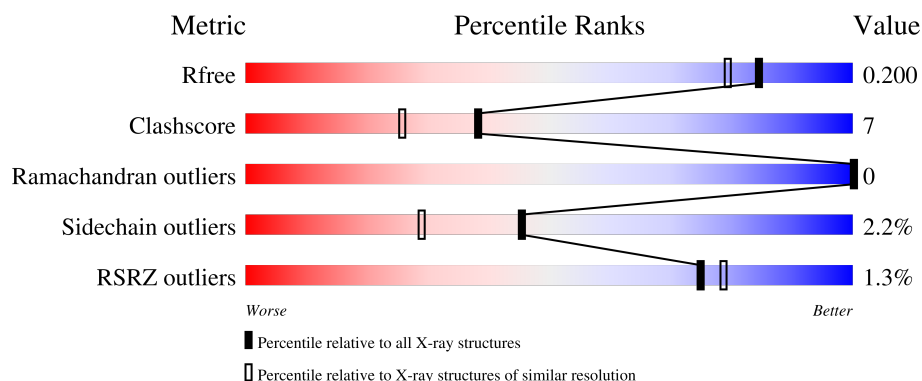
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	385	0% 81% 17% .
1	B	385	0% 82% 16% .
1	C	385	2% 78% 16% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	A	503	-	-	X	-
4	DMS	A	504	-	-	X	-
4	DMS	A	505	-	-	X	-
4	DMS	B	504	-	-	X	-
4	DMS	C	504	-	-	X	-

2 Entry composition [i](#)

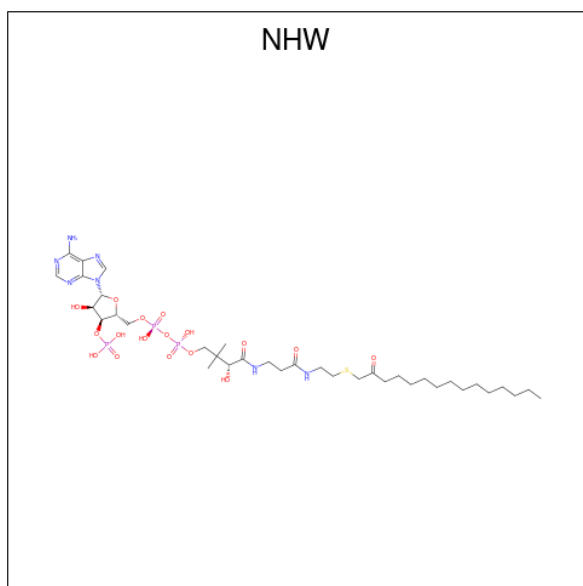
There are 8 unique types of molecules in this entry. The entry contains 11694 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

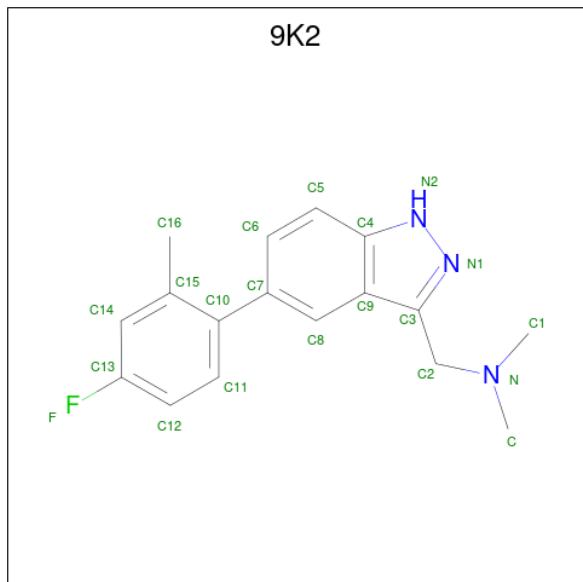
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	27	0
			3344	2179	543	610	12			
1	B	385	Total	C	N	O	S	0	26	0
			3329	2175	532	610	12			
1	C	368	Total	C	N	O	S	0	29	0
			3209	2096	509	593	11			

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



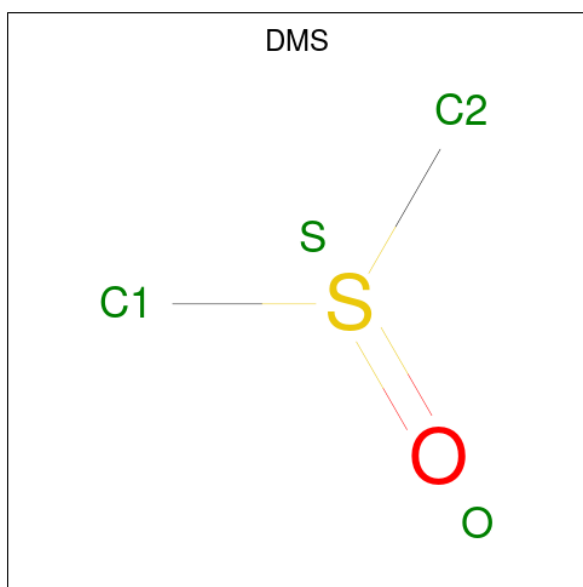
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		
2	C	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		

- Molecule 3 is 1-[5-(4-fluoranyl-2-methyl-phenyl)-1 {H}-indazol-3-yl]- {N}, {N}-dimethyl-methanamine (CCD ID: 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 (CCD ID: 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	A	1	Total C O S 4 2 1 1	0	0
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	B	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
4	C	1	Total C O S 4 2 1 1	0	0

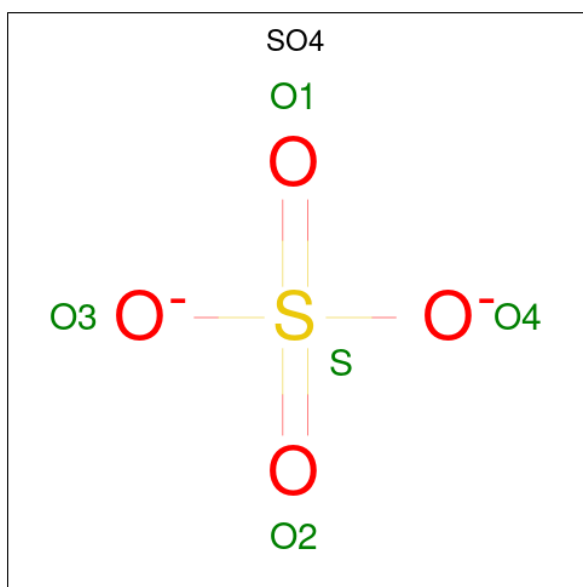
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is SULFATE ION (CCD ID: 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	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

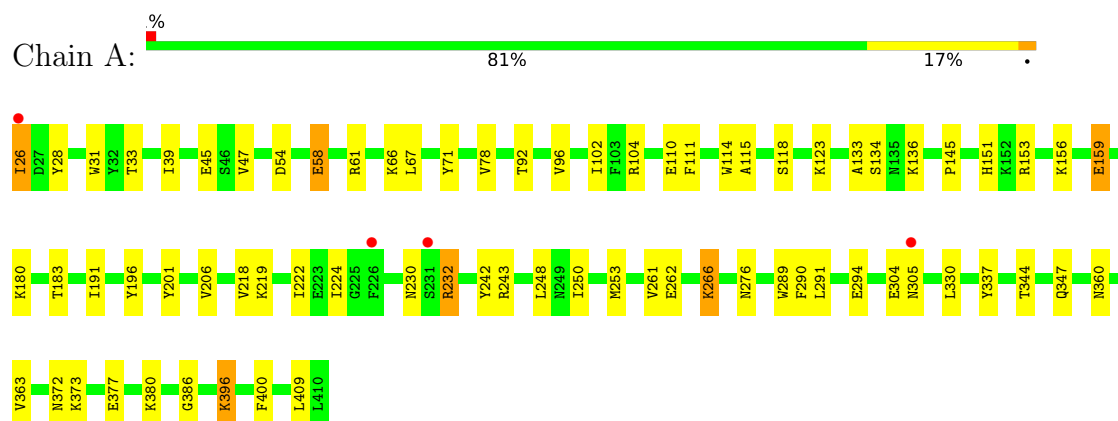
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	547	Total	O	0	0
			547	547		
8	B	527	Total	O	0	0
			527	527		
8	C	425	Total	O	0	0
			425	425		

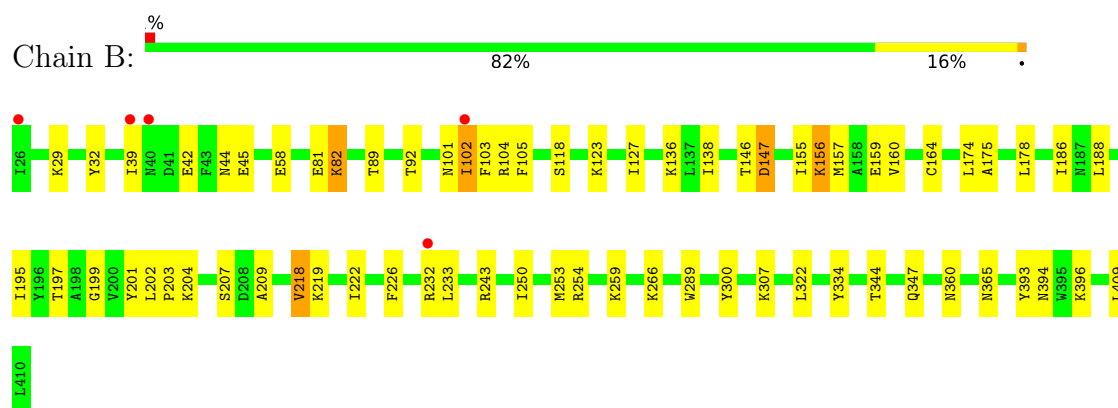
3 Residue-property plots [i](#)

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.

