



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:49 PM BST

PDB ID : 5NTC
Title : Crystal structure of mouse CARM1 in complex with inhibitor SA0678
Authors : Cura, V.; Marechal, N.; Mailliot, J.; Troffer-Charlier, N.; Hassenboehler, P.;
Wurtz, J.M.; Bonnefond, L.; Cavarelli, J.
Deposited on : 2017-04-27
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

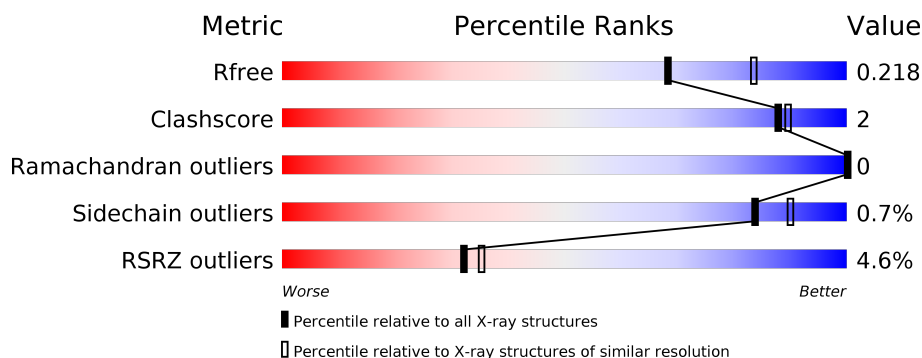
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	371	 2% 90% 6%
1	B	371	 2% 86% 10%
1	C	371	 9% 87% 7% 6%
1	D	371	 4% 85% 5% 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	502	-	-	-	X
2	EDO	B	504	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22816 atoms, of which 11025 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 Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	350	5539	1807	2740	463	515	14	0	2	0
1	B	333	5330	1740	2642	443	490	15	0	2	0
1	C	348	5513	1799	2729	461	510	14	0	2	0
1	D	333	5326	1737	2640	445	489	15	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	UNP Q9WVG6
C	128	HIS	-	expression tag	UNP Q9WVG6
C	129	MET	-	expression tag	UNP Q9WVG6
D	127	GLY	-	expression tag	UNP Q9WVG6
D	128	HIS	-	expression tag	UNP Q9WVG6
D	129	MET	-	expression tag	UNP Q9WVG6

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



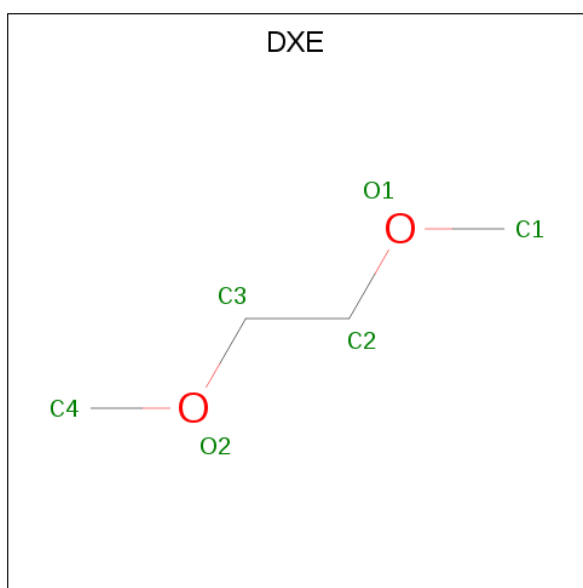
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



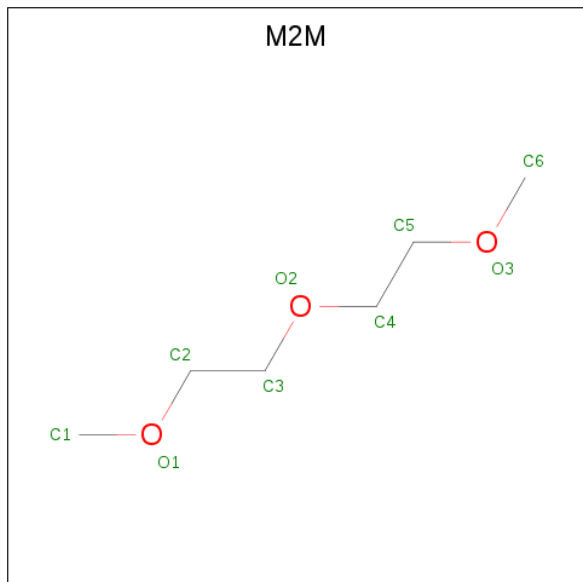
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	17	4	10	3	0	0
3	D	1	17	4	10	3	0	0

- Molecule 4 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: $C_4H_{10}O_2$).



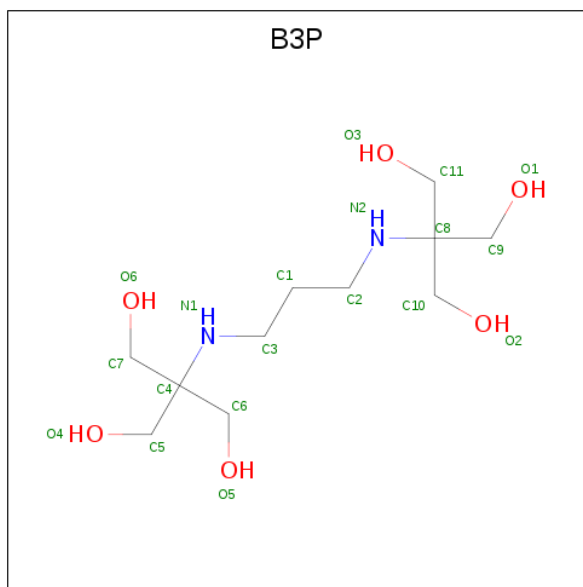
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	16	4	10	2	0	0
4	C	1	16	4	10	2	0	0

- Molecule 5 is 1-METHOXY-2-(2-METHOXYETHOXY)ETHANE (three-letter code: M2M) (formula: $C_6H_{14}O_3$).



