



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 12:49 pm GMT

PDB ID : 4B13
Title : Plasmodium vivax N-myristoyltransferase with a bound benzofuran inhibitor (compound 25)
Authors : Yu, Z.; Brannigan, J.A.; Moss, D.K.; Brzozowski, A.M.; Wilkinson, A.J.; Holder, A.A.; Tate, E.W.; Leatherbarrow, R.J.
Deposited on : 2012-07-06
Resolution : 1.58 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

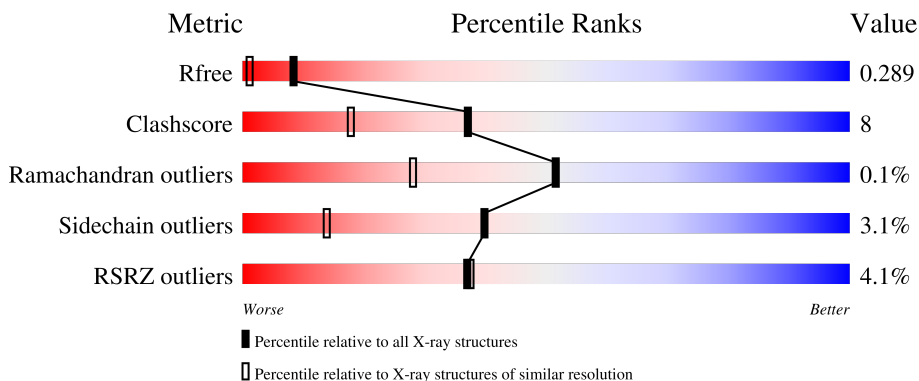
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 7 unique types of molecules in this entry. The entry contains 11104 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.

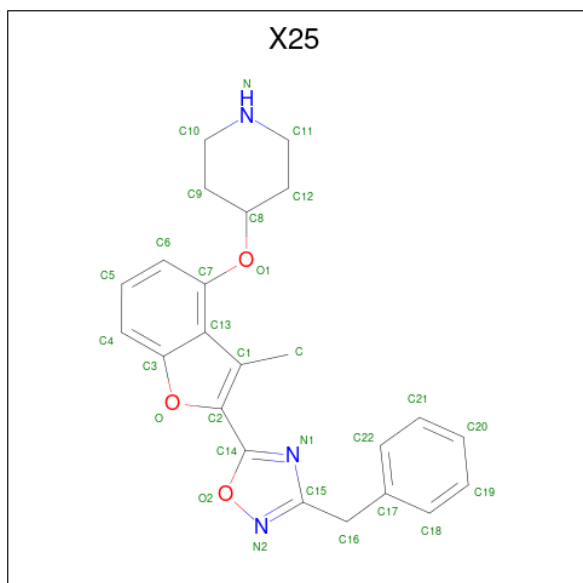
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	Total 3255	C 2117	N 528	O 598	S 12	0	11	0
1	B	385	Total 3251	C 2112	N 529	O 597	S 13	0	12	0
1	C	368	Total 3155	C 2059	N 503	O 582	S 11	0	17	0

There are 3 discrepancies between the modelled and reference sequences:

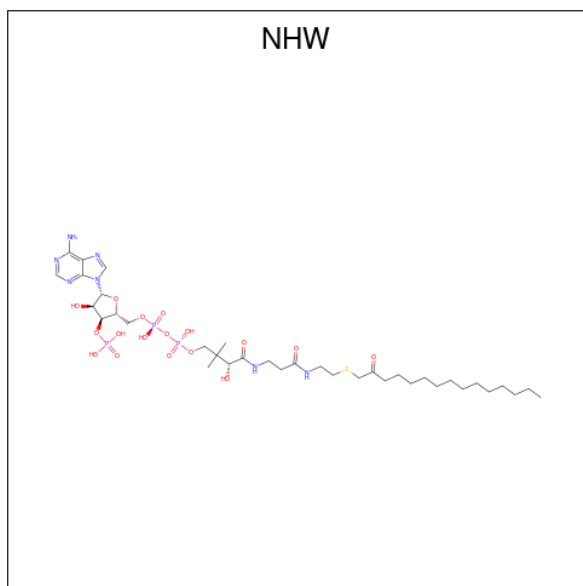
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP A5K1A2
B	26	MET	-	expression tag	UNP A5K1A2
C	26	MET	-	expression tag	UNP A5K1A2

- Molecule 2 is 4-{{2-(3-benzyl-1,2,4-oxadiazol-5-yl)-3-methyl-1-benzofuran-4-yl}oxy}piperidine (three-letter code: X25) (formula: C₂₃H₂₃N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	29	23	3	3	0	0
2	B	1	29	23	3	3	0	0
2	C	1	29	23	3	3	0	0

- Molecule 3 is 2-oxopentadecyl-CoA (three-letter code: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



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

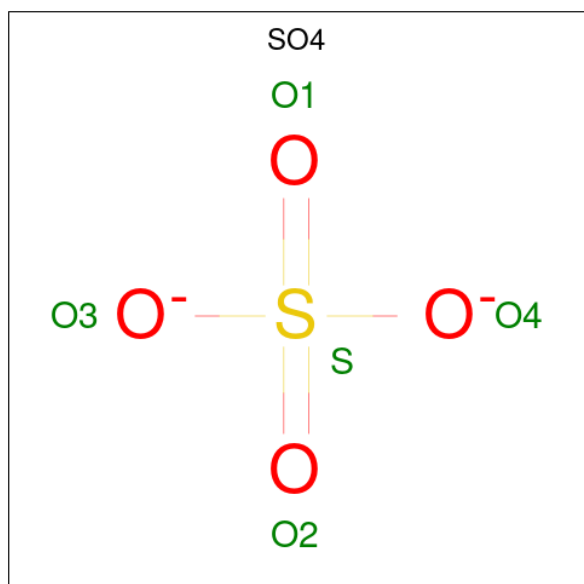
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

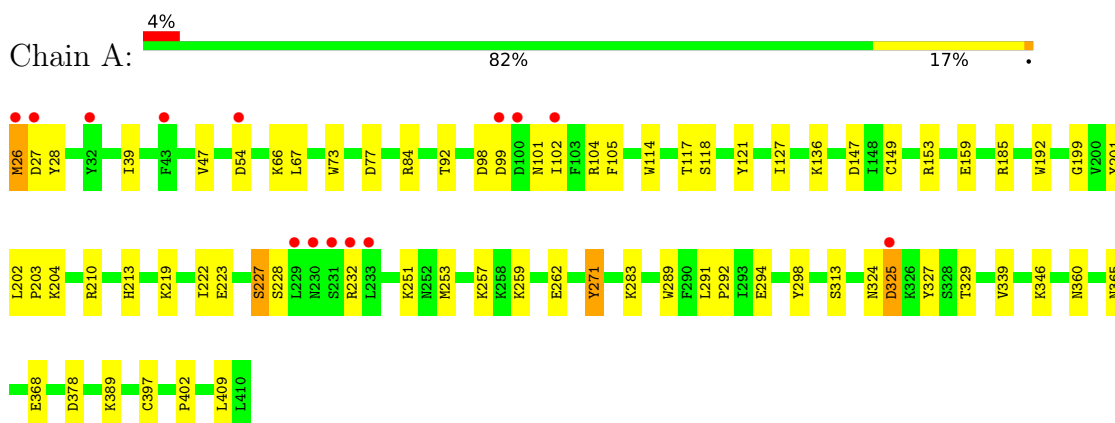
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	415	Total O 415 415	0	0
7	B	392	Total O 392 392	0	0
7	C	346	Total O 346 346	0	0

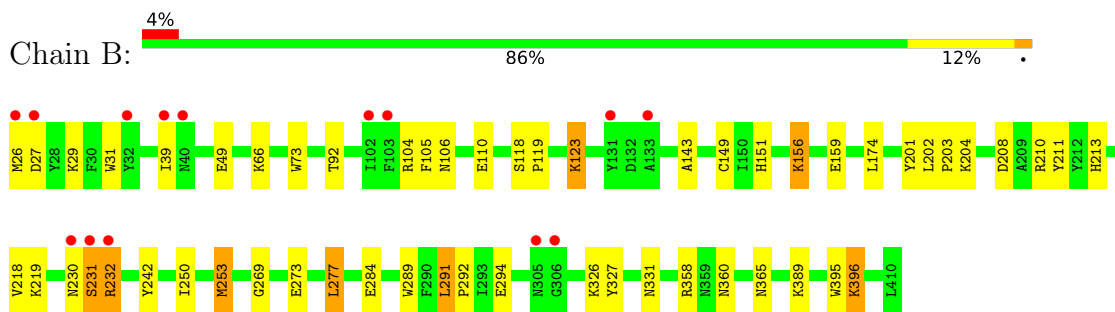
3 Residue-property plots [i](#)

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.