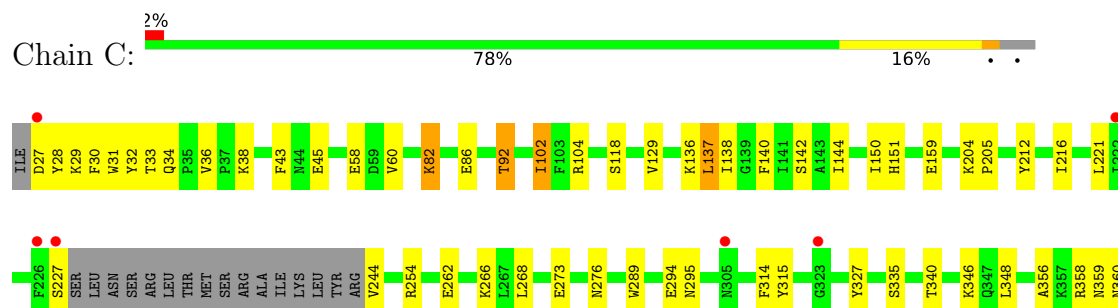
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase



E368	K373	D378	D385	K396	F400	A401	I407	V408	L409	L410
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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 121.98Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.67 – 1.69 100.67 – 1.69	Depositor EDS
% Data completeness (in resolution range)	98.9 (100.67-1.69) 98.9 (100.67-1.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.174 , 0.200 0.173 , 0.200	Depositor DCC
R_{free} test set	7002 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.9	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	0.95	EDS
Total number of atoms	11694	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, DMS, 9K2, NHW, SO4

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	1.58	21/3488 (0.6%)	1.27	9/4721 (0.2%)
1	B	1.58	23/3484 (0.7%)	1.29	8/4713 (0.2%)
1	C	1.55	20/3359 (0.6%)	1.25	8/4546 (0.2%)
All	All	1.57	64/10331 (0.6%)	1.27	25/13980 (0.2%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	ALA	N-CA	9.53	1.56	1.46
1	B	186	ILE	C-O	8.15	1.33	1.24
1	B	207	SER	N-CA	7.92	1.56	1.46
1	B	155	ILE	C-O	7.75	1.31	1.24
1	C	82	LYS	CA-C	7.27	1.62	1.52
1	B	188	LEU	N-CA	6.59	1.55	1.46
1	B	82	LYS	CA-C	6.57	1.61	1.52
1	A	363	VAL	N-CA	6.56	1.53	1.46
1	A	337	TYR	N-CA	6.43	1.54	1.46
1	A	386	GLY	N-CA	6.40	1.52	1.45
1	A	71	TYR	N-CA	6.36	1.53	1.46
1	C	356	ALA	C-O	6.31	1.31	1.24
1	B	45	GLU	C-O	-6.28	1.16	1.24
1	A	180	LYS	C-O	6.14	1.31	1.24
1	B	203	PRO	CA-C	6.14	1.58	1.52
1	A	159	GLU	CD-OE1	6.03	1.36	1.25
1	C	221	LEU	C-O	5.98	1.31	1.24
1	B	147[A]	ASP	C-O	5.96	1.31	1.24
1	B	147[B]	ASP	C-O	5.96	1.31	1.24
1	C	401	ALA	CA-C	5.96	1.59	1.53
1	C	129	VAL	C-O	5.94	1.30	1.24
1	C	268	LEU	N-CA	5.91	1.53	1.46
1	B	393	TYR	C-O	5.86	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	ALA	N-CA	5.85	1.53	1.46
1	C	60	VAL	N-CA	5.83	1.53	1.46
1	B	259	LYS	N-CA	5.78	1.53	1.46
1	C	407	ILE	N-CA	5.75	1.53	1.46
1	C	36	VAL	N-CA	5.74	1.51	1.46
1	C	315	TYR	C-O	5.73	1.31	1.23
1	C	254	ARG	CZ-NH1	5.67	1.40	1.32
1	B	218	VAL	CA-CB	5.66	1.61	1.54
1	A	153	ARG	C-O	5.63	1.30	1.24
1	C	150	ILE	CA-CB	5.55	1.61	1.54
1	A	115	ALA	CA-CB	5.54	1.62	1.53
1	A	123	LYS	C-O	5.53	1.31	1.24
1	A	262	GLU	N-CA	5.50	1.53	1.46
1	A	54	ASP	N-CA	5.47	1.54	1.46
1	C	358	ARG	CZ-NH2	5.39	1.40	1.33
1	A	373	LYS	CA-C	5.38	1.60	1.52
1	A	33	THR	N-CA	5.31	1.53	1.46
1	A	133	ALA	N-CA	5.29	1.53	1.46
1	A	372	ASN	N-CA	5.27	1.52	1.46
1	B	164	CYS	C-O	5.24	1.30	1.23
1	B	195	ILE	CA-C	-5.24	1.46	1.52
1	B	202	LEU	C-O	-5.23	1.19	1.24
1	C	140	PHE	C-O	5.21	1.30	1.23
1	C	314	PHE	CA-CB	5.21	1.63	1.53
1	C	368	GLU	N-CA	5.21	1.52	1.46
1	A	261	VAL	CA-C	5.21	1.59	1.52
1	B	138	ILE	CA-CB	5.20	1.60	1.54
1	A	111	PHE	N-CA	5.15	1.52	1.46
1	C	327	TYR	N-CA	5.14	1.52	1.46
1	B	89	THR	C-O	5.12	1.30	1.24
1	B	160	VAL	N-CA	5.11	1.52	1.46
1	A	96	VAL	C-O	-5.10	1.18	1.24
1	B	157	MET	C-O	5.10	1.30	1.23
1	C	335	SER	C-O	5.10	1.29	1.23
1	C	373	LYS	C-O	-5.08	1.18	1.24
1	A	196	TYR	N-CA	5.06	1.52	1.46
1	B	334	TYR	N-CA	5.05	1.52	1.46
1	B	394	ASN	C-O	5.04	1.30	1.23
1	A	96	VAL	CA-CB	5.03	1.59	1.54
1	C	142	SER	N-CA	5.01	1.52	1.45
1	A	61	ARG	CZ-NH1	5.01	1.39	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	LYS	CA-C-N	-8.09	111.43	119.76
1	C	204	LYS	C-N-CA	-8.09	111.43	119.76
1	C	216	ILE	N-CA-C	-7.62	104.32	111.48
1	A	183	THR	N-CA-C	-6.94	103.64	111.14
1	B	199	GLY	N-CA-C	-6.79	106.23	114.66
1	B	101	ASN	N-CA-C	6.67	120.60	111.54
1	B	396	LYS	N-CA-CB	-6.58	99.71	110.43
1	A	290	PHE	N-CA-C	6.49	121.86	113.88
1	B	204	LYS	CA-C-N	-6.15	113.64	119.85
1	B	204	LYS	C-N-CA	-6.15	113.64	119.85
1	C	82	LYS	N-CA-C	6.08	117.58	111.07
1	A	396	LYS	N-CA-CB	-5.64	101.71	110.57
1	A	291	LEU	CA-C-N	-5.50	114.30	119.85
1	A	291	LEU	C-N-CA	-5.50	114.30	119.85
1	A	67	LEU	CA-C-N	-5.47	114.74	120.38
1	A	67	LEU	C-N-CA	-5.47	114.74	120.38
1	A	380	LYS	CD-CE-NZ	-5.37	94.72	111.90
1	C	92	THR	N-CA-C	-5.30	105.50	111.28
1	A	114	TRP	N-CA-CB	-5.27	102.37	110.01
1	C	273	GLU	N-CA-C	5.16	118.36	111.75
1	B	127	ILE	CA-C-N	-5.11	117.17	122.69
1	B	127	ILE	C-N-CA	-5.11	117.17	122.69
1	C	205	PRO	N-CA-C	5.02	118.97	111.14
1	C	396	LYS	N-CA-CB	-5.01	102.70	110.57
1	B	203	PRO	O-C-N	-5.00	117.73	123.03

