



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 6TW6 / pdb_00006tw6
Title : Plasmodium vivax N-myristoyltransferase with bound indazole inhibitor IMP-923
Authors : Brannigan, J.A.
Deposited on : 2020-01-12
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

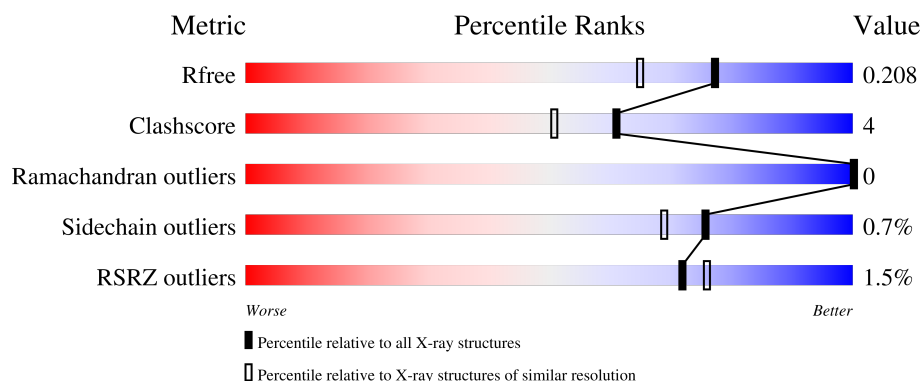
1 Overall quality at a glance

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	AAA	388	92% 7% .
1	BBB	388	90% 9% ..
1	CCC	388	2% 86% 8% 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11986 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.

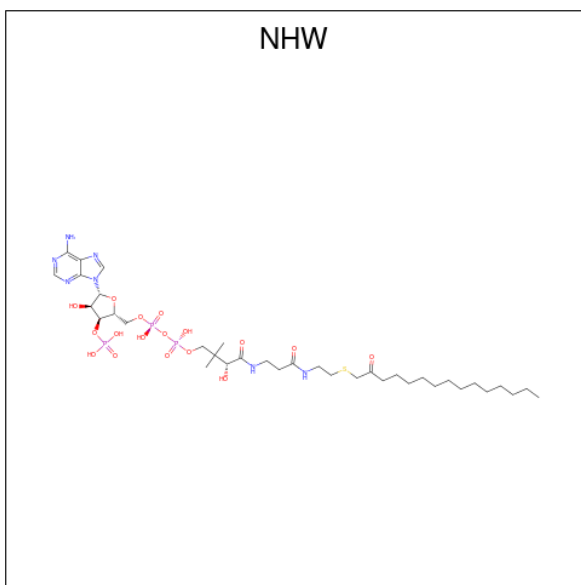
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	385	Total	C	N	O	S	0	41	0
			3427	2243	550	621	13			
1	BBB	385	Total	C	N	O	S	0	41	0
			3408	2236	541	618	13			
1	CCC	367	Total	C	N	O	S	0	33	0
			3233	2118	514	590	11			

There are 12 discrepancies between the modelled and reference sequences:

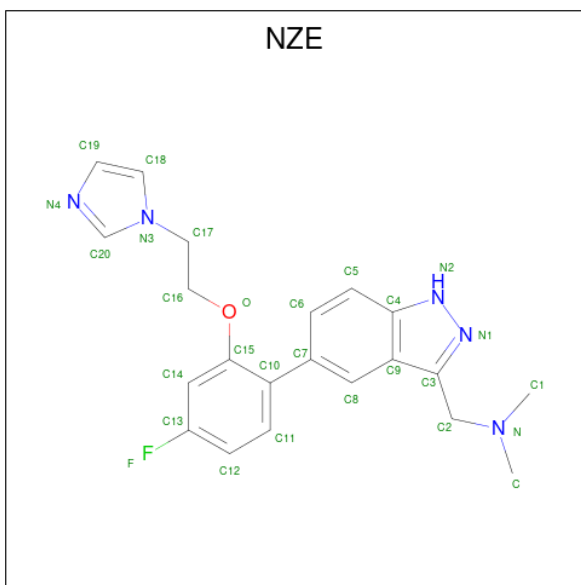
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	23	GLY	-	expression tag	UNP A5K1A2
AAA	24	PRO	-	expression tag	UNP A5K1A2
AAA	25	HIS	-	expression tag	UNP A5K1A2
AAA	26	MET	-	expression tag	UNP A5K1A2
BBB	23	GLY	-	expression tag	UNP A5K1A2
BBB	24	PRO	-	expression tag	UNP A5K1A2
BBB	25	HIS	-	expression tag	UNP A5K1A2
BBB	26	MET	-	expression tag	UNP A5K1A2
CCC	23	GLY	-	expression tag	UNP A5K1A2
CCC	24	PRO	-	expression tag	UNP A5K1A2
CCC	25	HIS	-	expression tag	UNP A5K1A2
CCC	26	MET	-	expression tag	UNP A5K1A2

- 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	AAA	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	BBB	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	CCC	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

- Molecule 3 is [(5-{4-fluoro-2-[2-(1H-imidazol-1-yl)ethoxy]phenyl}-1H-indazol-3-yl)methyl]dimethylamine (CCD ID: NZE) (formula: $C_{21}H_{22}FN_5O$) (labeled as "Ligand of Interest" by depositor).

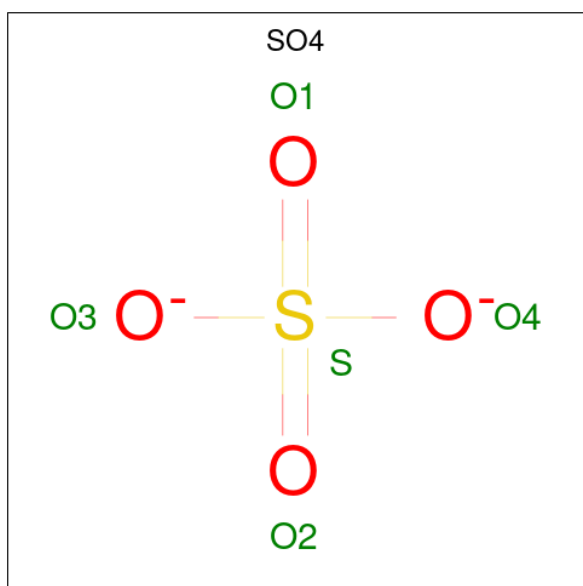


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	F	N	O	0	0
			28	21	1	5	1		
3	BBB	1	Total	C	F	N	O	0	0
			28	21	1	5	1		
3	CCC	1	Total	C	F	N	O	0	0
			28	21	1	5	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Mg	0	0
			1	1		
4	BBB	1	Total	Mg	0	0
			1	1		
4	CCC	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

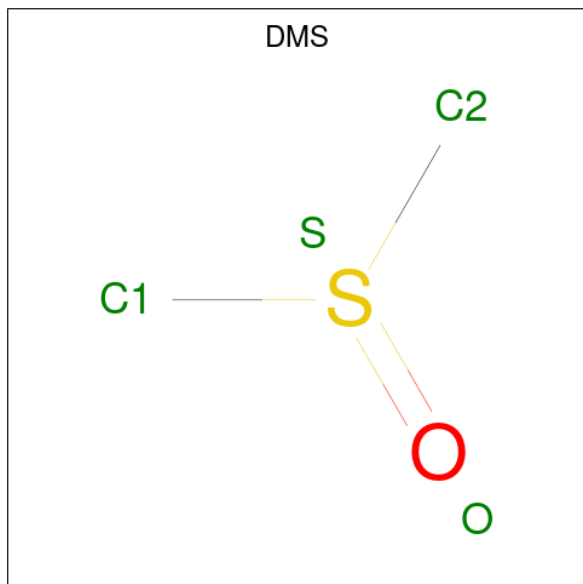


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Cl 1 1	0	0
6	BBB	1	Total Cl 1 1	0	0
6	CCC	1	Total Cl 1 1	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total C O S 4 2 1 1	0	0
7	BBB	1	Total C O S 4 2 1 1	0	0
7	CCC	1	Total C O S 4 2 1 1	0	0
7	CCC	1	Total C O S 4 2 1 1	0	0

