



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:42 AM UTC

PDB ID : 5O4V / pdb_00005o4v
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 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

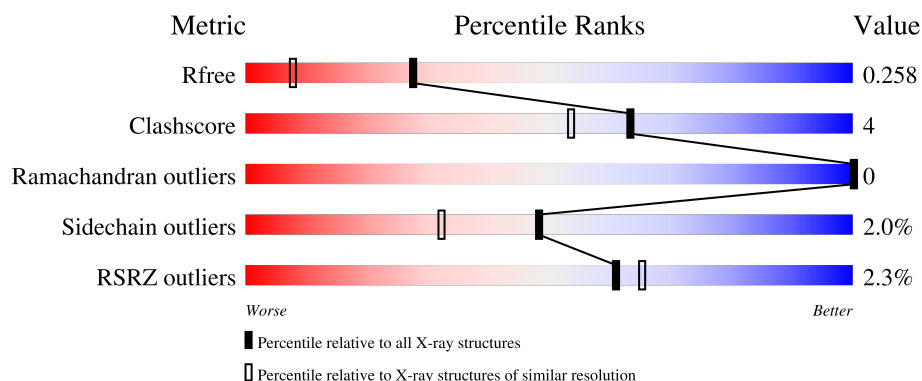
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	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	
1	B	385	
1	C	385	

2 Entry composition [i](#)

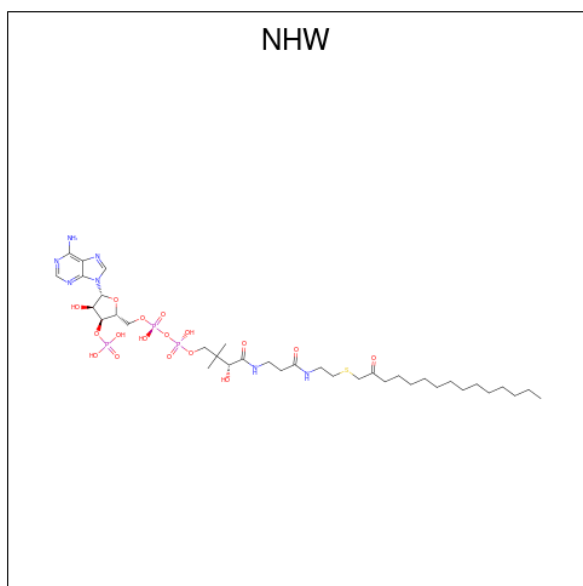
There are 9 unique types of molecules in this entry. The entry contains 11374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

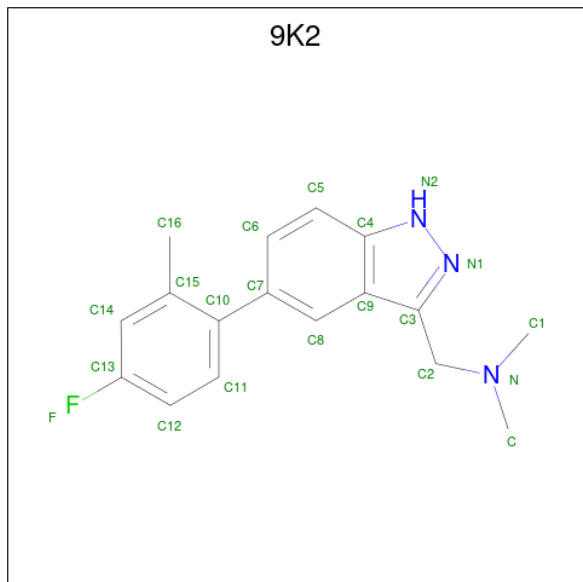
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	23	0
			3319	2160	542	605	12			
1	B	385	Total	C	N	O	S	0	26	0
			3333	2180	538	603	12			
1	C	368	Total	C	N	O	S	0	29	0
			3208	2099	509	589	11			

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



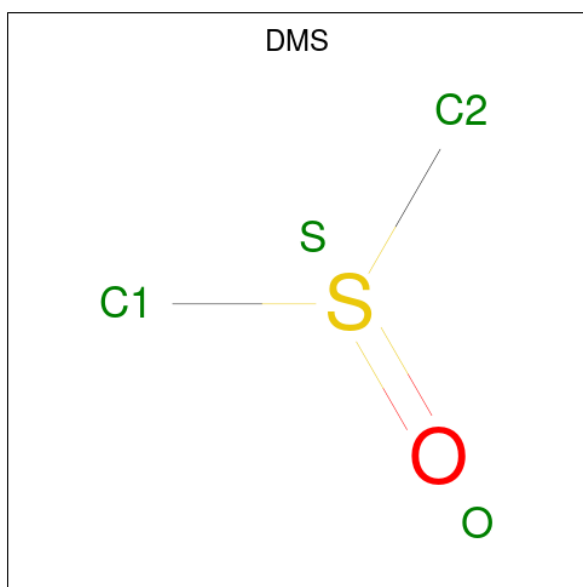
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

- 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	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		

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

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

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

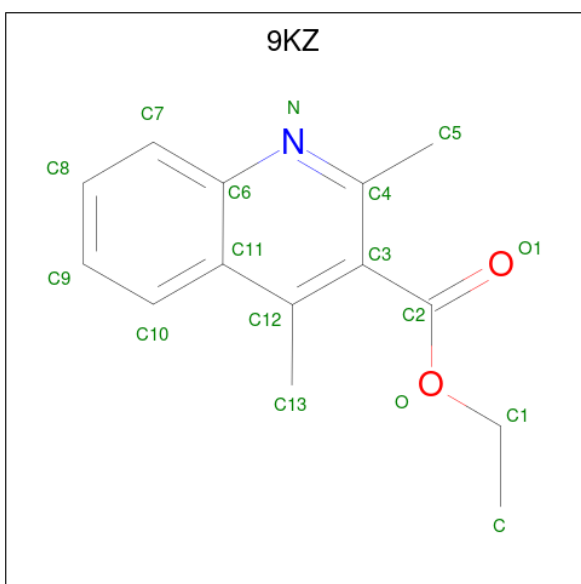
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

- 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	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 (CCD ID: 9KZ) (formula: C₁₄H₁₅NO₂).



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		

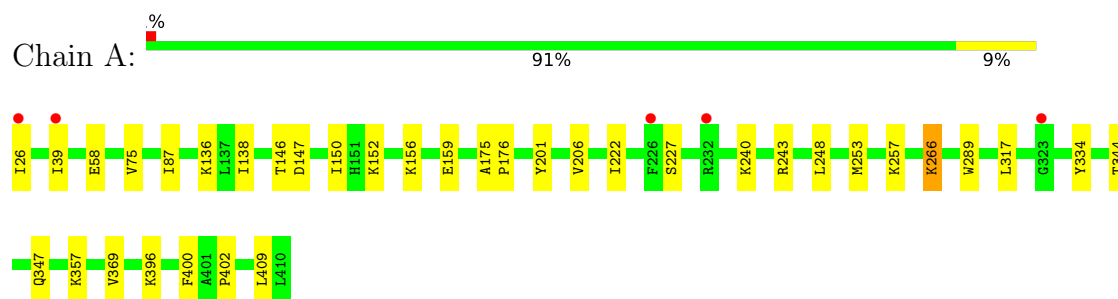
- Molecule 9 is water.