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	3344	0	3382	42	0
1	B	3329	0	3381	45	0
1	C	3209	0	3233	43	0
2	A	64	0	60	0	0
2	B	64	0	60	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	12	0	18	12	0
4	B	12	0	18	9	0
4	C	8	0	12	17	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	15	0	0	0	0
7	C	5	0	0	0	0
8	A	547	0	0	12	0
8	B	527	0	0	11	0
8	C	425	0	0	9	0
All	All	11694	0	10224	141	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 (141) 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:365:ASN:HD21	4:B:504:DMS:H13	1.14	1.11
1:C:159[A]:GLU:OE2	4:C:504:DMS:H21	1.51	1.09
1:C:30:PHE:O	1:C:33[A]:THR:HG22	1.58	1.01
1:C:410:LEU:H	4:C:504:DMS:H13	1.23	1.00
1:C:151:HIS:CE1	1:C:276[A]:ASN:HD21	1.79	1.00
1:A:110:GLU:HG3	8:A:1025:HOH:O	1.62	0.98
1:A:230:ASN:OD1	1:A:232:ARG:HG3	1.64	0.95
1:B:102[A]:ILE:HG13	1:B:103:PHE:CE2	2.06	0.91
1:C:159[A]:GLU:OE2	4:C:504:DMS:C2	2.19	0.91
1:B:102[B]:ILE:HG23	1:B:103:PHE:CD2	2.07	0.90
1:B:32[A]:TYR:CD1	8:B:967:HOH:O	2.29	0.85
1:C:151:HIS:CE1	1:C:276[A]:ASN:ND2	2.44	0.84
1:B:159[A]:GLU:OE2	4:B:505:DMS:H13	1.80	0.82
1:C:410:LEU:N	4:C:504:DMS:H13	1.94	0.82
1:C:276[A]:ASN:ND2	1:C:400:PHE:CE1	2.47	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:504:DMS:H11	8:C:805:HOH:O	1.81	0.80
4:C:503:DMS:H22	8:C:889:HOH:O	1.81	0.80
1:B:365:ASN:ND2	4:B:504:DMS:H13	1.95	0.80
1:B:102[B]:ILE:HG23	1:B:103:PHE:CE2	2.18	0.78
4:A:505:DMS:H13	8:A:650:HOH:O	1.84	0.77
1:C:262[B]:GLU:HG2	1:C:266[B]:LYS:HE3	1.65	0.77
4:C:504:DMS:C1	8:C:805:HOH:O	2.36	0.74
1:C:159[A]:GLU:OE2	4:C:504:DMS:S	2.47	0.73
1:C:276[A]:ASN:ND2	1:C:400:PHE:CD1	2.57	0.73
1:C:410:LEU:HG	4:C:504:DMS:C1	2.18	0.73
1:B:344:THR:OG1	1:B:347[B]:GLN:HG3	1.89	0.71
1:C:410:LEU:H	4:C:504:DMS:C1	2.01	0.71
4:A:503:DMS:H11	4:A:504:DMS:H12	1.73	0.69
1:C:410:LEU:HG	4:C:504:DMS:H13	1.74	0.69
4:A:503:DMS:C1	4:A:504:DMS:H12	2.23	0.69
1:A:377[B]:GLU:HG2	8:A:796:HOH:O	1.92	0.69
1:B:102[A]:ILE:HG13	1:B:103:PHE:CD2	2.29	0.67
4:B:504:DMS:H12	8:B:649:HOH:O	1.95	0.67
1:B:44[A]:ASN:OD1	8:B:602:HOH:O	2.14	0.66
1:A:66:LYS:HE2	8:A:872:HOH:O	1.94	0.66
1:A:360[A]:ASN:ND2	8:A:606:HOH:O	2.29	0.65
1:B:82:LYS:HE2	8:B:761:HOH:O	1.97	0.64
1:B:39:ILE:CD1	1:B:201:TYR:HE2	2.11	0.63
1:B:159[A]:GLU:OE2	4:B:505:DMS:S	2.56	0.63
1:A:58:GLU:O	1:A:58:GLU:HG3	1.97	0.62
1:B:159[A]:GLU:OE2	4:B:505:DMS:C1	2.47	0.62
1:C:262[B]:GLU:CG	1:C:266[B]:LYS:HE3	2.30	0.61
1:A:159:GLU:OE1	4:A:505:DMS:H12	2.01	0.60
1:A:243[B]:ARG:HD2	8:A:638:HOH:O	2.02	0.60
1:A:276[B]:ASN:ND2	1:A:400:PHE:CE2	2.67	0.59
1:C:359:ASN:O	1:C:360[B]:ASN:HB3	2.03	0.58
1:C:151:HIS:ND1	1:C:276[A]:ASN:OD1	2.36	0.57
1:A:266[B]:LYS:HG3	8:A:658:HOH:O	2.05	0.57
1:C:212:TYR:OH	1:C:373:LYS:HE2	2.04	0.57
1:C:144:ILE:HD11	4:C:504:DMS:C2	2.35	0.57
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.32	0.55
1:C:346:LYS:HE2	1:C:378:ASP:HB3	1.88	0.54
4:A:503:DMS:H13	4:A:504:DMS:C2	2.37	0.54
4:A:503:DMS:H13	4:A:504:DMS:H23	1.89	0.54
1:B:123:LYS:HB3	8:B:730:HOH:O	2.08	0.53
1:A:218[A]:VAL:HG21	1:A:242:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HD11	1:B:201:TYR:HE2	1.74	0.53
1:B:105:PHE:CZ	4:B:503:DMS:H23	2.44	0.52
1:A:159:GLU:OE2	1:A:409:LEU:HD22	2.09	0.51
1:A:134:SER:HB2	1:A:136:LYS:HD2	1.92	0.51
1:A:289:TRP:CZ2	4:A:505:DMS:H22	2.45	0.51
1:B:307:LYS:HD2	8:B:1111:HOH:O	2.09	0.51
1:B:39:ILE:HD12	1:B:201:TYR:HE2	1.76	0.51
1:A:28:TYR:HB3	1:A:31:TRP:HB2	1.93	0.50
1:C:360[A]:ASN:ND2	8:C:608:HOH:O	2.43	0.50
1:B:147[A]:ASP:OD1	1:B:156[A]:LYS:HE2	2.12	0.50
1:A:102[B]:ILE:HD11	8:A:1107:HOH:O	2.11	0.50
1:B:218:VAL:O	1:B:222[A]:ILE:HG12	2.11	0.50
1:C:340:THR:HB	1:C:348:LEU:HD22	1.93	0.50
1:A:344:THR:H	1:A:347:GLN:NE2	2.09	0.49
1:A:26:ILE:HD12	8:A:1063:HOH:O	2.12	0.49
1:A:344:THR:HG21	1:B:42[B]:GLU:HG3	1.92	0.49
1:A:102[B]:ILE:HD13	8:A:889:HOH:O	2.12	0.49
4:A:503:DMS:C1	4:A:504:DMS:H23	2.43	0.49
1:C:82:LYS:O	1:C:86[A]:GLU:HG3	2.12	0.49
1:A:330:LEU:HD23	4:A:504:DMS:H13	1.94	0.49
1:B:92:THR:O	1:B:104:ARG:HD2	2.13	0.49
1:B:197:THR:HG23	1:B:409[B]:LEU:HD12	1.94	0.49
1:C:138:ILE:HD12	1:C:138:ILE:C	2.37	0.49
1:B:146:THR:CA	1:B:156[A]:LYS:HZ2	2.26	0.48
1:C:92:THR:O	1:C:104:ARG:HD2	2.13	0.48
1:B:159[A]:GLU:HG3	1:B:409[A]:LEU:HD21	1.95	0.48
1:B:226:PHE:HE2	4:B:504:DMS:S	2.37	0.48
1:C:27:ASP:N	8:C:613:HOH:O	2.46	0.47
1:B:102[B]:ILE:CD1	1:B:322:LEU:O	2.63	0.47
1:B:147[B]:ASP:OD1	1:B:156[B]:LYS:HE3	2.15	0.47
1:B:32[A]:TYR:CE1	8:B:967:HOH:O	2.60	0.47
1:B:266[B]:LYS:HE2	8:B:1019:HOH:O	2.16	0.46
1:C:159[A]:GLU:OE2	4:C:504:DMS:H11	2.15	0.46
1:A:206[B]:VAL:HG12	1:A:400:PHE:CE2	2.51	0.46
1:C:144:ILE:HD11	4:C:504:DMS:H21	1.97	0.46
1:B:360:ASN:ND2	8:B:609:HOH:O	2.48	0.46
1:A:102[A]:ILE:HD12	8:A:651:HOH:O	2.16	0.45
1:A:344:THR:HG21	1:B:42[B]:GLU:CG	2.46	0.45
1:C:33[A]:THR:HG23	1:C:34:GLN:OE1	2.17	0.45
1:A:47:VAL:CG1	1:A:396:LYS:HG2	2.47	0.45
1:C:28:TYR:HB3	1:C:31:TRP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:GLU:HG3	1:C:295:ASN:N	2.32	0.44
1:C:359:ASN:O	1:C:360[B]:ASN:CB	2.65	0.44
1:C:32[A]:TYR:CE1	1:C:38[A]:LYS:HE2	2.52	0.44
1:A:304:GLU:O	1:A:305[A]:ASN:HB2	2.16	0.44
1:A:118:SER:HB3	1:A:289:TRP:CZ2	2.53	0.44
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.52	0.44
1:A:218[A]:VAL:CG2	1:A:242:TYR:HB2	2.47	0.44
4:C:504:DMS:H12	8:C:805:HOH:O	2.13	0.44
1:A:39:ILE:HD12	1:A:201:TYR:HE2	1.82	0.44
1:B:365:ASN:HD21	4:B:504:DMS:C1	2.05	0.43
4:A:503:DMS:C1	4:A:504:DMS:C1	2.96	0.43
1:B:39:ILE:CD1	1:B:201:TYR:CE2	2.98	0.43
4:A:505:DMS:C1	8:A:650:HOH:O	2.57	0.42
1:B:146:THR:HA	1:B:156[A]:LYS:NZ	2.33	0.42
1:A:250:ILE:HB	1:A:253[B]:MET:HG2	2.01	0.42
1:A:330:LEU:CD2	4:A:504:DMS:H13	2.48	0.42
1:C:136:LYS:HE2	8:C:907:HOH:O	2.19	0.42
1:A:248:LEU:HD13	1:A:253[B]:MET:HB2	2.00	0.42
1:B:29[B]:LYS:HA	1:B:29[B]:LYS:HD2	1.89	0.42
1:C:102[A]:ILE:HD11	8:C:888:HOH:O	2.19	0.42
1:A:250:ILE:O	1:A:253[B]:MET:HG2	2.20	0.42
1:B:250:ILE:HB	1:B:253[B]:MET:HG2	2.02	0.42
1:B:146:THR:CA	1:B:156[A]:LYS:NZ	2.82	0.42
1:C:346:LYS:HE2	1:C:378:ASP:CB	2.50	0.42
1:C:410:LEU:HG	4:C:504:DMS:H12	1.97	0.42
1:C:86[B]:GLU:HG3	1:C:137:LEU:HD22	2.02	0.42
1:C:28:TYR:OH	8:C:603:HOH:O	2.17	0.41
1:A:145:PRO:HB2	1:A:156[B]:LYS:HE3	2.00	0.41
1:A:156[B]:LYS:HG3	1:A:191:ILE:HG12	2.02	0.41
1:B:233:LEU:HA	1:B:233:LEU:HD12	1.88	0.41
1:C:43:PHE:CE1	1:C:396:LYS:HG3	2.56	0.41
1:B:174:LEU:O	1:B:178[B]:LEU:HD13	2.20	0.41
1:A:151[B]:HIS:HA	1:A:276[B]:ASN:OD1	2.21	0.41
1:A:45:GLU:HG3	8:B:724:HOH:O	2.21	0.40
1:A:92:THR:O	1:A:104[B]:ARG:HD2	2.20	0.40
1:A:110:GLU:H	1:A:110:GLU:CD	2.29	0.40
1:B:254:ARG:O	1:B:300:TYR:HA	2.20	0.40
1:C:159[A]:GLU:OE2	4:C:504:DMS:C1	2.69	0.40
1:B:118:SER:HB3	1:B:289:TRP:CZ2	2.56	0.40
1:B:243[B]:ARG:NH1	8:B:621:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/385 (106%)	397 (97%)	13 (3%)	0	100	100
1	B	409/385 (106%)	398 (97%)	11 (3%)	0	100	100
1	C	393/385 (102%)	382 (97%)	11 (3%)	0	100	100
All	All	1212/1155 (105%)	1177 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	378/351 (108%)	369 (98%)	9 (2%)	43	26
1	B	377/351 (107%)	368 (98%)	9 (2%)	43	26
1	C	364/351 (104%)	352 (97%)	12 (3%)	33	17
All	All	1119/1053 (106%)	1089 (97%)	30 (3%)	45	23