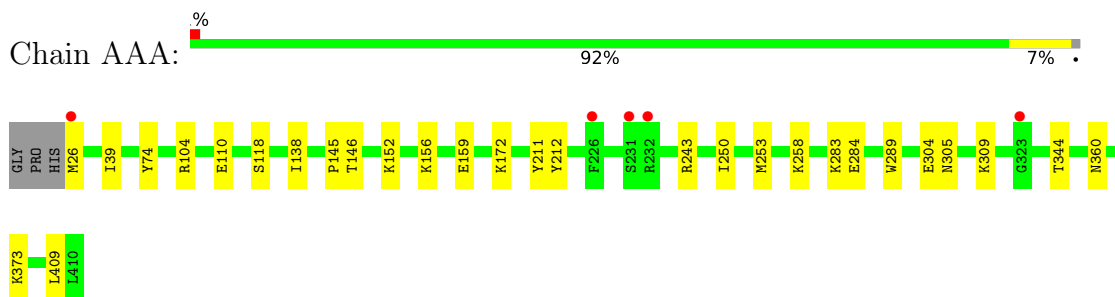
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	576	Total O 576 576	0	0
8	BBB	548	Total O 548 548	0	0
8	CCC	491	Total O 491 491	0	0

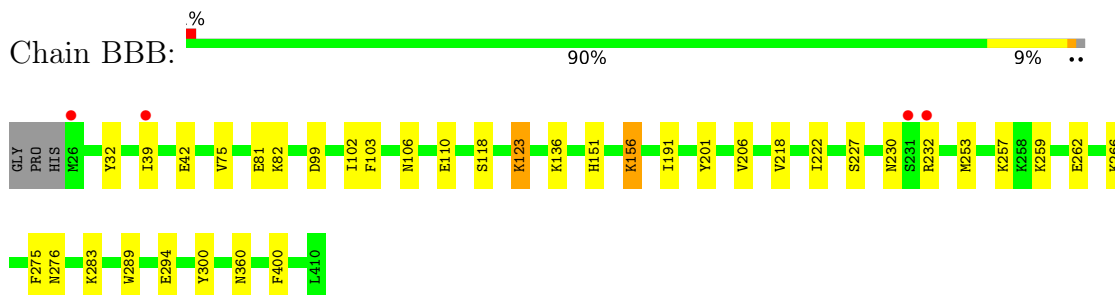
3 Residue-property plots [i](#)

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

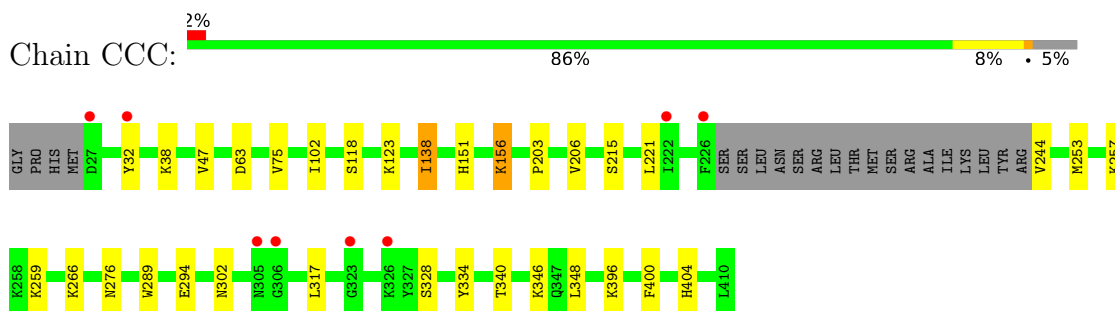
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase



- 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	57.61Å 121.78Å 178.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.38 – 1.70 50.38 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.38-1.70) 99.9 (50.38-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.168 , 0.208 0.168 , 0.208	Depositor DCC
R_{free} test set	6960 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11986	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	AAA	0.63	0/3617	0.96	2/4884 (0.0%)
1	BBB	0.67	2/3606 (0.1%)	0.96	2/4869 (0.0%)
1	CCC	0.65	3/3393 (0.1%)	0.96	3/4586 (0.1%)
All	All	0.65	5/10616 (0.0%)	0.96	7/14339 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	156[A]	LYS	C-O	6.05	1.31	1.24
1	BBB	156[B]	LYS	C-O	6.05	1.31	1.24
1	CCC	404	HIS	CE1-NE2	5.53	1.38	1.32
1	CCC	156[A]	LYS	C-O	5.52	1.30	1.24
1	CCC	156[B]	LYS	C-O	5.52	1.30	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	138	ILE	N-CA-C	-5.79	107.48	113.10
1	BBB	99	ASP	CA-CB-CG	5.48	118.08	112.60
1	AAA	74	TYR	CA-C-N	-5.40	115.62	122.43
1	AAA	74	TYR	C-N-CA	-5.40	115.62	122.43
1	BBB	275	PHE	CA-CB-CG	-5.08	108.72	113.80
1	CCC	203	PRO	CB-CA-C	-5.03	106.82	111.40
1	CCC	63	ASP	CA-CB-CG	5.01	117.61	112.60