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		

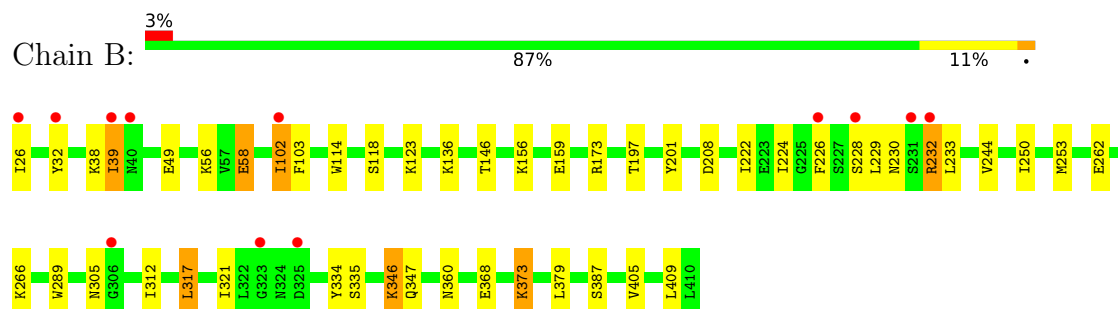
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

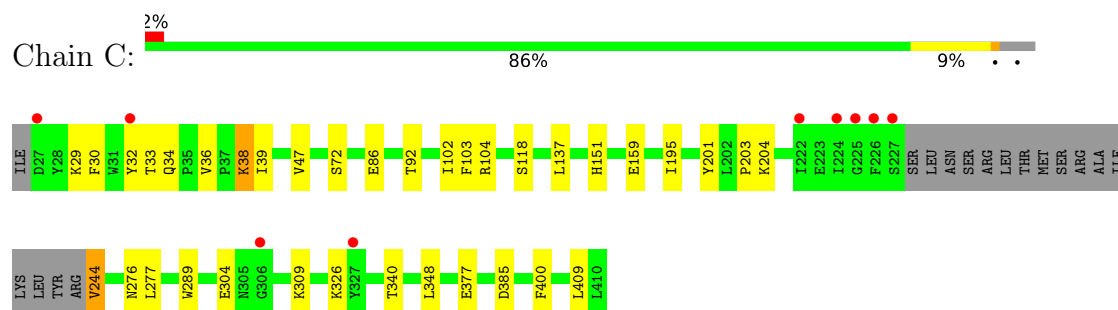
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



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• 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 89.53 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (89.53-1.70) 98.6 (89.53-1.70)	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 , 0.258	Depositor DCC
R_{free} test set	6874 reflections (4.94%)	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)	0.32 , 30.3	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: NHW, 9KZ, CL, 9K2, SO4, DMS, MG

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	1.14	1/3453 (0.0%)	1.05	2/4671 (0.0%)
1	B	1.15	5/3491 (0.1%)	1.08	6/4716 (0.1%)
1	C	1.12	1/3361 (0.0%)	1.02	2/4546 (0.0%)
All	All	1.14	7/10305 (0.1%)	1.05	10/13933 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	347	GLN	C-O	-6.91	1.16	1.24
1	B	335	SER	C-O	5.84	1.30	1.23
1	A	150	ILE	C-O	5.27	1.29	1.24
1	B	405	VAL	C-O	5.21	1.30	1.24
1	C	277	LEU	C-O	-5.18	1.17	1.23
1	B	173	ARG	CA-CB	5.13	1.61	1.53
1	B	49	GLU	N-CA	5.01	1.51	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	SER	N-CA-C	7.38	120.44	108.41
1	B	49	GLU	CA-C-N	-6.82	113.28	120.03
1	B	49	GLU	C-N-CA	-6.82	113.28	120.03
1	B	317	LEU	CA-C-N	-6.42	114.02	120.31
1	B	317	LEU	C-N-CA	-6.42	114.02	120.31
1	A	396	LYS	N-CA-CB	-6.09	100.51	110.43
1	C	36	VAL	CA-C-N	-5.61	114.47	120.03
1	C	36	VAL	C-N-CA	-5.61	114.47	120.03
1	B	114	TRP	N-CA-C	5.56	117.02	111.07
1	A	87	ILE	N-CA-C	-5.52	105.34	110.53

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	24	0
1	B	3333	0	3413	33	0
1	C	3208	0	3250	22	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	3	0
4	B	4	0	6	2	0
4	C	4	0	6	1	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	6	0
9	B	411	0	0	2	0
9	C	350	0	0	2	0
All	All	11374	0	10218	82	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 (82) 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:123[B]:LYS:HD3	1:B:123[B]:LYS:H	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:A:159[A]:GLU:OE1	4:A:503:DMS:H12	1.81	0.81
1:C:159[A]:GLU:OE2	4:C:503:DMS:H11	1.82	0.80
1:C:32[A]:TYR:CD1	1:C:38[A]:LYS:HE2	2.19	0.77
1:B:197:THR:HG23	1:B:409[B]:LEU:HD12	1.70	0.72
4:A:503:DMS:H13	9:A:645:HOH:O	1.88	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
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:A:146:THR:HG21	1:A:159[A]:GLU:HG3	1.80	0.62
1:B:146:THR:C	1:B:156[A]:LYS:HE3	2.24	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:A:152[B]:LYS:HD2	9:A:608:HOH:O	2.04	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206[B]:VAL:HG22	1:A:400:PHE:CE2	2.48	0.47
1:A:289:TRP:CZ2	4:A:503:DMS:H22	2.49	0.47
1:B:146:THR:CA	1:B:156[A]:LYS:HE3	2.44	0.47
1:B:289:TRP:CZ2	4:B:503:DMS:H12	2.49	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:32[B]:TYR:CD1	1:B:38[B]:LYS:HE3	2.50	0.46
1:B:317:LEU:HB3	1:B:334:TYR:CE1	2.51	0.46
1:C:159[A]:GLU:HG3	1:C:195:ILE:HG23	1.98	0.46
1:B:373[A]:LYS:HZ3	1:B:373[A]:LYS:HG2	1.67	0.46
1:A:266[A]:LYS:HB3	1:A:266[A]:LYS:HE3	1.46	0.45
1:B:262:GLU:HG3	1:B:266[A]:LYS:HE3	1.98	0.45
1:B:208:ASP:OD1	1:B:387:SER:OG	2.34	0.45
8:A:508:9KZ:C1	8:A:508:9KZ:C5	2.95	0.44
1:C:304[B]:GLU:OE1	1:C:309:LYS:NZ	2.49	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:138:ILE:C	1:A:138:ILE:HD12	2.43	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:253[B]:MET:HE2	1:B:312:ILE:HD12	1.99	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
4:B:503:DMS:H11	9:B:606:HOH:O	2.19	0.42
1:C:377[A]:GLU:HA	1:C:377[A]:GLU:OE1	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:HD13	1:B:39:ILE:HA	1.89	0.41
1:C:159[A]:GLU:CD	1:C:409:LEU:HD22	2.45	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

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	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

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%)	368 (98%)	6 (2%)	55	41
1	B	377/351 (107%)	366 (97%)	11 (3%)	37	20
1	C	364/351 (104%)	355 (98%)	9 (2%)	42	24
All	All	1115/1053 (106%)	1089 (98%)	26 (2%)	48	27

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	58	GLU
1	A	136	LYS
1	A	240	LYS
1	A	266[A]	LYS