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	58	GLU
1	A	219	LYS
1	A	224	ILE
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	266[A]	LYS
1	A	266[B]	LYS
1	A	294[A]	GLU
1	A	294[B]	GLU
1	B	58	GLU
1	B	81	GLU
1	B	102[A]	ILE
1	B	102[B]	ILE
1	B	136	LYS
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	219	LYS
1	B	232	ARG
1	C	29	LYS
1	C	45	GLU
1	C	58[A]	GLU
1	C	58[B]	GLU
1	C	102[A]	ILE
1	C	102[B]	ILE
1	C	137	LEU
1	C	227	SER
1	C	244	VAL
1	C	385[A]	ASP
1	C	385[B]	ASP
1	C	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	249	ASN
1	A	347	GLN
1	A	350	GLN
1	A	359	ASN
1	A	372	ASN
1	B	34	GLN
1	B	40	ASN
1	B	106	ASN
1	B	187	ASN
1	B	193	GLN
1	B	249	ASN
1	B	274	GLN

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Mol	Chain	Res	Type
1	B	359	ASN
1	B	360	ASN
1	B	371	GLN
1	B	372	ASN
1	C	55	ASN
1	C	101	ASN
1	C	193	GLN
1	C	320	GLN
1	C	331	ASN
1	C	359	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	B	503	-	3,3,3	0.84	0	3,3,3	1.06	0
3	9K2	B	502	-	23,23,23	1.87	9 (39%)	30,33,33	2.54	12 (40%)
4	DMS	A	503	-	3,3,3	0.55	0	3,3,3	1.60	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NHW	C	501	5	64,66,66	1.86	10 (15%)	87,92,92	1.82	16 (18%)
3	9K2	C	502	-	23,23,23	2.40	9 (39%)	30,33,33	2.39	9 (30%)
4	DMS	B	504	-	3,3,3	0.64	0	3,3,3	1.33	0
4	DMS	B	505	-	3,3,3	0.41	0	3,3,3	2.22	2 (66%)
4	DMS	C	504	-	3,3,3	0.86	0	3,3,3	1.81	1 (33%)
7	SO4	A	508	-	4,4,4	0.62	0	6,6,6	1.70	2 (33%)
3	9K2	A	502	-	23,23,23	2.01	9 (39%)	30,33,33	3.17	14 (46%)
7	SO4	A	510	-	4,4,4	1.30	1 (25%)	6,6,6	1.22	1 (16%)
4	DMS	A	504	-	3,3,3	0.27	0	3,3,3	1.44	0
4	DMS	C	503	-	3,3,3	0.39	0	3,3,3	1.60	1 (33%)
4	DMS	A	505	-	3,3,3	0.86	0	3,3,3	2.14	2 (66%)
2	NHW	B	501	5	64,66,66	1.57	13 (20%)	87,92,92	1.56	18 (20%)
7	SO4	A	509	-	4,4,4	1.06	0	6,6,6	0.51	0
2	NHW	A	501	5	64,66,66	1.46	13 (20%)	87,92,92	1.66	18 (20%)
7	SO4	C	507	-	4,4,4	1.26	0	6,6,6	0.31	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	-	-	0/8/8/8	0/3/3/3
2	NHW	C	501	5	-	2/65/81/81	0/3/3/3
3	9K2	C	502	-	-	0/8/8/8	0/3/3/3
3	9K2	A	502	-	-	0/8/8/8	0/3/3/3
2	NHW	B	501	5	-	3/65/81/81	0/3/3/3
2	NHW	A	501	5	-	1/65/81/81	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NHW	P1A-O3A	9.00	1.69	1.59
3	C	502	9K2	C2-C3	7.40	1.60	1.51
2	B	501	NHW	P2A-O3A	-5.34	1.53	1.59
2	C	501	NHW	P3X-O3X	4.63	1.67	1.59
3	A	502	9K2	C9-C4	-4.55	1.35	1.41
2	C	501	NHW	O4X-C4X	4.27	1.54	1.45
3	A	502	9K2	C8-C7	3.74	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	9K2	C3-N1	3.72	1.36	1.29
2	A	501	NHW	O4X-C4X	3.63	1.53	1.45
2	B	501	NHW	O10-C10	3.31	1.48	1.42
2	A	501	NHW	C8A-N7A	3.20	1.37	1.31
3	C	502	9K2	C10-C7	-3.19	1.43	1.49
3	C	502	9K2	C5-C6	3.18	1.44	1.38
3	C	502	9K2	C3-N1	3.06	1.35	1.29
2	C	501	NHW	C5A-N7A	-3.00	1.33	1.39
2	A	501	NHW	P2A-O3A	-2.99	1.56	1.59
3	B	502	9K2	C12-C11	2.98	1.43	1.38
3	A	502	9K2	C5-C6	-2.96	1.34	1.38
2	C	501	NHW	C8A-N7A	2.94	1.37	1.31
2	C	501	NHW	O2X-C2X	2.86	1.50	1.43
3	A	502	9K2	C2-C3	2.82	1.54	1.51
2	A	501	NHW	O4X-C1X	2.73	1.48	1.42
2	B	501	NHW	CP-S1	2.69	1.88	1.81
2	C	501	NHW	CP-C1M	2.69	1.55	1.51
3	C	502	9K2	C12-C13	2.69	1.42	1.37
2	B	501	NHW	O4X-C4X	2.68	1.51	1.45
3	A	502	9K2	C12-C11	2.68	1.43	1.38
2	B	501	NHW	CP-C1M	2.67	1.55	1.51
3	B	502	9K2	C2-C3	2.63	1.54	1.51
2	C	501	NHW	O10-C10	2.61	1.46	1.42
3	A	502	9K2	C3-N1	2.57	1.34	1.29
3	B	502	9K2	C8-C7	2.54	1.44	1.39
2	B	501	NHW	C5X-C4X	2.52	1.59	1.51
2	A	501	NHW	CP-C1M	2.48	1.55	1.51
3	B	502	9K2	C14-C15	2.48	1.43	1.39
2	B	501	NHW	C8A-N9A	-2.46	1.33	1.37
2	B	501	NHW	P3X-O8A	-2.45	1.45	1.54
3	C	502	9K2	C8-C7	2.44	1.44	1.39
2	A	501	NHW	P3X-O7A	2.41	1.63	1.54
3	B	502	9K2	C2-N	-2.37	1.41	1.47
7	A	510	SO4	O1-S	2.36	1.58	1.44
2	A	501	NHW	C5A-N7A	-2.34	1.34	1.39
2	B	501	NHW	P3X-O3X	2.34	1.63	1.59
3	A	502	9K2	C5-C4	2.33	1.43	1.39
3	C	502	9K2	N2-N1	2.31	1.42	1.36
3	B	502	9K2	C5-C6	2.30	1.42	1.38
3	C	502	9K2	C12-C11	2.30	1.42	1.38
2	B	501	NHW	C4A-N9A	-2.28	1.33	1.37
2	A	501	NHW	C7-C6	2.26	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NHW	O1M-C1M	2.24	1.25	1.21
2	A	501	NHW	C3-N4	2.22	1.51	1.46
3	C	502	9K2	C8-C9	2.22	1.43	1.39
3	A	502	9K2	C8-C9	2.20	1.43	1.39
2	C	501	NHW	C13-C11	-2.20	1.49	1.53
2	A	501	NHW	C4A-N9A	-2.15	1.33	1.37
2	C	501	NHW	C8A-N9A	-2.15	1.33	1.37
2	A	501	NHW	C5X-C4X	2.15	1.58	1.51
3	B	502	9K2	C9-C4	-2.14	1.38	1.41
3	B	502	9K2	C10-C7	-2.11	1.45	1.49
2	B	501	NHW	C2A-N1A	-2.11	1.30	1.33
2	A	501	NHW	C3M-C2M	2.10	1.59	1.52
3	A	502	9K2	C10-C7	-2.08	1.45	1.49
2	B	501	NHW	C13-C11	2.06	1.58	1.53
2	B	501	NHW	P1A-O3A	2.04	1.61	1.59