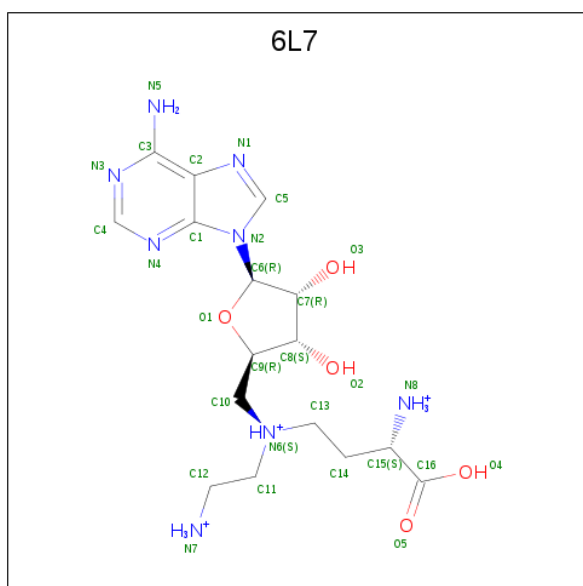
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	23	6	14	3	0	0

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total	C	H	N	O	0	0
			45	11	26	2	6		
6	B	1	Total	C	H	N	O	0	0
			45	11	26	2	6		
6	D	1	Total	C	H	N	O	0	0
			45	11	26	2	6		

- Molecule 7 is [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl-(2-azaniumylethyl)-[(3 {S})-3-azaniumyl-4-oxidanyl-4-oxidanylidene-butyl]azanium (three-letter code: 6L7) (formula: C₁₆H₂₉N₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	A	1	Total	C	H	N	O	0	0
			57	16	28	8	5		
7	B	1	Total	C	H	N	O	0	0
			57	16	28	8	5		
7	C	1	Total	C	H	N	O	0	0
			57	16	28	8	5		
7	D	1	Total	C	H	N	O	0	0
			57	16	28	8	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	216	Total	O	0	0
			216	216		
8	B	164	Total	O	0	0
			164	164		

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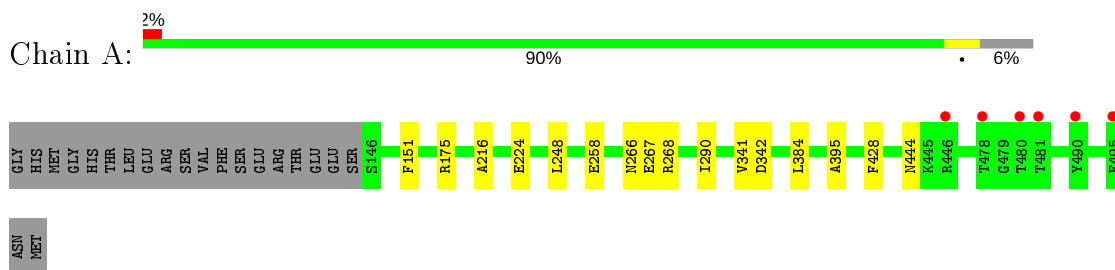
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	97	Total O 97 97	0	0
8	D	97	Total O 97 97	0	0

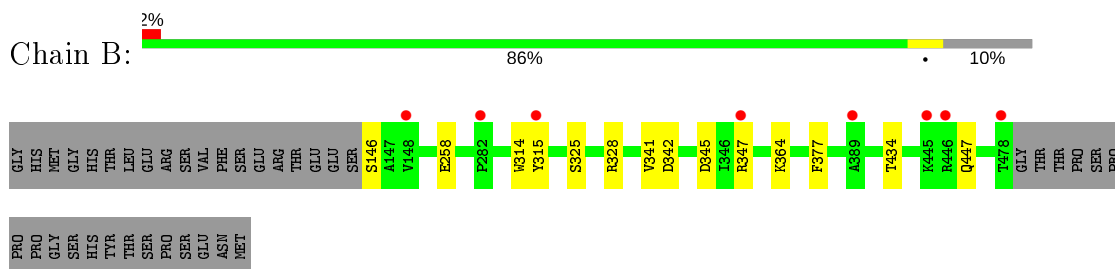
3 Residue-property plots [i](#)

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.

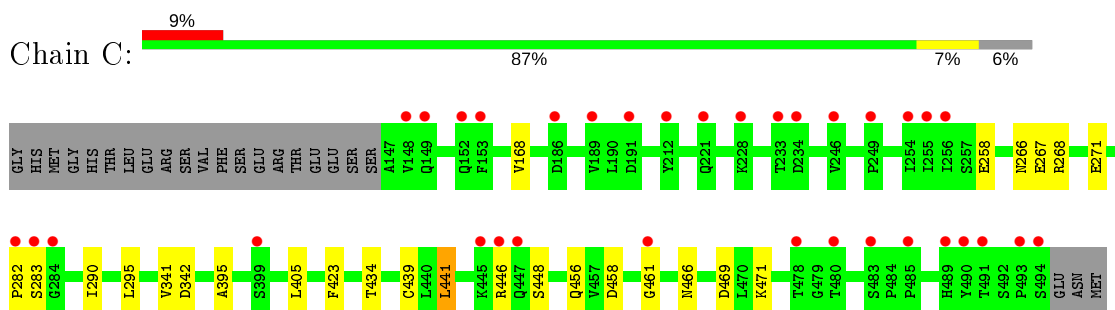
- Molecule 1: Histone-arginine methyltransferase CARM1



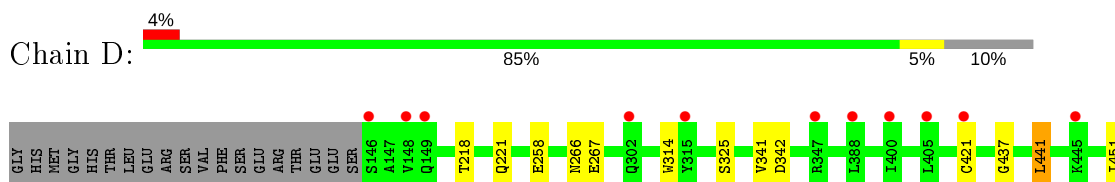
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.91Å 99.15Å 206.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.25 19.94 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.94-2.25) 99.4 (19.94-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.07 (at 2.26Å)	Xtrriage
Refinement program	PHENIX dev_1951	Depositor
R, R_{free}	0.178 , 0.216 0.179 , 0.218	Depositor DCC
R_{free} test set	3640 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.238	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22816	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6017e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: B3P, EDO, M2M, DXE, PEG, 6L7

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	0.29	0/2892	0.51	0/3928
1	B	0.29	0/2758	0.52	0/3739
1	C	0.28	0/2877	0.53	0/3908
1	D	0.29	0/2756	0.53	0/3736
All	All	0.29	0/11283	0.52	0/15311

There are no bond length outliers.

There are no bond angle outliers.

