



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:31 AM UTC

PDB ID : 4C68 / pdb_00004c68
Title : Plasmodium vivax N-myristoyltransferase in complex with a peptidomimetic inhibitor
Authors : Olaleye, T.O.; Brannigan, J.A.; Goncalves, V.; Roberts, S.M.; Leatherbarrow, R.J.; Wilkinson, A.J.; Tate, E.W.
Deposited on : 2013-09-17
Resolution : 1.38 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

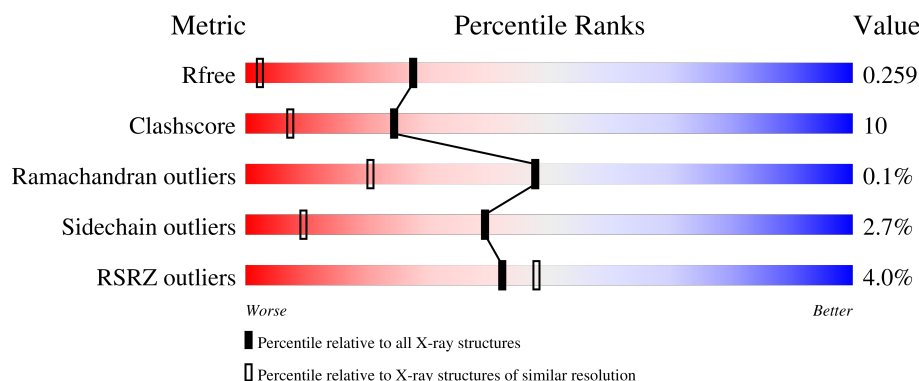
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	384	
1	B	384	
1	C	384	

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
2	FMT	A	997	-	-	X	-
3	DMS	A	999	-	X	-	-
3	DMS	B	1414	-	-	X	-
3	DMS	C	999	-	-	X	-

2 Entry composition [i](#)

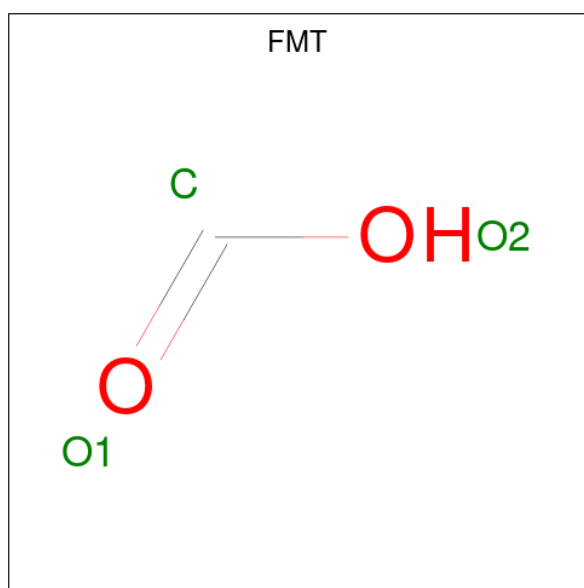
There are 9 unique types of molecules in this entry. The entry contains 11510 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

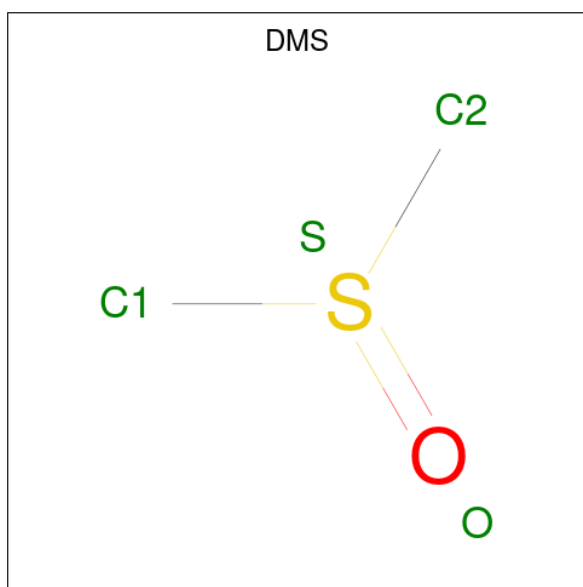
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	32	0
			3375	2199	543	619	14			
1	B	384	Total	C	N	O	S	0	20	0
			3319	2162	534	611	12			
1	C	370	Total	C	N	O	S	0	18	0
			3191	2082	511	587	11			

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



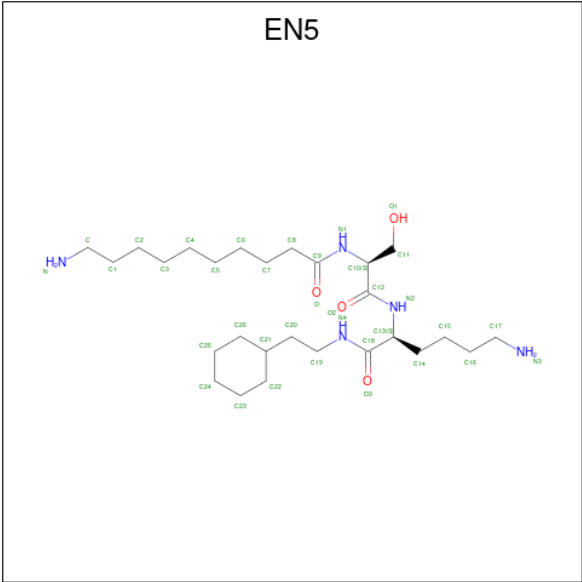
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



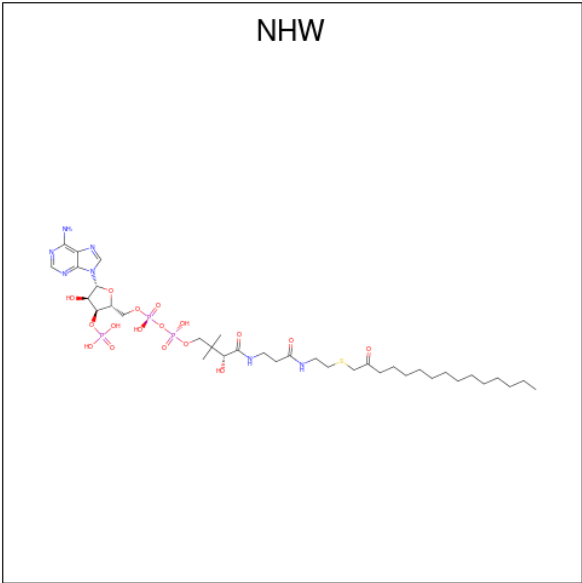
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is N-(10-aminodecanoyl)-L-seryl-N-(2-cyclohexylethyl)-L-lysineamide (CCD ID: EN5) (formula: C₂₇H₅₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			72	54	10	8		
4	B	1	Total	C	N	O	0	0
			36	27	5	4		

- Molecule 5 is 2-oxopentadecyl-CoA (CCD ID: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



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

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

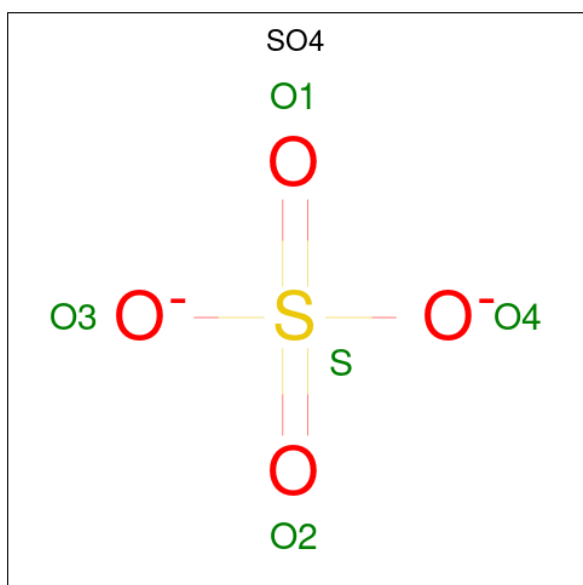
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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	3	Total	Cl	0	0
			3	3		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

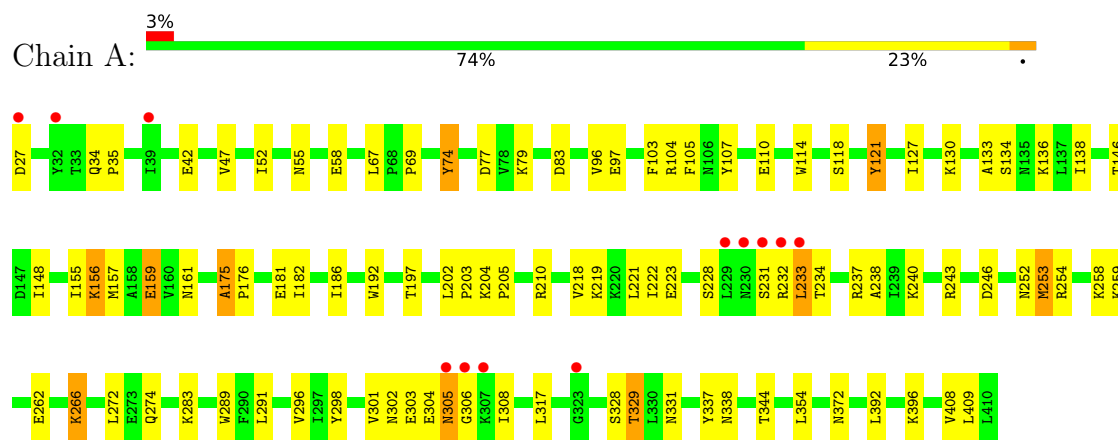
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	479	Total	O	0	0
			479	479		
9	B	453	Total	O	0	0
			453	453		
9	C	357	Total	O	0	0
			357	357		

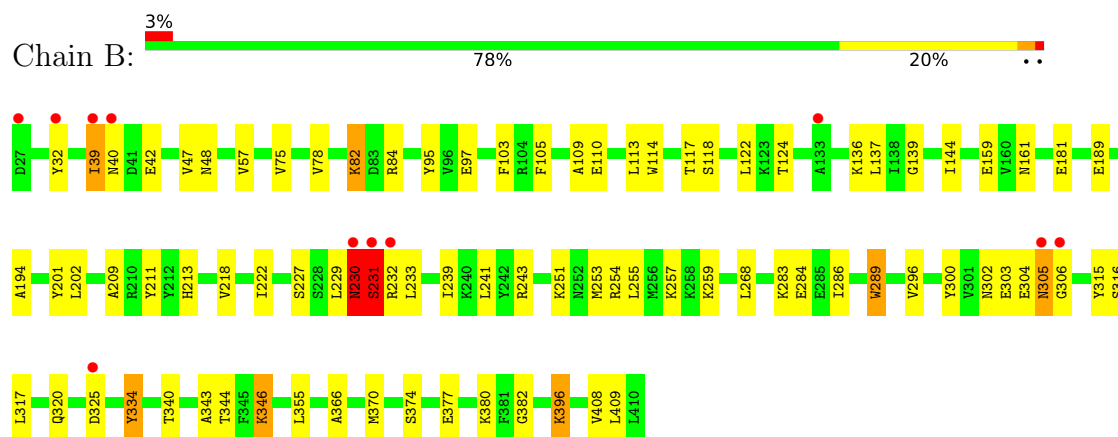
3 Residue-property plots

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.