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Mol	Chain	Res	Type
1	A	266[B]	LYS
1	B	26	ILE
1	B	39	ILE
1	B	58	GLU
1	B	102	ILE
1	B	136	LYS
1	B	232	ARG
1	B	244	VAL
1	B	346[A]	LYS
1	B	346[B]	LYS
1	B	373[A]	LYS
1	B	373[B]	LYS
1	C	29	LYS
1	C	38[A]	LYS
1	C	38[B]	LYS
1	C	47	VAL
1	C	72[A]	SER
1	C	72[B]	SER
1	C	244	VAL
1	C	326	LYS
1	C	385	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	249	ASN
1	A	347	GLN
1	A	350	GLN
1	A	372	ASN
1	B	34	GLN
1	B	55	ASN
1	B	249	ASN
1	B	274	GLN
1	B	359	ASN
1	B	360	ASN
1	C	120	ASN
1	C	320	GLN
1	C	371	GLN
1	C	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	A	503	-	3,3,3	0.58	0	3,3,3	1.88	1 (33%)
7	SO4	A	507	-	4,4,4	0.54	0	6,6,6	0.86	0
3	9K2	A	502	-	23,23,23	1.64	8 (34%)	30,33,33	2.44	9 (30%)
8	9KZ	A	508	-	18,18,18	3.26	8 (44%)	24,25,25	2.33	9 (37%)
4	DMS	C	503	-	3,3,3	0.61	0	3,3,3	1.06	0
7	SO4	A	506	-	4,4,4	0.53	0	6,6,6	0.14	0
2	NHW	A	501	5	64,66,66	1.33	8 (12%)	87,92,92	1.66	15 (17%)
2	NHW	C	501	5	64,66,66	1.37	8 (12%)	87,92,92	1.73	14 (16%)
3	9K2	B	502	-	23,23,23	1.58	4 (17%)	30,33,33	2.48	13 (43%)
2	NHW	B	501	5	64,66,66	1.16	4 (6%)	87,92,92	1.56	11 (12%)
4	DMS	B	503	-	3,3,3	0.50	0	3,3,3	1.15	0
7	SO4	B	506	-	4,4,4	0.33	0	6,6,6	1.14	1 (16%)
8	9KZ	C	507	-	18,18,18	2.55	5 (27%)	24,25,25	2.28	8 (33%)
3	9K2	C	502	-	23,23,23	1.81	6 (26%)	30,33,33	2.61	12 (40%)
7	SO4	C	506	-	4,4,4	0.45	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	9KZ	B	507	-	18,18,18	2.57	7 (38%)	24,25,25	2.10	7 (29%)

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	A	502	-	-	1/8/8/8	0/3/3/3
8	9KZ	A	508	-	-	2/7/7/7	0/2/2/2
2	NHW	A	501	5	-	4/65/81/81	0/3/3/3
2	NHW	C	501	5	-	3/65/81/81	0/3/3/3
3	9K2	B	502	-	-	1/8/8/8	0/3/3/3
2	NHW	B	501	5	-	4/65/81/81	0/3/3/3
8	9KZ	C	507	-	-	0/7/7/7	0/2/2/2
3	9K2	C	502	-	-	1/8/8/8	0/3/3/3
8	9KZ	B	507	-	-	1/7/7/7	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	508	9KZ	C3-C12	10.96	1.47	1.38
8	C	507	9KZ	C3-C12	8.41	1.45	1.38
8	B	507	9KZ	C3-C12	7.15	1.44	1.38
2	C	501	NHW	P1A-O3A	4.85	1.64	1.59
2	C	501	NHW	P2A-O3A	-4.74	1.54	1.59
2	A	501	NHW	P2A-O3A	-4.43	1.54	1.59
8	B	507	9KZ	C11-C6	4.06	1.48	1.42
8	A	508	9KZ	C3-C4	3.89	1.48	1.41
3	C	502	9K2	C3-N1	3.81	1.36	1.29
8	B	507	9KZ	C3-C4	3.79	1.48	1.41
3	C	502	9K2	C10-C7	-3.76	1.42	1.49
2	A	501	NHW	C4A-N3A	3.73	1.41	1.34
3	B	502	9K2	C10-C7	-3.64	1.42	1.49
3	B	502	9K2	C3-N1	3.62	1.36	1.29
8	A	508	9KZ	C11-C6	3.46	1.47	1.42
8	A	508	9KZ	O-C2	3.40	1.41	1.33
2	B	501	NHW	P2A-O3A	3.34	1.63	1.59
8	C	507	9KZ	C6-N	-3.25	1.32	1.37
2	A	501	NHW	C8A-N7A	3.08	1.37	1.31
8	B	507	9KZ	O1-C2	-3.04	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	9K2	C9-C3	-2.96	1.38	1.45
3	C	502	9K2	C5-C6	2.86	1.43	1.38
2	B	501	NHW	P1A-O3A	2.85	1.62	1.59
3	A	502	9K2	C9-C4	-2.84	1.37	1.41
3	A	502	9K2	C14-C13	2.84	1.42	1.37
8	A	508	9KZ	C7-C6	-2.79	1.37	1.41
3	A	502	9K2	C8-C7	2.70	1.44	1.39
8	A	508	9KZ	C4-N	2.65	1.35	1.32
2	A	501	NHW	C14-C11	2.64	1.59	1.53
3	A	502	9K2	C3-N1	2.60	1.34	1.29
3	A	502	9K2	C12-C13	2.60	1.42	1.37
2	C	501	NHW	O4X-C4X	2.57	1.50	1.45
2	B	501	NHW	C4A-N9A	-2.49	1.32	1.37
8	B	507	9KZ	O-C2	2.48	1.39	1.33
8	B	507	9KZ	C6-N	-2.36	1.33	1.37
8	A	508	9KZ	C9-C10	2.33	1.41	1.36
2	C	501	NHW	C2-C3	2.32	1.60	1.51
8	B	507	9KZ	C7-C6	-2.27	1.38	1.41
8	C	507	9KZ	C3-C4	2.25	1.45	1.41
3	C	502	9K2	N2-N1	2.25	1.42	1.36
2	A	501	NHW	C7-C6	2.22	1.58	1.51
2	A	501	NHW	C6-C5	2.22	1.55	1.51
2	A	501	NHW	O10-C10	2.21	1.46	1.42
2	A	501	NHW	C3M-C2M	2.21	1.60	1.52
3	A	502	9K2	C5-C6	2.21	1.42	1.38
3	C	502	9K2	C2-C3	2.20	1.54	1.51
2	C	501	NHW	P3X-O3X	2.20	1.63	1.59
3	B	502	9K2	C5-C6	2.13	1.42	1.38
2	B	501	NHW	P3X-O3X	2.12	1.63	1.59
2	C	501	NHW	P2A-O5A	-2.12	1.43	1.50
2	C	501	NHW	CP-C1M	2.10	1.54	1.51
8	C	507	9KZ	C11-C6	2.09	1.45	1.42
2	C	501	NHW	C5A-N7A	-2.07	1.35	1.39
8	C	507	9KZ	C10-C11	-2.07	1.38	1.42
3	C	502	9K2	C8-C9	2.05	1.43	1.39
8	A	508	9KZ	C12-C11	2.03	1.48	1.42
3	A	502	9K2	C12-C11	2.01	1.42	1.38
3	A	502	9K2	C10-C7	-2.00	1.45	1.49