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	2799	2740	2729	9	0
1	B	2688	2642	2640	8	0
1	C	2784	2729	2718	15	0
1	D	2686	2640	2638	11	0
2	A	12	6	18	0	0
2	B	20	12	30	1	0
2	C	16	12	24	1	0
2	D	4	0	6	0	0
3	A	7	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	10	10	0	0
4	A	6	10	10	0	0
4	C	6	10	10	0	0
5	A	9	14	14	0	0
6	A	19	26	26	1	0
6	B	19	26	26	0	0
6	D	19	26	26	0	0
7	A	29	28	0	0	0
7	B	29	28	0	0	0
7	C	29	28	0	0	0
7	D	29	28	0	0	0
8	A	216	0	0	2	0
8	B	164	0	0	0	0
8	C	97	0	0	1	0
8	D	97	0	0	0	0
All	All	11791	11025	10935	44	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 2.

All (44) 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:C:446:ARG:NH2	1:C:469:ASP:OD1	1.97	0.98
1:A:224:GLU:OE1	8:A:601:HOH:O	2.08	0.72
1:B:364:LYS:HB3	2:B:504:EDO:H12	1.74	0.70
1:A:267:GLU:O	6:A:507:B3P:O3	2.12	0.68
1:C:268:ARG:NH1	1:C:271:GLU:OE2	2.37	0.58
1:B:315:TYR:HD1	1:B:328:ARG:HD2	1.73	0.53
1:C:446:ARG:HH12	1:C:471:LYS:HB3	1.74	0.52
1:C:456:GLN:HE21	1:C:461:GLY:HA2	1.75	0.52
1:D:451:ILE:HD11	1:D:470:LEU:HD11	1.92	0.51
2:C:504:EDO:H11	8:C:631:HOH:O	2.10	0.51
1:C:446:ARG:NH1	1:C:471:LYS:HB3	2.29	0.48
1:A:175:ARG:NH1	8:A:605:HOH:O	2.39	0.47
1:B:146:SER:HA	1:B:447:GLN:NE2	2.29	0.47
1:D:218:THR:O	1:D:221:GLN:HG2	2.14	0.47
1:C:266:ASN:O	1:C:267:GLU:HB2	2.14	0.47
1:B:315:TYR:CD1	1:B:328:ARG:HD2	2.49	0.46
1:B:345:ASP:CG	1:B:347:ARG:HE	2.19	0.45
1:A:341:VAL:O	1:A:342:ASP:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:NH1	1:A:444:ASN:O	2.49	0.45
1:A:266:ASN:O	1:A:267:GLU:HB2	2.17	0.44
1:D:421:CYS:O	1:D:421:CYS:SG	2.75	0.43
1:C:441:LEU:CD1	1:C:441:LEU:N	2.81	0.43
1:D:421:CYS:SG	1:D:453:ILE:HD13	2.58	0.43
1:A:384:LEU:HD21	1:A:428:PHE:CZ	2.54	0.43
1:C:423:PHE:HA	1:C:466:ASN:ND2	2.33	0.42
1:A:290:ILE:HG13	1:A:395:ALA:HB3	2.00	0.42
1:D:477:TYR:O	1:D:478:THR:C	2.57	0.42
1:C:434:THR:OG1	1:C:458:ASP:HB2	2.19	0.42
1:A:151:PHE:CE1	1:A:216:ALA:HB3	2.54	0.42
1:D:341:VAL:O	1:D:342:ASP:HB3	2.20	0.42
1:B:341:VAL:O	1:B:342:ASP:HB3	2.19	0.41
1:C:439:CYS:SG	1:C:441:LEU:HD11	2.59	0.41
1:D:314:TRP:O	1:D:325:SER:HA	2.20	0.41
1:D:266:ASN:O	1:D:267:GLU:HB2	2.21	0.41
1:C:282:PRO:O	1:C:283:SER:OG	2.27	0.41
1:C:341:VAL:O	1:C:342:ASP:HB3	2.20	0.41
1:C:168:VAL:HG12	1:C:405:LEU:CD1	2.51	0.41
1:C:448:SER:CB	1:C:471:LYS:HB2	2.51	0.41
1:B:314:TRP:O	1:B:325:SER:HA	2.20	0.40
1:D:441:LEU:HD12	1:D:441:LEU:N	2.35	0.40
1:D:437:GLY:HA3	1:D:454:VAL:O	2.21	0.40
1:B:377:PHE:O	1:B:434:THR:HA	2.22	0.40
1:C:290:ILE:HG12	1:C:395:ALA:HB3	2.03	0.40
1:D:441:LEU:HG	1:D:451:ILE:HG12	2.03	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	350/371 (94%)	341 (97%)	9 (3%)	0	100	100
1	B	333/371 (90%)	324 (97%)	9 (3%)	0	100	100
1	C	348/371 (94%)	338 (97%)	10 (3%)	0	100	100
1	D	333/371 (90%)	322 (97%)	11 (3%)	0	100	100
All	All	1364/1484 (92%)	1325 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	306/323 (95%)	304 (99%)	2 (1%)	84	90
1	B	291/323 (90%)	290 (100%)	1 (0%)	92	95
1	C	304/323 (94%)	301 (99%)	3 (1%)	76	84
1	D	291/323 (90%)	289 (99%)	2 (1%)	84	90
All	All	1192/1292 (92%)	1184 (99%)	8 (1%)	84	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	LEU
1	A	258	GLU
1	B	258	GLU
1	C	258	GLU
1	C	295	LEU
1	C	441	LEU
1	D	258	GLU
1	D	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	456	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](#)

25 ligands are modelled in this entry.