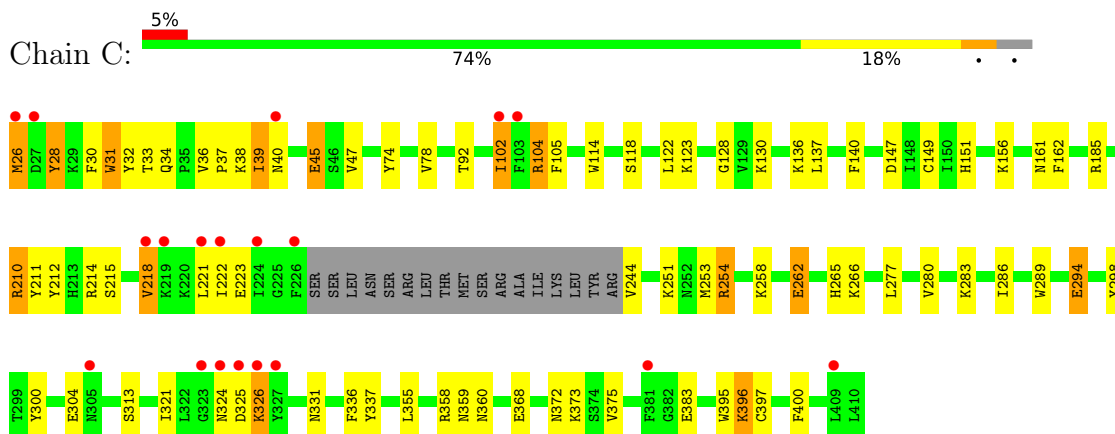
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.32Å 119.13Å 178.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.51 – 1.58 37.48 – 1.58	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.51-1.58) 98.3 (37.48-1.58)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.58Å)	Xtrriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.238 , 0.291 0.236 , 0.289	Depositor DCC
R_{free} test set	8223 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtrriage
Anisotropy	0.597	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11104	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: CL, NHW, SO4, X25, 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	1.03	2/3356 (0.1%)	1.07	6/4543 (0.1%)
1	B	1.00	3/3361 (0.1%)	1.07	10/4549 (0.2%)
1	C	0.99	5/3269 (0.2%)	1.06	9/4425 (0.2%)
All	All	1.01	10/9986 (0.1%)	1.07	25/13517 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	TRP	CD2-CE2	7.83	1.50	1.41
1	B	395	TRP	CD2-CE2	6.72	1.49	1.41
1	B	31	TRP	CD2-CE2	6.47	1.49	1.41
1	B	73	TRP	CD2-CE2	5.81	1.48	1.41
1	C	395	TRP	CD2-CE2	5.52	1.48	1.41
1	A	114	TRP	CD2-CE2	5.49	1.48	1.41
1	C	31	TRP	CD2-CE2	5.35	1.47	1.41
1	C	337	TYR	CG-CD1	5.29	1.46	1.39
1	C	114	TRP	CD2-CE2	5.19	1.47	1.41
1	C	140	PHE	CG-CD1	5.06	1.46	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	B	210	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	358	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	208	ASP	CB-CG-OD1	6.88	124.50	118.30
1	A	84	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	291	LEU	CB-CG-CD2	-6.56	99.84	111.00
1	C	358	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	C	39	ILE	CG1-CB-CG2	-6.17	97.82	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	210	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	77	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	185	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	26	MET	CG-SD-CE	5.56	109.09	100.20
1	A	271	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	B	210	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	254	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	253	MET	CA-CB-CG	5.40	122.49	113.30
1	C	122	LEU	CA-CB-CG	5.33	127.57	115.30
1	B	202	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	B	358	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	174	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	B	105	PHE	CB-CG-CD1	5.13	124.39	120.80
1	B	277	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	C	210	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	C	104	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3255	0	3255	47	0
1	B	3251	0	3255	39	0
1	C	3155	0	3145	65	1
2	A	29	0	23	4	0
2	B	29	0	23	1	0
2	C	29	0	23	2	0
3	A	64	0	60	1	0
3	B	64	0	60	1	0
3	C	64	0	60	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	5	0	0	0	0
7	A	415	0	0	9	1
7	B	392	0	0	12	0
7	C	346	0	0	13	0
All	All	11104	0	9904	155	1

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 8.