All (100) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	507	9KZ	C4-N-C6	7.29	125.12	118.42
3	C	502	9K2	C-N-C2	6.71	121.35	110.38
3	A	502	9K2	C1-N-C2	6.68	121.30	110.38
3	A	502	9K2	C-N-C2	6.33	120.74	110.38
8	A	508	9KZ	C3-C4-N	-6.06	118.92	122.55
2	B	501	NHW	N3A-C2A-N1A	-6.02	119.47	128.58
2	C	501	NHW	C5A-C4A-N3A	-5.66	118.93	126.72
3	B	502	9K2	C1-N-C2	5.59	119.51	110.38
2	C	501	NHW	N3A-C2A-N1A	-5.44	120.34	128.58
2	A	501	NHW	N3A-C2A-N1A	-5.34	120.50	128.58
3	B	502	9K2	C-N-C2	5.23	118.94	110.38
3	C	502	9K2	C2-C3-N1	5.19	125.67	119.81
3	C	502	9K2	C1-N-C2	5.03	118.61	110.38
8	B	507	9KZ	C3-C4-N	-4.72	119.73	122.55
2	C	501	NHW	C2-S1-CP	-4.65	94.06	101.72
3	B	502	9K2	C-N-C1	4.53	121.33	109.72
3	B	502	9K2	C4-N2-N1	-4.47	108.58	111.90
8	A	508	9KZ	C4-N-C6	4.45	122.51	118.42
2	C	501	NHW	N3A-C4A-N9A	4.44	134.72	127.17
3	C	502	9K2	C4-N2-N1	-4.43	108.61	111.90
2	A	501	NHW	C5A-C4A-N3A	-4.39	120.68	126.72
8	B	507	9KZ	C4-N-C6	4.31	122.38	118.42
2	A	501	NHW	N9A-C8A-N7A	-4.25	107.91	113.94
3	A	502	9K2	C15-C14-C13	4.24	122.14	119.26
2	C	501	NHW	P3X-O3X-C3X	-4.19	112.25	123.43
2	C	501	NHW	C2A-N3A-C4A	4.16	121.99	111.83
2	A	501	NHW	O2A-P1A-O3A	4.06	118.25	107.27
3	A	502	9K2	C12-C13-C14	-4.01	117.93	123.23
8	B	507	9KZ	O-C2-C3	3.98	121.23	112.35
2	B	501	NHW	C5A-C4A-N3A	-3.93	121.31	126.72
2	A	501	NHW	C4A-N9A-C8A	3.83	109.76	105.74
3	C	502	9K2	C-N-C1	3.75	119.32	109.72
8	A	508	9KZ	O-C2-C3	3.65	120.48	112.35
2	B	501	NHW	C2A-N3A-C4A	3.64	120.72	111.83
2	B	501	NHW	C4A-N9A-C8A	3.56	109.47	105.74
8	C	507	9KZ	O-C2-C3	3.56	120.27	112.35
2	C	501	NHW	N9A-C8A-N7A	-3.48	109.00	113.94
3	C	502	9K2	C15-C14-C13	3.47	121.62	119.26
2	C	501	NHW	O1M-C1M-CP	-3.44	117.26	122.17
2	B	501	NHW	N9A-C8A-N7A	-3.42	109.08	113.94
2	B	501	NHW	P3X-O3X-C3X	-3.42	114.30	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NHW	N3A-C4A-N9A	3.35	132.87	127.17
2	A	501	NHW	C5A-N7A-C8A	3.31	108.65	103.45
2	A	501	NHW	N3A-C4A-N9A	3.29	132.76	127.17
2	B	501	NHW	O2A-P1A-O3A	3.18	115.87	107.27
2	A	501	NHW	C2A-N3A-C4A	3.15	119.53	111.83
8	C	507	9KZ	C5-C4-C3	-3.15	118.20	122.23
3	B	502	9K2	C7-C10-C15	3.13	128.58	122.53
8	A	508	9KZ	C10-C11-C6	3.12	121.83	118.36
3	C	502	9K2	C8-C9-C3	-3.10	129.24	136.17
8	B	507	9KZ	C3-C12-C11	-3.06	114.34	117.50
3	A	502	9K2	F-C13-C14	3.03	122.58	118.28
2	A	501	NHW	C4A-C5A-N7A	-3.02	107.13	110.58
3	C	502	9K2	C8-C9-C4	2.99	122.30	119.39
8	B	507	9KZ	C5-C4-N	2.98	121.34	116.94
3	B	502	9K2	F-C13-C14	2.98	122.51	118.28
2	C	501	NHW	CP-C1M-C2M	2.94	121.77	115.55
3	A	502	9K2	C-N-C1	2.91	117.19	109.72
3	B	502	9K2	C12-C13-C14	-2.88	119.44	123.23
8	C	507	9KZ	C7-C6-N	2.87	122.88	118.69
8	C	507	9KZ	O-C2-O1	-2.86	117.95	123.67
8	A	508	9KZ	C12-C11-C6	-2.82	116.22	118.52
2	C	501	NHW	C3-N4-C5	2.80	128.04	122.82
3	B	502	9K2	C2-C3-N1	2.77	122.94	119.81
8	A	508	9KZ	C12-C3-C2	-2.76	115.72	119.93
8	B	507	9KZ	C5-C4-C3	-2.72	118.75	122.23
8	C	507	9KZ	C11-C6-N	-2.69	119.95	122.80
3	B	502	9K2	C16-C15-C14	-2.69	114.83	119.57
2	C	501	NHW	C4A-N9A-C8A	2.61	108.48	105.74
3	C	502	9K2	C12-C13-C14	-2.58	119.82	123.23
2	A	501	NHW	C14-C11-C10	2.56	113.14	108.77
2	A	501	NHW	C2A-N1A-C6A	2.56	122.93	118.73
8	A	508	9KZ	C7-C6-C11	-2.55	116.39	119.13
4	A	503	DMS	O-S-C1	2.54	119.20	106.49
2	B	501	NHW	O3A-P1A-O1A	-2.51	103.15	110.70
3	B	502	9K2	C11-C10-C7	-2.47	113.80	118.70
2	A	501	NHW	C5X-C4X-C3X	-2.47	106.17	114.38
3	C	502	9K2	C5-C4-C9	-2.45	119.82	122.19
3	B	502	9K2	C5-C4-C9	-2.45	119.82	122.19
2	A	501	NHW	O3A-P1A-O1A	-2.44	103.37	110.70
8	C	507	9KZ	C5-C4-N	2.44	120.54	116.94
2	A	501	NHW	C2-S1-CP	-2.40	97.77	101.72
3	B	502	9K2	C8-C9-C3	-2.37	130.88	136.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	9K2	C7-C10-C15	2.35	127.08	122.53
8	A	508	9KZ	O-C1-C	2.33	116.75	108.40
8	B	507	9KZ	C9-C8-C7	2.28	123.45	120.40
2	C	501	NHW	C2-C3-N4	-2.26	107.69	112.41
3	A	502	9K2	C11-C10-C15	-2.26	116.60	119.30
2	C	501	NHW	C5A-N7A-C8A	2.24	106.98	103.45
3	C	502	9K2	C5-C6-C7	2.22	123.97	121.12
2	C	501	NHW	O2A-P1A-O3A	2.21	113.25	107.27
2	B	501	NHW	C13-C11-C10	2.19	112.50	108.77
8	C	507	9KZ	C3-C4-N	-2.18	121.24	122.55
3	A	502	9K2	C2-C3-C9	2.09	132.18	126.25
2	B	501	NHW	C2-C3-N4	-2.06	108.11	112.41
3	B	502	9K2	C11-C12-C13	2.06	120.49	118.38
8	A	508	9KZ	C1-O-C2	-2.04	111.88	116.45
2	A	501	NHW	C6-C7-N8	-2.03	107.67	112.00
7	B	506	SO4	O4-S-O1	2.02	120.13	109.56
3	C	502	9K2	C11-C10-C15	-2.01	116.90	119.30

There are no chirality outliers.

All (17) torsion outliers are listed below:

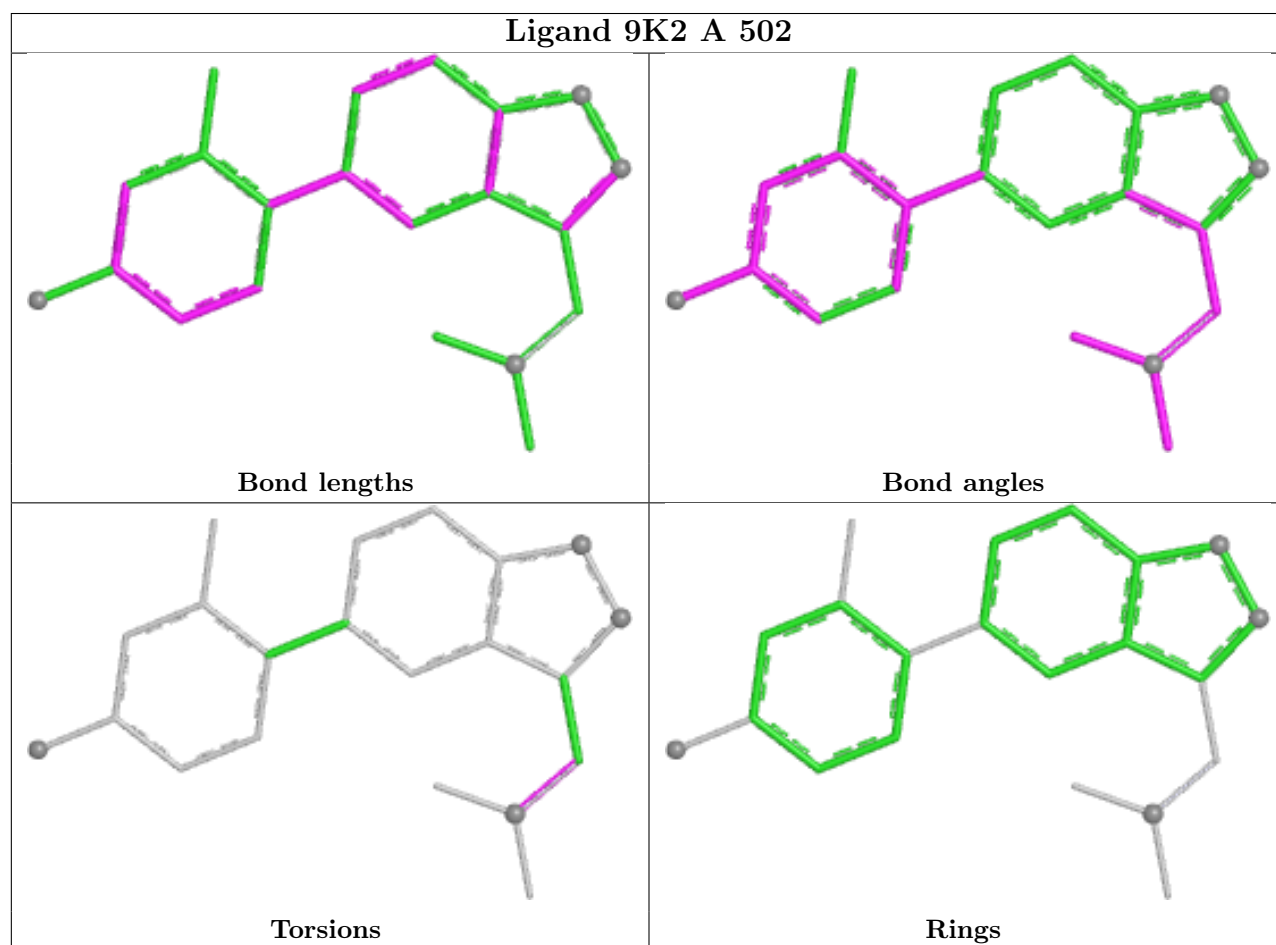
Mol	Chain	Res	Type	Atoms
8	A	508	9KZ	C3-C2-O-C1
8	A	508	9KZ	O1-C2-O-C1
8	B	507	9KZ	C-C1-O-C2
3	B	502	9K2	C3-C2-N-C1
2	A	501	NHW	C7M-C8M-C9M-CAM
2	C	501	NHW	C6-C7-N8-C9
3	A	502	9K2	C3-C2-N-C1
3	C	502	9K2	C3-C2-N-C
2	C	501	NHW	C4M-C5M-C6M-C7M
2	A	501	NHW	P2A-O3A-P1A-O1A
2	B	501	NHW	P2A-O3A-P1A-O2A
2	A	501	NHW	C11-C12-O6A-P2A
2	B	501	NHW	C11-C12-O6A-P2A
2	B	501	NHW	C4M-C5M-C6M-C7M
2	A	501	NHW	C4M-C5M-C6M-C7M
2	B	501	NHW	P2A-O3A-P1A-O1A
2	C	501	NHW	P2A-O3A-P1A-O1A

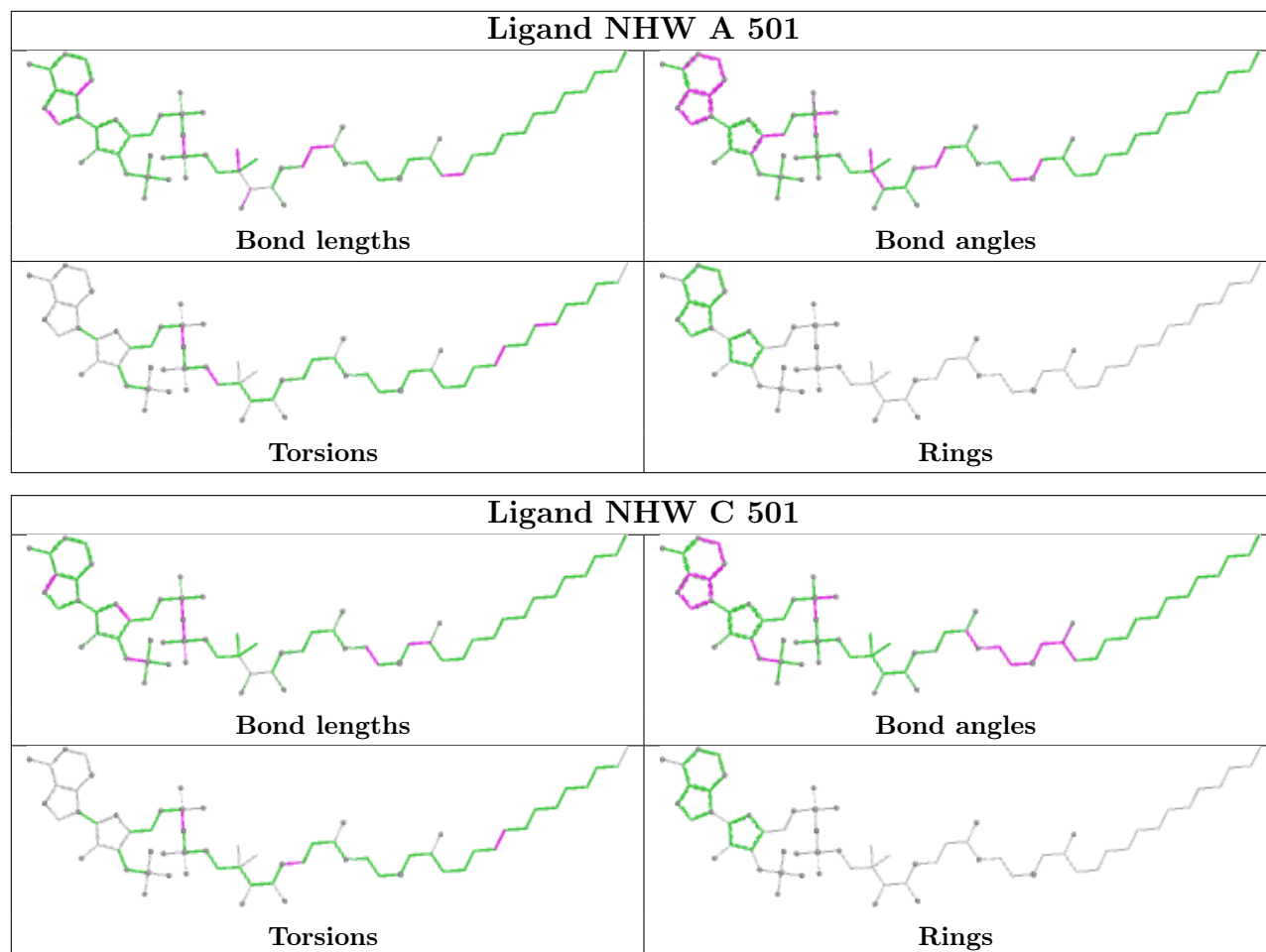
There are no ring outliers.