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	AAA	3427	0	3520	33	0
1	BBB	3408	0	3520	33	0
1	CCC	3233	0	3287	21	0
2	AAA	64	0	60	0	0
2	BBB	64	0	60	0	0
2	CCC	64	0	60	0	0
3	AAA	28	0	0	0	0
3	BBB	28	0	0	0	0
3	CCC	28	0	0	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
5	AAA	5	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
7	AAA	4	0	6	0	0
7	BBB	4	0	6	0	0
7	CCC	8	0	8	2	0
8	AAA	576	0	0	9	0
8	BBB	548	0	0	14	0
8	CCC	491	0	0	6	0
All	All	11986	0	10527	87	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 (87) 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:AAA:304[A]:GLU:OE1	1:AAA:309[A]:LYS:HE2	1.46	1.12
1:CCC:151[A]:HIS:CE1	1:CCC:276[A]:ASN:OD1	2.22	0.93
1:AAA:243[A]:ARG:HD3	8:AAA:837:HOH:O	1.68	0.93
1:AAA:146:THR:HG21	1:AAA:159[B]:GLU:HG3	1.55	0.89
1:AAA:159[A]:GLU:CD	1:AAA:409[A]:LEU:HD22	1.97	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:304[A]:GLU:OE1	1:AAA:309[A]:LYS:CE	2.23	0.85
1:AAA:26:MET:HA	1:AAA:26:MET:HE2	1.59	0.84
1:BBB:82[B]:LYS:HG3	8:BBB:649:HOH:O	1.80	0.81
1:BBB:110[A]:GLU:HG2	8:BBB:1034:HOH:O	1.80	0.81
1:AAA:146:THR:CG2	1:AAA:159[B]:GLU:HG3	2.10	0.81
1:AAA:110:GLU:HG3	8:AAA:1085:HOH:O	1.81	0.80
1:BBB:32[A]:TYR:CD1	8:BBB:994:HOH:O	2.37	0.76
1:BBB:156[B]:LYS:HE2	1:BBB:191:ILE:HD11	1.68	0.75
7:CCC:506:DMS:H11	8:CCC:641:HOH:O	1.90	0.71
1:CCC:151[A]:HIS:ND1	1:CCC:276[A]:ASN:ND2	2.39	0.69
1:CCC:32[A]:TYR:CE1	1:CCC:38:LYS:HE3	2.28	0.69
1:AAA:159[A]:GLU:OE2	1:AAA:409[A]:LEU:HD22	1.92	0.68
1:AAA:159[A]:GLU:CD	1:AAA:409[A]:LEU:CD2	2.69	0.64
1:BBB:206[B]:VAL:HG22	1:BBB:400:PHE:CE1	2.33	0.63
1:AAA:146:THR:HG21	1:AAA:159[B]:GLU:CG	2.27	0.62
1:CCC:257[B]:LYS:HD3	1:CCC:259[B]:LYS:HE2	1.82	0.61
1:BBB:262[A]:GLU:OE2	1:BBB:266[A]:LYS:NZ	2.30	0.61
1:BBB:266[B]:LYS:HE2	8:BBB:1045:HOH:O	2.01	0.60
1:CCC:215:SER:HB3	1:CCC:221:LEU:HD12	1.83	0.60
1:AAA:360[A]:ASN:ND2	8:AAA:611:HOH:O	2.36	0.59
1:BBB:82[B]:LYS:HD2	8:BBB:649:HOH:O	2.03	0.57
1:CCC:156[A]:LYS:HE2	8:CCC:994:HOH:O	2.05	0.57
1:CCC:266[B]:LYS:HG3	8:CCC:909:HOH:O	2.05	0.57
1:AAA:104[B]:ARG:NH2	8:AAA:609:HOH:O	2.32	0.57
1:AAA:258[A]:LYS:HG3	8:AAA:978:HOH:O	2.05	0.56
1:AAA:159[A]:GLU:OE1	1:AAA:409[A]:LEU:CD2	2.52	0.56
1:AAA:243[B]:ARG:HD3	8:AAA:837:HOH:O	2.06	0.56
1:AAA:159[A]:GLU:OE1	1:AAA:409[A]:LEU:HD21	2.06	0.55
1:BBB:102[B]:ILE:HG13	1:BBB:103:PHE:CE2	2.41	0.55
1:BBB:32[A]:TYR:CE1	8:BBB:994:HOH:O	2.59	0.54
1:AAA:344:THR:HG21	1:BBB:42[A]:GLU:HG2	1.89	0.54
1:AAA:344:THR:HG21	1:BBB:42[A]:GLU:CG	2.39	0.53
1:CCC:47:VAL:CG1	1:CCC:396[A]:LYS:HG2	2.39	0.53
1:BBB:230:ASN:OD1	1:BBB:232:ARG:HG2	2.10	0.52
1:BBB:136:LYS:NZ	8:BBB:612:HOH:O	2.42	0.51
1:AAA:284[B]:GLU:HG2	8:AAA:635:HOH:O	2.11	0.51
1:CCC:47:VAL:HG11	1:CCC:396[A]:LYS:HG2	1.92	0.50
1:BBB:257:LYS:HE3	8:BBB:774:HOH:O	2.11	0.50
1:AAA:146:THR:HG22	1:AAA:159[B]:GLU:HG3	1.93	0.50
1:BBB:259[B]:LYS:HE3	8:BBB:1023:HOH:O	2.11	0.50
1:BBB:39:ILE:HD11	1:BBB:201:TYR:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:266[A]:LYS:HG3	8:BBB:977:HOH:O	2.11	0.49
1:BBB:82[B]:LYS:CD	8:BBB:649:HOH:O	2.58	0.49
1:BBB:294[B]:GLU:HG2	8:BBB:1047:HOH:O	2.12	0.48
1:BBB:262[B]:GLU:HG3	1:BBB:283[B]:LYS:HE3	1.95	0.48
1:AAA:26:MET:HA	1:AAA:26:MET:CE	2.37	0.48
1:BBB:360:ASN:ND2	8:BBB:614:HOH:O	2.45	0.47
1:CCC:151[A]:HIS:CE1	1:CCC:276[A]:ASN:CG	2.92	0.47
1:AAA:145:PRO:HB2	1:AAA:156[B]:LYS:HE3	1.96	0.46
7:CCC:506:DMS:H21	8:CCC:641:HOH:O	2.15	0.46
1:BBB:253[A]:MET:HG3	1:BBB:300:TYR:HB3	1.97	0.46
1:AAA:250:ILE:HB	1:AAA:253[B]:MET:HG2	1.97	0.46
1:BBB:230:ASN:OD1	1:BBB:232:ARG:CG	2.64	0.46
1:CCC:346:LYS:HE2	8:CCC:1026:HOH:O	2.15	0.45
1:BBB:75:VAL:HG12	1:BBB:123[B]:LYS:HE2	1.98	0.45
1:CCC:118:SER:HB3	1:CCC:289:TRP:CZ2	2.51	0.45
1:AAA:172:LYS:HG2	8:AAA:736:HOH:O	2.17	0.45
1:AAA:138:ILE:HD12	1:AAA:138:ILE:C	2.42	0.44
1:CCC:215:SER:CB	1:CCC:221:LEU:HD12	2.48	0.44
1:CCC:138:ILE:C	1:CCC:138:ILE:HD12	2.42	0.44
1:CCC:317:LEU:HB3	1:CCC:334:TYR:CE1	2.52	0.44
1:AAA:118:SER:HB3	1:AAA:289:TRP:CZ2	2.54	0.43
1:CCC:32[A]:TYR:CD1	1:CCC:38:LYS:HE3	2.54	0.43
1:CCC:75:VAL:HG12	1:CCC:123[B]:LYS:HE2	2.00	0.43
1:BBB:218:VAL:O	1:BBB:222[A]:ILE:HG12	2.18	0.43
1:BBB:151[B]:HIS:HA	1:BBB:276[B]:ASN:OD1	2.19	0.43
1:CCC:102:ILE:HG23	8:CCC:633:HOH:O	2.17	0.43
1:BBB:82[B]:LYS:CG	8:BBB:649:HOH:O	2.49	0.43
1:BBB:276[B]:ASN:ND2	1:BBB:400:PHE:CE1	2.87	0.42
1:AAA:304[A]:GLU:CB	1:AAA:309[A]:LYS:HE2	2.50	0.42
1:BBB:156[B]:LYS:HG2	1:BBB:191:ILE:HG12	2.02	0.42
1:BBB:102[B]:ILE:HG13	1:BBB:103:PHE:CD2	2.55	0.41
1:AAA:39:ILE:HD13	1:AAA:39:ILE:HA	1.77	0.41
1:AAA:212:TYR:OH	1:AAA:373[B]:LYS:HE2	2.21	0.41
1:AAA:283[A]:LYS:NZ	8:AAA:626:HOH:O	2.51	0.41
1:CCC:340:THR:HB	1:CCC:348:LEU:HD22	2.01	0.41
1:BBB:222[A]:ILE:HD13	1:BBB:227:SER:HB2	2.02	0.41
1:BBB:118:SER:HB3	1:BBB:289:TRP:CZ2	2.56	0.40
1:CCC:206[B]:VAL:HG22	1:CCC:400:PHE:CE2	2.57	0.40
1:CCC:253[B]:MET:SD	1:CCC:302:ASN:HB2	2.61	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	AAA	424/388 (109%)	415 (98%)	9 (2%)	0	100	100
1	BBB	424/388 (109%)	416 (98%)	8 (2%)	0	100	100
1	CCC	396/388 (102%)	385 (97%)	11 (3%)	0	100	100
All	All	1244/1164 (107%)	1216 (98%)	28 (2%)	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	AAA	392/353 (111%)	391 (100%)	1 (0%)	86	83
1	BBB	392/353 (111%)	388 (99%)	4 (1%)	68	58
1	CCC	367/353 (104%)	363 (99%)	4 (1%)	65	54
All	All	1151/1059 (109%)	1142 (99%)	9 (1%)	76	65

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	211	TYR
1	BBB	81	GLU
1	BBB	106	ASN
1	BBB	123[A]	LYS
1	BBB	123[B]	LYS

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Mol	Chain	Res	Type
1	CCC	244	VAL
1	CCC	294[A]	GLU
1	CCC	294[B]	GLU
1	CCC	328	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	DMS	CCC	505	7	3,3,3	0.22	0	3,3,3	0.24	0
5	SO4	AAA	504	-	4,4,4	0.43	0	6,6,6	0.41	0
2	NHW	BBB	501	4	64,66,66	1.47	9 (14%)	87,92,92	1.42	12 (13%)
7	DMS	BBB	505	-	3,3,3	0.85	0	3,3,3	0.44	0
3	NZE	AAA	502	-	31,31,31	1.50	5 (16%)	40,43,43	2.12	15 (37%)
2	NHW	CCC	501	4	64,66,66	1.52	9 (14%)	87,92,92	1.78	13 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NHW	AAA	501	4	64,66,66	1.28	7 (10%)	87,92,92	1.69	18 (20%)
3	NZE	CCC	502	-	31,31,31	1.73	5 (16%)	40,43,43	1.86	14 (35%)
7	DMS	AAA	506	-	3,3,3	0.53	0	3,3,3	0.38	0
3	NZE	BBB	502	-	31,31,31	1.87	8 (25%)	40,43,43	2.07	13 (32%)
7	DMS	CCC	506	7	3,3,3	0.38	0	3,3,3	0.11	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
2	NHW	BBB	501	4	-	4/65/81/81	0/3/3/3
3	NZE	AAA	502	-	-	0/14/14/14	0/4/4/4
2	NHW	CCC	501	4	-	3/65/81/81	0/3/3/3
2	NHW	AAA	501	4	-	1/65/81/81	0/3/3/3
3	NZE	CCC	502	-	-	0/14/14/14	0/4/4/4
3	NZE	BBB	502	-	-	0/14/14/14	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	501	NHW	P1A-O3A	6.79	1.66	1.59
3	BBB	502	NZE	C10-C15	5.85	1.52	1.40
3	CCC	502	NZE	C9-C4	5.46	1.48	1.41
2	BBB	501	NHW	P2A-O3A	-4.92	1.54	1.59
3	BBB	502	NZE	C9-C4	4.71	1.47	1.41
3	CCC	502	NZE	C10-C15	4.59	1.49	1.40
2	BBB	501	NHW	P1A-O3A	4.40	1.64	1.59
2	CCC	501	NHW	P2A-O3A	-3.97	1.55	1.59
2	BBB	501	NHW	P3X-O3X	3.40	1.65	1.59
3	AAA	502	NZE	C10-C15	3.35	1.47	1.40
2	AAA	501	NHW	CP-C1M	3.12	1.56	1.51
2	BBB	501	NHW	CP-C1M	2.96	1.56	1.51
3	AAA	502	NZE	C3-N1	2.90	1.35	1.29
3	AAA	502	NZE	C9-C4	2.89	1.45	1.41
3	BBB	502	NZE	C3-N1	2.85	1.35	1.29
2	CCC	501	NHW	P3X-O3X	2.83	1.64	1.59
2	AAA	501	NHW	O4X-C4X	2.74	1.51	1.45
2	BBB	501	NHW	C12-C11	2.73	1.57	1.52
2	CCC	501	NHW	C1X-N9A	2.65	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	502	NZE	N2-N1	2.62	1.42	1.36
3	CCC	502	NZE	C20-N4	2.56	1.38	1.32
2	BBB	501	NHW	C8A-N7A	2.55	1.36	1.31
2	AAA	501	NHW	C7-C6	2.54	1.59	1.51
2	AAA	501	NHW	P1A-O3A	2.50	1.62	1.59
2	CCC	501	NHW	C2A-N3A	-2.49	1.29	1.33
2	AAA	501	NHW	C12-C11	2.43	1.56	1.52
3	AAA	502	NZE	C18-C19	2.40	1.40	1.35
3	CCC	502	NZE	C3-N1	2.40	1.34	1.29
2	BBB	501	NHW	C6-C5	2.34	1.56	1.51
2	BBB	501	NHW	O10-C10	2.29	1.46	1.42
2	CCC	501	NHW	P2A-O5A	-2.28	1.42	1.50
3	BBB	502	NZE	C20-N4	2.27	1.38	1.32
3	BBB	502	NZE	C6-C5	2.25	1.42	1.38
3	AAA	502	NZE	C20-N4	2.22	1.37	1.32
3	BBB	502	NZE	C18-C19	2.18	1.40	1.35
3	BBB	502	NZE	C12-C13	2.14	1.41	1.37
2	CCC	501	NHW	C5X-C4X	2.09	1.57	1.51
2	AAA	501	NHW	O2X-C2X	2.08	1.48	1.43
2	CCC	501	NHW	CP-S1	2.07	1.86	1.81
2	CCC	501	NHW	C3-N4	2.05	1.50	1.46
2	AAA	501	NHW	C5A-N7A	-2.03	1.35	1.39
3	CCC	502	NZE	C2-C3	2.02	1.53	1.51
2	BBB	501	NHW	CP-S1	2.01	1.86	1.81