All (155) 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:A:257:LYS:HE3	1:A:259:LYS:HE2	1.27	1.16
1:B:151[B]:HIS:HE1	7:B:2028:HOH:O	1.38	1.06
1:C:30:PHE:O	1:C:33[A]:THR:HG22	1.60	1.02
1:C:147:ASP:OD1	1:C:156:LYS:HE3	1.63	0.98
1:B:232:ARG:HH11	1:B:232:ARG:HG2	1.28	0.94
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:CA	1.98	0.92
1:C:102:ILE:HG13	7:C:2105:HOH:O	1.70	0.92
1:B:39:ILE:HD11	1:B:201:TYR:HE2	1.37	0.90
1:C:40:ASN:HB2	7:C:2010:HOH:O	1.76	0.84
1:C:326[B]:LYS:HG2	7:C:2287:HOH:O	1.79	0.82
1:A:105:PHE:HZ	2:A:1411:X25:HC2	1.45	0.82
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:HA	1.62	0.81
1:C:262[B]:GLU:HG3	1:C:283:LYS:HE3	1.68	0.74
1:B:232:ARG:HG2	1:B:232:ARG:NH1	2.01	0.72
1:C:262[A]:GLU:HG2	1:C:283:LYS:HE3	1.71	0.72
1:C:331:ASN:HB3	7:C:2288:HOH:O	1.91	0.70
1:A:257:LYS:HE3	1:A:259:LYS:CE	2.13	0.70
1:C:28:TYR:CE2	1:C:39:ILE:HG13	2.26	0.69
1:C:147:ASP:OD1	1:C:156:LYS:CE	2.41	0.69
1:B:294:GLU:OE2	7:B:2309:HOH:O	2.12	0.68
1:C:32[A]:TYR:CE1	1:C:38:LYS:HE3	2.29	0.67
1:C:325:ASP:H	1:C:326[A]:LYS:HZ1	1.40	0.67
1:A:105:PHE:CZ	2:A:1411:X25:HC2	2.29	0.66
1:A:66:LYS:HE3	7:A:2084:HOH:O	1.97	0.65
1:C:45[B]:GLU:OE2	1:C:151:HIS:HE1	1.79	0.65
1:C:304[B]:GLU:HG2	7:C:2231:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:VAL:O	7:C:2263:HOH:O	2.15	0.64
1:C:32[B]:TYR:CE2	1:C:38:LYS:HD2	2.33	0.64
1:A:127:ILE:HD11	1:A:185:ARG:HD2	1.78	0.64
1:B:49[B]:GLU:HB2	7:B:2176:HOH:O	1.97	0.64
1:A:257:LYS:CE	1:A:259:LYS:HE2	2.17	0.63
1:C:254:ARG:HA	7:C:2232:HOH:O	1.99	0.62
1:B:156[A]:LYS:HA	1:B:156[A]:LYS:CE	2.29	0.62
1:C:123:LYS:HB3	7:C:2073:HOH:O	2.00	0.61
1:B:123:LYS:HD3	7:B:2155:HOH:O	2.02	0.60
1:C:33[A]:THR:HG23	1:C:34:GLN:OE1	2.02	0.59
1:B:213:HIS:HB2	7:B:2219:HOH:O	2.02	0.59
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.23	0.59
1:C:223:GLU:OE2	1:C:326[B]:LYS:HE2	2.03	0.59
1:C:214[B]:ARG:HD2	1:C:215:SER:N	2.19	0.58
1:B:92:THR:O	1:B:104:ARG:HD2	2.04	0.58
1:B:230[A]:ASN:OD1	1:B:231:SER:N	2.36	0.58
1:C:45[B]:GLU:OE2	1:C:151:HIS:CE1	2.57	0.57
1:C:214[B]:ARG:HD2	1:C:214[B]:ARG:C	2.24	0.57
1:B:39:ILE:HD11	1:B:201:TYR:CE2	2.29	0.56
1:B:156[A]:LYS:CA	1:B:156[A]:LYS:CE	2.81	0.56
1:B:232:ARG:HH11	1:B:232:ARG:CG	2.11	0.56
1:C:262[B]:GLU:CG	1:C:283:LYS:HE3	2.35	0.55
1:A:325:ASP:OD1	1:A:325:ASP:N	2.27	0.55
1:A:26:MET:CE	1:A:27:ASP:HB2	2.37	0.55
1:B:26:MET:HA	7:B:2001:HOH:O	2.07	0.55
1:C:325:ASP:N	1:C:326[A]:LYS:HZ1	2.05	0.54
1:B:156[A]:LYS:HG2	7:B:2168:HOH:O	2.08	0.53
1:C:212:TYR:CE2	1:C:383:GLU:HG3	2.43	0.53
1:A:222[A]:ILE:HD13	1:A:227:SER:HB2	1.90	0.53
1:A:118:SER:HB3	1:A:289:TRP:CZ2	2.45	0.52
1:C:265:HIS:HA	1:C:286:ILE:HG13	1.91	0.52
1:A:39:ILE:HD12	1:A:201:TYR:HE2	1.75	0.52
1:C:92:THR:O	1:C:104:ARG:HD2	2.10	0.51
1:A:219:LYS:NZ	1:A:223:GLU:OE2	2.44	0.51
1:C:105:PHE:HZ	2:C:1411:X25:HC2	1.75	0.51
1:A:368:GLU:O	1:A:402:PRO:HB2	2.10	0.50
1:A:26:MET:SD	1:A:27:ASP:N	2.85	0.50
1:C:161:ASN:HB3	1:C:162:PHE:CD2	2.47	0.50
1:C:321:ILE:HG22	1:C:324:ASN:HB3	1.94	0.50
1:C:36:VAL:HB	1:C:37:PRO:HD2	1.94	0.49
1:B:218:VAL:HG21	1:B:242:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLU:HA	1:A:283:LYS:HE3	1.94	0.49
1:A:365:ASN:HB3	2:A:1411:X25:H4	1.94	0.49
1:A:329:THR:HG23	7:A:2149:HOH:O	2.12	0.49
2:C:1411:X25:C	2:C:1411:X25:N1	2.74	0.49
1:A:98:ASP:OD1	1:A:102:ILE:N	2.47	0.48
1:B:365:ASN:HB3	2:B:1411:X25:H4	1.95	0.48
1:C:128:GLY:HA3	1:C:137:LEU:HD11	1.95	0.48
1:A:294:GLU:HG3	7:A:2341:HOH:O	2.12	0.48
1:A:360[B]:ASN:ND2	7:A:2384:HOH:O	2.26	0.48
1:C:298:TYR:O	1:C:313:SER:HA	2.14	0.48
1:B:151[B]:HIS:CE1	7:B:2028:HOH:O	2.27	0.48
1:A:92:THR:O	1:A:104:ARG:HD2	2.14	0.48
1:A:346:LYS:HE3	1:A:378:ASP:HB3	1.95	0.48
1:C:47:VAL:O	1:C:397:CYS:HA	2.14	0.48
1:A:28:TYR:CE1	1:A:203:PRO:HD3	2.49	0.47
1:C:215:SER:OG	1:C:221:LEU:CD1	2.62	0.47
1:C:321:ILE:HG23	7:C:2105:HOH:O	2.14	0.47
1:A:26:MET:HE3	1:A:27:ASP:H	1.78	0.47
1:C:36:VAL:HB	1:C:37:PRO:CD	2.44	0.47
1:A:117:THR:HA	1:A:121[A]:TYR:CD2	2.50	0.47
1:B:326:LYS:HD3	1:B:327:TYR:CE2	2.50	0.47
3:B:1412:NHW:C2A	3:B:1412:NHW:H5MA	2.44	0.47
1:A:26:MET:HB3	7:A:2013:HOH:O	2.13	0.47
1:C:294[A]:GLU:HA	1:C:294[A]:GLU:OE1	2.14	0.47
1:C:210:ARG:NH2	1:C:373:LYS:HE2	2.30	0.46
1:C:253:MET:HG3	1:C:300:TYR:HB3	1.97	0.46
1:B:219:LYS:HB3	7:B:2231:HOH:O	2.15	0.46
1:C:400:PHE:N	1:C:400:PHE:CD1	2.83	0.46
1:B:149:CYS:O	1:B:277:LEU:HA	2.15	0.46
1:C:254:ARG:O	1:C:300:TYR:HA	2.16	0.46
1:A:26:MET:CB	7:A:2013:HOH:O	2.63	0.46
1:A:67:LEU:HD11	1:A:73:TRP:CE2	2.51	0.45
1:A:149:CYS:HA	1:A:153:ARG:O	2.16	0.45
1:A:202:LEU:O	1:A:204:LYS:HA	2.16	0.45
1:B:27:ASP:HB3	1:B:29:LYS:HE3	1.98	0.45
1:C:258:LYS:HD2	7:C:2239:HOH:O	2.16	0.45
2:A:1411:X25:O1	2:A:1411:X25:HC1	2.16	0.45
1:A:67:LEU:HD11	1:A:73:TRP:CD2	2.52	0.45
1:A:127:ILE:CD1	1:A:185:ARG:HD2	2.44	0.45
1:A:26:MET:HE3	1:A:27:ASP:HB2	1.99	0.45
1:A:324:ASN:HB3	1:A:327:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:TYR:O	1:A:313:SER:HA	2.17	0.45
1:B:143:ALA:HA	1:B:159:GLU:O	2.17	0.44
1:A:159:GLU:OE2	1:A:409:LEU:HD22	2.17	0.44
3:A:1412:NHW:H8A	7:A:2413:HOH:O	2.17	0.44
1:B:110[B]:GLU:H	1:B:110[B]:GLU:CD	2.21	0.44
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.82	0.44
1:C:39:ILE:HG23	1:C:39:ILE:HD12	1.59	0.44
1:A:98:ASP:O	1:A:101:ASN:N	2.30	0.44
1:B:66:LYS:HE3	7:B:2081:HOH:O	2.18	0.44
1:B:119:PRO:CG	1:B:284[A]:GLU:HG3	2.48	0.44
1:C:214[B]:ARG:HG2	1:C:214[B]:ARG:NH1	2.32	0.44
1:C:74:TYR:CD1	1:C:130:LYS:HE3	2.53	0.43
1:B:269:GLY:O	1:B:273:GLU:HG3	2.18	0.43
1:C:214[B]:ARG:HG2	1:C:214[B]:ARG:HH11	1.81	0.43
1:C:149:CYS:O	1:C:277:LEU:HA	2.18	0.43
1:B:118:SER:HB3	1:B:289:TRP:CZ2	2.53	0.42
1:B:203:PRO:HA	1:B:204:LYS:HA	1.90	0.42
1:A:291:LEU:HA	1:A:292:PRO:HD3	1.93	0.42
1:C:360:ASN:HA	7:C:2208:HOH:O	2.18	0.42
1:C:396:LYS:O	1:C:396:LYS:HG2	2.18	0.42
1:A:271:TYR:CD2	1:A:339:VAL:HG22	2.54	0.42
1:B:291:LEU:HA	1:B:292:PRO:HD3	1.89	0.42
1:B:250:ILE:O	1:B:253[B]:MET:HG2	2.19	0.42
1:A:199:GLY:O	1:A:389:LYS:NZ	2.37	0.42
1:C:34:GLN:NE2	7:C:2007:HOH:O	2.52	0.42
1:C:218:VAL:O	1:C:222:ILE:HG12	2.20	0.42
1:C:47:VAL:HG12	1:C:396:LYS:HG2	2.02	0.42
1:C:215:SER:OG	1:C:221:LEU:HD13	2.19	0.42
1:C:359:ASN:O	1:C:360:ASN:HB2	2.19	0.42
1:A:28:TYR:CD1	1:A:203:PRO:HD3	2.54	0.41
1:C:251:LYS:HG2	7:C:2223:HOH:O	2.20	0.41
1:C:28:TYR:HA	3:C:1412:NHW:P3X	2.60	0.41
1:C:215:SER:CB	1:C:221:LEU:HD12	2.51	0.41
1:B:389:LYS:N	1:B:389:LYS:HD2	2.36	0.41
1:A:47:VAL:O	1:A:397:CYS:HA	2.20	0.41
1:C:28:TYR:HB3	1:C:31:TRP:HB2	2.01	0.41
1:C:221:LEU:HD23	1:C:221:LEU:HA	1.79	0.41
1:C:372:ASN:O	1:C:375:VAL:HG22	2.19	0.41
1:A:219:LYS:HD3	7:A:2258:HOH:O	2.19	0.41
1:C:300:TYR:CD2	1:C:355:LEU:HD13	2.55	0.41
1:A:39:ILE:CD1	1:A:201:TYR:HE2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.56	0.40
1:A:213:HIS:HB2	7:A:2249:HOH:O	2.22	0.40
1:B:331:ASN:ND2	7:B:2331:HOH:O	2.54	0.40
1:B:360:ASN:ND2	7:B:2355:HOH:O	2.54	0.40
1:C:32[B]:TYR:CD2	1:C:38:LYS:HD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:MET:CE	7:A:2180:HOH:O[4_456]	1.63	0.57

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	394/385 (102%)	385 (98%)	9 (2%)	0	100	100
1	B	395/385 (103%)	384 (97%)	11 (3%)	0	100	100
1	C	380/385 (99%)	367 (97%)	12 (3%)	1 (0%)	41	21
All	All	1169/1155 (101%)	1136 (97%)	32 (3%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	368	GLU

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/351 (103%)	352 (97%)	10 (3%)	43	17
1	B	363/351 (103%)	352 (97%)	11 (3%)	41	15
1	C	352/351 (100%)	332 (94%)	20 (6%)	20	4
All	All	1077/1053 (102%)	1036 (96%)	41 (4%)	40	9

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	99	ASP
1	A	136	LYS
1	A	147	ASP
1	A	227	SER
1	A	228	SER
1	A	232	ARG
1	A	251[A]	LYS
1	A	251[B]	LYS
1	A	325	ASP
1	B	106	ASN
1	B	123	LYS
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	211	TYR
1	B	231	SER
1	B	232	ARG
1	B	253[A]	MET
1	B	253[B]	MET
1	B	396[A]	LYS
1	B	396[B]	LYS
1	C	26	MET
1	C	28	TYR
1	C	45[A]	GLU
1	C	45[B]	GLU
1	C	78[A]	VAL
1	C	78[B]	VAL
1	C	102	ILE
1	C	136	LYS
1	C	211	TYR

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Mol	Chain	Res	Type
1	C	218	VAL
1	C	244	VAL
1	C	262[A]	GLU
1	C	262[B]	GLU
1	C	266	LYS
1	C	294[A]	GLU
1	C	294[B]	GLU
1	C	326[A]	LYS
1	C	326[B]	LYS
1	C	336	PHE
1	C	396	LYS