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	9K2	C1-N-C2	8.80	124.77	110.38
3	A	502	9K2	C-N-C2	7.05	121.91	110.38
3	A	502	9K2	C1-N-C2	6.99	121.80	110.38
2	C	501	NHW	C5A-C4A-N3A	-6.78	117.39	126.72
3	A	502	9K2	C4-N2-N1	-6.75	106.89	111.90
3	B	502	9K2	C-N-C2	6.40	120.84	110.38
2	C	501	NHW	N3A-C2A-N1A	-6.14	119.29	128.58
3	B	502	9K2	C15-C14-C13	-5.86	115.27	119.26
2	A	501	NHW	C5A-C4A-N3A	-5.46	119.19	126.72
3	A	502	9K2	C2-C3-N1	5.36	125.86	119.81
2	B	501	NHW	N3A-C2A-N1A	-5.20	120.71	128.58
2	A	501	NHW	O1M-C1M-CP	-5.04	114.98	122.17
2	C	501	NHW	C2A-N3A-C4A	4.71	123.34	111.83
3	A	502	9K2	C15-C14-C13	4.70	122.45	119.26
3	B	502	9K2	C4-N2-N1	-4.33	108.68	111.90
2	C	501	NHW	N3A-C4A-N9A	4.13	134.20	127.17
3	B	502	9K2	C-N-C1	3.94	119.80	109.72
2	B	501	NHW	C5A-C4A-N3A	-3.90	121.35	126.72
2	A	501	NHW	C13-C11-C12	-3.87	101.84	108.22
3	A	502	9K2	C12-C13-C14	-3.79	118.22	123.23
3	A	502	9K2	C3-N1-N2	3.71	112.91	105.03
3	C	502	9K2	C-N-C2	3.64	116.33	110.38
2	C	501	NHW	O1M-C1M-CP	-3.62	117.01	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NHW	C4A-C5A-N7A	-3.51	106.57	110.58
3	C	502	9K2	C8-C9-C3	-3.51	128.32	136.17
3	A	502	9K2	C7-C10-C15	3.50	129.28	122.53
2	C	501	NHW	C5A-N7A-C8A	3.48	108.92	103.45
2	B	501	NHW	C4A-C5A-N7A	-3.34	106.77	110.58
2	A	501	NHW	CP-C1M-C2M	3.32	122.58	115.55
3	B	502	9K2	C8-C9-C3	-3.27	128.86	136.17
2	C	501	NHW	P3X-O3X-C3X	-3.23	114.81	123.43
2	B	501	NHW	N9A-C8A-N7A	-3.19	109.41	113.94
2	C	501	NHW	C2A-N1A-C6A	3.15	123.90	118.73
3	C	502	9K2	C8-C9-C4	3.10	122.41	119.39
2	C	501	NHW	N9A-C8A-N7A	-3.09	109.56	113.94
3	B	502	9K2	C14-C15-C10	3.08	123.43	118.62
3	B	502	9K2	C16-C15-C14	-3.05	114.20	119.57
2	B	501	NHW	O2A-P1A-O3A	3.00	115.39	107.27
2	A	501	NHW	N9A-C8A-N7A	-2.95	109.75	113.94
3	A	502	9K2	C9-C4-N2	2.92	108.69	106.59
2	A	501	NHW	C5A-C4A-N9A	2.92	109.00	105.81
2	A	501	NHW	C6A-C5A-C4A	2.92	121.16	117.18
4	C	504	DMS	O-S-C1	2.91	121.05	106.49
3	B	502	9K2	C8-C9-C4	2.90	122.21	119.39
3	C	502	9K2	C14-C15-C10	2.89	123.12	118.62
2	B	501	NHW	C4A-N9A-C8A	2.87	108.75	105.74
3	A	502	9K2	C5-C6-C7	2.83	124.75	121.12
2	A	501	NHW	C4A-C5A-N7A	-2.82	107.36	110.58
2	B	501	NHW	O4X-C1X-C2X	-2.81	100.61	106.62
4	A	505	DMS	O-S-C1	2.80	120.50	106.49
2	B	501	NHW	P3X-O3X-C3X	-2.80	115.96	123.43
3	B	502	9K2	C1-N-C2	2.79	114.94	110.38
2	A	501	NHW	N3A-C4A-N9A	2.71	131.77	127.17
2	A	501	NHW	C14-C11-C13	2.70	114.58	109.20
4	B	505	DMS	O-S-C1	2.69	119.96	106.49
3	A	502	9K2	C11-C10-C7	-2.68	113.37	118.70
3	A	502	9K2	C8-C9-C3	-2.67	130.20	136.17
2	B	501	NHW	C2A-N3A-C4A	2.63	118.25	111.83
2	B	501	NHW	C5A-N7A-C8A	2.62	107.56	103.45
2	B	501	NHW	C2A-N1A-C6A	2.62	123.03	118.73
2	A	501	NHW	O2A-P1A-O3A	2.57	114.22	107.27
2	B	501	NHW	O4A-P2A-O5A	2.56	124.33	112.44
2	A	501	NHW	C6-C7-N8	-2.53	106.61	112.00
3	B	502	9K2	C5-C4-C9	-2.53	119.74	122.19
7	A	508	SO4	O4-S-O1	2.51	122.66	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	DMS	O-S-C2	2.49	118.94	106.49
2	A	501	NHW	C2-C3-N4	-2.46	107.29	112.41
2	B	501	NHW	O5-C5-N4	2.42	127.78	123.03
2	B	501	NHW	C5X-C4X-C3X	-2.41	106.36	114.38
2	C	501	NHW	C5A-C4A-N9A	2.39	108.41	105.81
2	A	501	NHW	C5X-C4X-C3X	-2.37	106.49	114.38
3	A	502	9K2	F-C13-C12	2.36	122.33	118.55
3	C	502	9K2	C5-C6-C7	2.36	124.15	121.12
3	C	502	9K2	C6-C7-C10	2.35	124.81	120.91
3	A	502	9K2	C8-C9-C4	2.34	121.66	119.39
4	B	505	DMS	C2-S-C1	-2.33	86.47	98.42
7	A	510	SO4	O4-S-O2	-2.30	97.54	109.56
2	C	501	NHW	O8A-P3X-O9A	2.25	119.60	110.83
4	A	503	DMS	O-S-C1	2.24	117.71	106.49
3	C	502	9K2	C-N-C1	2.23	115.42	109.72
2	A	501	NHW	O8A-P3X-O9A	2.20	119.42	110.83
2	C	501	NHW	O4A-P2A-O3A	-2.20	101.32	107.27
3	B	502	9K2	C3-N1-N2	2.20	109.69	105.03
3	B	502	9K2	C7-C10-C15	2.15	126.68	122.53
2	B	501	NHW	O4X-C1X-N9A	-2.14	103.97	108.09
3	C	502	9K2	C16-C15-C14	-2.13	115.81	119.57
2	A	501	NHW	C5A-N7A-C8A	2.12	106.79	103.45
4	A	505	DMS	C2-S-C1	-2.10	87.67	98.42
7	A	508	SO4	O3-S-O2	2.10	120.52	109.56
2	C	501	NHW	O6A-C12-C11	-2.10	107.18	110.55
2	C	501	NHW	C6-C5-N4	-2.08	112.55	116.34
2	A	501	NHW	O4X-C4X-C5X	-2.07	102.70	109.33
2	B	501	NHW	C6A-C5A-N7A	2.06	136.07	132.09
2	C	501	NHW	O4X-C4X-C5X	-2.03	102.84	109.33
2	A	501	NHW	O4A-P2A-O3A	-2.02	101.81	107.27
2	B	501	NHW	N3A-C4A-N9A	2.01	130.59	127.17
2	B	501	NHW	C4M-C3M-C2M	-2.00	105.77	113.13

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	NHW	C6-C7-N8-C9
2	B	501	NHW	C6-C7-N8-C9
2	A	501	NHW	P2A-O3A-P1A-O1A
2	B	501	NHW	P2A-O3A-P1A-O1A
2	C	501	NHW	C11-C12-O6A-P2A

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Mol	Chain	Res	Type	Atoms
2	B	501	NHW	P2A-O3A-P1A-O2A