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	501	NHW	N3A-C2A-N1A	-6.01	119.48	128.58
2	CCC	501	NHW	C5A-C4A-N3A	-5.75	118.80	126.72
2	CCC	501	NHW	O4X-C1X-C2X	-5.21	95.47	106.62
2	BBB	501	NHW	N3A-C2A-N1A	-5.09	120.88	128.58
2	AAA	501	NHW	C5A-C4A-N3A	-5.05	119.77	126.72
2	CCC	501	NHW	P3X-O3X-C3X	-4.89	110.37	123.43
3	BBB	502	NZE	C8-C9-C4	4.89	124.15	119.39
2	CCC	501	NHW	O4X-C4X-C5X	-4.89	93.67	109.33
3	AAA	502	NZE	C2-C3-N1	4.75	125.18	119.81
3	BBB	502	NZE	C11-C10-C15	4.62	124.10	117.40
2	AAA	501	NHW	C4A-C5A-N7A	-4.60	105.33	110.58
3	AAA	502	NZE	C11-C12-C13	-4.55	113.70	118.38
2	CCC	501	NHW	C2A-N3A-C4A	4.52	122.86	111.83
3	BBB	502	NZE	C5-C4-C9	-4.50	117.84	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	501	NHW	C5A-C4A-N3A	-4.34	120.73	126.72
3	AAA	502	NZE	C11-C10-C15	4.14	123.41	117.40
2	CCC	501	NHW	N3A-C4A-N9A	4.00	133.97	127.17
3	AAA	502	NZE	C12-C13-C14	3.79	128.24	123.23
2	AAA	501	NHW	C6-C5-N4	-3.72	109.56	116.34
3	CCC	502	NZE	C2-C3-N1	3.68	123.97	119.81
3	BBB	502	NZE	C16-O-C15	3.68	126.56	117.69
2	AAA	501	NHW	C5A-N7A-C8A	3.65	109.18	103.45
3	AAA	502	NZE	C6-C7-C8	3.47	123.01	118.23
2	AAA	501	NHW	N9A-C8A-N7A	-3.45	109.03	113.94
2	AAA	501	NHW	O1M-C1M-CP	-3.37	117.37	122.17
3	CCC	502	NZE	C8-C9-C4	3.33	122.64	119.39
3	CCC	502	NZE	C11-C10-C15	3.32	122.22	117.40
2	AAA	501	NHW	CP-C1M-C2M	3.30	122.52	115.55
3	BBB	502	NZE	C6-C7-C8	3.26	122.72	118.23
3	CCC	502	NZE	C3-N1-N2	3.23	111.88	105.03
2	AAA	501	NHW	N3A-C2A-N1A	-3.17	123.78	128.58
3	BBB	502	NZE	C9-C8-C7	-3.14	114.99	120.82
3	BBB	502	NZE	C8-C9-C3	-3.14	129.15	136.17
3	BBB	502	NZE	C7-C10-C15	-3.10	116.14	122.42
2	BBB	501	NHW	C2A-N3A-C4A	3.10	119.41	111.83
3	CCC	502	NZE	C6-C7-C8	2.94	122.28	118.23
2	AAA	501	NHW	C2-S1-CP	-2.94	96.87	101.72
3	BBB	502	NZE	F-C13-C12	-2.92	113.88	118.55
3	AAA	502	NZE	C14-C15-C10	-2.92	114.97	120.75
2	BBB	501	NHW	P3X-O3X-C3X	-2.91	115.66	123.43
3	CCC	502	NZE	C8-C7-C10	-2.90	115.74	120.61
2	BBB	501	NHW	O2A-P1A-O3A	2.90	115.11	107.27
3	AAA	502	NZE	C16-O-C15	2.89	124.65	117.69
2	AAA	501	NHW	C5A-C4A-N9A	2.88	108.95	105.81
3	CCC	502	NZE	C7-C10-C15	-2.86	116.63	122.42
2	CCC	501	NHW	C5A-N7A-C8A	2.83	107.90	103.45
2	CCC	501	NHW	N9A-C8A-N7A	-2.81	109.95	113.94
3	AAA	502	NZE	F-C13-C12	-2.76	114.13	118.55
2	AAA	501	NHW	C2A-N3A-C4A	2.74	118.52	111.83
3	CCC	502	NZE	C5-C4-C9	-2.72	119.55	122.19
3	CCC	502	NZE	C9-C8-C7	-2.72	115.77	120.82
2	AAA	501	NHW	C6A-C5A-C4A	2.72	120.89	117.18
3	AAA	502	NZE	C7-C10-C15	-2.71	116.94	122.42
2	BBB	501	NHW	N3A-C4A-N9A	2.66	131.69	127.17
3	AAA	502	NZE	C9-C8-C7	-2.62	115.95	120.82
3	AAA	502	NZE	C3-N1-N2	2.61	110.57	105.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	502	NZE	C1-N-C2	2.55	114.55	110.38
2	CCC	501	NHW	C4A-C5A-N7A	-2.50	107.73	110.58
3	CCC	502	NZE	C-N-C2	2.48	114.43	110.38
2	AAA	501	NHW	P3X-O3X-C3X	-2.48	116.82	123.43
3	BBB	502	NZE	C12-C13-C14	2.46	126.49	123.23
3	AAA	502	NZE	C8-C7-C10	-2.46	116.48	120.61
3	CCC	502	NZE	C16-O-C15	2.43	123.56	117.69
3	AAA	502	NZE	C8-C9-C4	2.43	121.75	119.39
2	AAA	501	NHW	C2-C3-N4	-2.39	107.42	112.41
2	BBB	501	NHW	C2A-N1A-C6A	2.39	122.66	118.73
2	AAA	501	NHW	N3A-C4A-N9A	2.38	131.21	127.17
3	BBB	502	NZE	C12-C11-C10	-2.36	116.27	120.33
2	CCC	501	NHW	C2A-N1A-C6A	2.34	122.58	118.73
2	BBB	501	NHW	O4X-C1X-C2X	-2.31	101.67	106.62
3	CCC	502	NZE	C4-N2-N1	-2.31	110.19	111.90
3	CCC	502	NZE	C8-C9-C3	-2.27	131.09	136.17
2	AAA	501	NHW	C14-C11-C12	-2.24	104.53	108.22
3	BBB	502	NZE	C2-C3-N1	2.21	122.31	119.81
2	BBB	501	NHW	O3A-P1A-O1A	-2.20	104.09	110.70
2	BBB	501	NHW	O5-C5-N4	2.20	127.34	123.03
2	BBB	501	NHW	N9A-C8A-N7A	-2.17	110.85	113.94
2	AAA	501	NHW	C14-C11-C13	2.16	113.52	109.20
3	AAA	502	NZE	C19-C18-N3	2.16	110.12	106.57
2	AAA	501	NHW	O4A-P2A-O3A	-2.14	101.49	107.27
2	BBB	501	NHW	O6A-C12-C11	-2.12	107.14	110.55
2	CCC	501	NHW	C3M-C2M-C1M	-2.12	109.22	114.59
3	BBB	502	NZE	C3-N1-N2	2.10	109.49	105.03
2	CCC	501	NHW	C2-C3-N4	-2.01	108.21	112.41
3	CCC	502	NZE	C14-C15-C10	-2.00	116.78	120.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