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	6L7	C	506	-	24,31,31	0.93	0	23,44,44	1.08	3 (13%)
2	EDO	C	504	-	3,3,3	0.48	0	2,2,2	0.46	0
2	EDO	C	501	-	3,3,3	0.49	0	2,2,2	0.48	0
7	6L7	D	504	-	24,31,31	0.84	0	23,44,44	0.98	2 (8%)
5	M2M	A	506	-	8,8,8	0.58	0	7,7,7	0.46	0
2	EDO	B	502	-	3,3,3	0.48	0	2,2,2	0.47	0
2	EDO	B	503	-	3,3,3	0.47	0	2,2,2	0.48	0
6	B3P	B	506	-	18,18,18	0.18	0	21,23,23	0.39	0
7	6L7	A	508	-	24,31,31	0.84	0	23,44,44	1.25	3 (13%)
4	DXE	A	505	-	5,5,5	0.42	0	4,4,4	0.30	0
2	EDO	B	505	-	3,3,3	0.47	0	2,2,2	0.46	0
2	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.50	0
2	EDO	D	501	-	3,3,3	0.48	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	6L7	B	507	-	24,31,31	0.88	0	23,44,44	1.33	3 (13%)
2	EDO	A	501	-	3,3,3	0.48	0	2,2,2	0.45	0
3	PEG	A	504	-	6,6,6	0.47	0	5,5,5	0.60	0
2	EDO	A	503	-	3,3,3	0.48	0	2,2,2	0.48	0
6	B3P	D	503	-	18,18,18	0.29	0	21,23,23	0.44	0
3	PEG	D	502	-	6,6,6	0.47	0	5,5,5	0.45	0
2	EDO	C	502	-	3,3,3	0.48	0	2,2,2	0.54	0
6	B3P	A	507	-	18,18,18	0.27	0	21,23,23	0.41	0
4	DXE	C	505	-	5,5,5	0.44	0	4,4,4	0.25	0
2	EDO	B	501	-	3,3,3	0.47	0	2,2,2	0.48	0
2	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.46	0
2	EDO	C	503	-	3,3,3	0.47	0	2,2,2	0.48	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
7	6L7	C	506	-	-	9/12/36/36	0/3/3/3
2	EDO	C	504	-	-	1/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-
7	6L7	D	504	-	-	5/12/36/36	0/3/3/3
5	M2M	A	506	-	-	4/6/6/6	-
2	EDO	B	502	-	-	1/1/1/1	-
2	EDO	B	503	-	-	0/1/1/1	-
6	B3P	B	506	-	-	6/28/28/28	-
7	6L7	A	508	-	-	7/12/36/36	0/3/3/3
4	DXE	A	505	-	-	3/3/3/3	-
2	EDO	B	505	-	-	0/1/1/1	-
2	EDO	A	502	-	-	1/1/1/1	-
2	EDO	D	501	-	-	0/1/1/1	-
7	6L7	B	507	-	-	10/12/36/36	0/3/3/3
2	EDO	A	501	-	-	1/1/1/1	-
3	PEG	A	504	-	-	4/4/4/4	-
2	EDO	A	503	-	-	1/1/1/1	-
6	B3P	D	503	-	-	7/28/28/28	-
3	PEG	D	502	-	-	1/4/4/4	-
2	EDO	C	502	-	-	1/1/1/1	-
6	B3P	A	507	-	-	5/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DXE	C	505	-	-	1/3/3/3	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	B	504	-	-	0/1/1/1	-
2	EDO	C	503	-	-	0/1/1/1	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	507	6L7	C12-C11-N6	3.51	121.31	113.23
7	A	508	6L7	C12-C11-N6	3.30	120.81	113.23
7	B	507	6L7	C13-N6-C10	3.23	119.65	111.96
7	C	506	6L7	C12-C11-N6	3.01	120.15	113.23
7	A	508	6L7	C13-N6-C10	2.81	118.65	111.96
7	D	504	6L7	C13-N6-C10	2.37	117.60	111.96
7	C	506	6L7	C13-N6-C10	2.26	117.35	111.96
7	D	504	6L7	C2-C3-N5	2.20	123.69	120.35
7	A	508	6L7	C2-C3-N5	2.14	123.61	120.35
7	C	506	6L7	C2-C3-N5	2.12	123.57	120.35
7	B	507	6L7	C2-C3-N5	2.10	123.55	120.35

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	506	6L7	N6-C10-C9-C8
7	C	506	6L7	N6-C10-C9-O1
7	C	506	6L7	N6-C11-C12-N7
7	C	506	6L7	C13-C14-C15-C16
7	C	506	6L7	C13-C14-C15-N8
7	D	504	6L7	N6-C10-C9-C8
7	D	504	6L7	N6-C10-C9-O1
7	D	504	6L7	N6-C13-C14-C15
6	B	506	B3P	C5-C4-N1-C3
6	B	506	B3P	C6-C4-N1-C3
7	A	508	6L7	N6-C10-C9-C8
7	A	508	6L7	N6-C10-C9-O1
7	A	508	6L7	C9-C10-N6-C13
7	A	508	6L7	C13-C14-C15-C16
7	B	507	6L7	N6-C10-C9-C8
7	B	507	6L7	N6-C10-C9-O1

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Mol	Chain	Res	Type	Atoms
7	B	507	6L7	C9-C10-N6-C13
7	B	507	6L7	C13-C14-C15-C16
7	B	507	6L7	C13-C14-C15-N8
6	A	507	B3P	N1-C4-C7-O6
6	A	507	B3P	C5-C4-C7-O6
6	A	507	B3P	C6-C4-C7-O6
7	B	507	6L7	C12-C11-N6-C10
7	C	506	6L7	C12-C11-N6-C10
7	A	508	6L7	C12-C11-N6-C10
6	D	503	B3P	C3-C1-C2-N2
3	D	502	PEG	O2-C3-C4-O4
4	A	505	DXE	O1-C2-C3-O2
5	A	506	M2M	O2-C4-C5-O3
6	A	507	B3P	C2-C1-C3-N1
3	A	504	PEG	O2-C3-C4-O4
2	C	504	EDO	O1-C1-C2-O2
7	C	506	6L7	C9-C10-N6-C13
7	D	504	6L7	C9-C10-N6-C13
4	C	505	DXE	O1-C2-C3-O2
7	B	507	6L7	C14-C13-N6-C10
2	A	501	EDO	O1-C1-C2-O2
2	C	502	EDO	O1-C1-C2-O2
5	A	506	M2M	C5-C4-O2-C3
6	D	503	B3P	C11-C8-N2-C2
2	B	502	EDO	O1-C1-C2-O2
2	A	502	EDO	O1-C1-C2-O2
7	B	507	6L7	C14-C13-N6-C11
7	B	507	6L7	C12-C11-N6-C13
5	A	506	M2M	C3-C2-O1-C1
6	B	506	B3P	C7-C4-N1-C3
7	C	506	6L7	C14-C13-N6-C10
6	D	503	B3P	C2-C1-C3-N1
6	B	506	B3P	C7-C4-C5-O4
6	D	503	B3P	C5-C4-C6-O5
6	D	503	B3P	C11-C8-C9-O1
3	A	504	PEG	C1-C2-O2-C3
3	A	504	PEG	C4-C3-O2-C2
7	C	506	6L7	C12-C11-N6-C13
7	A	508	6L7	C12-C11-N6-C13
6	B	506	B3P	O3-C11-C8-C10
6	D	503	B3P	C9-C8-N2-C2
3	A	504	PEG	O1-C1-C2-O2