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	34	GLN
1	A	40	ASN
1	A	106	ASN
1	A	193	GLN
1	A	371	GLN
1	B	34	GLN
1	B	106	ASN
1	B	295	ASN
1	B	320	GLN
1	B	331	ASN
1	B	360	ASN
1	B	371	GLN
1	C	34	GLN
1	C	151	HIS
1	C	320	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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
6	SO4	B	1413	-	4,4,4	0.28	0	6,6,6	0.45	0
3	NHW	A	1412	5	58,66,66	1.28	7 (12%)	70,92,92	1.61	12 (17%)
2	X25	B	1411	-	25,33,33	1.52	3 (12%)	25,46,46	2.87	12 (48%)
2	X25	A	1411	-	25,33,33	1.67	5 (20%)	25,46,46	2.80	9 (36%)
3	NHW	C	1412	5	58,66,66	1.49	5 (8%)	70,92,92	1.39	9 (12%)
3	NHW	B	1412	5	58,66,66	1.45	7 (12%)	70,92,92	1.54	8 (11%)
2	X25	C	1411	-	25,33,33	1.26	3 (12%)	25,46,46	2.48	11 (44%)

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	NHW	A	1412	5	-	2/61/81/81	0/3/3/3
2	X25	B	1411	-	-	3/8/20/20	0/5/5/5
2	X25	A	1411	-	-	3/8/20/20	0/5/5/5
3	NHW	C	1412	5	-	3/61/81/81	0/3/3/3
3	NHW	B	1412	5	-	3/61/81/81	0/3/3/3
2	X25	C	1411	-	-	4/8/20/20	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1412	NHW	P3X-O3X	7.78	1.74	1.59
3	B	1412	NHW	O4X-C4X	5.09	1.56	1.45
2	B	1411	X25	C1-C13	-4.85	1.35	1.40
3	B	1412	NHW	P3X-O3X	4.61	1.68	1.59
2	A	1411	X25	C1-C13	-4.53	1.36	1.40
3	A	1412	NHW	O4X-C4X	3.81	1.53	1.45
3	B	1412	NHW	C6-C5	3.61	1.58	1.51
2	A	1411	X25	C16-C15	-3.49	1.45	1.50
2	A	1411	X25	C-C1	-3.45	1.43	1.51
2	B	1411	X25	C13-C3	-3.24	1.36	1.43
2	A	1411	X25	C7-C13	-3.23	1.35	1.42
3	B	1412	NHW	CP-C1M	2.94	1.56	1.51
2	B	1411	X25	C7-C13	-2.93	1.36	1.42
2	C	1411	X25	C1-C13	-2.89	1.37	1.40
2	C	1411	X25	C13-C3	-2.79	1.37	1.43
2	C	1411	X25	C7-C13	-2.75	1.36	1.42
3	C	1412	NHW	P2A-O4A	-2.71	1.42	1.55
3	A	1412	NHW	P3X-O8A	2.70	1.65	1.54
3	A	1412	NHW	P3X-O3X	2.59	1.64	1.59
3	C	1412	NHW	CP-C1M	2.32	1.55	1.51
2	A	1411	X25	C13-C3	-2.24	1.38	1.43
3	A	1412	NHW	P3X-O7A	-2.19	1.46	1.54
3	B	1412	NHW	O6A-C12	2.14	1.50	1.43
3	A	1412	NHW	C7-N8	2.14	1.51	1.46
3	A	1412	NHW	O6A-C12	-2.05	1.37	1.43
3	A	1412	NHW	O1M-C1M	2.04	1.25	1.21
3	C	1412	NHW	P1A-O2A	-2.03	1.45	1.55
3	C	1412	NHW	C14-C11	-2.03	1.49	1.53
3	B	1412	NHW	C6A-C5A	-2.03	1.35	1.43
3	B	1412	NHW	C7-N8	2.00	1.50	1.46

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1412	NHW	N3A-C2A-N1A	-7.28	117.31	128.68
2	A	1411	X25	C1-C13-C3	-7.20	98.06	110.65
3	A	1412	NHW	N3A-C2A-N1A	-6.54	118.45	128.68
2	A	1411	X25	C15-C16-C17	-6.19	97.42	114.17
2	B	1411	X25	C15-C16-C17	-5.87	98.28	114.17
2	C	1411	X25	C1-C13-C3	-5.74	100.62	110.65
2	B	1411	X25	O1-C8-C12	5.43	120.30	108.31
2	B	1411	X25	C4-C3-C13	5.32	126.68	117.84
3	C	1412	NHW	N3A-C2A-N1A	-5.21	120.54	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1411	X25	O1-C8-C12	5.03	119.43	108.31
2	B	1411	X25	C1-C13-C3	-4.93	102.03	110.65
2	C	1411	X25	C15-C16-C17	-4.58	101.78	114.17
3	A	1412	NHW	O1M-C1M-CP	-4.39	115.91	122.17
2	C	1411	X25	C16-C15-N2	4.27	129.62	122.94
2	B	1411	X25	C12-C11-N	4.23	119.21	110.64
2	B	1411	X25	C11-N-C10	3.94	121.66	110.34
3	B	1412	NHW	C2A-N1A-C6A	3.88	125.39	118.75
3	A	1412	NHW	C13-C11-C10	3.88	115.55	108.82
2	C	1411	X25	C11-N-C10	3.84	121.38	110.34
2	A	1411	X25	C11-N-C10	3.72	121.04	110.34
2	A	1411	X25	C12-C11-N	3.68	118.08	110.64
3	B	1412	NHW	O6A-C12-C11	-3.53	104.87	110.55
2	A	1411	X25	O1-C8-C9	3.52	116.08	108.31
3	A	1412	NHW	O4X-C1X-C2X	-3.39	101.97	106.93
3	C	1412	NHW	O4X-C4X-C5X	-3.35	98.34	109.37
2	A	1411	X25	C6-C7-C13	-3.28	114.50	120.61
2	B	1411	X25	C20-C21-C22	3.18	125.03	120.19
2	C	1411	X25	C12-C11-N	3.16	117.05	110.64
2	B	1411	X25	O1-C8-C9	3.16	115.29	108.31
2	C	1411	X25	O1-C8-C12	3.15	115.27	108.31
3	A	1412	NHW	C7-N8-C9	3.00	127.93	122.59
2	C	1411	X25	C4-C3-C13	2.97	122.77	117.84
3	A	1412	NHW	C14-C11-C10	-2.92	103.75	108.82
2	B	1411	X25	C5-C6-C7	2.84	124.24	119.89
3	B	1412	NHW	O1M-C1M-CP	-2.78	118.20	122.17
3	B	1412	NHW	C10-C9-N8	-2.76	111.08	116.58
3	B	1412	NHW	C4M-C3M-C2M	-2.63	103.73	113.19
3	A	1412	NHW	C2A-N1A-C6A	2.62	123.24	118.75
3	A	1412	NHW	C5X-C4X-C3X	-2.59	105.81	114.40
3	C	1412	NHW	O7A-P3X-O9A	2.53	120.59	110.68
3	C	1412	NHW	C13-C11-C10	2.48	113.13	108.82
3	A	1412	NHW	O6A-C12-C11	-2.47	106.58	110.55
3	C	1412	NHW	N6A-C6A-N1A	2.45	123.67	118.57
2	A	1411	X25	C5-C6-C7	2.44	123.64	119.89
2	C	1411	X25	C6-C7-C13	-2.42	116.10	120.61
3	C	1412	NHW	C5A-C6A-N6A	-2.41	116.69	120.35
3	C	1412	NHW	C14-C11-C13	-2.40	104.27	109.17
3	B	1412	NHW	C2X-C3X-C4X	-2.38	99.01	103.22
2	B	1411	X25	C16-C15-N1	2.36	129.15	122.54
2	A	1411	X25	C4-C3-C13	2.30	121.66	117.84
3	B	1412	NHW	N6A-C6A-N1A	2.30	123.34	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1412	NHW	C5X-C4X-C3X	-2.25	106.94	114.40
3	A	1412	NHW	CP-C1M-C2M	2.21	120.27	115.52
3	A	1412	NHW	C1X-N9A-C4A	-2.19	122.79	126.64
2	B	1411	X25	O1-C7-C6	-2.14	120.72	124.59
2	C	1411	X25	O1-C7-C6	-2.11	120.76	124.59
3	A	1412	NHW	C3-N4-C5	-2.11	118.92	122.84
2	B	1411	X25	C6-C7-C13	-2.05	116.79	120.61
2	C	1411	X25	C15-N1-C14	2.03	104.75	102.02
2	C	1411	X25	C21-C20-C19	-2.03	116.17	119.93
3	C	1412	NHW	P2A-O3A-P1A	-2.01	125.92	132.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1411	X25	C6-C7-O1-C8
3	A	1412	NHW	C6-C7-N8-C9
2	C	1411	X25	C9-C8-O1-C7
3	C	1412	NHW	C6-C7-N8-C9
3	A	1412	NHW	C9M-CAM-CBM-CCM
2	A	1411	X25	C13-C7-O1-C8
2	B	1411	X25	C13-C7-O1-C8
2	C	1411	X25	C13-C7-O1-C8
2	A	1411	X25	C9-C8-O1-C7
2	B	1411	X25	C9-C8-O1-C7
2	C	1411	X25	C12-C8-O1-C7
3	B	1412	NHW	C6-C7-N8-C9
3	C	1412	NHW	C9M-CAM-CBM-CCM
3	B	1412	NHW	C7M-C8M-C9M-CAM
2	A	1411	X25	C6-C7-O1-C8
2	C	1411	X25	C6-C7-O1-C8
3	B	1412	NHW	C2-C3-N4-C5
3	C	1412	NHW	C5X-O5X-P1A-O1A

There are no ring outliers.