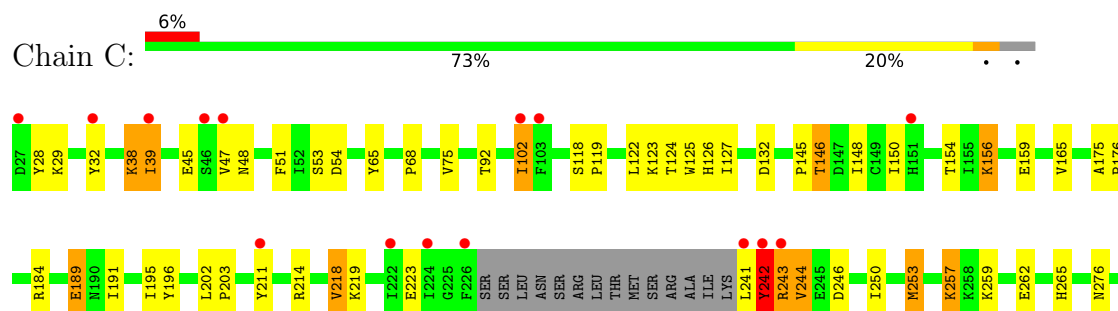
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE

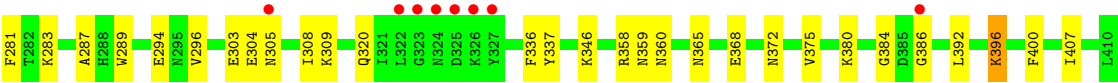


• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



• 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	57.33Å 121.43Å 178.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.97 – 1.38 41.97 – 1.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.97-1.38) 100.0 (41.97-1.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.38Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.220 , 0.260 0.219 , 0.259	Depositor DCC
R_{free} test set	12849 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11510	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, SO4, CL, NHW, EN5, DMS, FMT

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	1.59	26/3531 (0.7%)	1.43	22/4770 (0.5%)
1	B	1.60	30/3433 (0.9%)	1.46	25/4642 (0.5%)
1	C	1.54	31/3307 (0.9%)	1.38	19/4477 (0.4%)
All	All	1.58	87/10271 (0.8%)	1.42	66/13889 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	4
All	All	0	7

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243[A]	ARG	CA-C	10.78	1.67	1.52
1	C	243[B]	ARG	CA-C	10.78	1.67	1.52
1	B	284[A]	GLU	CA-C	10.71	1.66	1.52
1	B	284[B]	GLU	CA-C	10.71	1.66	1.52
1	B	283[A]	LYS	CA-C	9.81	1.65	1.52
1	B	283[B]	LYS	CA-C	9.81	1.65	1.52
1	B	48	ASN	C-O	-9.26	1.14	1.23
1	C	203	PRO	C-O	9.13	1.32	1.23
1	A	254	ARG	C-O	-8.75	1.12	1.23
1	A	253[A]	MET	CA-C	8.49	1.64	1.52
1	A	253[B]	MET	CA-C	8.49	1.64	1.52
1	B	95	TYR	C-O	-8.14	1.15	1.23
1	B	268	LEU	C-O	-8.10	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	ASN	C-O	-7.98	1.14	1.24
1	A	392	LEU	CA-C	-7.50	1.43	1.52
1	A	104	ARG	C-O	-7.47	1.15	1.24
1	A	159	GLU	C-O	-7.33	1.15	1.24
1	B	343	ALA	C-O	-7.19	1.14	1.24
1	C	287	ALA	C-O	7.05	1.32	1.24
1	C	202	LEU	C-N	6.99	1.40	1.33
1	A	233	LEU	C-O	-6.78	1.16	1.24
1	B	366	ALA	C-O	6.75	1.32	1.23
1	A	69	PRO	CA-C	6.74	1.60	1.52
1	A	205	PRO	C-O	6.69	1.31	1.23
1	C	407	ILE	N-CA	6.52	1.54	1.46
1	C	246	ASP	C-O	-6.41	1.16	1.24
1	B	161	ASN	C-O	6.27	1.31	1.23
1	A	246	ASP	C-O	-6.25	1.16	1.24
1	A	83	ASP	N-CA	6.23	1.53	1.46
1	B	202	LEU	C-O	-6.23	1.18	1.24
1	B	181	GLU	C-O	-6.21	1.16	1.24
1	B	334	TYR	N-CA	6.18	1.53	1.46
1	C	296	VAL	C-O	-6.17	1.16	1.24
1	C	358	ARG	C-O	-6.13	1.16	1.24
1	C	392	LEU	CA-C	-6.12	1.45	1.52
1	B	315	TYR	N-CA	6.07	1.52	1.45
1	B	139	GLY	N-CA	6.07	1.52	1.45
1	C	154	THR	N-CA	6.03	1.53	1.46
1	C	165	VAL	C-O	5.99	1.30	1.24
1	C	253[A]	MET	C-O	5.97	1.31	1.23
1	C	253[B]	MET	C-O	5.97	1.31	1.23
1	C	196	TYR	N-CA	5.95	1.53	1.46
1	C	48	ASN	C-O	-5.92	1.18	1.23
1	B	113	LEU	C-O	-5.85	1.17	1.24
1	C	195	ILE	C-O	5.83	1.29	1.24
1	C	184	ARG	N-CA	-5.82	1.39	1.46
1	C	150	ILE	CA-CB	5.78	1.61	1.54
1	C	336	PHE	N-CA	5.78	1.53	1.46
1	C	65	TYR	CA-C	-5.77	1.45	1.52
1	A	175	ALA	C-O	-5.76	1.16	1.24
1	B	286	ILE	CA-C	5.69	1.59	1.52
1	A	298	TYR	C-O	5.68	1.30	1.24
1	A	308	ILE	C-O	-5.68	1.17	1.24
1	A	133	ALA	N-CA	5.67	1.53	1.46
1	B	194	ALA	C-O	5.64	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	189	GLU	N-CA	-5.60	1.38	1.46
1	B	289	TRP	N-CA	5.60	1.53	1.46
1	B	78	VAL	C-O	-5.58	1.16	1.24
1	C	346	LYS	C-O	5.55	1.30	1.24
1	A	337	TYR	C-O	-5.53	1.17	1.24
1	C	375	VAL	CA-CB	5.50	1.60	1.54
1	A	234	THR	C-O	5.49	1.31	1.23
1	A	259	LYS	N-CA	5.48	1.53	1.46
1	C	365	ASN	N-CA	-5.46	1.39	1.46
1	A	77	ASP	C-O	5.45	1.30	1.23
1	B	82	LYS	CA-C	5.42	1.59	1.52
1	A	34	GLN	CD-OE1	5.39	1.33	1.23
1	B	377	GLU	C-O	-5.38	1.17	1.24
1	C	380	LYS	C-O	-5.35	1.16	1.23
1	B	316	SER	CA-C	-5.35	1.46	1.52
1	B	408	VAL	C-O	5.34	1.30	1.24
1	C	384	GLY	N-CA	5.32	1.50	1.45
1	A	181	GLU	C-O	5.32	1.30	1.24
1	A	221	LEU	N-CA	-5.29	1.39	1.46
1	A	161	ASN	CA-C	-5.28	1.46	1.52
1	B	57	VAL	C-O	5.24	1.30	1.24
1	C	368	GLU	C-O	-5.24	1.17	1.24
1	C	337	TYR	CA-C	5.22	1.58	1.52
1	C	148	ILE	CA-CB	5.21	1.60	1.54
1	B	340	THR	C-O	5.20	1.30	1.23
1	A	296	VAL	N-CA	-5.13	1.40	1.46
1	B	370	MET	C-O	-5.13	1.17	1.24
1	C	126	HIS	C-O	5.12	1.29	1.23
1	B	320	GLN	C-O	-5.11	1.17	1.23
1	B	374	SER	N-CA	5.10	1.52	1.46
1	A	274	GLN	CA-C	5.07	1.59	1.52
1	B	209	ALA	C-O	5.06	1.29	1.24