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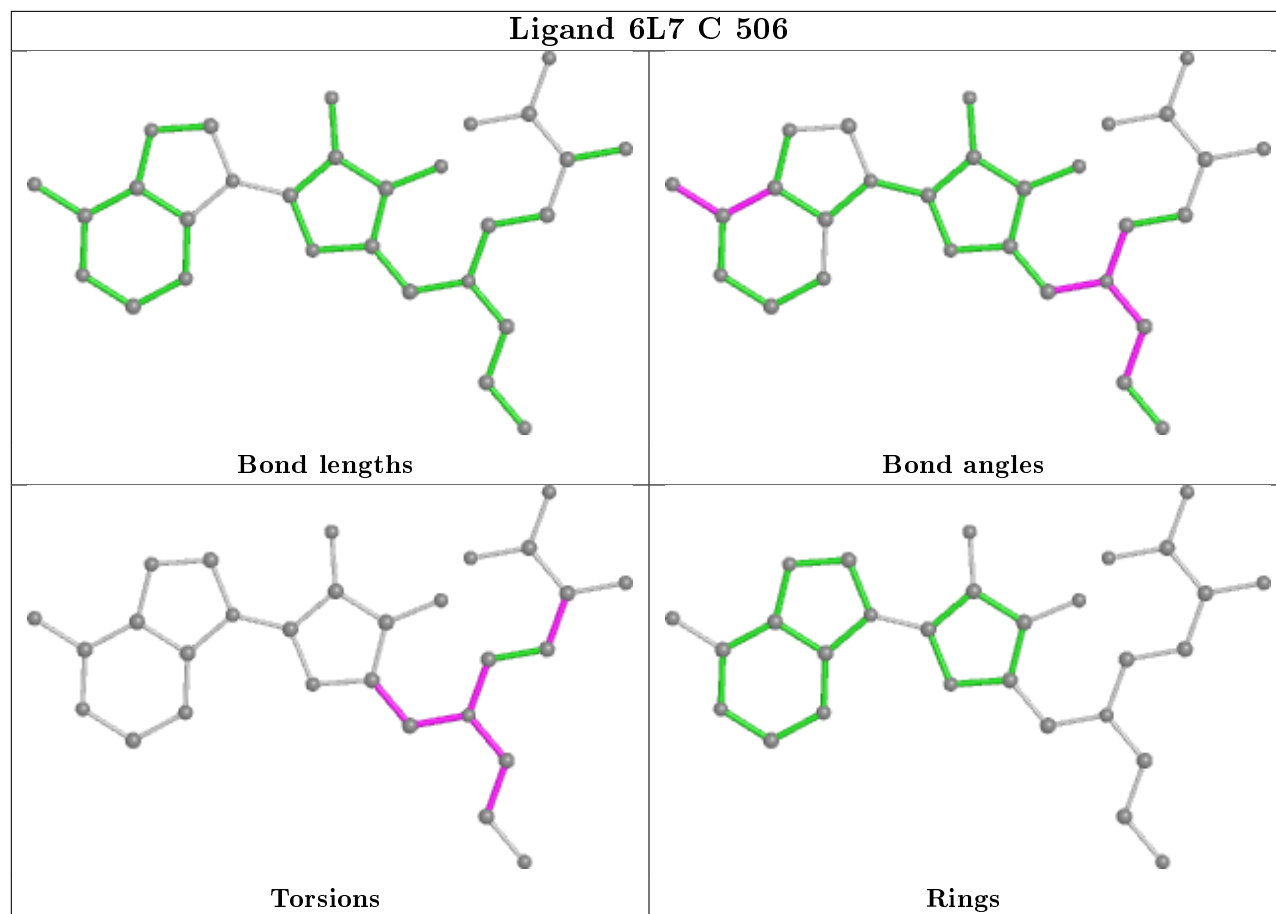
Mol	Chain	Res	Type	Atoms
5	A	506	M2M	O1-C2-C3-O2
2	A	503	EDO	O1-C1-C2-O2
6	B	506	B3P	N1-C4-C5-O4
6	D	503	B3P	N1-C4-C6-O5
7	A	508	6L7	C13-C14-C15-N8
7	D	504	6L7	N6-C11-C12-N7
7	B	507	6L7	N6-C11-C12-N7
4	A	505	DXE	C3-C2-O1-C1
2	B	501	EDO	O1-C1-C2-O2
6	A	507	B3P	C5-C4-N1-C3
4	A	505	DXE	C2-C3-O2-C4

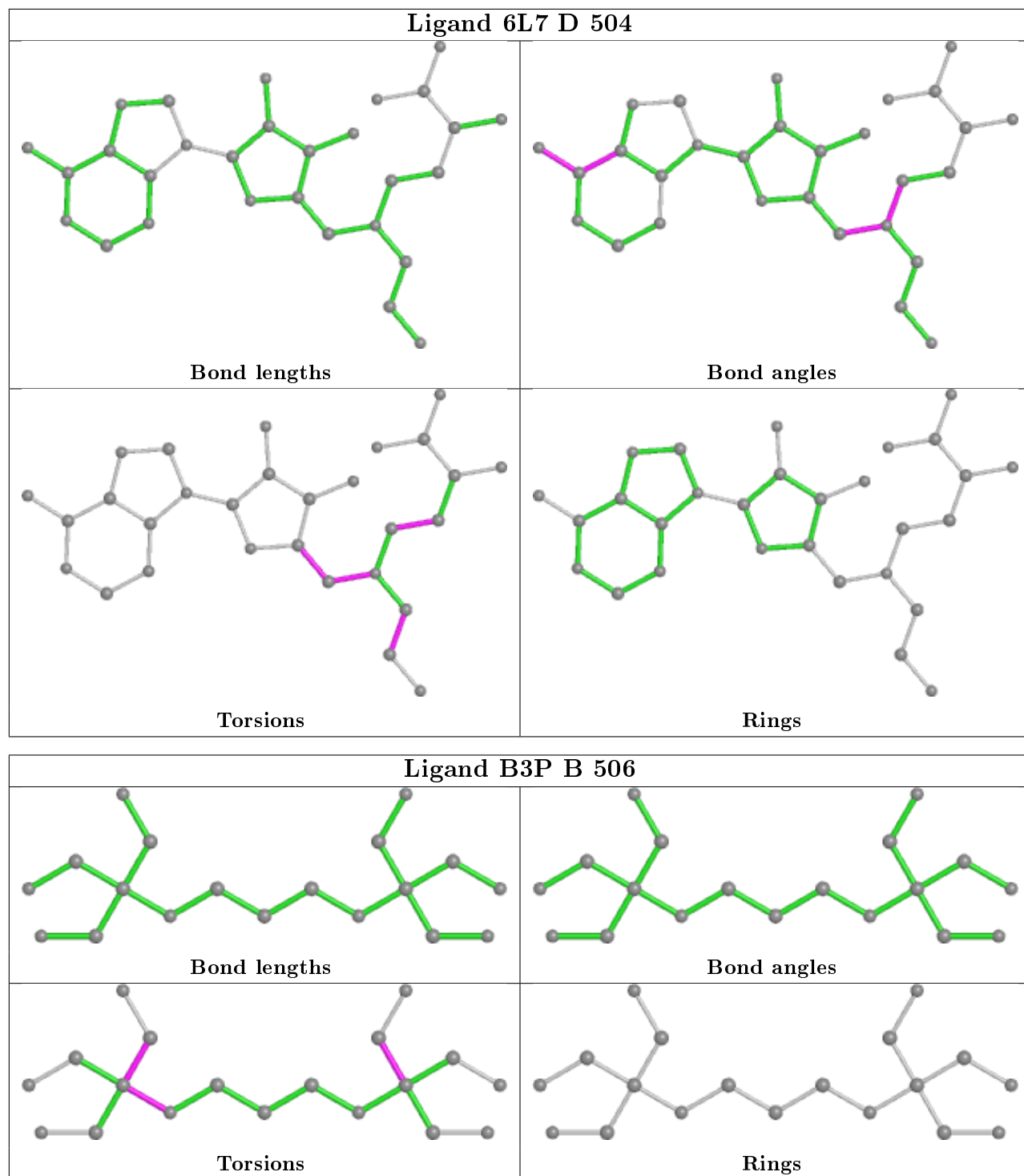
There are no ring outliers.