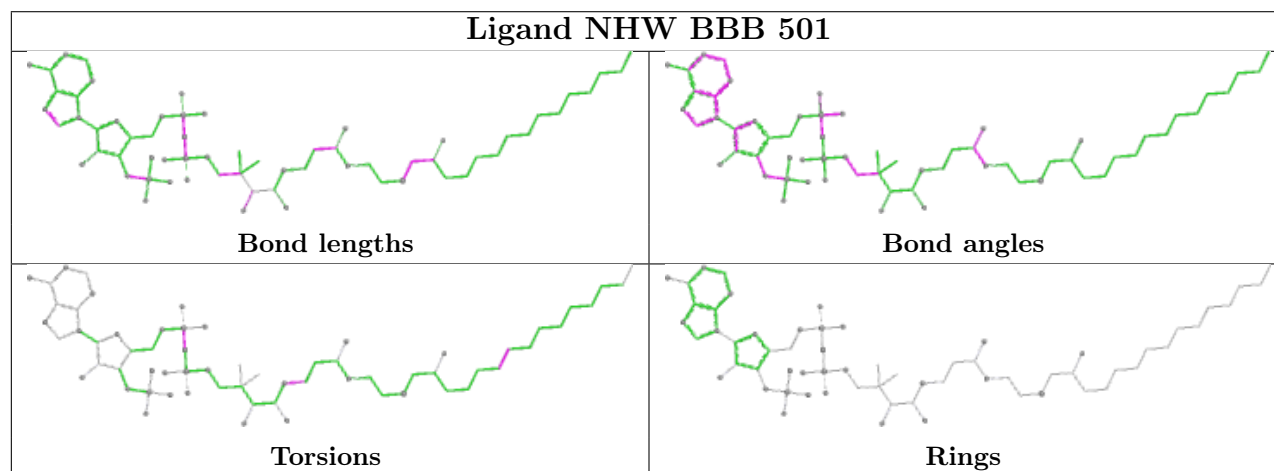
Mol	Chain	Res	Type	Atoms
2	BBB	501	NHW	C4M-C5M-C6M-C7M
2	BBB	501	NHW	C6-C7-N8-C9
2	AAA	501	NHW	C4M-C5M-C6M-C7M
2	BBB	501	NHW	P2A-O3A-P1A-O1A
2	BBB	501	NHW	P2A-O3A-P1A-O2A
2	CCC	501	NHW	P2A-O3A-P1A-O1A
2	CCC	501	NHW	C6-C7-N8-C9
2	CCC	501	NHW	P2A-O3A-P1A-O2A

There are no ring outliers.

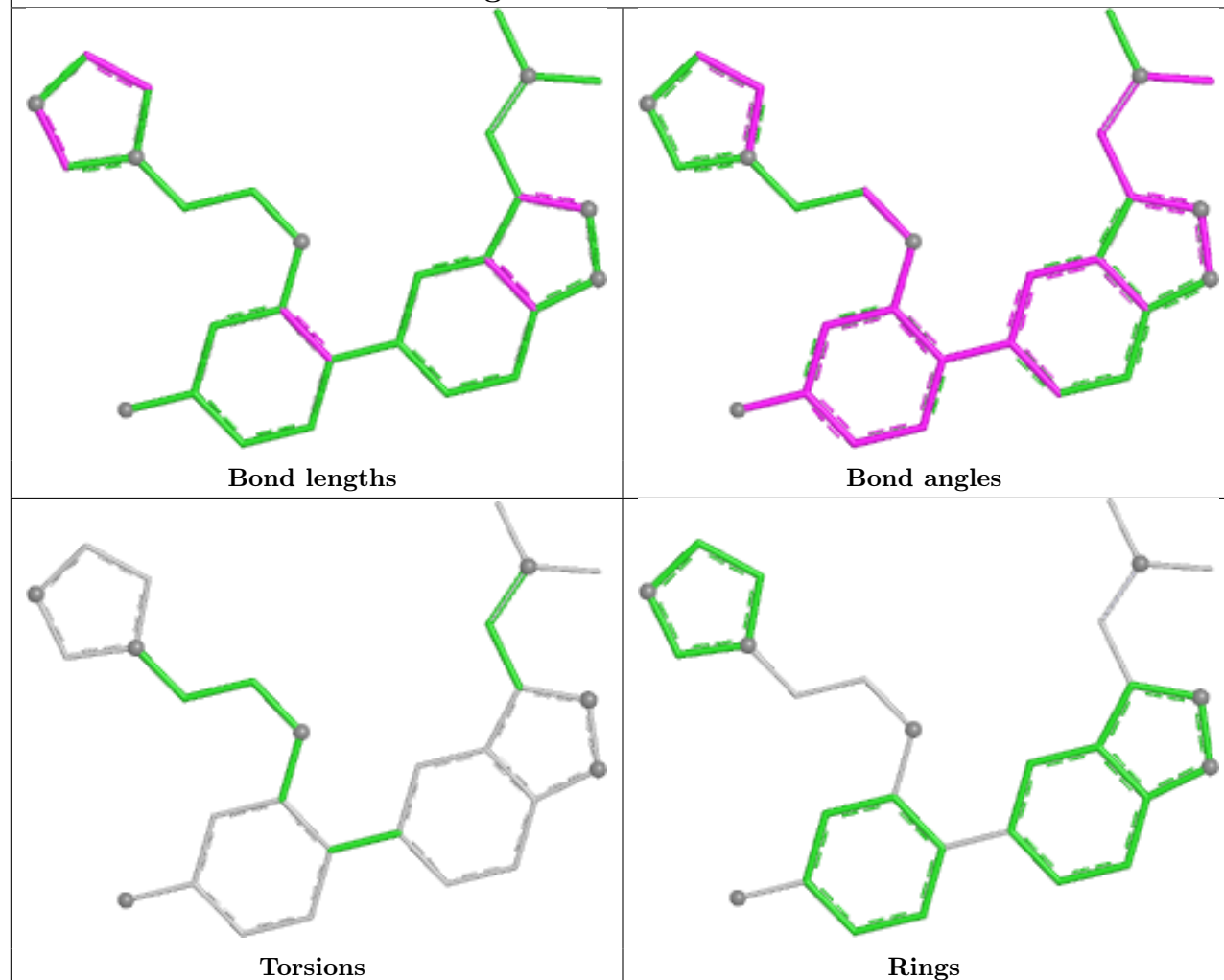
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	CCC	506	DMS	2	0

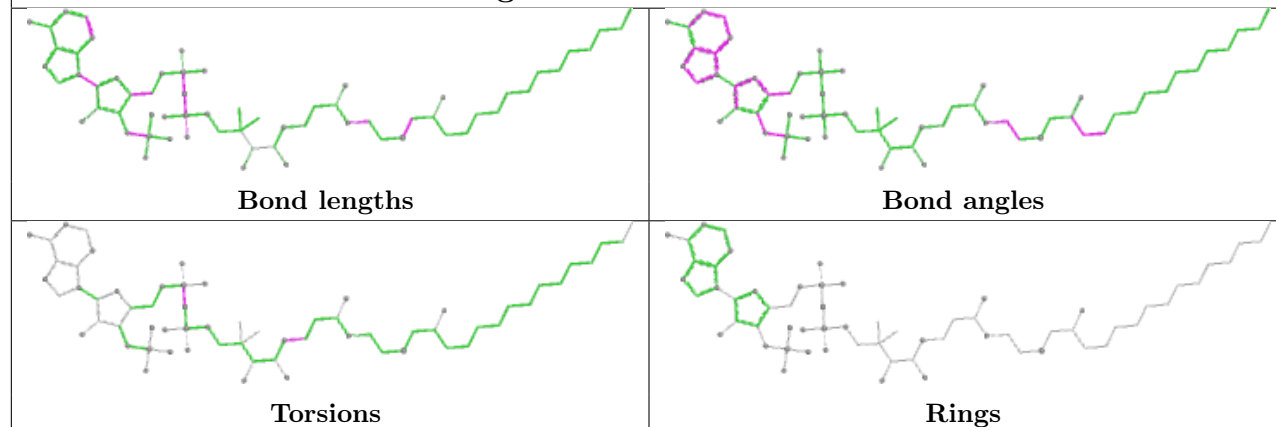
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