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	SER	N-CA-C	-9.00	101.44	111.07
1	B	283[A]	LYS	CA-C-O	8.47	129.53	120.55
1	B	283[B]	LYS	CA-C-O	8.47	129.53	120.55
1	B	284[A]	GLU	CA-C-O	8.43	129.49	120.55
1	B	284[B]	GLU	CA-C-O	8.43	129.49	120.55
1	B	283[A]	LYS	O-C-N	7.84	130.43	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283[B]	LYS	O-C-N	7.84	130.43	122.12
1	A	232	ARG	N-CA-C	-7.83	102.77	113.18
1	B	325	ASP	N-CA-C	7.42	119.36	111.28
1	C	243[A]	ARG	CA-C-N	-6.98	114.10	123.10
1	C	243[A]	ARG	C-N-CA	-6.98	114.10	123.10
1	C	243[B]	ARG	CA-C-N	-6.98	114.10	123.10
1	C	243[B]	ARG	C-N-CA	-6.98	114.10	123.10
1	A	253[A]	MET	CB-CA-C	-6.78	99.33	109.90
1	A	253[B]	MET	CB-CA-C	-6.78	99.33	109.90
1	C	244	VAL	N-CA-C	6.72	118.27	108.53
1	A	252	ASN	CA-C-N	-6.66	111.16	121.02
1	A	252	ASN	C-N-CA	-6.66	111.16	121.02
1	A	121	TYR	CA-C-O	6.55	128.49	121.55
1	A	372	ASN	N-CA-C	6.33	118.18	111.28
1	B	283[A]	LYS	N-CA-C	6.25	118.09	111.28
1	B	283[B]	LYS	N-CA-C	6.25	118.09	111.28
1	B	230	ASN	N-CA-C	-5.99	98.03	110.80
1	B	218	VAL	N-CA-C	5.95	116.13	110.42
1	C	304	GLU	CB-CA-C	-5.94	100.29	110.16
1	B	114	TRP	N-CA-C	5.93	118.22	111.11
1	A	67	LEU	CA-C-N	-5.89	114.31	120.38
1	A	67	LEU	C-N-CA	-5.89	114.31	120.38
1	C	372	ASN	N-CA-C	5.81	117.61	111.28
1	B	231	SER	CB-CA-C	5.74	119.89	110.88
1	C	102	ILE	CB-CA-C	-5.72	104.64	110.88
1	C	309	LYS	N-CA-C	5.71	120.52	113.50
1	A	74	TYR	CA-C-N	-5.68	115.62	122.90
1	A	74	TYR	C-N-CA	-5.68	115.62	122.90
1	C	132	ASP	N-CA-C	5.64	118.19	111.71
1	A	253[A]	MET	CA-C-O	5.62	127.33	120.92
1	A	253[B]	MET	CA-C-O	5.62	127.33	120.92
1	B	251	LYS	N-CA-C	5.62	118.17	111.71
1	A	354	LEU	N-CA-C	5.58	117.37	111.28
1	B	239	ILE	N-CA-C	-5.51	105.00	110.62
1	C	184	ARG	N-CA-C	5.47	117.68	111.11
1	A	291	LEU	CA-C-N	-5.45	114.16	119.78
1	A	291	LEU	C-N-CA	-5.45	114.16	119.78
1	A	96	VAL	CB-CA-C	-5.44	102.99	111.26
1	A	305	ASN	CB-CA-C	-5.44	104.01	111.73
1	A	114	TRP	N-CA-C	5.32	117.50	111.11
1	A	202	LEU	O-C-N	5.32	125.12	121.71
1	B	325	ASP	N-CA-CB	5.29	117.89	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	PHE	N-CA-C	-5.27	105.62	111.36
1	C	38	LYS	N-CA-C	-5.23	103.49	110.55
1	B	255	LEU	CA-C-O	5.22	126.89	121.15
1	B	137	LEU	CB-CA-C	5.20	118.58	110.67
1	B	396	LYS	N-CA-CB	-5.18	102.43	110.57
1	B	144	ILE	N-CA-C	-5.18	104.94	109.19
1	C	218	VAL	N-CA-C	5.16	115.78	110.36
1	C	127	ILE	N-CA-C	5.14	115.25	107.80
1	B	284[A]	GLU	N-CA-C	5.12	116.86	111.28
1	B	284[B]	GLU	N-CA-C	5.12	116.86	111.28
1	C	242	TYR	CA-CB-CG	5.10	123.09	113.90
1	B	40	ASN	N-CA-C	5.10	119.19	112.92
1	A	272	LEU	N-CA-C	5.09	118.59	112.38
1	C	68	PRO	CA-C-N	5.05	125.29	119.83
1	C	68	PRO	C-N-CA	5.05	125.29	119.83
1	A	186	ILE	N-CA-C	-5.05	105.62	110.72
1	B	117	THR	CB-CA-C	-5.03	103.03	111.13
1	C	336	PHE	CB-CA-C	5.01	120.38	110.42

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	ASN	Peptide
1	B	231	SER	Peptide,Mainchain
1	C	242	TYR	Peptide
1	C	243[A]	ARG	Mainchain
1	C	243[B]	ARG	Mainchain

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	3375	0	3417	65	0
1	B	3319	0	3326	68	0
1	C	3191	0	3182	56	0
2	A	3	0	2	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	12	4	0
3	B	8	0	12	18	0
3	C	4	0	6	4	0
4	A	72	0	106	4	0
4	B	36	0	53	8	0
5	A	64	0	60	0	0
5	B	64	0	60	0	0
5	C	64	0	60	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	5	0	0	0	0
9	A	479	0	0	8	0
9	B	453	0	0	7	0
9	C	357	0	0	3	0
All	All	11510	0	10296	203	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 10.