6 monomers are involved in 10 short contacts:

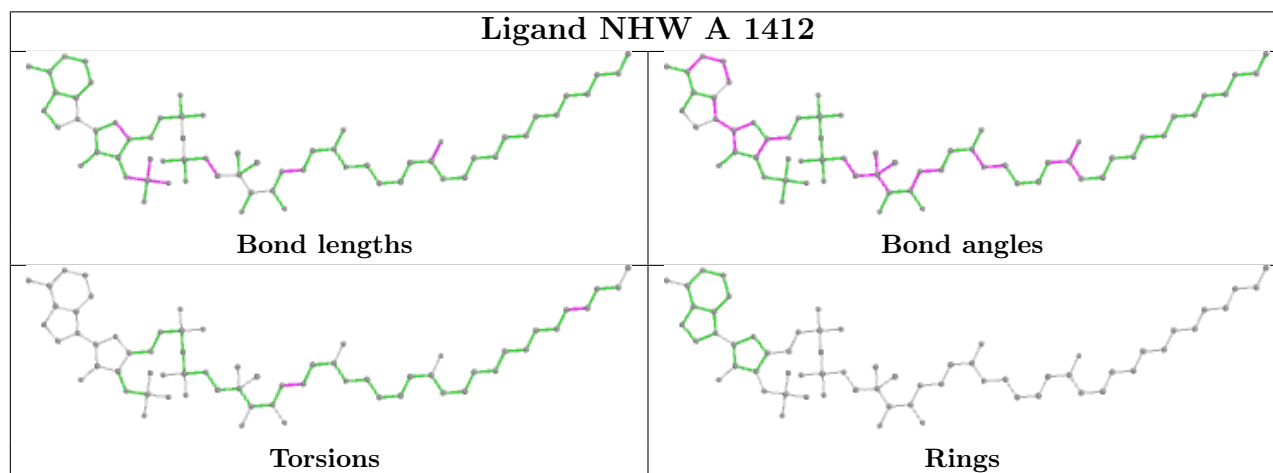
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1412	NHW	1	0
2	B	1411	X25	1	0
2	A	1411	X25	4	0

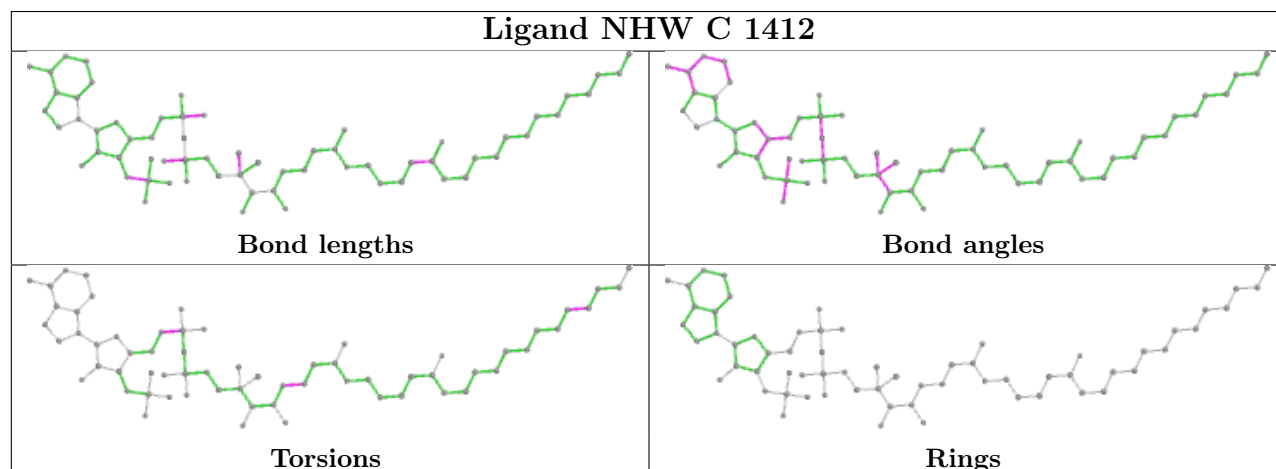
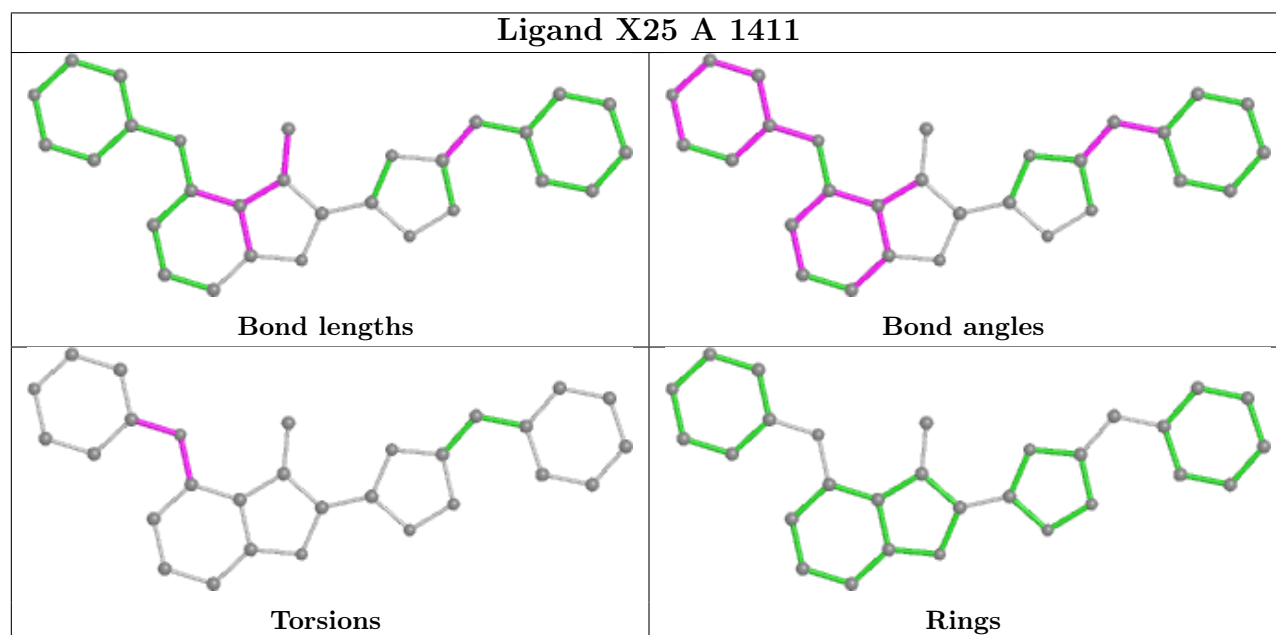
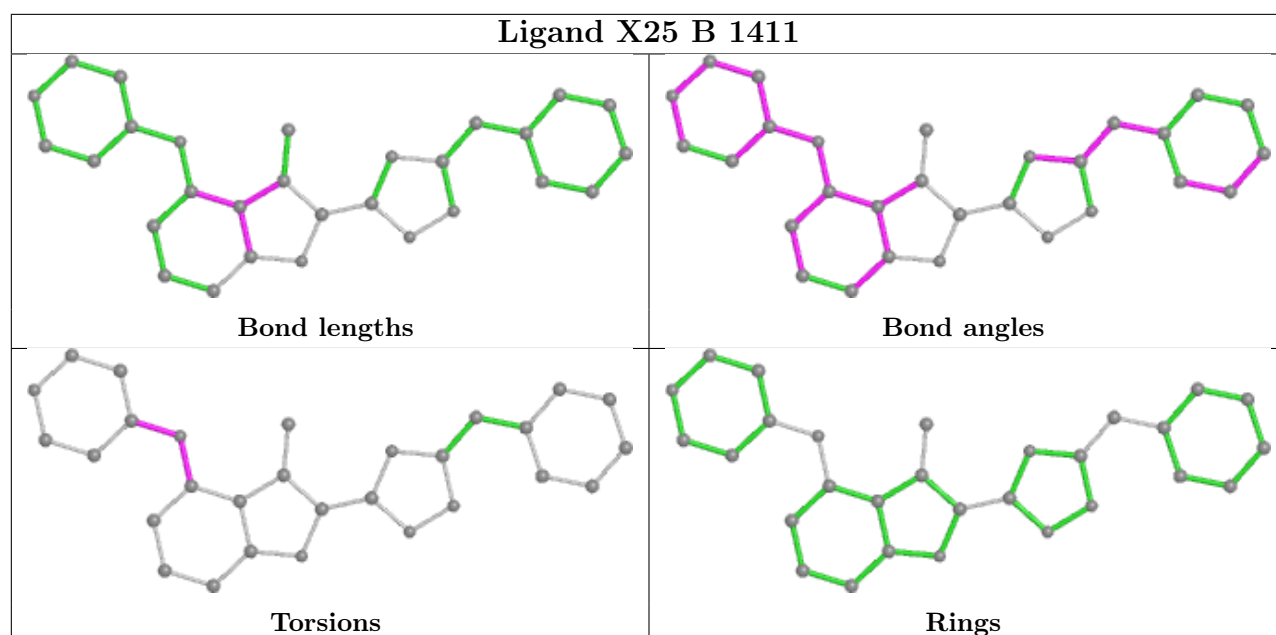
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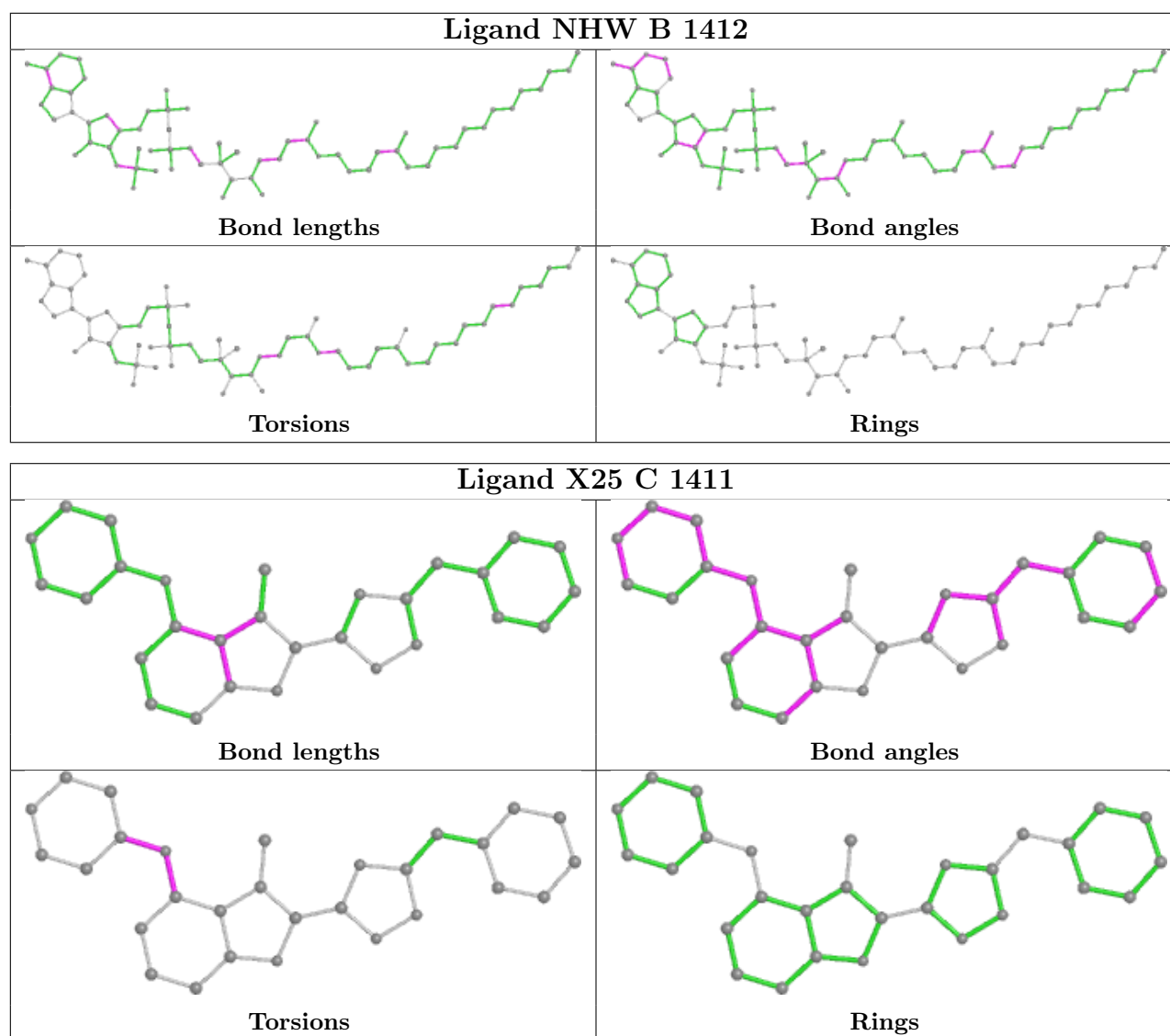
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1412	NHW	1	0
3	B	1412	NHW	1	0
2	C	1411	X25	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.29	14 (3%) 42 44	7, 12, 27, 65	13 (3%)
1	B	385/385 (100%)	0.34	14 (3%) 42 44	8, 13, 27, 49	13 (3%)
1	C	368/385 (95%)	0.44	19 (5%) 27 27	9, 14, 30, 40	11 (2%)
All	All	1138/1155 (98%)	0.36	47 (4%) 37 37	7, 13, 28, 65	37 (3%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ARG	5.8
1	B	232	ARG	5.5
1	C	222	ILE	5.2
1	C	26	MET	4.9
1	B	231	SER	4.5
1	C	326[A]	LYS	4.4
1	A	230	ASN	4.4
1	A	26	MET	4.4
1	C	323	GLY	4.2
1	C	325	ASP	4.2
1	A	99	ASP	4.1
1	B	131	TYR	3.8
1	B	133	ALA	3.8
1	B	26	MET	3.8
1	B	305	ASN	3.6
1	A	231	SER	3.5
1	A	102	ILE	3.4
1	A	229	LEU	3.3
1	B	230[A]	ASN	3.2
1	B	102	ILE	3.2
1	B	39	ILE	3.1
1	C	27	ASP	3.1
1	C	327	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	100	ASP	2.9
1	A	325	ASP	2.9
1	C	305	ASN	2.8
1	B	32	TYR	2.8
1	C	221	LEU	2.7
1	A	32	TYR	2.6
1	C	40	ASN	2.6
1	B	27	ASP	2.6
1	C	409	LEU	2.6
1	C	224	ILE	2.5
1	A	27	ASP	2.5
1	B	306	GLY	2.4
1	C	226[A]	PHE	2.4
1	C	102	ILE	2.4
1	C	218	VAL	2.4
1	C	324	ASN	2.4
1	A	43	PHE	2.1
1	C	219	LYS	2.1
1	B	40	ASN	2.1
1	C	103	PHE	2.1
1	C	381	PHE	2.1
1	A	233	LEU	2.1
1	B	103	PHE	2.0
1	A	54	ASP	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 [i](#)