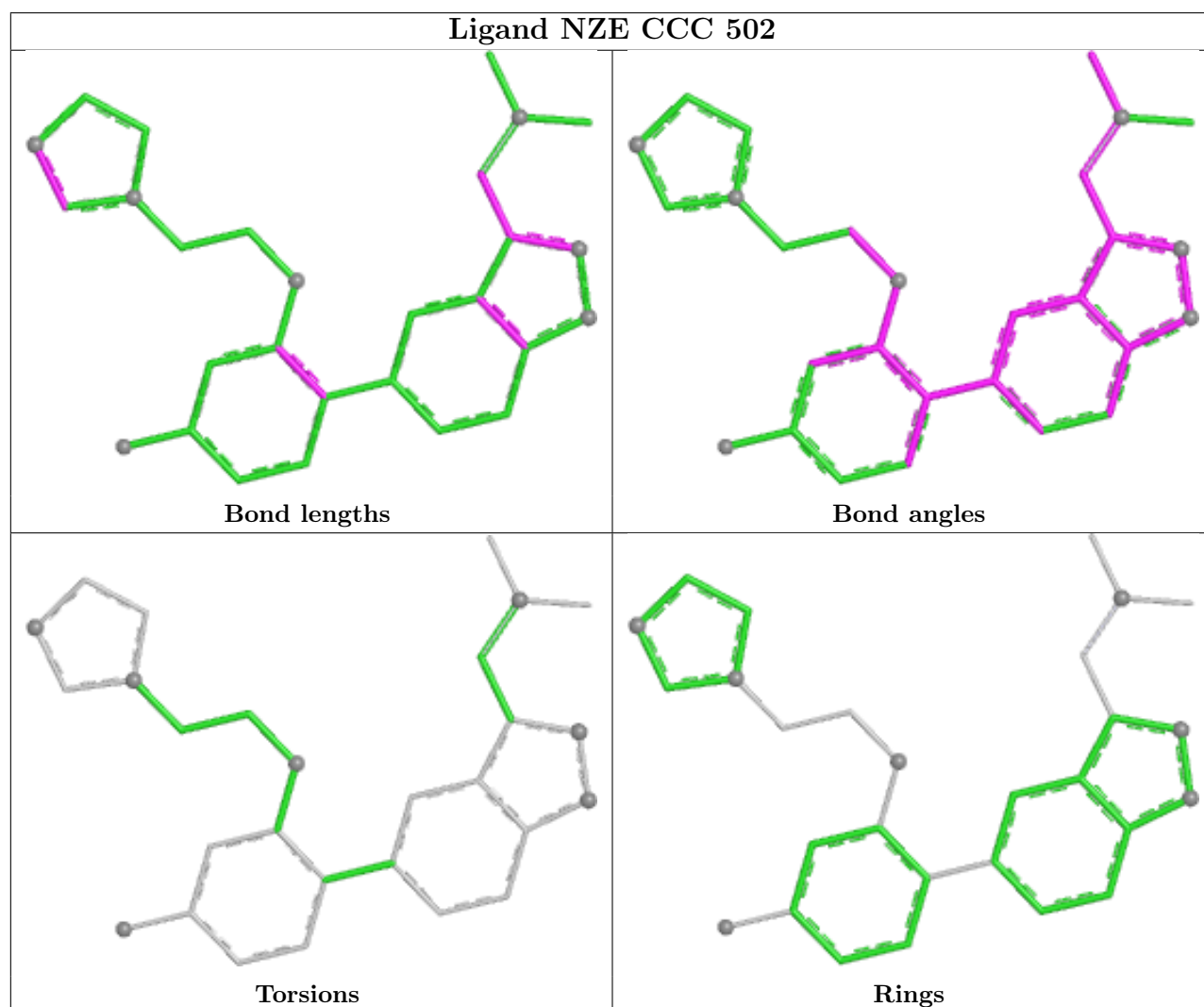
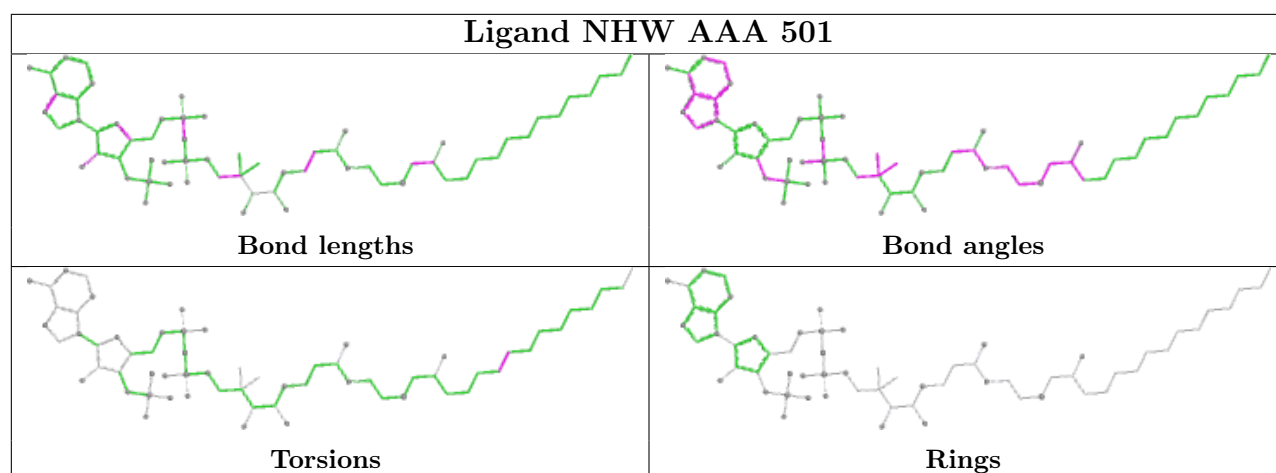