All (203) 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:257[B]:LYS:HD2	1:B:259[B]:LYS:NZ	1.27	1.42
1:B:257[B]:LYS:CD	1:B:259[B]:LYS:HZ2	1.49	1.25
1:B:257[B]:LYS:CD	1:B:259[B]:LYS:NZ	2.01	1.23
1:B:231:SER:N	1:B:233:LEU:H	1.39	1.19
1:B:231:SER:H	1:B:233:LEU:N	1.45	1.13
1:B:75[B]:VAL:HG22	9:B:2196:HOH:O	1.51	1.08
4:B:1000:EN5:H11A	3:B:1414:DMS:H12	1.32	1.06
4:B:1000:EN5:H8A	3:B:1414:DMS:H23	1.32	1.06
1:A:408:VAL:HG13	2:A:997:FMT:H	1.39	1.04
3:A:1415:DMS:H22	9:A:2397:HOH:O	1.55	1.04
1:B:257[B]:LYS:CE	1:B:259[B]:LYS:HZ1	1.70	1.04
4:A:1000[A]:EN5:HN	4:A:1000[A]:EN5:H3	1.21	1.02
1:A:136[B]:LYS:HD3	9:A:2211:HOH:O	1.67	0.95
1:C:145:PRO:HB2	1:C:156[A]:LYS:HE3	1.46	0.94
1:C:122[B]:LEU:HD11	1:C:189:GLU:HG3	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:SER:N	1:B:233:LEU:N	2.05	0.93
1:B:257[B]:LYS:HE3	1:B:259[B]:LYS:HZ1	1.33	0.92
1:A:134:SER:HB2	1:A:136[A]:LYS:HE3	1.50	0.92
1:A:283[B]:LYS:HB2	1:A:283[B]:LYS:NZ	1.83	0.89
1:B:159:GLU:OE2	3:B:999:DMS:H13	1.71	0.88
1:C:122[B]:LEU:HD12	1:C:125:TRP:NE1	1.88	0.88
1:A:253[A]:MET:HE2	1:A:302:ASN:N	1.88	0.88
1:A:283[B]:LYS:HB2	1:A:283[B]:LYS:HZ1	1.41	0.83
1:A:253[A]:MET:HE2	1:A:301:VAL:C	2.04	0.83
1:C:122[B]:LEU:HD12	1:C:125:TRP:CE2	2.14	0.83
1:C:211[B]:TYR:CD2	1:C:386:GLY:O	2.34	0.80
1:C:32[A]:TYR:CE1	1:C:38:LYS:HE3	2.16	0.80
1:A:253[A]:MET:CE	1:A:302:ASN:N	2.46	0.79
1:A:240[B]:LYS:HD3	1:A:243[B]:ARG:NH1	1.98	0.78
4:A:1000[A]:EN5:HN	4:A:1000[A]:EN5:C3	1.97	0.77
1:B:257[B]:LYS:CE	1:B:259[B]:LYS:NZ	2.40	0.77
1:C:265:HIS:ND1	1:C:283[A]:LYS:HG2	2.00	0.77
1:A:262:GLU:HG3	9:A:2356:HOH:O	1.86	0.75
1:A:58[A]:GLU:H	1:A:58[A]:GLU:CD	1.95	0.75
1:B:105:PHE:CZ	3:B:1414:DMS:H22	2.21	0.74
1:C:257:LYS:HE2	1:C:259:LYS:CE	2.17	0.74
1:C:32[A]:TYR:CD1	1:C:38:LYS:HE3	2.23	0.74
1:A:156[B]:LYS:HE3	9:A:2235:HOH:O	1.87	0.73
1:B:159:GLU:CD	1:B:409[A]:LEU:HD22	2.12	0.73
1:B:159:GLU:CD	1:B:409[A]:LEU:CD2	2.62	0.73
1:C:257:LYS:HE2	1:C:259:LYS:HE2	1.67	0.73
4:A:1000[A]:EN5:H3	4:A:1000[A]:EN5:N	2.01	0.73
1:C:159:GLU:OE2	3:C:999:DMS:H23	1.89	0.72
1:A:253[A]:MET:CE	1:A:301:VAL:C	2.63	0.72
1:A:303:GLU:OE2	1:A:306:GLY:HA2	1.91	0.71
1:C:219:LYS:O	1:C:223:GLU:HG3	1.91	0.71
1:B:257[B]:LYS:CD	1:B:259[B]:LYS:HZ1	1.86	0.70
1:A:283[B]:LYS:NZ	1:A:283[B]:LYS:CB	2.54	0.69
1:C:211[B]:TYR:CD2	1:C:386:GLY:C	2.71	0.69
1:B:257[B]:LYS:HE3	1:B:259[B]:LYS:NZ	2.05	0.68
1:B:230:ASN:ND2	1:B:231:SER:OG	2.27	0.68
1:C:211[B]:TYR:HD2	1:C:386:GLY:O	1.77	0.67
1:B:231:SER:H	1:B:233:LEU:CA	2.07	0.67
1:B:304[B]:GLU:O	1:B:305:ASN:ND2	2.28	0.66
1:B:230:ASN:C	1:B:233:LEU:H	2.05	0.65
1:A:253[A]:MET:CE	1:A:302:ASN:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:HIS:HE1	3:B:1414:DMS:H13	1.61	0.65
1:A:134:SER:HB2	1:A:136[A]:LYS:CE	2.26	0.64
1:C:281:PHE:HE1	3:C:999:DMS:H12	1.63	0.64
1:C:122[B]:LEU:HD11	1:C:189:GLU:CG	2.24	0.64
1:C:145:PRO:O	1:C:146[A]:THR:HG22	1.98	0.64
1:B:222:ILE:HD12	1:B:229:LEU:HG	1.78	0.64
1:A:148:ILE:HG13	1:A:157[B]:MET:HE2	1.78	0.63
1:A:42[A]:GLU:HG2	1:B:344:THR:HG21	1.79	0.62
1:C:145:PRO:CB	1:C:156[A]:LYS:HE3	2.25	0.62
3:B:999:DMS:H23	9:B:2396:HOH:O	2.00	0.61
1:C:257:LYS:HE2	1:C:259:LYS:NZ	2.16	0.60
1:B:105:PHE:CE1	3:B:1414:DMS:H22	2.35	0.60
1:B:110[A]:GLU:HG3	1:B:296:VAL:HG21	1.83	0.60
1:A:197:THR:HG23	1:A:409:LEU:HD12	1.83	0.60
1:C:257:LYS:CE	1:C:259:LYS:HE2	2.32	0.59
4:B:1000:EN5:H8A	3:B:1414:DMS:C2	2.20	0.59
1:A:253[A]:MET:HE2	1:A:302:ASN:CA	2.34	0.58
1:B:229:LEU:C	1:B:230:ASN:OD1	2.47	0.58
1:C:211[B]:TYR:CE2	1:C:386:GLY:HA3	2.39	0.58
1:C:218:VAL:HG22	1:C:242:TYR:CE2	2.39	0.58
1:B:47:VAL:CG1	1:B:396:LYS:HG2	2.34	0.58
1:B:211[A]:TYR:CG	3:B:1414:DMS:H11	2.39	0.57
1:A:118:SER:HB3	1:A:289:TRP:CZ2	2.39	0.57
1:A:240[B]:LYS:HD3	1:A:243[B]:ARG:CZ	2.34	0.57
1:C:211[B]:TYR:CE2	1:C:386:GLY:C	2.82	0.57
1:B:243:ARG:HG3	9:B:2301:HOH:O	2.03	0.57
3:C:999:DMS:H13	9:C:2309:HOH:O	2.05	0.57
4:B:1000:EN5:C8	3:B:1414:DMS:H23	2.21	0.57
1:C:122[B]:LEU:HD12	1:C:125:TRP:CD1	2.40	0.56
1:A:253[A]:MET:HE3	1:A:302:ASN:HB2	1.87	0.55
1:B:124:THR:HG23	9:B:2195:HOH:O	2.05	0.55
4:B:1000:EN5:C11	3:B:1414:DMS:H12	2.22	0.55
1:C:156[B]:LYS:HE2	1:C:191:ILE:HD11	1.87	0.55
1:B:47:VAL:HG11	1:B:396:LYS:HG2	1.88	0.55
1:A:266:LYS:NZ	1:A:266:LYS:HB2	2.23	0.54
1:A:266:LYS:HB2	1:A:266:LYS:HZ2	1.72	0.54
1:B:231:SER:HB2	1:B:232:ARG:C	2.32	0.54
1:C:276:ASN:ND2	1:C:400:PHE:CE2	2.76	0.54
1:C:303[B]:GLU:HB3	1:C:308:ILE:HD13	1.90	0.54
4:B:1000:EN5:H1	9:B:2145:HOH:O	2.08	0.54
1:C:211[B]:TYR:HE2	1:C:386:GLY:HA3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PHE:HZ	3:B:1414:DMS:H22	1.67	0.54
1:C:265:HIS:HB3	1:C:283[A]:LYS:HD3	1.91	0.53
1:A:344:THR:HG21	1:B:42[B]:GLU:HG3	1.91	0.53
1:B:231:SER:H	1:B:233:LEU:CB	2.22	0.53
1:C:265:HIS:CB	1:C:283[A]:LYS:HD3	2.39	0.52
1:A:253[A]:MET:HE2	1:A:302:ASN:HB2	1.90	0.52
1:B:382:GLY:HA3	4:B:1000:EN5:H24	1.91	0.52
1:A:127:ILE:HG13	1:A:182:ILE:HD13	1.92	0.52
1:C:156[B]:LYS:HG2	1:C:191:ILE:HG12	1.91	0.52
1:A:146:THR:HG23	1:A:148:ILE:HG12	1.92	0.52
1:B:303:GLU:OE2	1:B:306:GLY:HA2	2.10	0.51
1:A:35:PRO:HB3	1:A:52:ILE:HD12	1.92	0.51
1:C:276:ASN:ND2	1:C:400:PHE:CD2	2.78	0.51
1:C:75:VAL:HG12	1:C:123:LYS:HE2	1.93	0.51
1:A:155:ILE:HB	1:A:157[B]:MET:SD	2.51	0.51
1:C:45:GLU:HA	1:C:45:GLU:OE1	2.12	0.50
1:A:210:ARG:HB3	9:A:2283:HOH:O	2.11	0.50
1:B:253[B]:MET:SD	1:B:302:ASN:HB2	2.51	0.50
1:A:127:ILE:HD11	1:A:182:ILE:HD12	1.93	0.50
1:A:134:SER:CB	1:A:136[A]:LYS:HE3	2.34	0.49
1:B:122:LEU:HD22	1:B:189:GLU:HG3	1.93	0.49
1:A:233:LEU:HG	1:A:238:ALA:HB2	1.94	0.49
3:A:999:DMS:H11	9:A:2412:HOH:O	2.12	0.49
1:B:105:PHE:HZ	3:B:1414:DMS:C2	2.26	0.49
1:A:328:SER:OG	1:A:329[A]:THR:HG22	2.13	0.48
1:C:250:ILE:HB	1:C:253[B]:MET:HG3	1.96	0.48
1:A:408:VAL:CG1	2:A:997:FMT:H	2.27	0.48
1:B:213:HIS:HE1	3:B:1414:DMS:C1	2.25	0.48
1:A:304:GLU:O	1:A:305:ASN:HB2	2.12	0.48
1:C:92:THR:HG21	9:C:2095:HOH:O	2.14	0.48
1:C:265:HIS:CE1	1:C:283[A]:LYS:HG2	2.49	0.48
1:A:74:TYR:CD2	1:A:130:LYS:HE3	2.49	0.48
1:B:32[B]:TYR:OH	1:B:39:ILE:HB	2.13	0.48
1:B:257[B]:LYS:HD2	1:B:259[B]:LYS:HZ2	0.54	0.48
1:C:262:GLU:HG3	1:C:283[A]:LYS:HE3	1.96	0.48
1:C:303[B]:GLU:HB3	1:C:308:ILE:CD1	2.44	0.48
1:C:359:ASN:O	1:C:360:ASN:HB3	2.14	0.48
3:A:999:DMS:C1	9:A:2412:HOH:O	2.61	0.47
1:B:39:ILE:CD1	1:B:201:TYR:HE2	2.27	0.47
1:A:148:ILE:CG1	1:A:157[B]:MET:HE2	2.45	0.47
1:A:47:VAL:CG1	1:A:396:LYS:HG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLU:OE2	1:B:409[A]:LEU:HD22	2.13	0.47
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.40	0.47
1:A:156[B]:LYS:C	1:A:157[B]:MET:HG3	2.39	0.46
4:A:1000[A]:EN5:C3	4:A:1000[A]:EN5:N	2.71	0.46
1:C:281:PHE:CE1	3:C:999:DMS:H12	2.47	0.46
1:A:134:SER:OG	1:A:136[B]:LYS:HB3	2.16	0.46
1:C:218:VAL:HG22	1:C:242:TYR:HE2	1.81	0.46
1:A:253[A]:MET:HE2	1:A:302:ASN:CB	2.45	0.46
1:B:231:SER:HB2	1:B:232:ARG:CB	2.46	0.46
1:A:253[A]:MET:HE1	1:A:302:ASN:N	2.28	0.45
1:C:257:LYS:HE3	1:C:257:LYS:HB2	1.50	0.45
1:B:211[A]:TYR:CD1	3:B:1414:DMS:H11	2.50	0.45
1:B:254:ARG:NH1	1:B:257[B]:LYS:HE2	2.32	0.45
3:B:1414:DMS:H21	9:B:2267:HOH:O	2.17	0.45
1:B:84:ARG:HD2	1:B:109:ALA:O	2.17	0.45
1:A:55:ASN:HB3	1:A:192:TRP:CZ3	2.51	0.45
1:B:229:LEU:O	1:B:230:ASN:OD1	2.35	0.45
1:A:97:GLU:HA	1:A:103:PHE:O	2.16	0.45
1:A:110[B]:GLU:H	1:A:110[B]:GLU:CD	2.23	0.45
1:A:107:TYR:CD1	1:A:317:LEU:HD13	2.52	0.45
1:A:47:VAL:HG12	1:A:396:LYS:HG2	1.99	0.45
1:B:289:TRP:CD2	3:B:999:DMS:H21	2.52	0.44
1:B:122:LEU:CD2	1:B:189:GLU:HG3	2.47	0.44
1:B:159:GLU:OE2	1:B:409[A]:LEU:CD2	2.65	0.44
1:B:241:LEU:HD12	1:B:380:LYS:HE2	1.99	0.44
1:C:47:VAL:HG11	1:C:396:LYS:HD2	2.00	0.44
1:A:218:VAL:O	1:A:222:ILE:HG12	2.17	0.44
1:B:75[B]:VAL:O	1:B:75[B]:VAL:HG12	2.17	0.44
1:B:230:ASN:HD22	1:B:231:SER:CB	2.30	0.44
1:B:227:SER:HB3	4:B:1000:EN5:H26	1.99	0.44
1:B:230:ASN:O	1:B:233:LEU:O	2.35	0.43
1:B:317:LEU:HB3	1:B:334:TYR:CE1	2.53	0.43
1:A:253[A]:MET:CE	1:A:302:ASN:CB	2.95	0.43
1:C:211[B]:TYR:CE2	1:C:386:GLY:CA	3.02	0.43
1:C:211[B]:TYR:HD2	1:C:386:GLY:C	2.21	0.43
1:C:265:HIS:ND1	1:C:283[A]:LYS:CG	2.74	0.43
1:A:79:LYS:HE3	1:A:121:TYR:OH	2.19	0.43
1:A:283[B]:LYS:CB	1:A:283[B]:LYS:HZ2	2.30	0.43
1:B:97:GLU:HA	1:B:103:PHE:O	2.19	0.43
1:C:360:ASN:HB2	9:C:2329:HOH:O	2.18	0.43
1:A:233:LEU:HD12	1:A:237[A]:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HD12	1:B:201:TYR:HE2	1.83	0.42
1:B:118:SER:HB3	1:B:289:TRP:CZ2	2.54	0.42
1:B:231:SER:CB	1:B:232:ARG:CB	2.97	0.42
1:A:243[B]:ARG:HE	1:A:243[B]:ARG:HB3	1.65	0.42
1:C:28:TYR:CE2	1:C:39:ILE:HG13	2.54	0.42
1:B:211[A]:TYR:CD2	3:B:1414:DMS:H11	2.53	0.42
1:A:138:ILE:C	1:A:138:ILE:HD12	2.45	0.42
1:A:175:ALA:HB3	1:A:176:PRO:HD3	2.02	0.41
1:C:175:ALA:HB3	1:C:176:PRO:HD3	2.02	0.41
1:A:105:PHE:HE1	3:A:1415:DMS:H21	1.85	0.41
1:A:228:SER:HB2	9:A:2309:HOH:O	2.20	0.41
1:B:304[B]:GLU:HG2	1:B:305:ASN:ND2	2.36	0.41
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.56	0.41
1:C:211[B]:TYR:CD2	1:C:386:GLY:CA	3.04	0.41
1:B:253[A]:MET:HG3	1:B:300:TYR:HB3	2.03	0.41
1:C:262:GLU:HA	1:C:283[A]:LYS:CD	2.51	0.41
1:A:219:LYS:O	1:A:223:GLU:HG3	2.22	0.40
1:C:250:ILE:HG22	1:C:253[B]:MET:HG2	2.03	0.40
1:A:203:PRO:HA	1:A:204:LYS:HA	1.94	0.40
1:B:300:TYR:CG	1:B:355:LEU:HD13	2.57	0.40
1:B:346[A]:LYS:HD3	9:B:2403:HOH:O	2.22	0.40
1:C:29:LYS:HD3	1:C:29:LYS:HA	1.87	0.40
1:C:124:THR:HG1	1:C:125:TRP:CD1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	413/384 (108%)	401 (97%)	12 (3%)	0	100	100
1	B	401/384 (104%)	390 (97%)	10 (2%)	1 (0%)	43	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	384/384 (100%)	372 (97%)	12 (3%)	0	100	100
All	All	1198/1152 (104%)	1163 (97%)	34 (3%)	1 (0%)	48	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	ASN