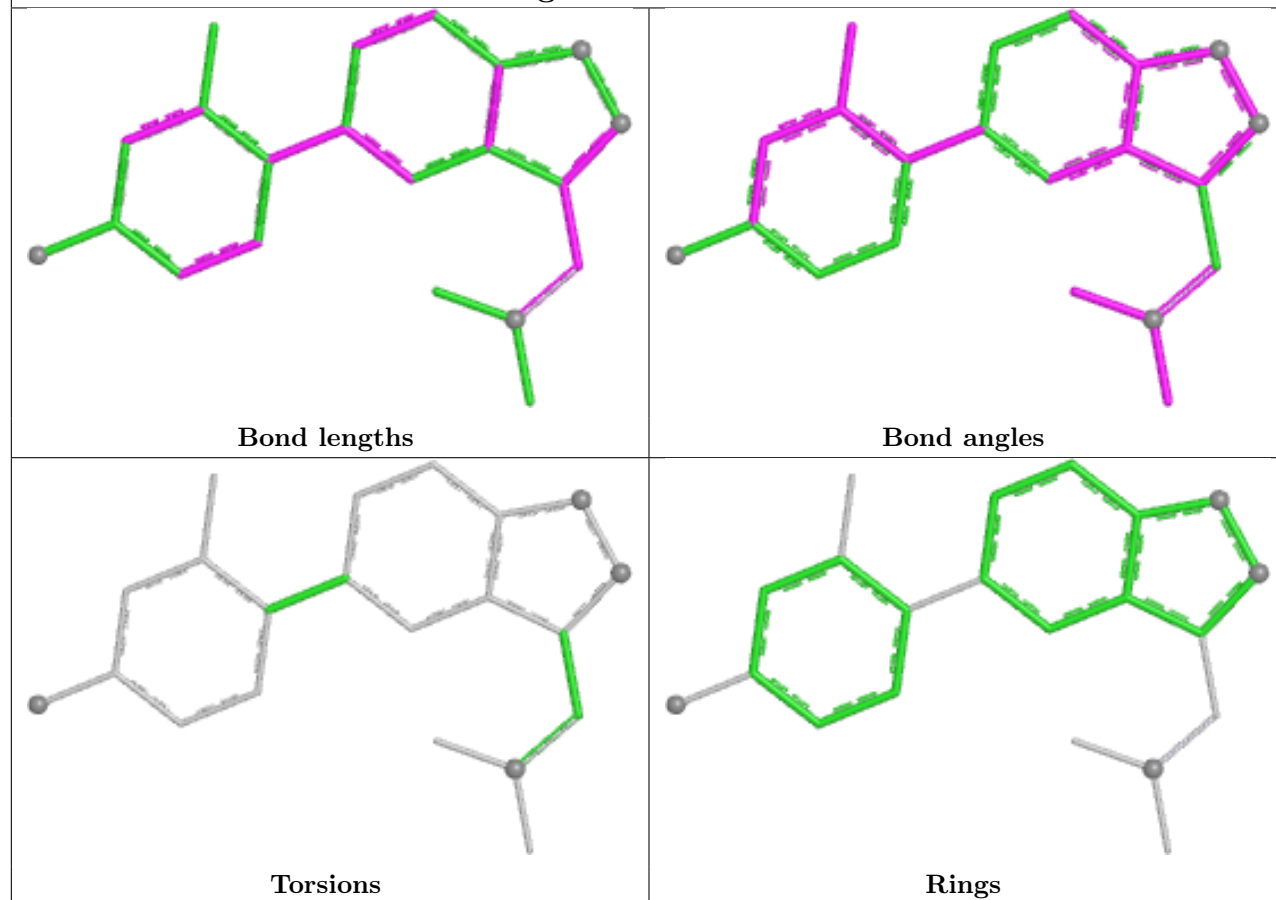
There are no ring outliers.

8 monomers are involved in 38 short contacts:

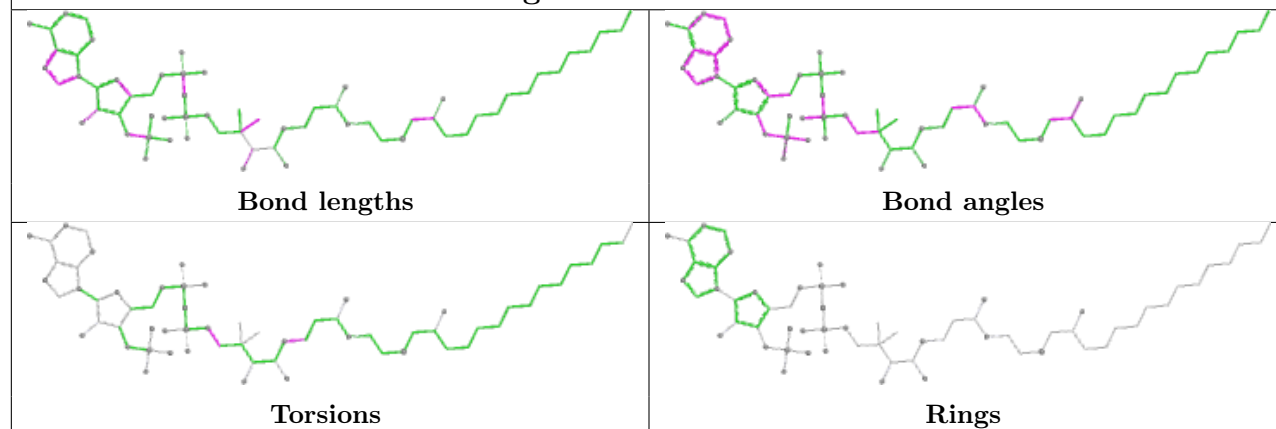
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	DMS	1	0
4	A	503	DMS	6	0
4	B	504	DMS	5	0
4	B	505	DMS	3	0
4	C	504	DMS	16	0
4	A	504	DMS	8	0
4	C	503	DMS	1	0
4	A	505	DMS	4	0

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.