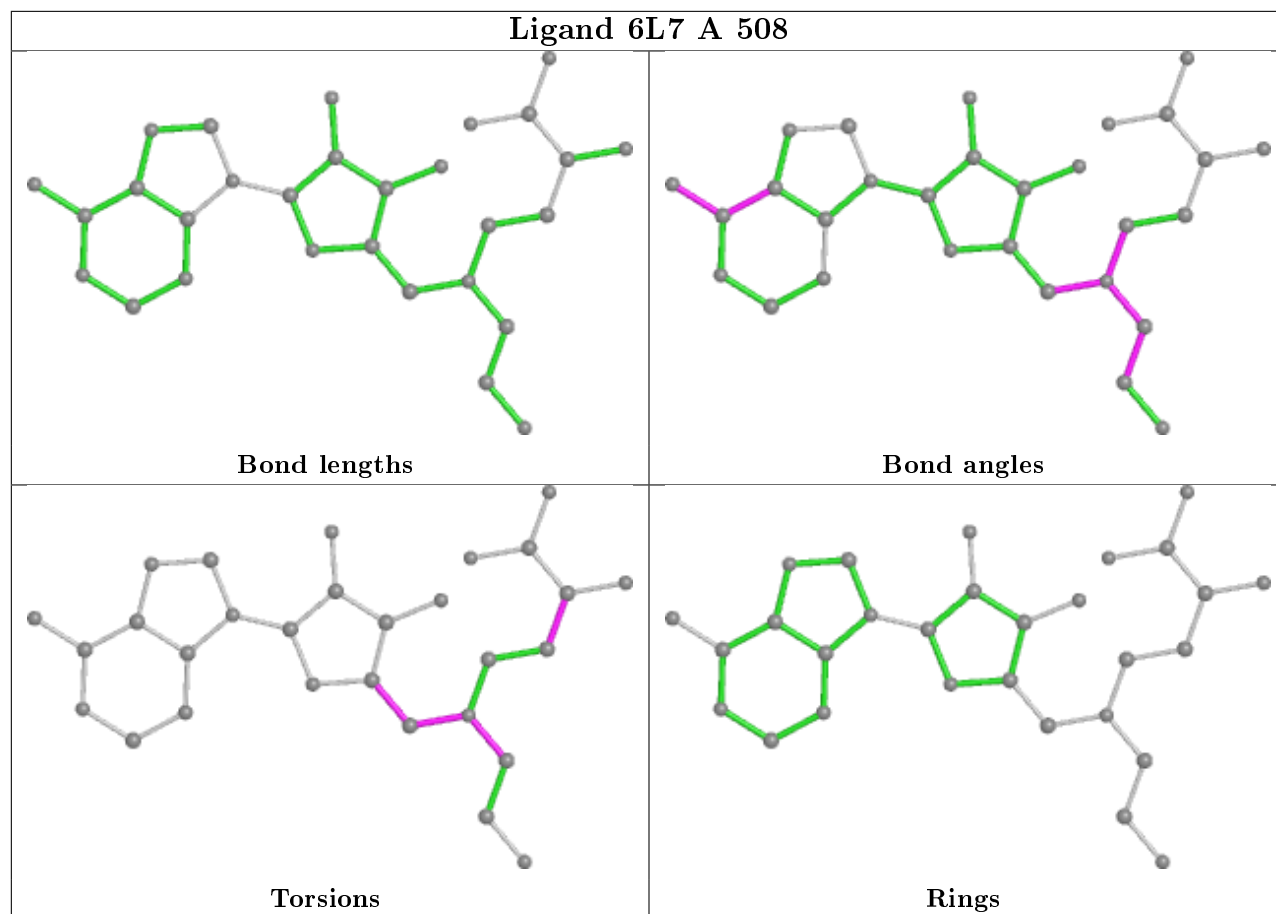
3 monomers are involved in 3 short contacts:

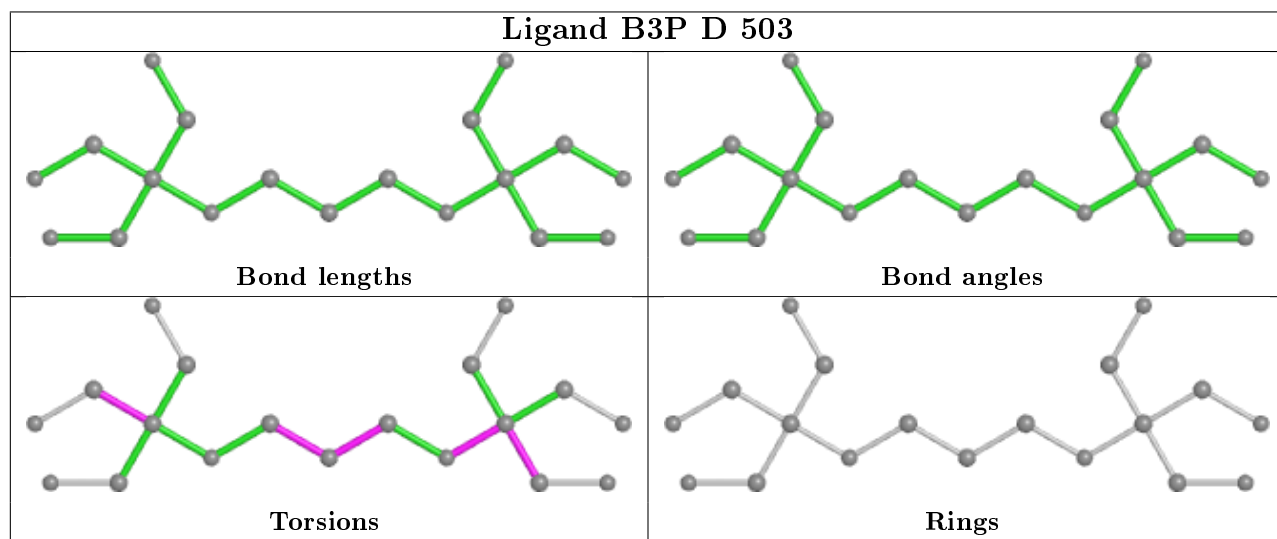
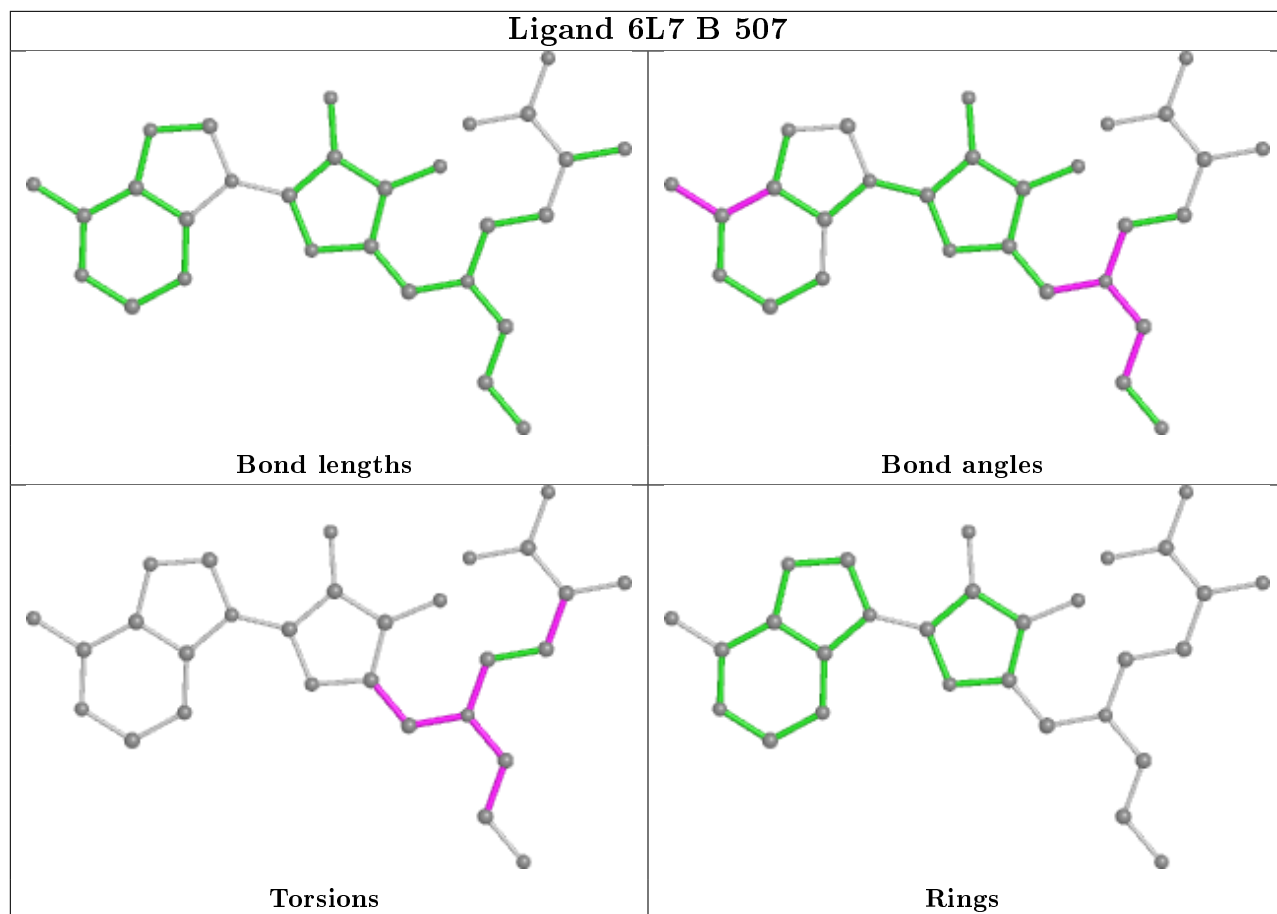
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	504	EDO	1	0
6	A	507	B3P	1	0
2	B	504	EDO	1	0