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	382/350 (109%)	370 (97%)	12 (3%)	35	7
1	B	370/350 (106%)	362 (98%)	8 (2%)	45	14
1	C	355/350 (101%)	336 (95%)	19 (5%)	20	2
All	All	1107/1050 (105%)	1068 (96%)	39 (4%)	39	6

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27[A]	ASP
1	A	27[B]	ASP
1	A	156[B]	LYS
1	A	156[C]	LYS
1	A	231	SER
1	A	258[A]	LYS
1	A	258[B]	LYS
1	A	266	LYS
1	A	329[A]	THR
1	A	329[B]	THR
1	A	331[A]	ASN
1	A	331[B]	ASN
1	B	39	ILE
1	B	82	LYS

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Mol	Chain	Res	Type
1	B	136[A]	LYS
1	B	136[B]	LYS
1	B	230	ASN
1	B	305	ASN
1	B	346[A]	LYS
1	B	346[B]	LYS
1	C	39	ILE
1	C	53	SER
1	C	54[A]	ASP
1	C	54[B]	ASP
1	C	102	ILE
1	C	119	PRO
1	C	146[A]	THR
1	C	146[B]	THR
1	C	156[A]	LYS
1	C	156[B]	LYS
1	C	214[A]	ARG
1	C	214[B]	ARG
1	C	241	LEU
1	C	244	VAL
1	C	257	LYS
1	C	294	GLU
1	C	305	ASN
1	C	320	GLN
1	C	396	LYS

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	40	ASN
1	A	101	ASN
1	A	187	ASN
1	A	249	ASN
1	A	350	GLN
1	A	359	ASN
1	A	372	ASN
1	B	44	ASN
1	B	151	HIS
1	B	187	ASN
1	B	230	ASN
1	B	249	ASN

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Mol	Chain	Res	Type
1	B	350	GLN
1	B	371	GLN
1	B	372	ASN
1	C	34	GLN
1	C	249	ASN
1	C	302	ASN
1	C	350	GLN
1	C	359	ASN
1	C	360	ASN
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 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	EN5	A	1000[B]	-	36,36,36	1.19	3 (8%)	41,42,42	1.15	3 (7%)
3	DMS	B	999	-	3,3,3	0.91	0	3,3,3	2.13	1 (33%)
5	NHW	B	1411	-	64,66,66	1.75	10 (15%)	87,92,92	1.64	12 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMS	A	1415	-	3,3,3	0.64	0	3,3,3	1.61	1 (33%)
3	DMS	B	1414	-	3,3,3	0.80	0	3,3,3	2.58	2 (66%)
4	EN5	B	1000	-	36,36,36	0.99	1 (2%)	41,42,42	1.54	8 (19%)
5	NHW	C	1411	7	64,66,66	2.47	14 (21%)	87,92,92	1.81	24 (27%)
5	NHW	A	1411	7	64,66,66	1.52	13 (20%)	87,92,92	1.94	26 (29%)
2	FMT	A	997	-	2,2,2	1.72	1 (50%)	1,1,1	0.39	0
3	DMS	C	999	-	3,3,3	0.50	0	3,3,3	1.28	0
8	SO4	A	1414	-	4,4,4	0.55	0	6,6,6	1.42	1 (16%)
3	DMS	A	999	-	3,3,3	0.44	0	3,3,3	2.99	3 (100%)
4	EN5	A	1000[A]	-	36,36,36	1.18	3 (8%)	41,42,42	1.13	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EN5	A	1000[B]	-	-	5/39/47/47	0/1/1/1
5	NHW	B	1411	-	-	5/65/81/81	0/3/3/3
4	EN5	B	1000	-	-	7/39/47/47	0/1/1/1
5	NHW	C	1411	7	-	3/65/81/81	0/3/3/3
5	NHW	A	1411	7	-	1/65/81/81	0/3/3/3
4	EN5	A	1000[A]	-	-	4/39/47/47	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1411	NHW	P1A-O3A	9.94	1.70	1.59
5	C	1411	NHW	P2A-O3A	-8.56	1.50	1.59
5	C	1411	NHW	P3X-O3X	8.52	1.74	1.59
5	B	1411	NHW	P3X-O3X	6.88	1.71	1.59
5	B	1411	NHW	P1A-O3A	-5.96	1.53	1.59
5	C	1411	NHW	O4X-C4X	5.84	1.58	1.45
5	B	1411	NHW	O10-C10	4.61	1.50	1.42
4	A	1000[A]	EN5	O2-C12	-4.13	1.15	1.23
4	A	1000[B]	EN5	O2-C12	-4.13	1.15	1.23
4	A	1000[A]	EN5	O3-C18	-4.11	1.15	1.23
4	A	1000[B]	EN5	O3-C18	-4.11	1.15	1.23
5	C	1411	NHW	C8A-N9A	-3.93	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1411	NHW	C5A-N7A	-3.54	1.32	1.39
5	B	1411	NHW	CP-S1	3.49	1.90	1.81
5	B	1411	NHW	P2A-O5A	-3.11	1.40	1.50
5	A	1411	NHW	P1A-O2A	-3.11	1.40	1.55
5	A	1411	NHW	O1M-C1M	3.09	1.27	1.21
5	C	1411	NHW	CP-C1M	3.08	1.56	1.51
5	A	1411	NHW	C8A-N7A	3.04	1.37	1.31
5	B	1411	NHW	P3X-O7A	-3.02	1.43	1.54
5	A	1411	NHW	P3X-O8A	2.92	1.65	1.54
5	A	1411	NHW	CP-C1M	-2.91	1.46	1.51
5	C	1411	NHW	P3X-O7A	-2.83	1.44	1.54
5	C	1411	NHW	C8A-N7A	2.71	1.36	1.31
5	C	1411	NHW	C4A-N3A	2.71	1.39	1.34
5	A	1411	NHW	P1A-O3A	-2.67	1.56	1.59
4	A	1000[A]	EN5	O-C9	-2.63	1.18	1.23
5	A	1411	NHW	C13-C11	-2.62	1.48	1.53
5	A	1411	NHW	P3X-O3X	2.60	1.64	1.59
4	A	1000[B]	EN5	O-C9	-2.59	1.18	1.23
5	A	1411	NHW	P2A-O3A	2.53	1.62	1.59
5	A	1411	NHW	O4X-C4X	2.51	1.50	1.45
5	B	1411	NHW	P2A-O4A	-2.49	1.43	1.55
4	B	1000	EN5	O2-C12	2.43	1.28	1.23
5	B	1411	NHW	C4A-N9A	-2.35	1.32	1.37
5	B	1411	NHW	C5A-N7A	-2.31	1.34	1.39
5	C	1411	NHW	C2M-C1M	-2.27	1.44	1.51
5	A	1411	NHW	C4A-N3A	2.23	1.38	1.34
5	C	1411	NHW	C9-N8	-2.22	1.28	1.33
2	A	997	FMT	O2-C	2.22	1.40	1.28
5	B	1411	NHW	CP-C1M	-2.15	1.47	1.51
5	C	1411	NHW	CAM-C9M	2.11	1.62	1.51
5	A	1411	NHW	O4X-C1X	2.07	1.46	1.42
5	A	1411	NHW	C14-C11	-2.05	1.49	1.53
5	C	1411	NHW	C7-N8	-2.02	1.41	1.46