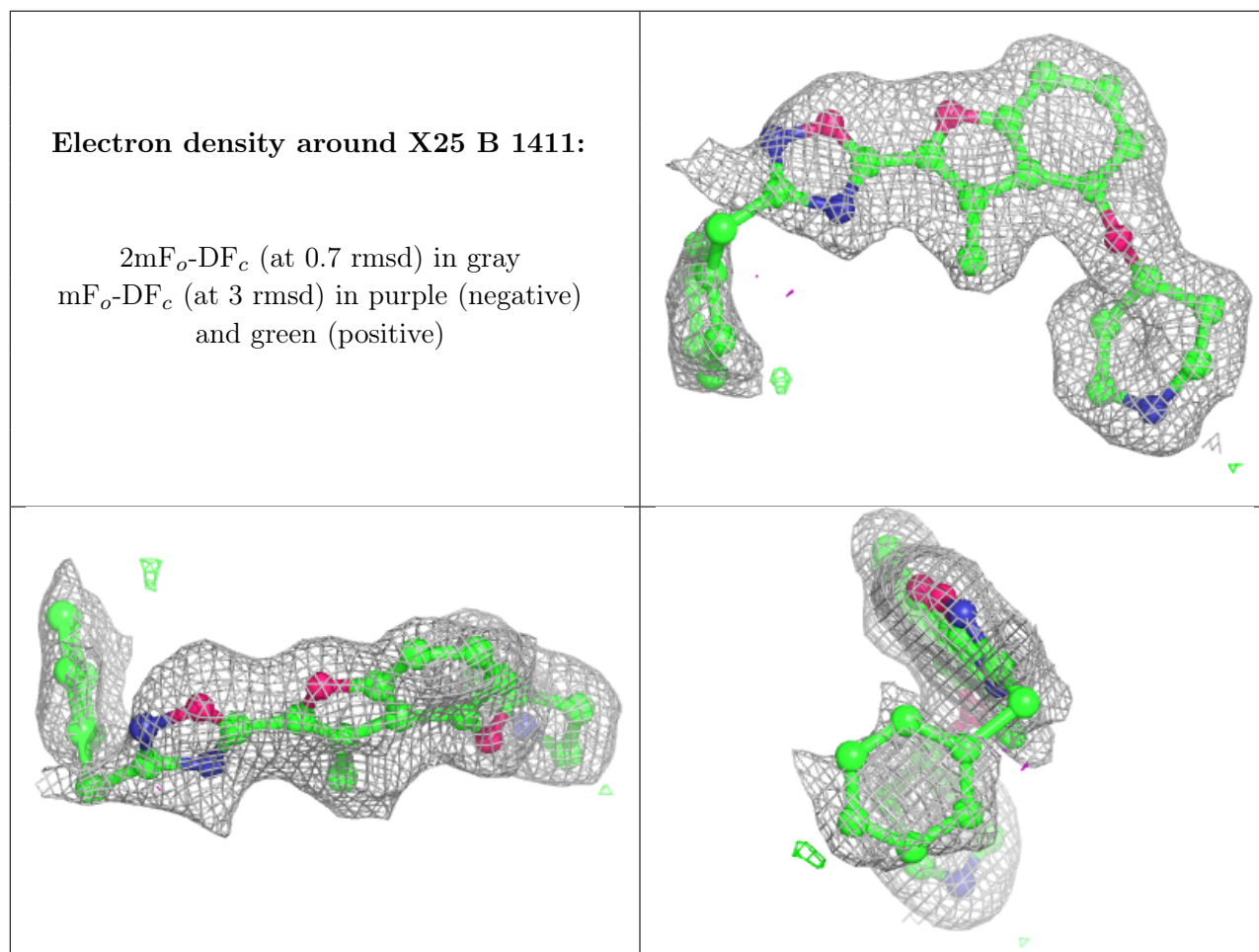
There are no monosaccharides in this entry.