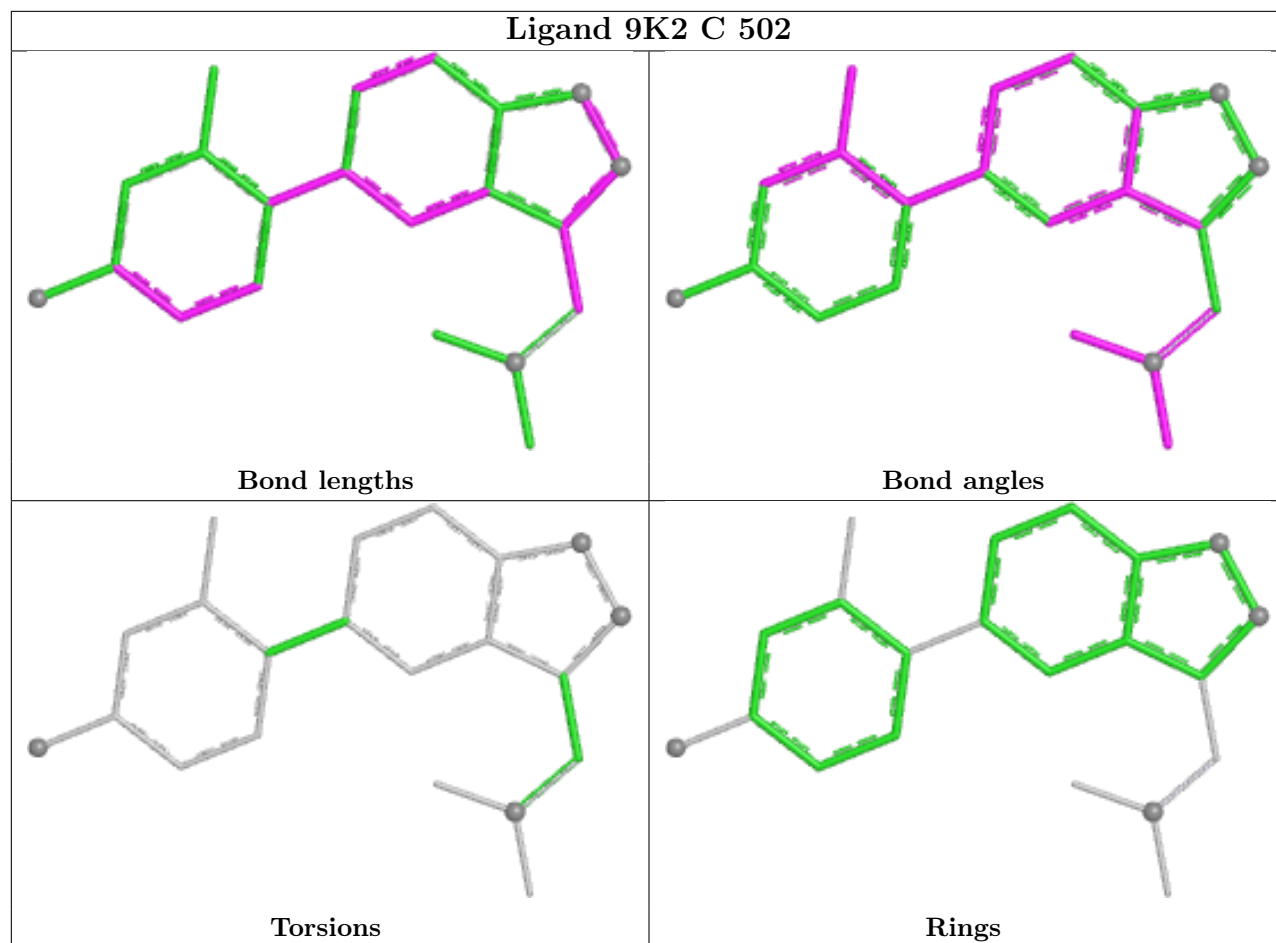
Ligand 9K2 B 502



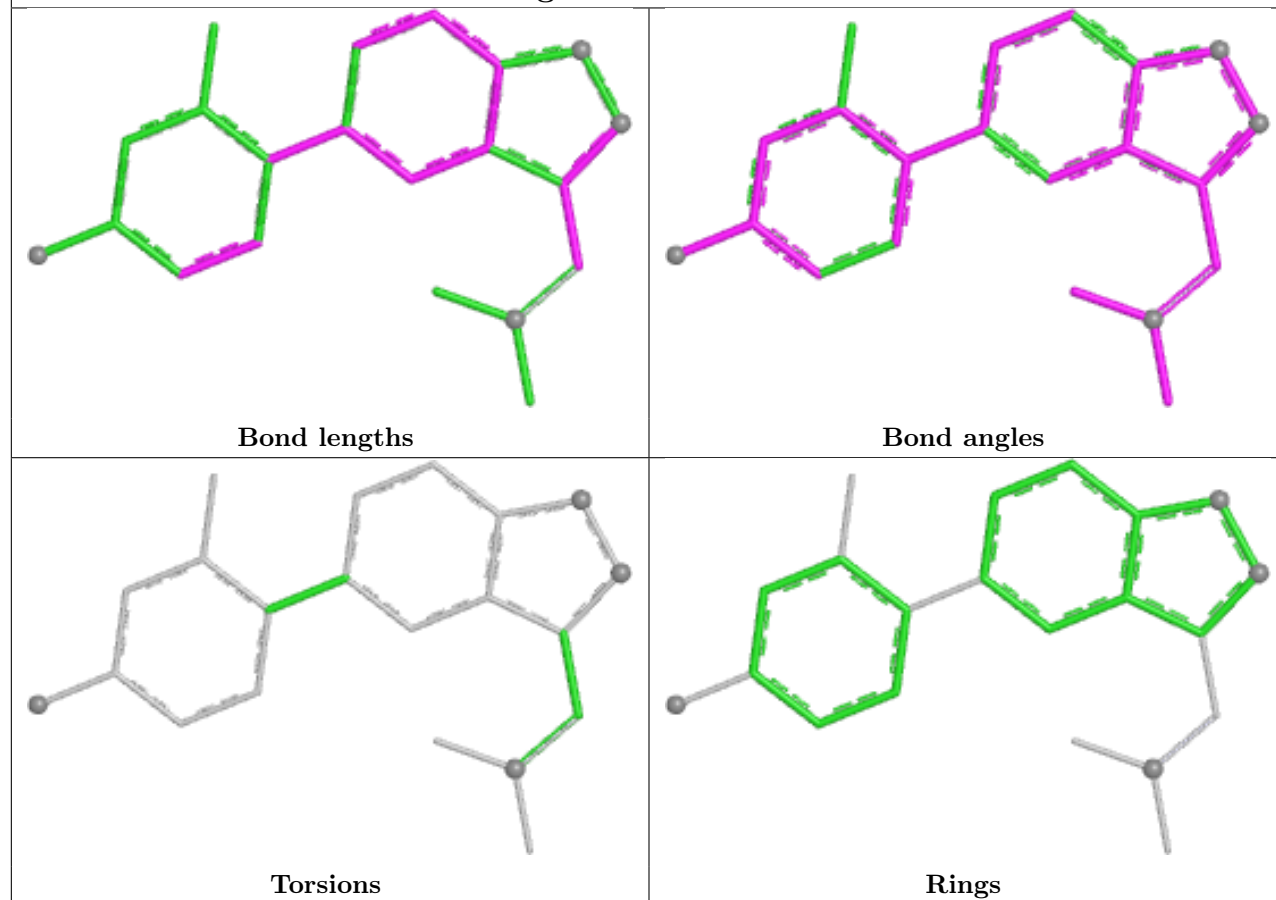
Ligand NHW C 501



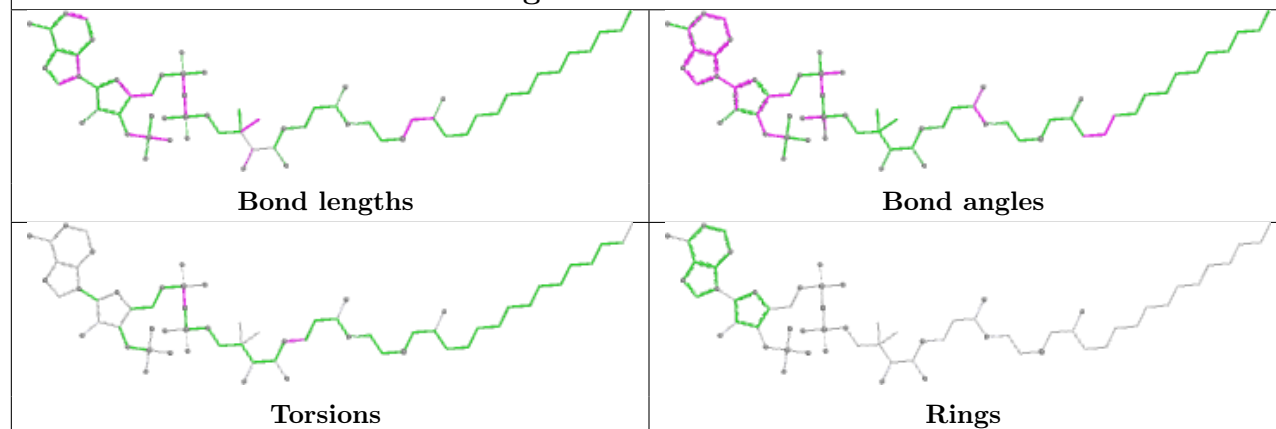
Ligand 9K2 C 502

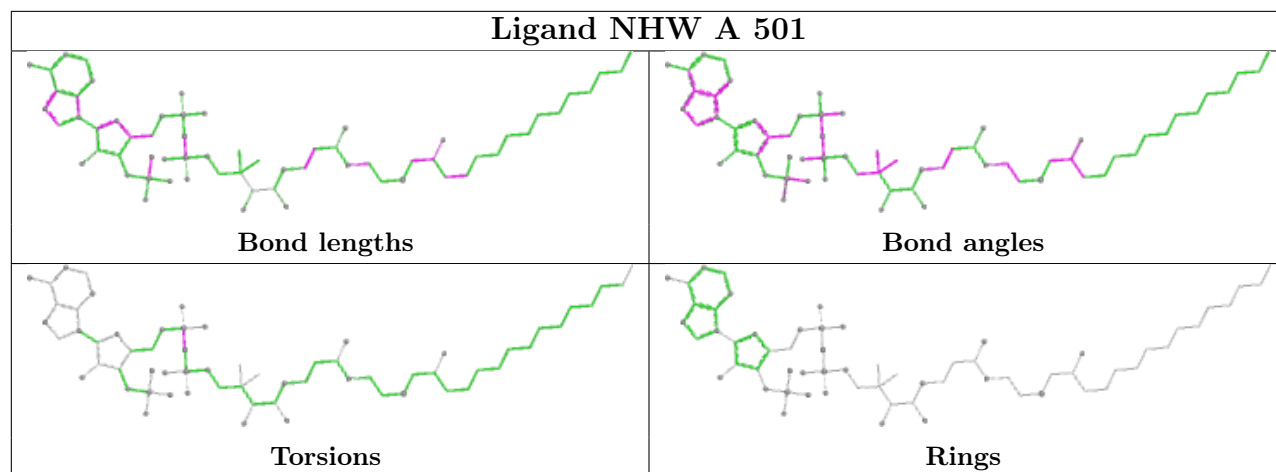


Ligand 9K2 A 502



Ligand NHW B 501





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%)	-0.60	4 (1%) 79 82	6, 11, 26, 58	40 (10%)
1	B	385/385 (100%)	-0.63	5 (1%) 75 79	4, 10, 27, 74	35 (9%)
1	C	368/385 (95%)	-0.52	6 (1%) 70 75	5, 12, 25, 67	40 (10%)
All	All	1138/1155 (98%)	-0.58	15 (1%) 75 79	4, 11, 26, 74	115 (10%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	ILE	4.0
1	C	227	SER	3.9
1	A	226	PHE	3.7
1	A	26	ILE	3.3
1	A	231	SER	3.1
1	B	102[A]	ILE	2.9
1	C	305[A]	ASN	2.7
1	B	39	ILE	2.4
1	B	40	ASN	2.3
1	C	222[A]	ILE	2.3
1	C	323	GLY	2.2
1	C	226	PHE	2.2
1	C	27	ASP	2.1
1	B	232	ARG	2.1
1	A	305[A]	ASN	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