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1411	NHW	C5A-C4A-N3A	-5.71	118.85	126.72
5	B	1411	NHW	N9A-C8A-N7A	-5.60	105.99	113.94
5	C	1411	NHW	C5A-C4A-N3A	-5.59	119.03	126.72
5	B	1411	NHW	C4A-N9A-C8A	5.44	111.45	105.74
5	A	1411	NHW	C13-C11-C12	-5.09	99.82	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1411	NHW	C14-C11-C10	5.01	117.32	108.77
5	B	1411	NHW	C6-C5-N4	-5.00	107.23	116.34
5	A	1411	NHW	O6A-C12-C11	-4.94	102.61	110.55
5	C	1411	NHW	N3A-C4A-N9A	4.89	135.49	127.17
5	C	1411	NHW	N9A-C8A-N7A	-4.76	107.18	113.94
4	B	1000	EN5	O-C9-C8	4.41	130.01	122.02
5	C	1411	NHW	C4A-N9A-C8A	4.16	110.10	105.74
5	C	1411	NHW	C5A-N7A-C8A	4.14	109.96	103.45
5	A	1411	NHW	O1M-C1M-CP	-3.93	116.56	122.17
4	A	1000[A]	EN5	C24-C23-C22	3.82	119.28	111.42
4	A	1000[B]	EN5	C24-C23-C22	3.82	119.28	111.42
5	A	1411	NHW	C6A-C5A-C4A	3.77	122.32	117.18
5	A	1411	NHW	O5-C5-C6	3.74	128.79	122.02
5	A	1411	NHW	C6-C7-N8	-3.55	104.45	112.00
3	B	999	DMS	O-S-C1	3.38	123.39	106.49
3	A	999	DMS	O-S-C2	3.35	123.28	106.49
5	B	1411	NHW	C5A-N7A-C8A	3.35	108.71	103.45
5	B	1411	NHW	P3X-O3X-C3X	-3.34	114.51	123.43
3	B	1414	DMS	C2-S-C1	3.30	115.35	98.42
4	B	1000	EN5	C8-C9-N1	-3.29	110.07	115.86
3	A	999	DMS	C2-S-C1	3.25	115.10	98.42
5	C	1411	NHW	O6A-C12-C11	3.23	115.73	110.55
4	B	1000	EN5	C26-C21-C22	3.19	117.08	109.29
5	C	1411	NHW	C2X-C1X-N9A	-3.19	105.39	113.30
5	A	1411	NHW	N3A-C4A-N9A	3.08	132.40	127.17
5	B	1411	NHW	C14-C11-C10	3.07	114.00	108.77
5	C	1411	NHW	C7-N8-C9	3.04	128.01	122.55
5	C	1411	NHW	C13-C11-C10	3.00	113.87	108.77
5	B	1411	NHW	O2A-P1A-O3A	2.93	115.18	107.27
5	C	1411	NHW	C4A-C5A-N7A	-2.92	107.25	110.58
5	B	1411	NHW	N3A-C2A-N1A	-2.91	124.17	128.58
5	B	1411	NHW	C2A-N1A-C6A	2.90	123.50	118.73
5	C	1411	NHW	O1M-C1M-CP	-2.88	118.06	122.17
5	A	1411	NHW	O9-C9-N8	2.88	129.07	122.98
4	B	1000	EN5	C3-C2-C1	2.80	128.53	114.37
5	C	1411	NHW	O3A-P2A-O5A	-2.76	102.42	110.70
3	A	1415	DMS	C2-S-C1	2.75	112.49	98.42
5	A	1411	NHW	C7-C6-C5	-2.70	107.89	112.39
5	C	1411	NHW	O4X-C1X-C2X	-2.70	100.84	106.62
5	A	1411	NHW	C5A-C4A-N9A	2.69	108.74	105.81
5	B	1411	NHW	O7A-P3X-O9A	2.68	121.27	110.83
5	A	1411	NHW	O4A-P2A-O5A	2.65	124.76	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1411	NHW	C7-N8-C9	2.63	127.27	122.55
5	A	1411	NHW	C4A-C5A-N7A	-2.62	107.59	110.58
5	C	1411	NHW	C2A-N3A-C4A	2.56	118.07	111.83
5	A	1411	NHW	C13-C11-C10	2.55	113.12	108.77
5	A	1411	NHW	P3X-O3X-C3X	-2.54	116.64	123.43
5	A	1411	NHW	C2-S1-CP	-2.50	97.59	101.72
5	A	1411	NHW	CP-C1M-C2M	2.50	120.83	115.55
4	B	1000	EN5	C18-C13-N2	-2.47	104.43	111.11
4	B	1000	EN5	C7-C8-C9	2.45	120.00	113.19
5	C	1411	NHW	C2-S1-CP	-2.38	97.80	101.72
5	C	1411	NHW	CP-C1M-C2M	2.35	120.52	115.55
4	B	1000	EN5	C14-C13-N2	-2.35	106.26	110.91
5	A	1411	NHW	C6-C5-N4	-2.33	112.09	116.34
3	B	1414	DMS	O-S-C2	2.33	118.15	106.49
5	A	1411	NHW	O3A-P1A-O1A	-2.32	103.71	110.70
4	A	1000[A]	EN5	C25-C26-C21	2.31	116.94	112.08
4	A	1000[B]	EN5	C25-C26-C21	2.31	116.94	112.08
5	A	1411	NHW	C3-N4-C5	2.29	127.08	122.82
5	C	1411	NHW	O5-C5-C6	-2.28	117.89	122.02
5	C	1411	NHW	O4A-P2A-O5A	2.27	123.01	112.44
5	C	1411	NHW	O4A-P2A-O3A	2.27	113.40	107.27
5	C	1411	NHW	C4A-N9A-C1X	-2.26	121.35	126.63
3	A	999	DMS	O-S-C1	2.25	117.77	106.49
5	C	1411	NHW	C6-C7-N8	-2.25	107.21	112.00
5	A	1411	NHW	O3X-C3X-C4X	-2.13	102.54	110.03
5	A	1411	NHW	O5-C5-N4	-2.12	118.86	123.03
5	B	1411	NHW	C2-S1-CP	2.12	105.21	101.72
5	B	1411	NHW	C13-C11-C10	2.11	112.36	108.77
5	C	1411	NHW	C2A-N1A-C6A	-2.10	115.28	118.73
4	A	1000[A]	EN5	C20-C21-C22	2.09	117.30	112.05
4	A	1000[B]	EN5	C20-C21-C22	2.09	117.30	112.05
4	B	1000	EN5	C14-C13-C18	2.08	115.20	110.11
5	A	1411	NHW	C2A-N3A-C4A	2.04	116.81	111.83
5	C	1411	NHW	O8A-P3X-O3X	-2.03	97.92	105.85
5	A	1411	NHW	O9-C9-C10	-2.02	115.25	120.89
5	C	1411	NHW	C5A-C6A-N1A	2.01	122.62	117.51
8	A	1414	SO4	O4-S-O2	2.01	120.06	109.56

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1411	NHW	C12-O6A-P2A-O5A
5	C	1411	NHW	C12-O6A-P2A-O5A
5	C	1411	NHW	C6-C7-N8-C9
4	B	1000	EN5	C1-C2-C3-C4
5	A	1411	NHW	C6-C7-N8-C9
4	A	1000[A]	EN5	N-C-C1-C2
4	B	1000	EN5	C-C1-C2-C3
4	B	1000	EN5	C4-C5-C6-C7
5	B	1411	NHW	C12-O6A-P2A-O3A
5	B	1411	NHW	C12-O6A-P2A-O4A
4	B	1000	EN5	N-C-C1-C2
4	A	1000[B]	EN5	C4-C5-C6-C7
4	A	1000[A]	EN5	C4-C5-C6-C7
4	B	1000	EN5	N2-C13-C18-O3
4	A	1000[B]	EN5	C1-C2-C3-C4
4	A	1000[B]	EN5	C2-C3-C4-C5
5	C	1411	NHW	C4M-C5M-C6M-C7M
4	A	1000[A]	EN5	N2-C13-C18-O3
4	A	1000[B]	EN5	N2-C13-C18-O3
4	A	1000[A]	EN5	N2-C13-C18-N4
4	A	1000[B]	EN5	N2-C13-C18-N4
5	B	1411	NHW	C11-C12-O6A-P2A
4	B	1000	EN5	N2-C13-C18-N4
4	B	1000	EN5	C6-C7-C8-C9
5	B	1411	NHW	P2A-O3A-P1A-O1A

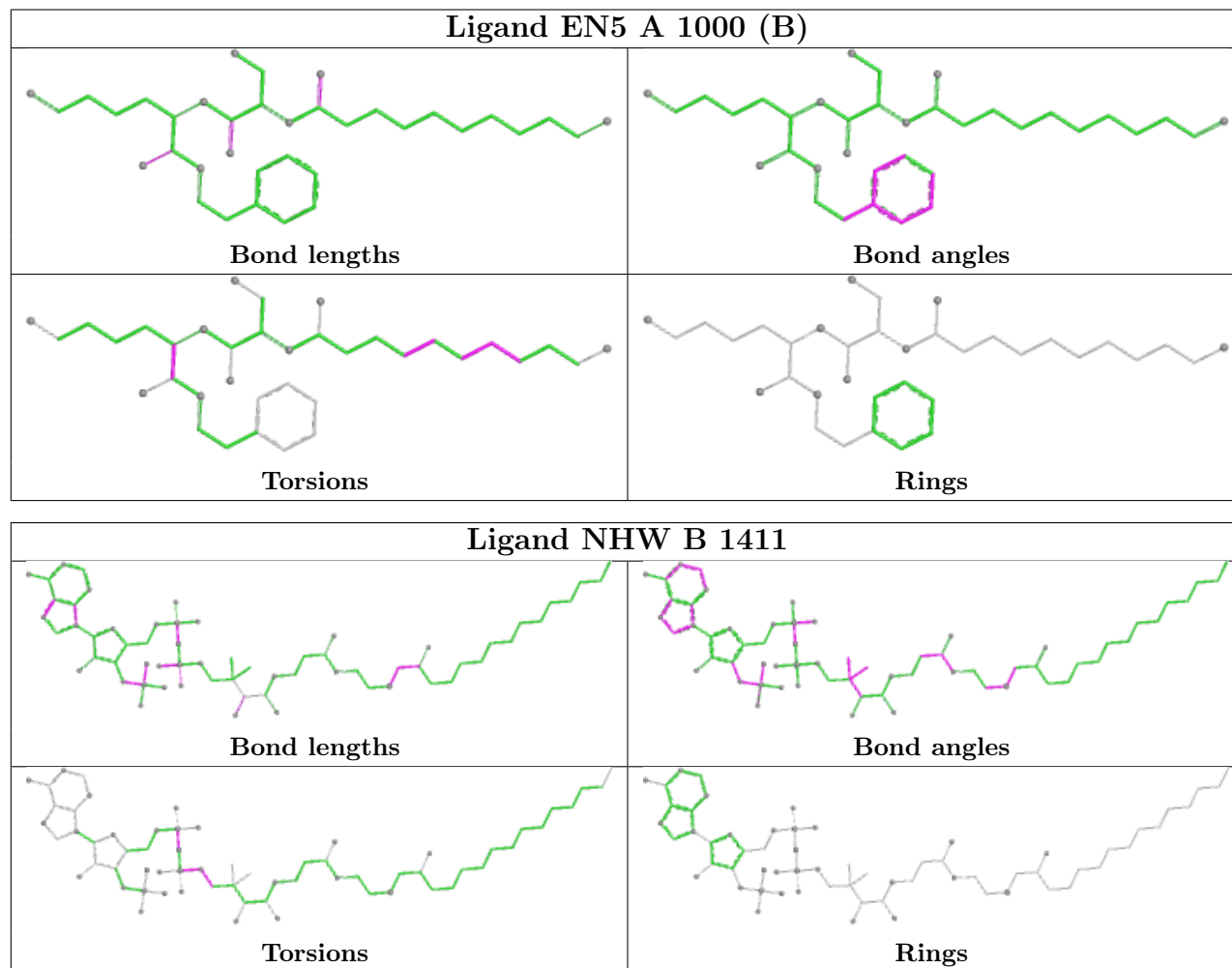
There are no ring outliers.