5 monomers are involved in 9 short contacts:

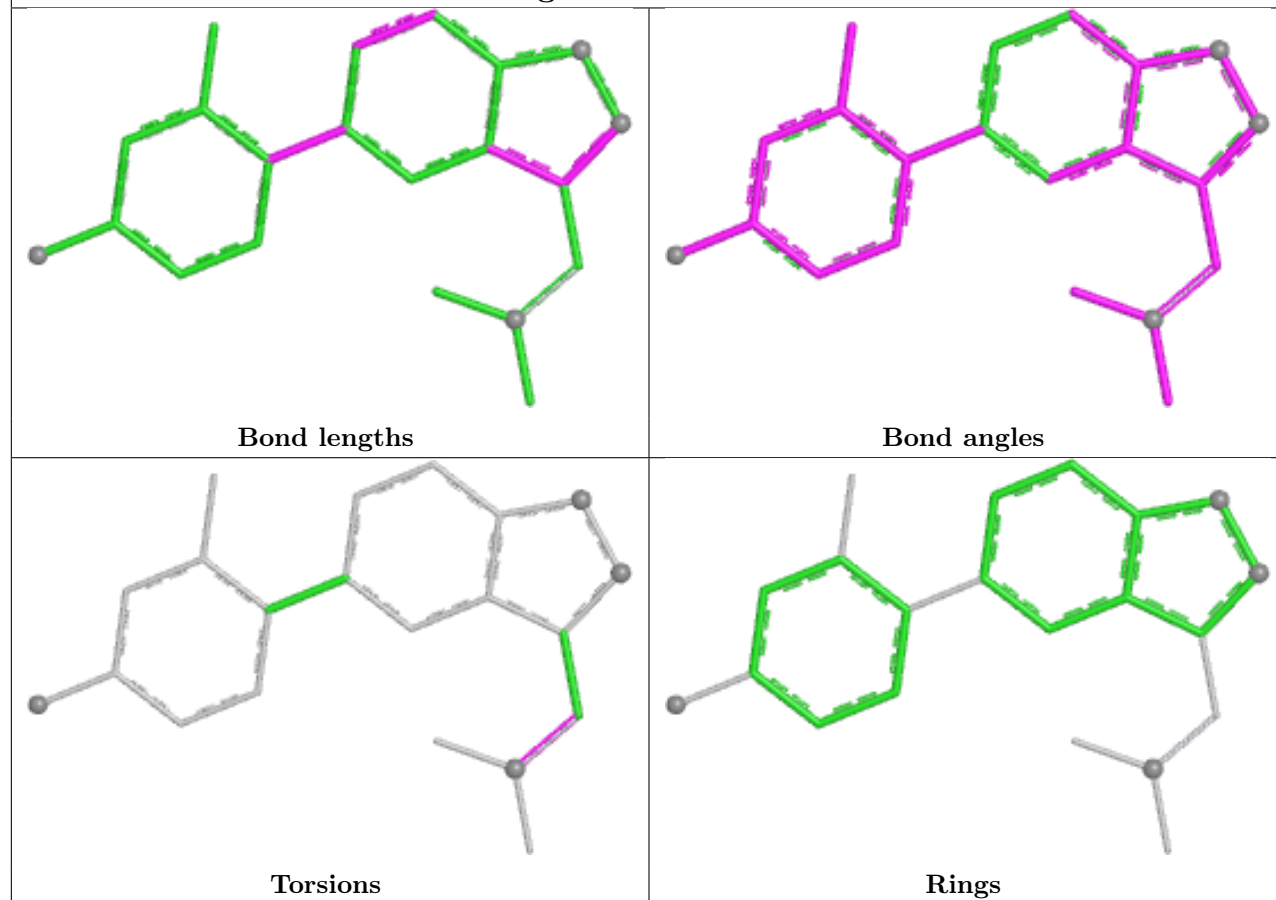
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	DMS	3	0
8	A	508	9KZ	1	0
4	C	503	DMS	1	0
4	B	503	DMS	2	0
8	B	507	9KZ	2	0