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.

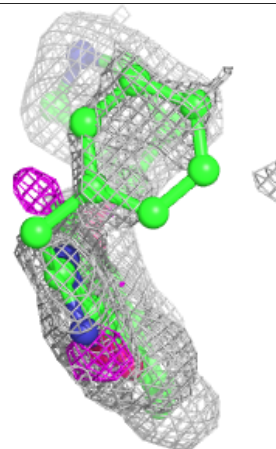
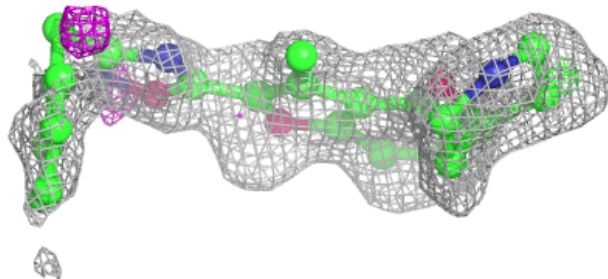
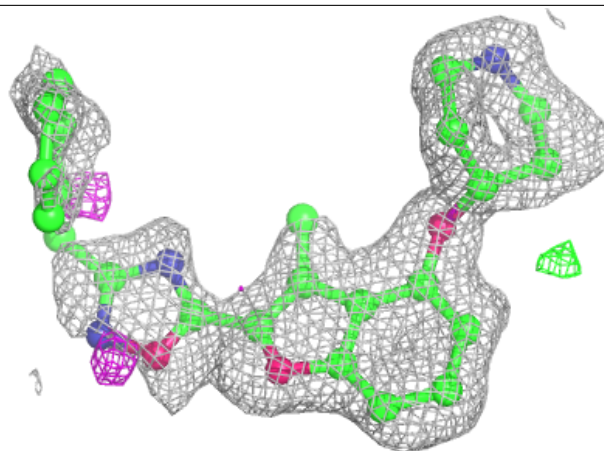
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	X25	B	1411	29/29	0.77	0.16	20,31,45,47	0
2	X25	A	1411	29/29	0.79	0.19	21,28,47,50	0
2	X25	C	1411	29/29	0.79	0.14	21,28,36,37	0
6	SO4	B	1413	5/5	0.88	0.11	37,40,44,45	0
5	MG	B	1415	1/1	0.92	0.08	25,25,25,25	0
3	NHW	A	1412	64/64	0.94	0.09	7,10,14,17	0
3	NHW	B	1412	64/64	0.95	0.09	8,13,15,18	0
3	NHW	C	1412	64/64	0.95	0.09	7,12,15,16	0
5	MG	A	1414	1/1	0.96	0.12	20,20,20,20	0
5	MG	C	1414	1/1	0.99	0.04	20,20,20,20	0
4	CL	B	1414	1/1	0.99	0.10	12,12,12,12	0
4	CL	A	1413	1/1	1.00	0.03	10,10,10,10	0
4	CL	C	1413	1/1	1.00	0.05	12,12,12,12	0

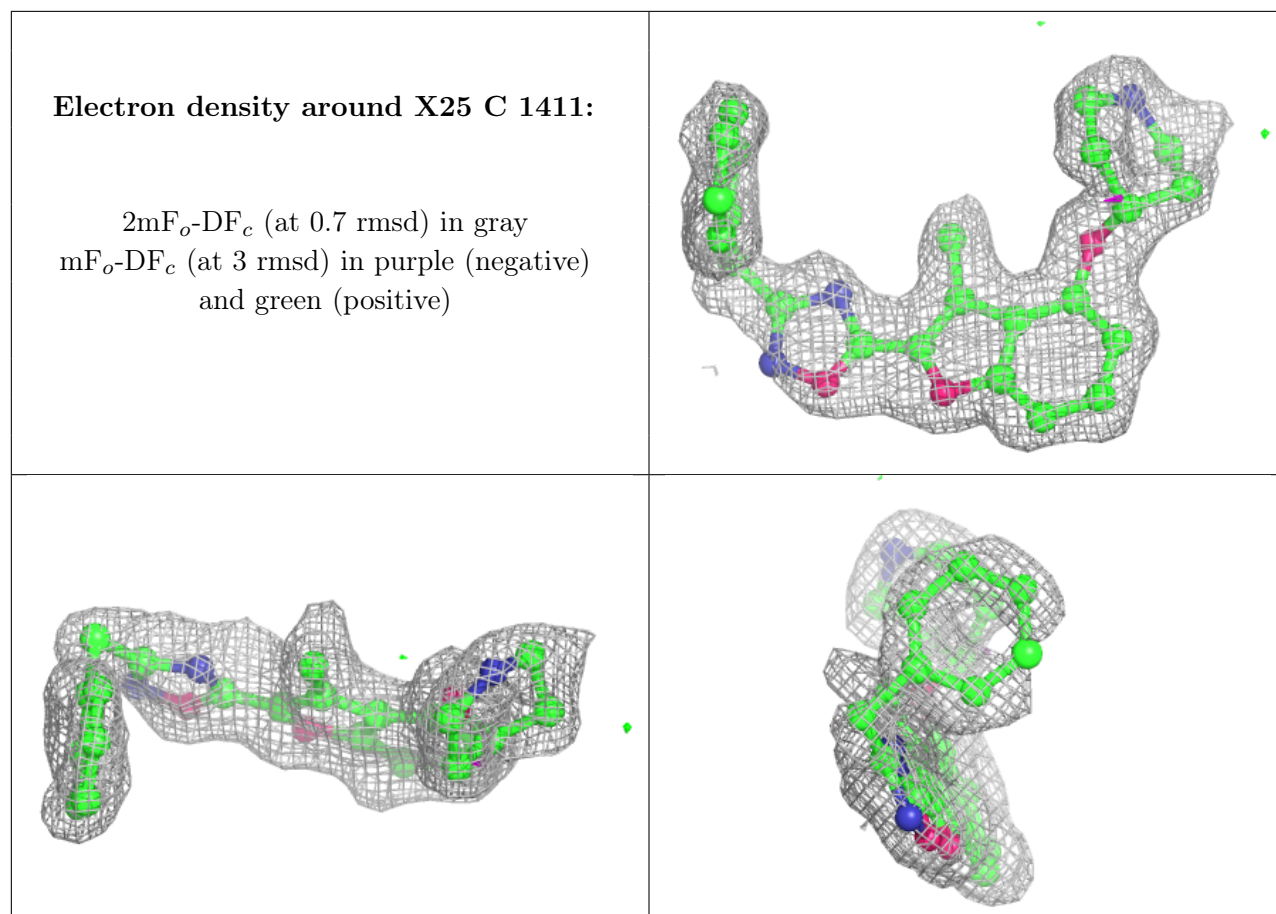
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