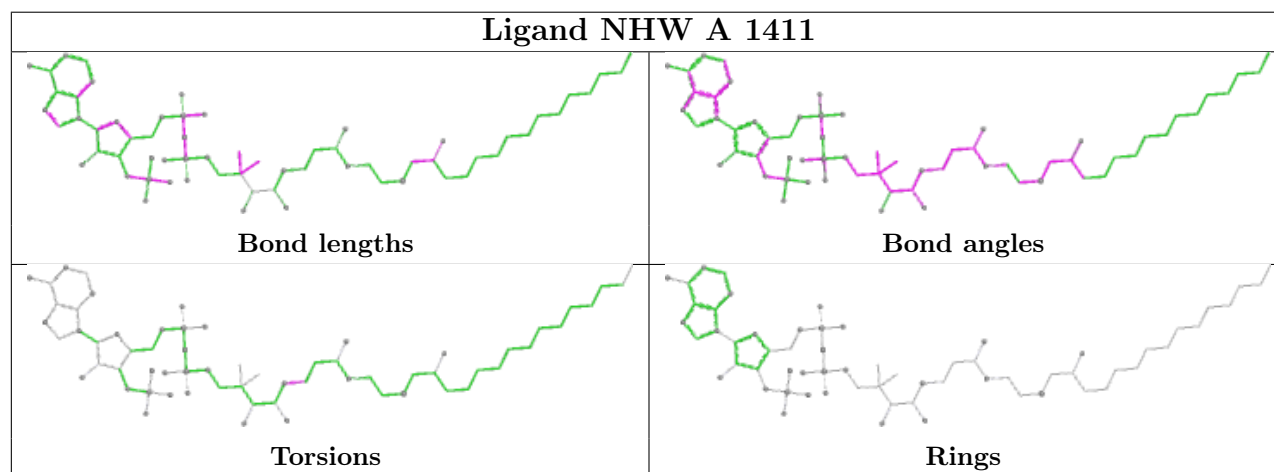
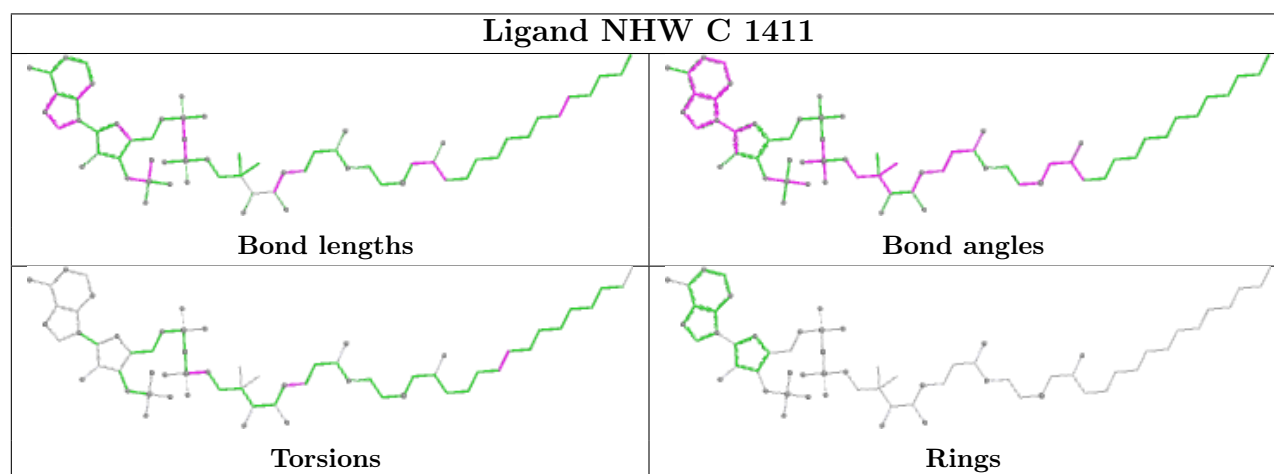
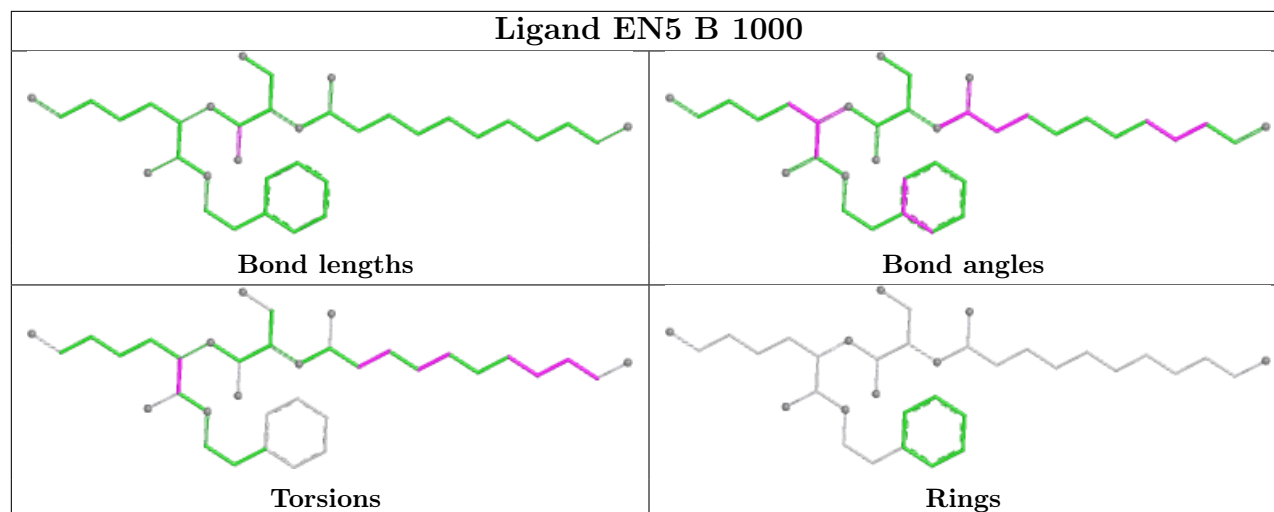
8 monomers are involved in 35 short contacts:

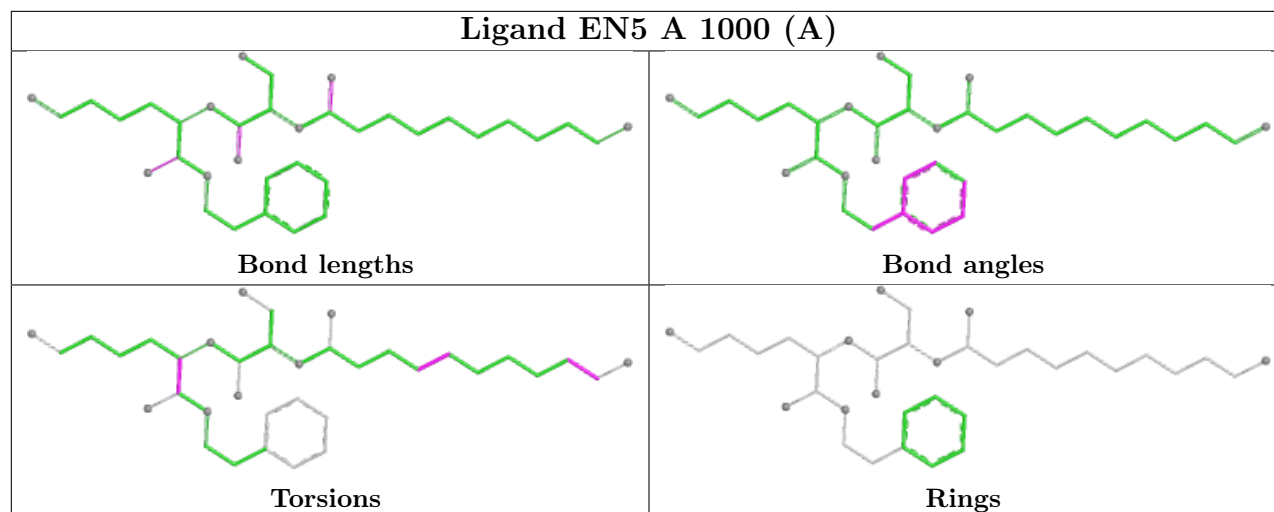
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	999	DMS	3	0
3	A	1415	DMS	2	0
3	B	1414	DMS	15	0
4	B	1000	EN5	8	0
2	A	997	FMT	2	0
3	C	999	DMS	4	0
3	A	999	DMS	2	0
4	A	1000[A]	EN5	4	0

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.







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	384/384 (100%)	0.16	12 (3%)	51 57	4, 11, 19, 31	43 (11%)
1	B	384/384 (100%)	-0.05	11 (2%)	53 59	5, 10, 20, 60	31 (8%)
1	C	370/384 (96%)	0.34	23 (6%)	26 31	5, 12, 24, 49	32 (8%)
All	All	1138/1152 (98%)	0.15	46 (4%)	42 48	4, 11, 23, 60	106 (9%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	241	LEU	18.0
1	C	242	TYR	17.4
1	A	231	SER	8.7
1	A	230	ASN	8.1
1	A	232	ARG	7.3
1	C	243[A]	ARG	6.3
1	C	323	GLY	5.0
1	B	231	SER	4.4
1	A	39	ILE	3.9
1	C	326	LYS	3.5
1	A	27[A]	ASP	3.5
1	B	230	ASN	3.3
1	A	306	GLY	3.2
1	B	232	ARG	3.1
1	C	27	ASP	3.0
1	B	32[A]	TYR	2.9
1	B	305	ASN	2.9
1	C	386	GLY	2.8
1	C	211[A]	TYR	2.8
1	C	222	ILE	2.8
1	C	305	ASN	2.7
1	B	325	ASP	2.7
1	C	327	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	46	SER	2.7
1	C	39	ILE	2.7
1	B	40	ASN	2.7
1	C	32[A]	TYR	2.7
1	A	229	LEU	2.6
1	A	233	LEU	2.6
1	A	305	ASN	2.6
1	B	27[A]	ASP	2.5
1	C	322	LEU	2.5
1	C	103	PHE	2.5
1	C	102	ILE	2.5
1	A	32[A]	TYR	2.3
1	C	151	HIS	2.2
1	A	307	LYS	2.2
1	C	325	ASP	2.1
1	C	224	ILE	2.1
1	B	133	ALA	2.1
1	C	47	VAL	2.1
1	A	323	GLY	2.1
1	C	324	ASN	2.1
1	B	39	ILE	2.1
1	B	306	GLY	2.1
1	C	226	PHE	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.