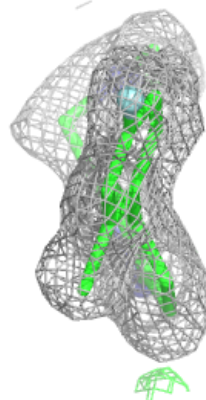
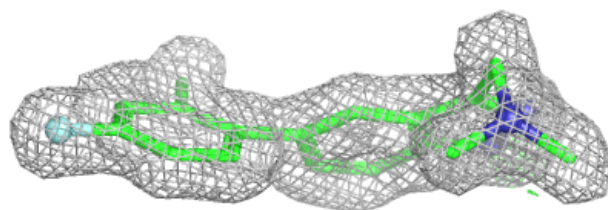
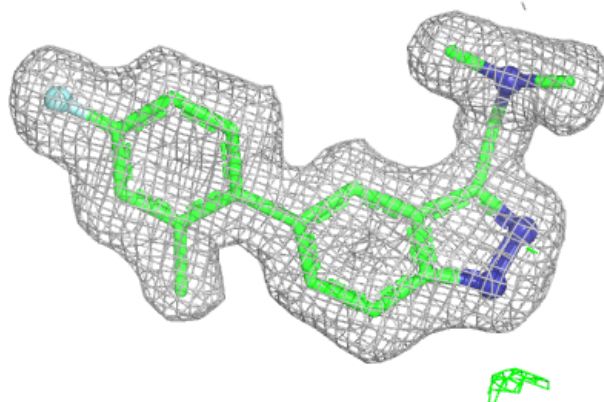
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	505	4/4	0.62	0.28	30,37,43,66	0
7	SO4	A	509	5/5	0.67	0.16	52,55,60,74	0
7	SO4	A	510	5/5	0.71	0.16	40,40,60,65	0
4	DMS	B	504	4/4	0.79	0.20	26,45,56,58	0
7	SO4	C	507	5/5	0.80	0.14	36,43,47,47	0
4	DMS	A	504	4/4	0.83	0.18	22,38,49,53	0
4	DMS	C	503	4/4	0.85	0.15	30,37,50,54	0
4	DMS	B	503	4/4	0.89	0.17	51,54,54,59	0
4	DMS	A	503	4/4	0.89	0.16	38,42,42,53	0
7	SO4	A	508	5/5	0.90	0.12	37,38,43,49	0
4	DMS	C	504	4/4	0.93	0.18	22,28,31,36	0
4	DMS	B	505	4/4	0.94	0.15	23,25,26,29	0
3	9K2	C	502	21/21	0.95	0.06	12,15,20,21	0
3	9K2	A	502	21/21	0.96	0.05	12,13,15,17	0
3	9K2	B	502	21/21	0.97	0.05	10,11,14,16	0
5	MG	B	506	1/1	0.99	0.06	22,22,22,22	0
5	MG	C	505	1/1	0.99	0.04	20,20,20,20	0
6	CL	B	507	1/1	0.99	0.01	9,9,9,9	0
6	CL	C	506	1/1	0.99	0.03	11,11,11,11	0
2	NHW	C	501	64/64	0.99	0.04	6,11,14,17	0
2	NHW	A	501	64/64	0.99	0.04	6,10,13,15	0
2	NHW	B	501	64/64	0.99	0.03	5,9,11,13	0
5	MG	A	506	1/1	0.99	0.05	17,17,17,17	0
6	CL	A	507	1/1	1.00	0.02	10,10,10,10	0

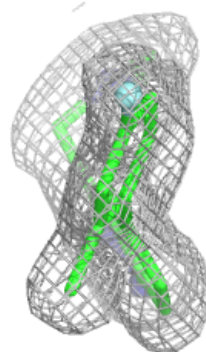
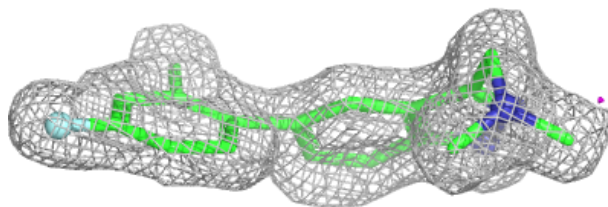
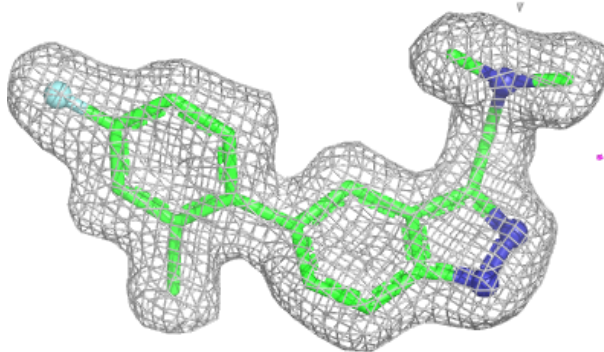
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

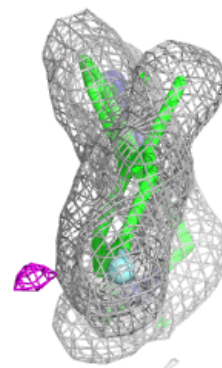
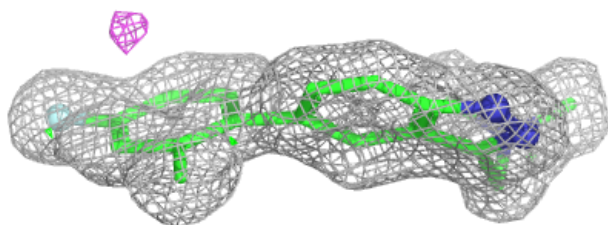
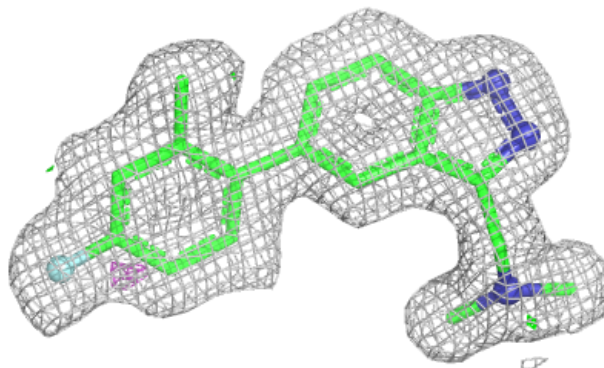
**Electron density around 9K2 A 502:**

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

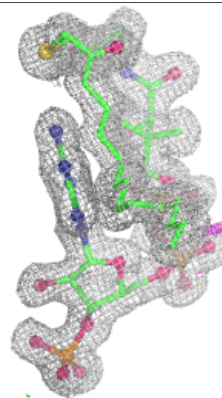
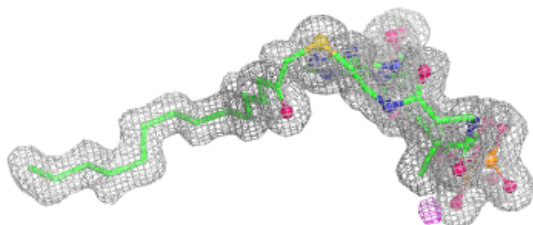
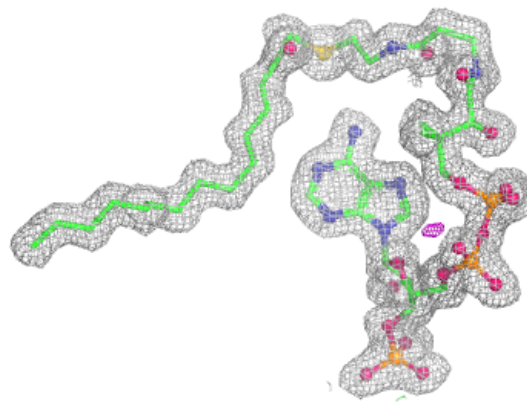


Electron density around 9K2 B 502:

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

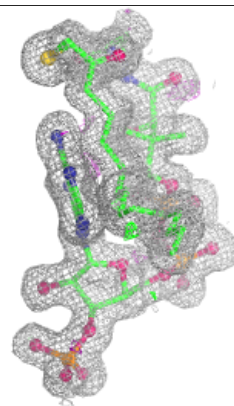
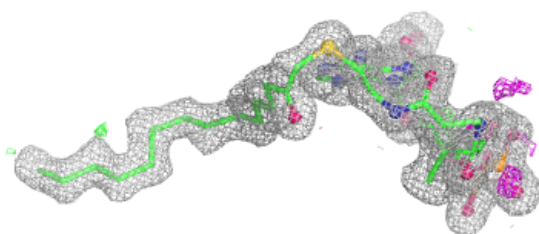
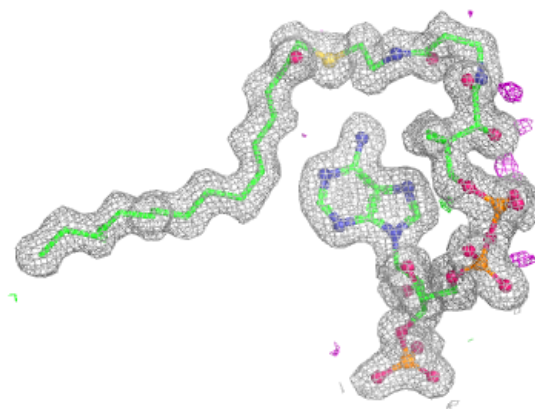
**Electron density around NHW C 501:**

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

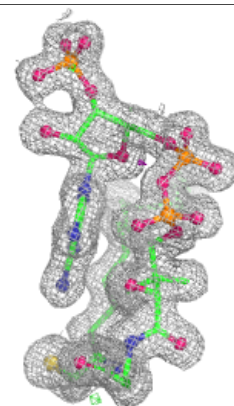
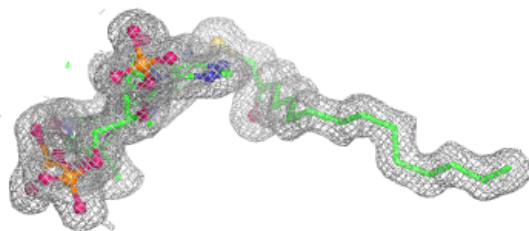
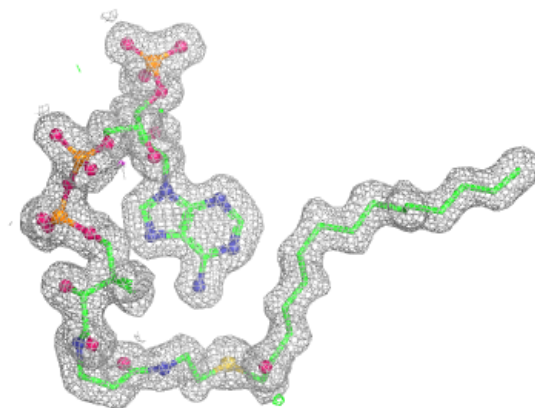


Electron density around NHW A 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.