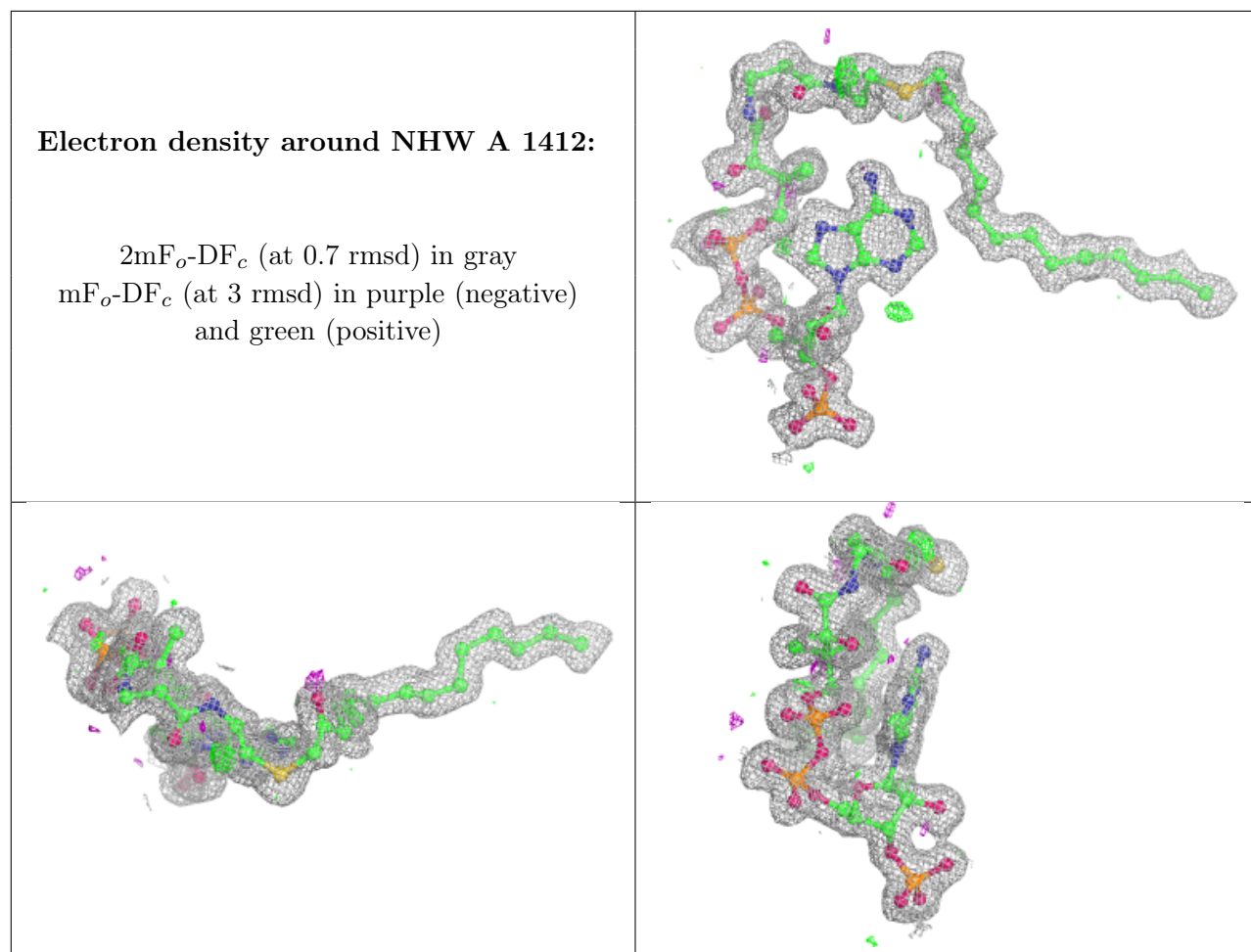


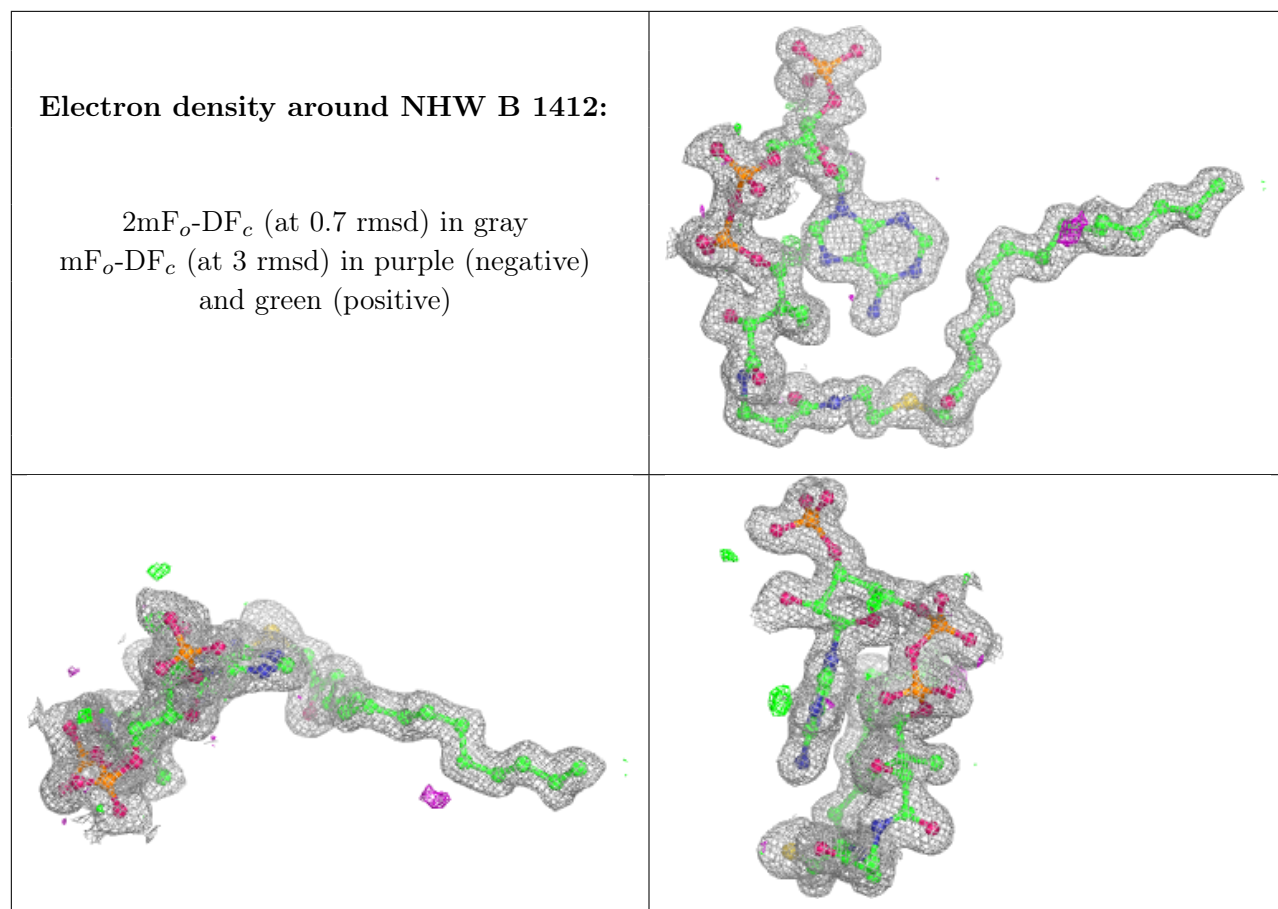
Electron density around X25 A 1411:

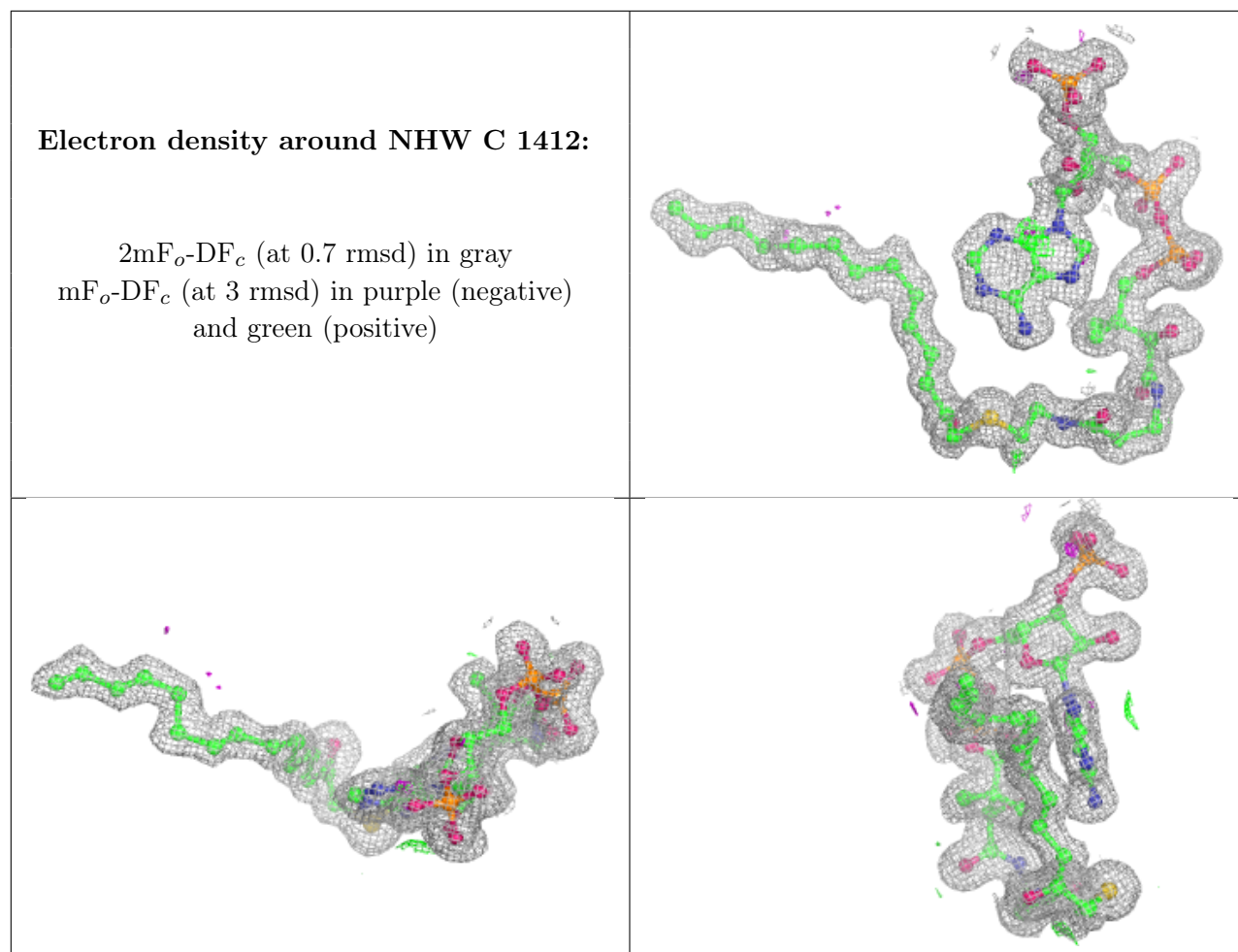
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)











6.5 Other polymers [i](#)

There are no such residues in this entry.