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

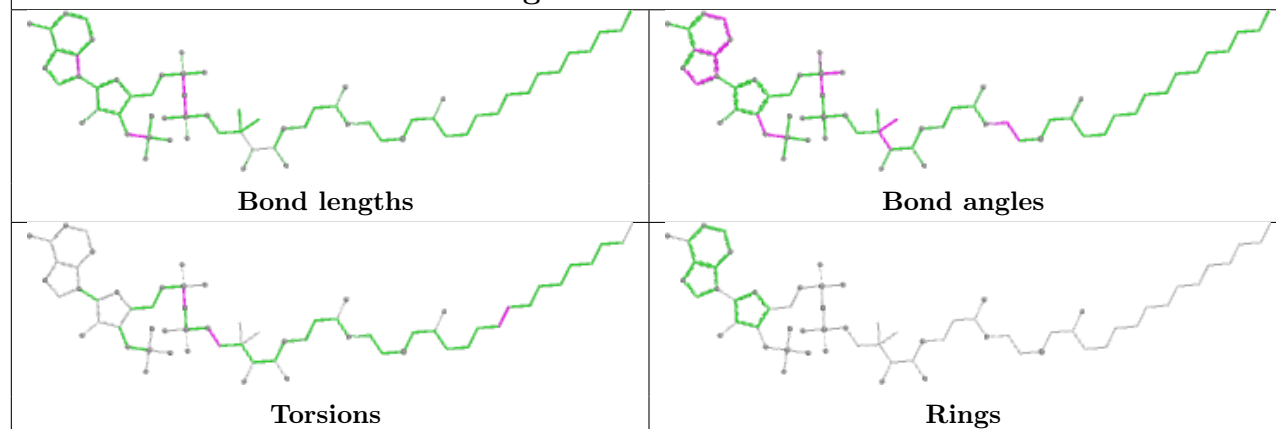


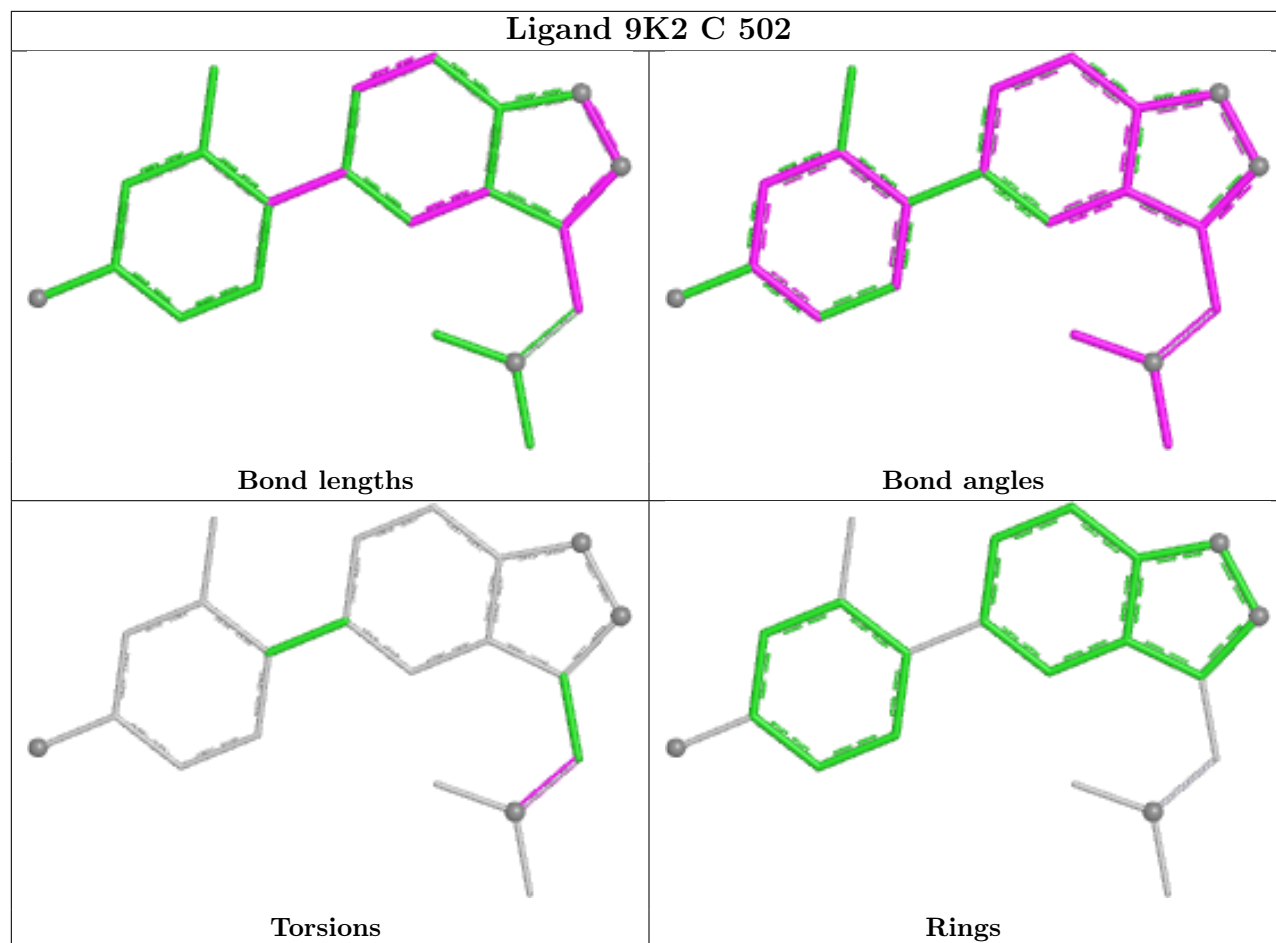


Ligand 9K2 B 502



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	385/385 (100%)	-0.05	5 (1%) 75 79	8, 18, 32, 59	36 (9%)
1	B	385/385 (100%)	-0.16	12 (3%) 51 55	9, 16, 31, 64	33 (8%)
1	C	368/385 (95%)	0.03	9 (2%) 59 64	8, 18, 33, 107	40 (10%)
All	All	1138/1155 (98%)	-0.06	26 (2%) 61 65	8, 17, 32, 107	109 (9%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	SER	6.8
1	C	226	PHE	6.0
1	A	26	ILE	5.2
1	B	26	ILE	4.5
1	C	27	ASP	3.6
1	C	222[A]	ILE	3.3
1	C	224	ILE	3.2
1	B	232	ARG	3.1
1	B	323	GLY	3.0
1	C	225	GLY	2.9
1	B	228	SER	2.8
1	A	226	PHE	2.8
1	C	32[A]	TYR	2.7
1	C	306	GLY	2.6
1	A	232	ARG	2.6
1	B	231	SER	2.5
1	A	39	ILE	2.3
1	A	323	GLY	2.3
1	B	226	PHE	2.3
1	B	325	ASP	2.2
1	B	40	ASN	2.2
1	B	39	ILE	2.2
1	B	32[A]	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	306	GLY	2.1
1	B	102	ILE	2.1
1	C	327	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	A	506	5/5	0.59	0.20	84,91,95,96	0
4	DMS	C	503	4/4	0.60	0.35	65,78,83,88	0
7	SO4	C	506	5/5	0.65	0.24	108,117,122,126	0
4	DMS	A	503	4/4	0.67	0.26	39,44,54,66	0
4	DMS	B	503	4/4	0.73	0.20	50,54,56,66	0
7	SO4	A	507	5/5	0.77	0.15	54,54,62,66	0
7	SO4	B	506	5/5	0.84	0.13	40,50,52,52	0
8	9KZ	B	507	17/17	0.91	0.09	16,19,28,33	0
3	9K2	C	502	21/21	0.92	0.08	20,22,26,31	0
3	9K2	B	502	21/21	0.93	0.07	18,20,22,24	0
8	9KZ	A	508	17/17	0.94	0.08	16,17,26,30	0
3	9K2	A	502	21/21	0.94	0.07	17,19,22,22	0
8	9KZ	C	507	17/17	0.94	0.08	19,20,31,31	0
2	NHW	C	501	64/64	0.97	0.05	11,16,20,24	0
5	MG	B	504	1/1	0.97	0.06	29,29,29,29	0
5	MG	C	504	1/1	0.97	0.05	27,27,27,27	0
2	NHW	A	501	64/64	0.97	0.05	11,15,19,22	0
2	NHW	B	501	64/64	0.97	0.05	11,14,17,18	0
5	MG	A	504	1/1	0.98	0.08	27,27,27,27	0
6	CL	B	505	1/1	0.99	0.02	16,16,16,16	0

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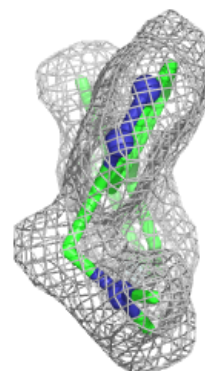
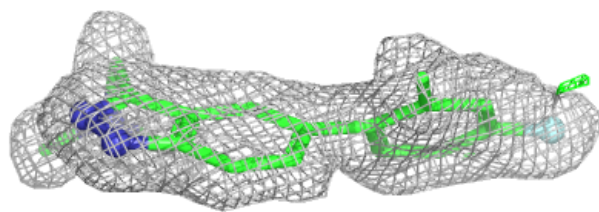
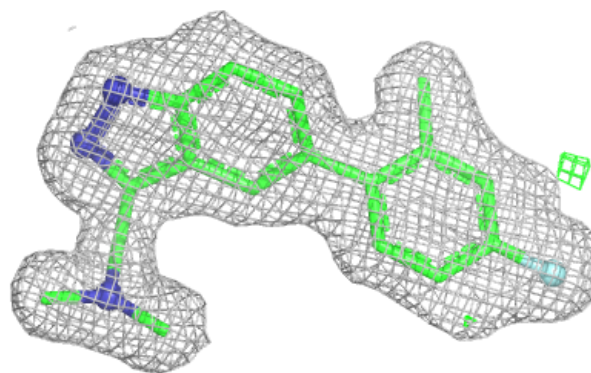
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	C	505	1/1	1.00	0.04	17,17,17,17	0
6	CL	A	505	1/1	1.00	0.04	17,17,17,17	0

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.

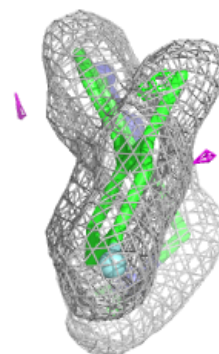
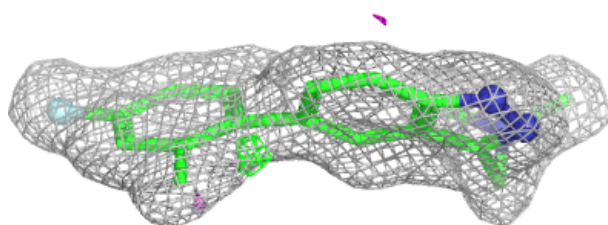
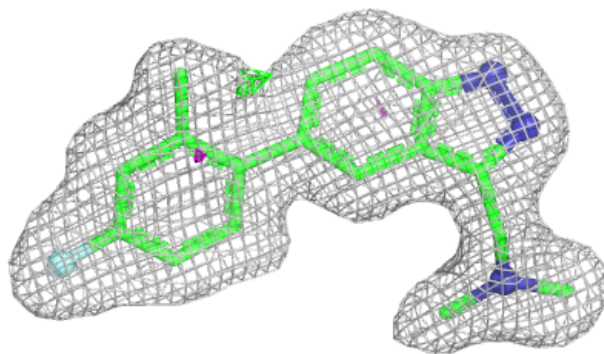
Electron density around 9K2 C 502:

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

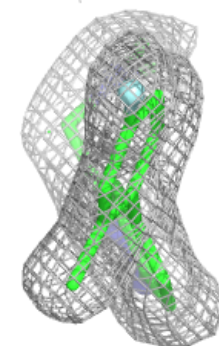
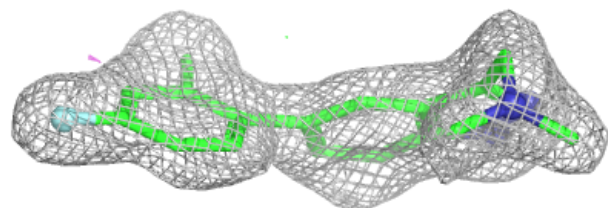
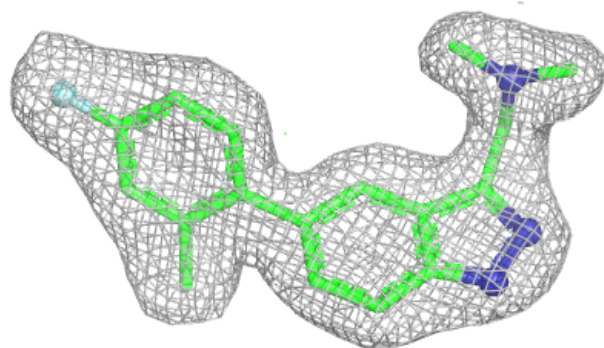


Electron density around 9K2 B 502:

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

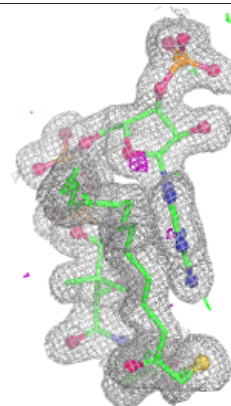
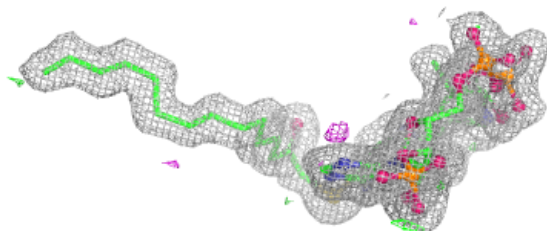
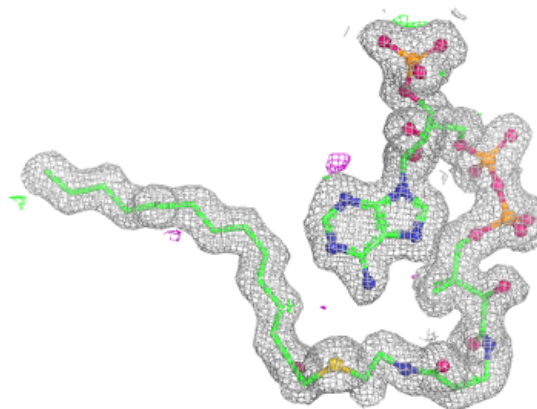
**Electron density around 9K2 A 502:**

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

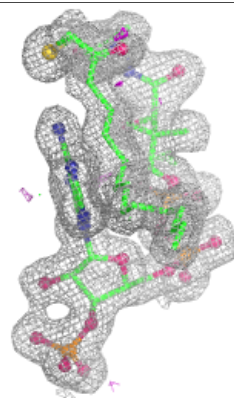
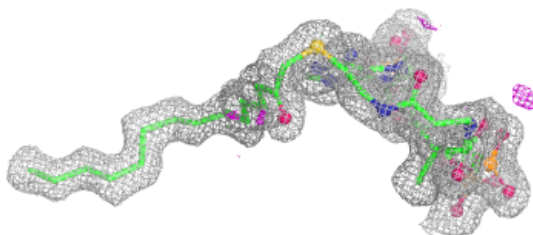
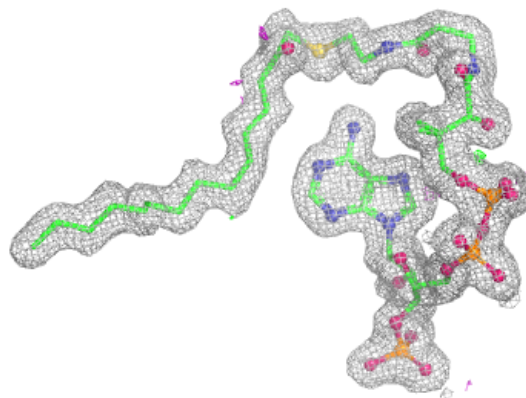


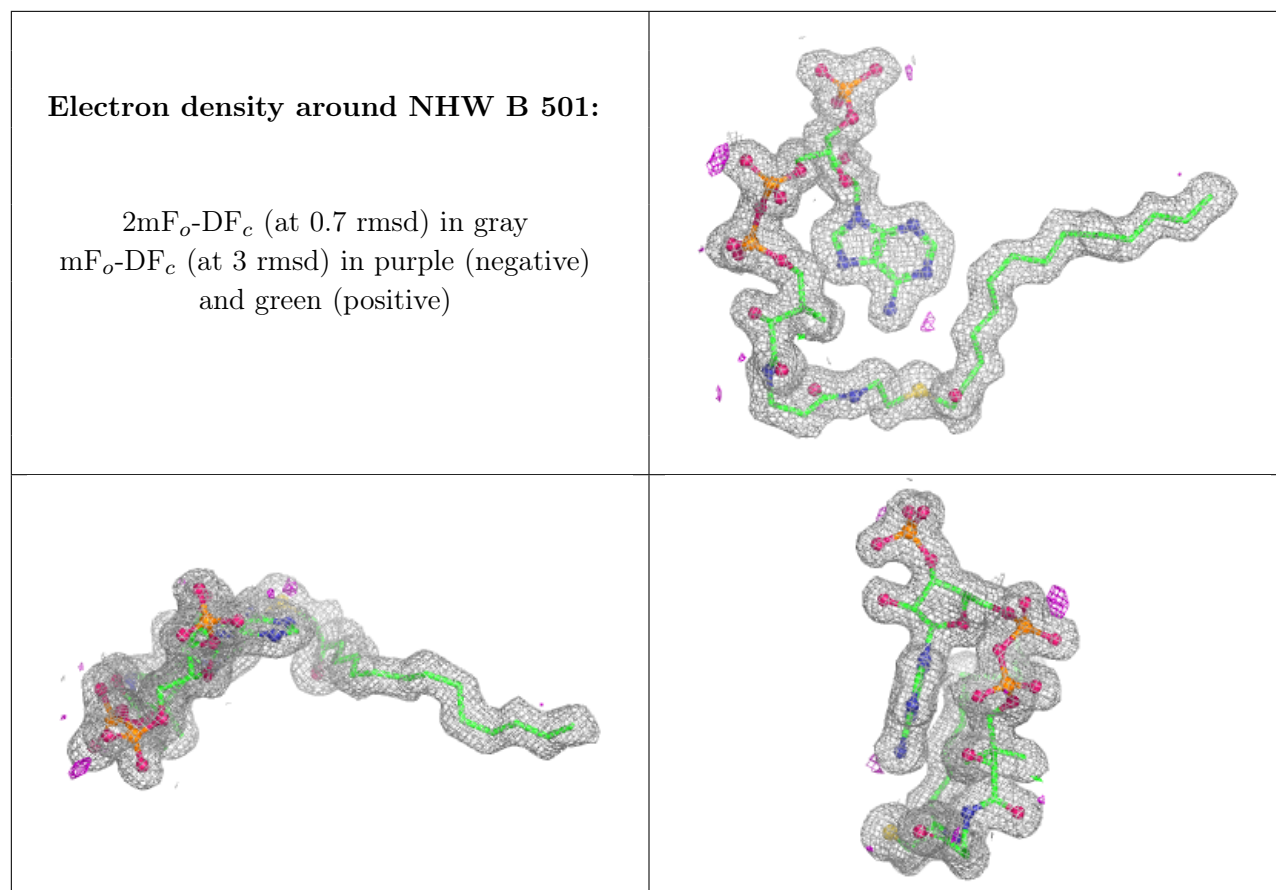
Electron density around NHW C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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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 ⓘ

There are no such residues in this entry.