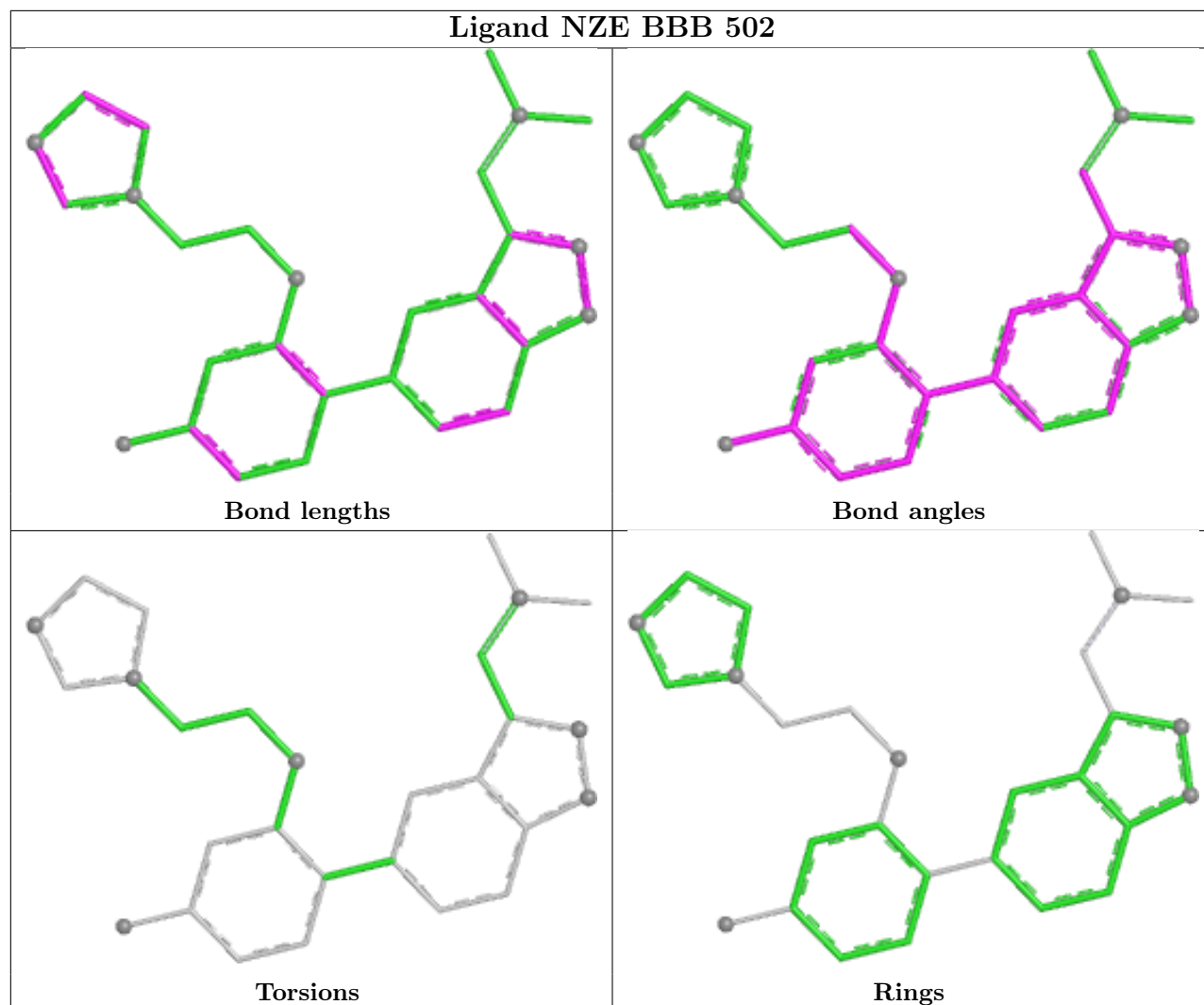
Ligand NZE AAA 502



Ligand NHW CCC 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	AAA	385/388 (99%)	-0.52	5 (1%) 75 79	6, 12, 23, 40	52 (13%)
1	BBB	385/388 (99%)	-0.58	4 (1%) 79 82	6, 11, 24, 42	55 (14%)
1	CCC	367/388 (94%)	-0.40	8 (2%) 62 66	6, 14, 27, 39	52 (14%)
All	All	1137/1164 (97%)	-0.50	17 (1%) 72 76	6, 12, 26, 42	159 (13%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	222	ILE	4.9
1	CCC	32[A]	TYR	4.5
1	BBB	232	ARG	4.2
1	AAA	26	MET	4.0
1	BBB	26	MET	3.6
1	AAA	232	ARG	2.9
1	CCC	323	GLY	2.8
1	AAA	226	PHE	2.8
1	CCC	27	ASP	2.6
1	AAA	231	SER	2.6
1	CCC	326[A]	LYS	2.5
1	CCC	305	ASN	2.3
1	CCC	306	GLY	2.3
1	AAA	323	GLY	2.2
1	BBB	231[A]	SER	2.1
1	BBB	39	ILE	2.0
1	CCC	226	PHE	2.0

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 ⓘ

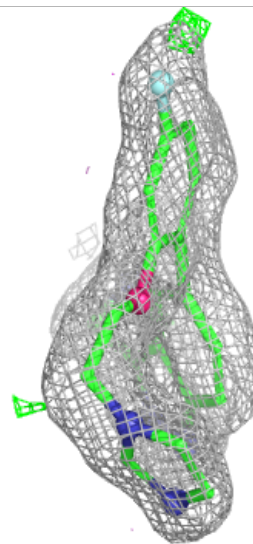
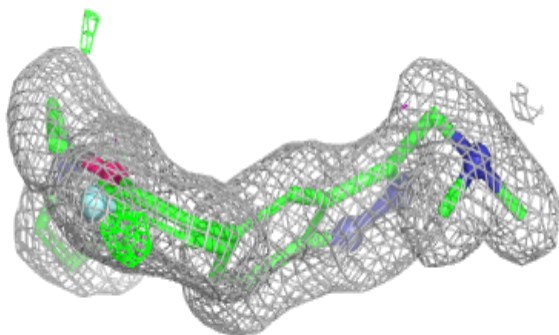
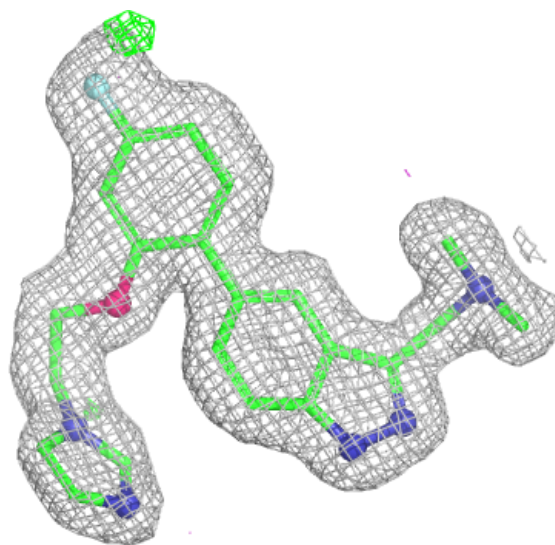
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	DMS	AAA	506	4/4	0.78	0.19	12,13,15,23	4
7	DMS	CCC	505	4/4	0.78	0.22	23,28,33,35	4
7	DMS	CCC	506	4/4	0.82	0.25	30,32,32,38	4
7	DMS	BBB	505	4/4	0.84	0.19	13,14,17,23	4
5	SO4	AAA	504	5/5	0.87	0.13	42,43,43,50	0
3	NZE	CCC	502	28/28	0.95	0.07	14,19,32,35	0
3	NZE	AAA	502	28/28	0.95	0.07	12,15,27,31	0
3	NZE	BBB	502	28/28	0.95	0.08	11,13,28,29	0
4	MG	BBB	503	1/1	0.98	0.04	22,22,22,22	0
2	NHW	CCC	501	64/64	0.99	0.04	8,12,16,18	0
2	NHW	AAA	501	64/64	0.99	0.04	7,11,13,15	0
4	MG	CCC	503	1/1	0.99	0.08	20,20,20,20	0
2	NHW	BBB	501	64/64	0.99	0.03	7,10,13,14	0
4	MG	AAA	503	1/1	1.00	0.02	19,19,19,19	0
6	CL	AAA	505	1/1	1.00	0.02	12,12,12,12	0
6	CL	BBB	504	1/1	1.00	0.01	11,11,11,11	0
6	CL	CCC	504	1/1	1.00	0.03	12,12,12,12	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.

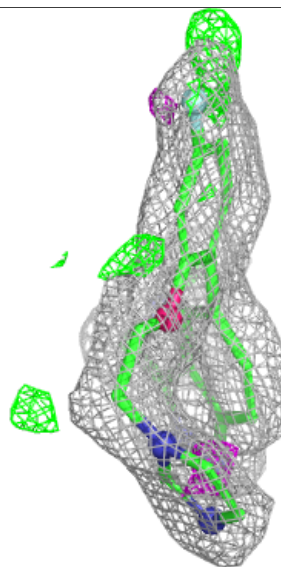
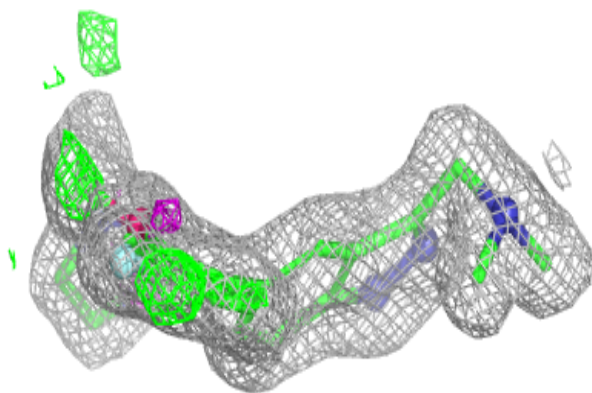
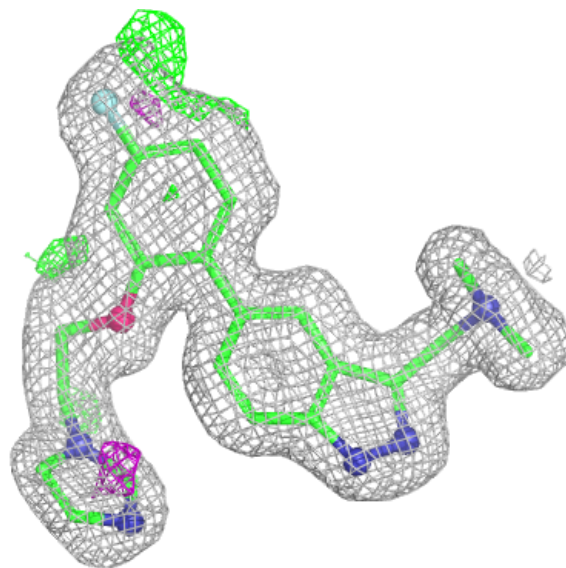
Electron density around NZE CCC 502:

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



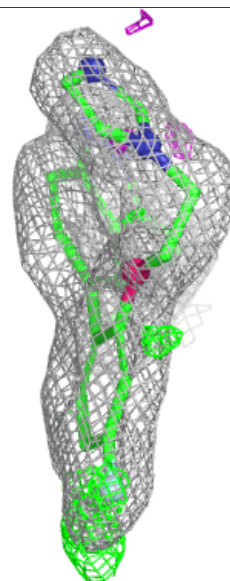
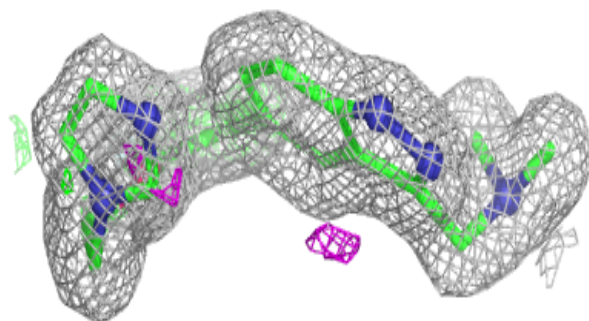
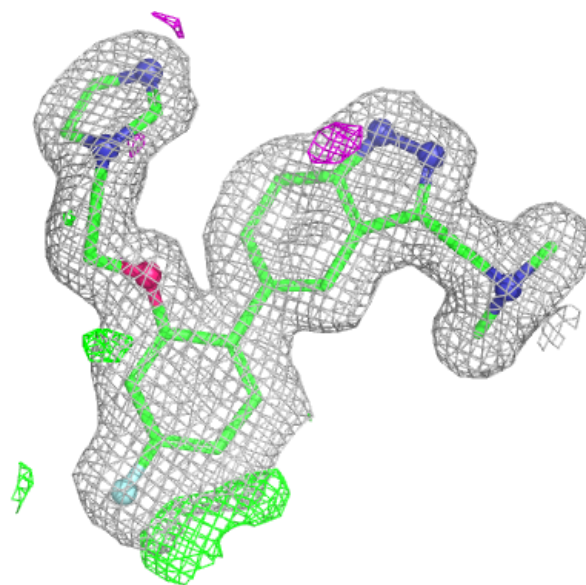
Electron density around NZE AAA 502:

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



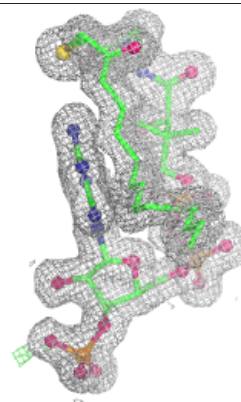
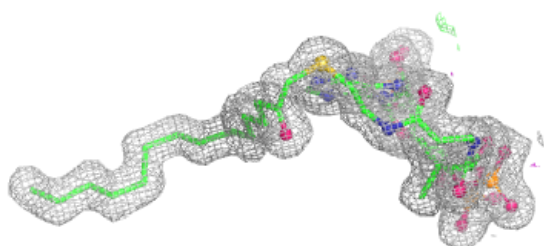
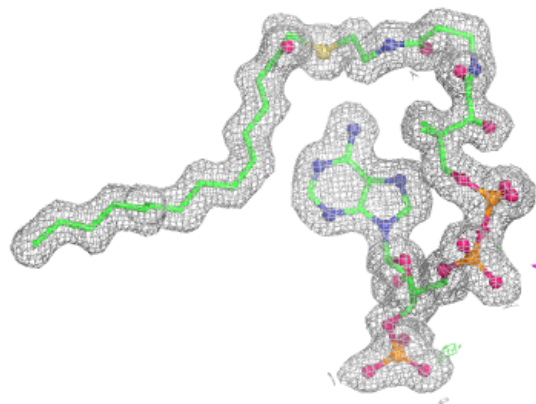
Electron density around NZE BBB 502:

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

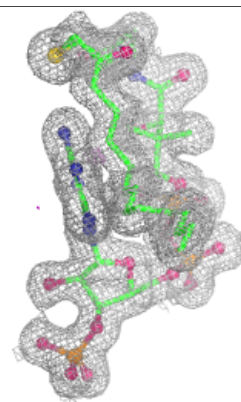
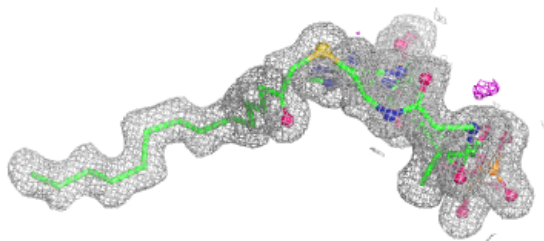
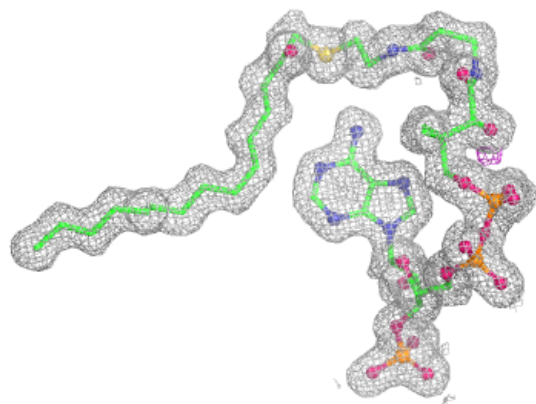


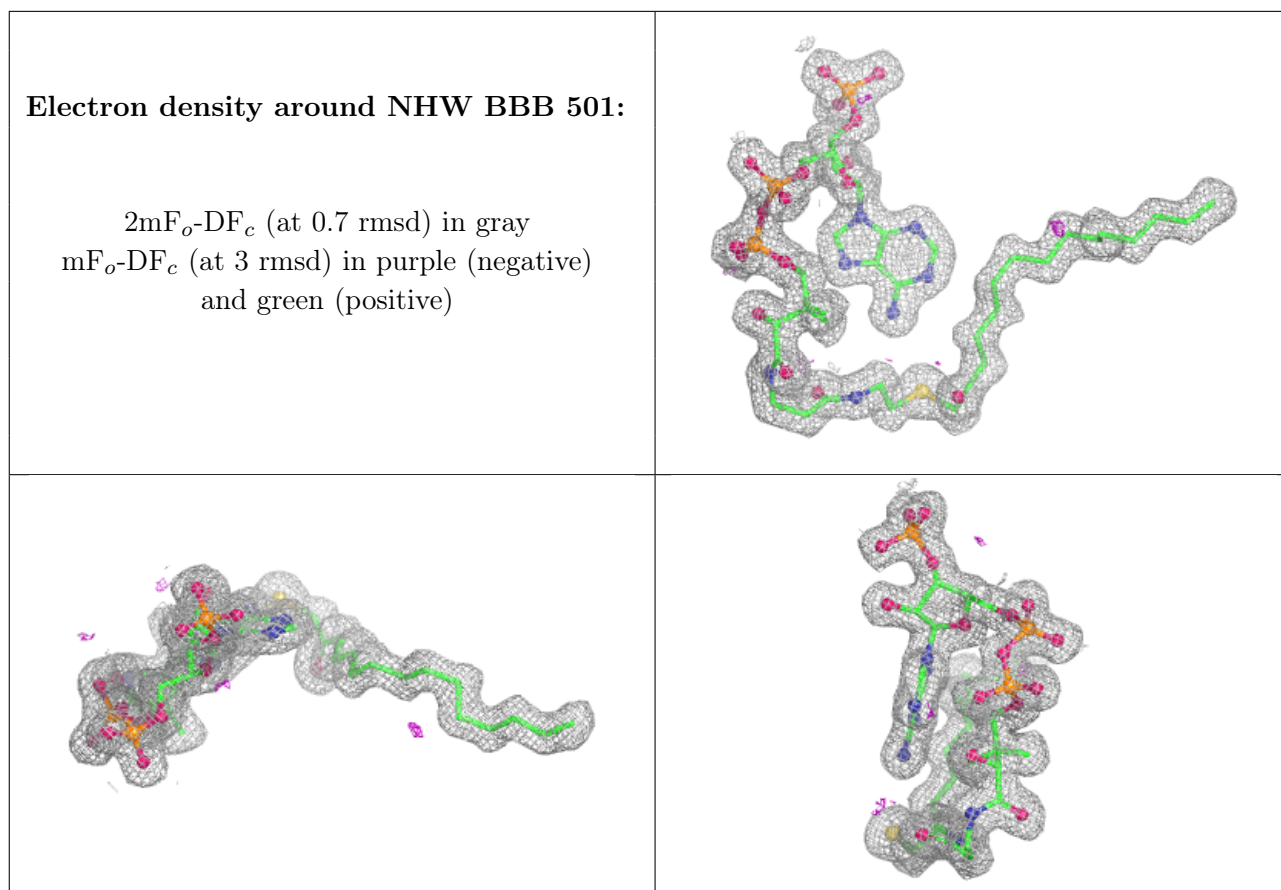
Electron density around NHW CCC 501:

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

**Electron density around NHW AAA 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.