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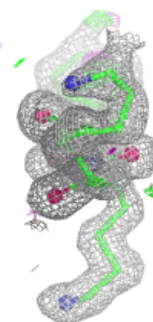
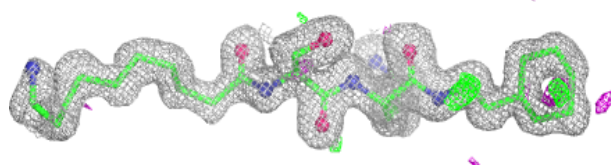
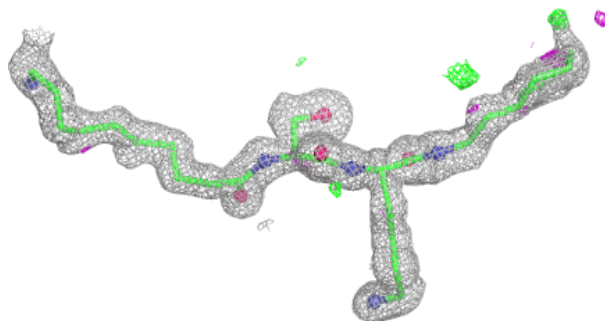
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMS	C	999	4/4	0.64	0.34	27,28,31,34	4
3	DMS	A	999	4/4	0.69	0.22	15,17,21,24	4
3	DMS	B	999	4/4	0.75	0.21	20,20,24,25	1
3	DMS	A	1415	4/4	0.76	0.21	23,24,25,27	4
6	CL	C	1414	1/1	0.83	0.18	54,54,54,54	0
3	DMS	B	1414	4/4	0.84	0.18	18,20,21,25	4
8	SO4	A	1414	5/5	0.88	0.12	31,36,38,43	0
4	EN5	A	1000[A]	36/36	0.91	0.09	14,16,18,19	36
4	EN5	A	1000[B]	36/36	0.91	0.09	16,19,22,23	36
4	EN5	B	1000	36/36	0.93	0.09	12,15,22,22	0
6	CL	C	1413	1/1	0.93	0.11	41,41,41,41	0
2	FMT	A	997	3/3	0.95	0.09	16,16,17,18	0
7	MG	A	1413	1/1	0.96	0.08	21,21,21,21	0
5	NHW	B	1411	64/64	0.98	0.04	5,8,11,14	0
5	NHW	C	1411	64/64	0.98	0.05	6,10,13,16	0
7	MG	C	1415	1/1	0.98	0.09	21,21,21,21	0
5	NHW	A	1411	64/64	0.98	0.05	6,8,11,14	0
6	CL	B	1412	1/1	0.99	0.02	9,9,9,9	0
7	MG	B	1413	1/1	0.99	0.04	21,21,21,21	0
6	CL	A	1412	1/1	1.00	0.03	8,8,8,8	0
6	CL	C	1412	1/1	1.00	0.05	10,10,10,10	0

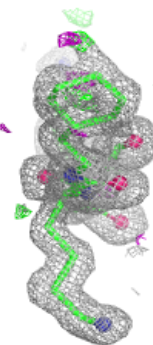
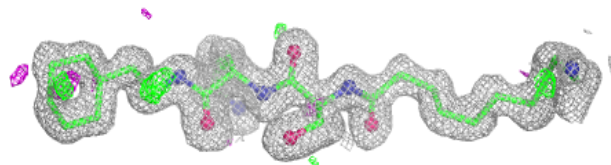
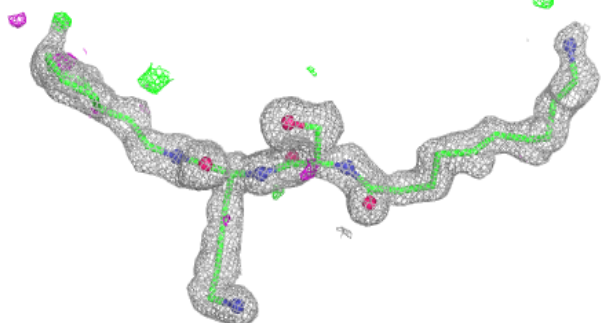
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EN5 A 1000 (A):

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

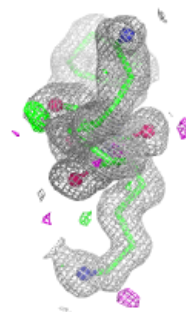
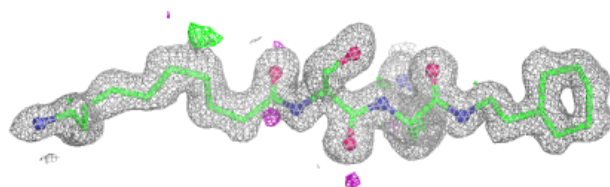
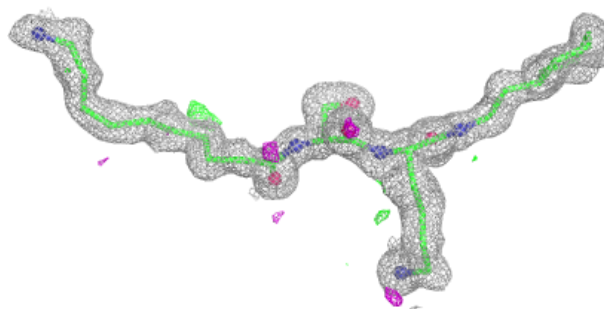
**Electron density around EN5 A 1000 (B):**

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

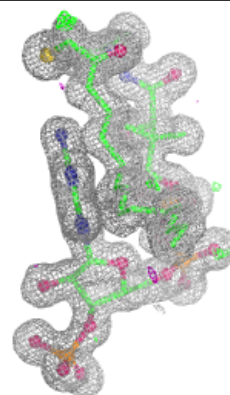
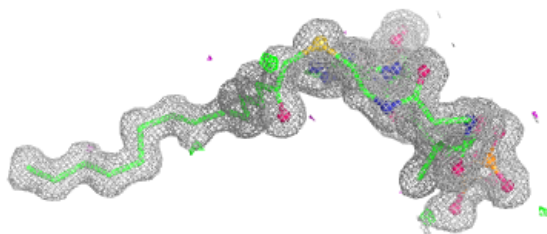
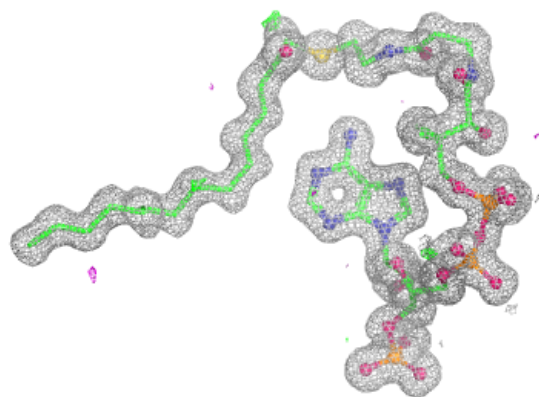


Electron density around EN5 B 1000:

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

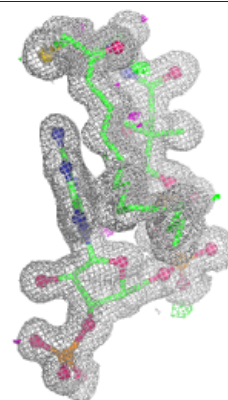
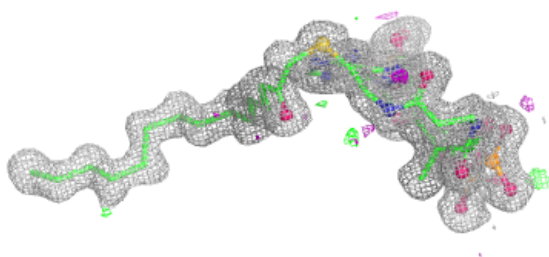
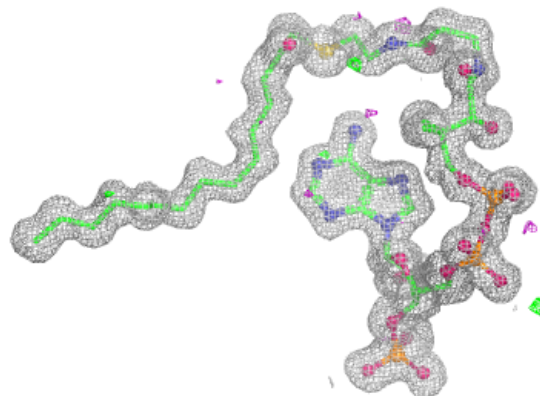
**Electron density around NHW B 1411:**

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

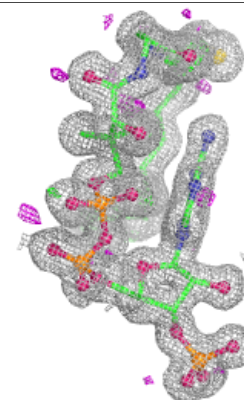
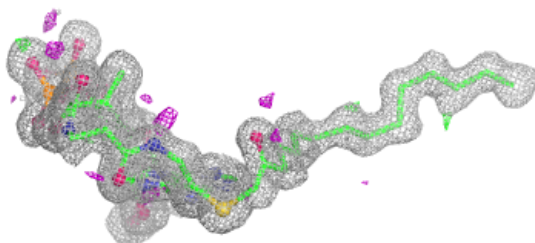
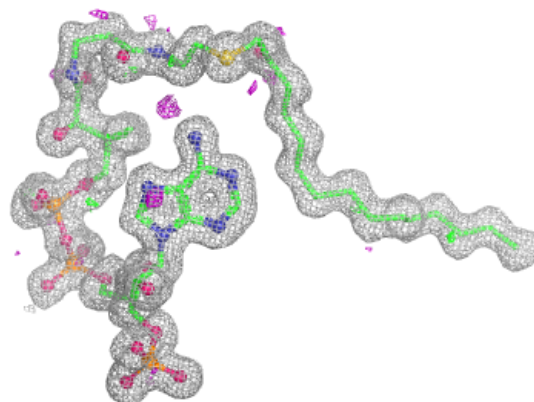


Electron density around NHW C 1411:

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

**Electron density around NHW A 1411:**

$2mF_o-DF_c$ (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.