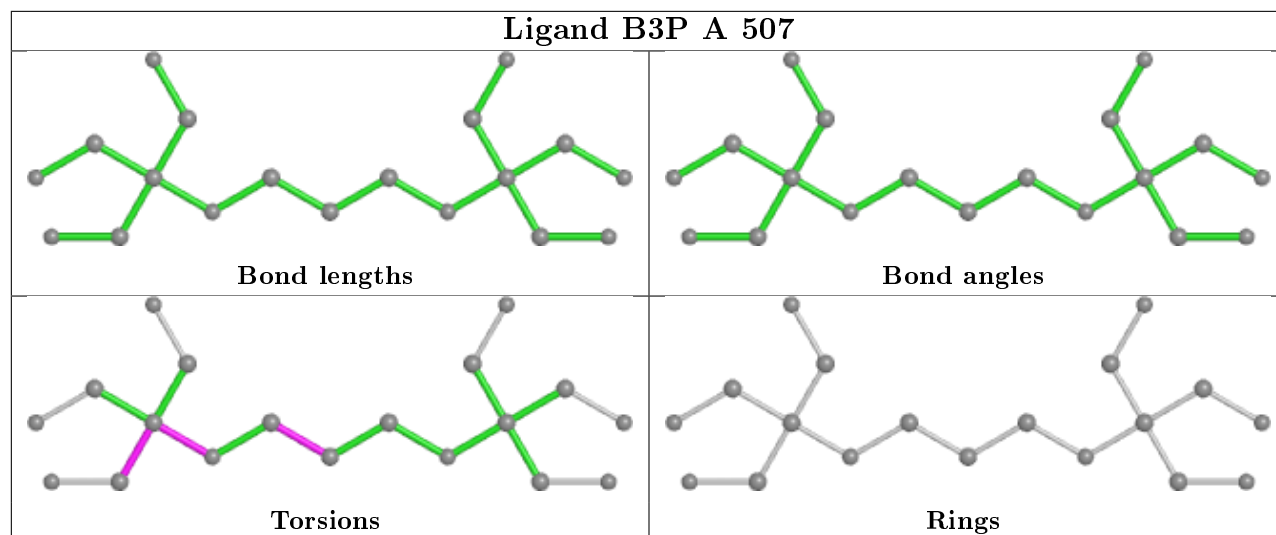
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/371 (94%)	-0.20	6 (1%) 70 73	18, 33, 56, 78	0
1	B	333/371 (89%)	-0.14	8 (2%) 59 62	21, 36, 58, 82	0
1	C	348/371 (93%)	0.36	34 (9%) 7 8	25, 52, 80, 105	0
1	D	333/371 (89%)	0.02	15 (4%) 33 36	29, 45, 66, 90	0
All	All	1364/1484 (91%)	0.01	63 (4%) 32 35	18, 42, 70, 105	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	490	TYR	6.2
1	D	477	TYR	5.7
1	C	491	THR	5.6
1	B	445	LYS	5.0
1	C	480	THR	5.0
1	B	478	THR	4.6
1	A	480	THR	4.3
1	C	284	GLY	4.3
1	C	153	PHE	4.1
1	C	489	HIS	4.0
1	D	478	THR	3.8
1	D	445	LYS	3.6
1	A	495	GLU	3.5
1	C	149	GLN	3.3
1	C	148	VAL	3.3
1	C	234	ASP	3.3
1	B	148	VAL	3.3
1	A	490	TYR	3.3
1	D	146	SER	3.1
1	D	475	PHE	3.1
1	C	282	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	446	ARG	3.0
1	C	447	GLN	2.9
1	C	256	ILE	2.9
1	C	246	VAL	2.9
1	C	478	THR	2.9
1	C	233	THR	2.8
1	D	347	ARG	2.8
1	C	461	GLY	2.8
1	B	315	TYR	2.7
1	C	283	SER	2.6
1	D	400	ILE	2.6
1	C	186	ASP	2.6
1	B	347	ARG	2.5
1	B	446	ARG	2.5
1	C	189	VAL	2.5
1	C	445	LYS	2.5
1	A	446	ARG	2.4
1	B	282	PRO	2.4
1	D	315	TYR	2.4
1	A	478	THR	2.4
1	D	148	VAL	2.4
1	D	302	GLN	2.3
1	C	221	GLN	2.3
1	D	421	CYS	2.3
1	D	463	LYS	2.3
1	B	389	ALA	2.2
1	D	405	LEU	2.2
1	D	149	GLN	2.2
1	C	191	ASP	2.1
1	D	388	LEU	2.1
1	C	152	GLN	2.1
1	C	228	LYS	2.1
1	C	494	SER	2.1
1	C	255	ILE	2.1
1	A	481	THR	2.0
1	C	399	SER	2.0
1	C	483	SER	2.0
1	C	254	ILE	2.0
1	C	249	PRO	2.0
1	C	485	PRO	2.0
1	C	493	PRO	2.0
1	C	212	TYR	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.

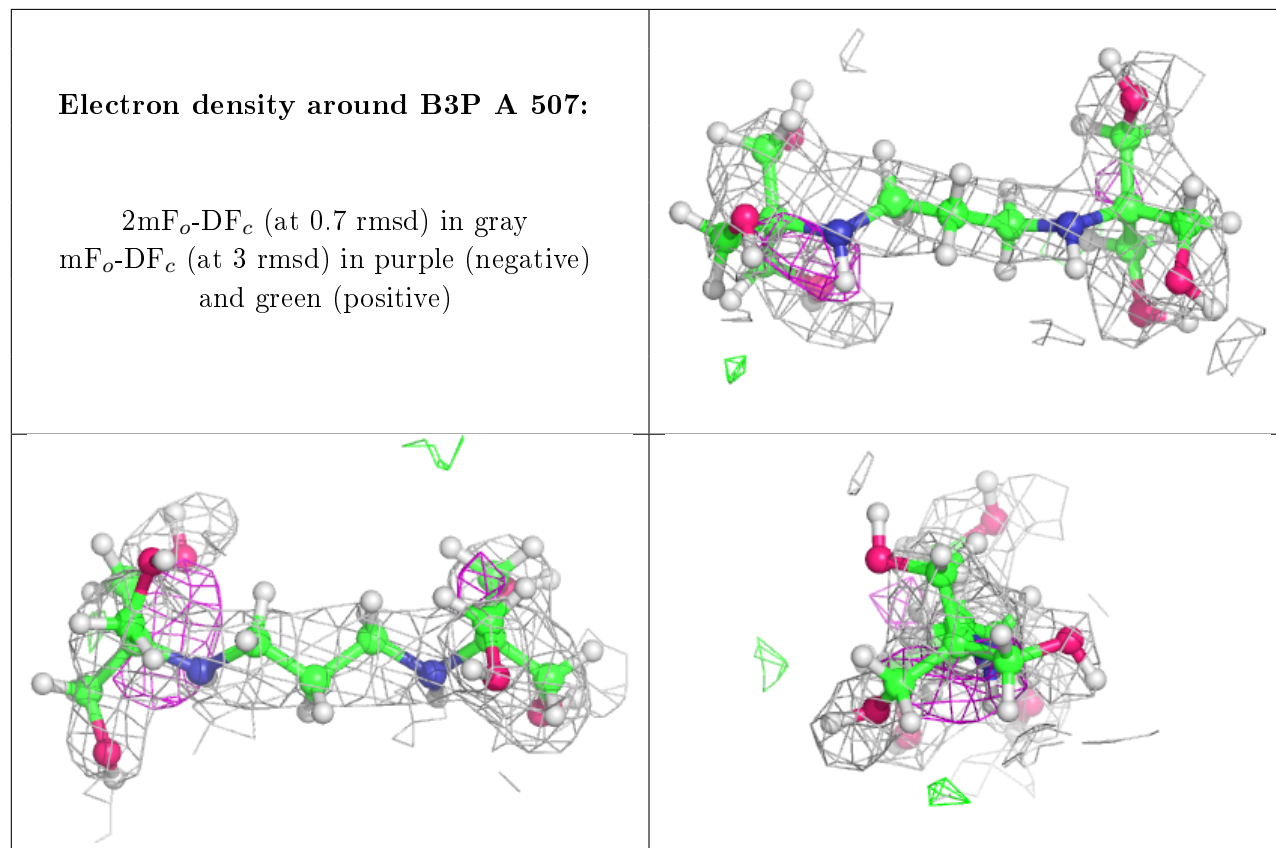
6.4 Ligands [i](#)

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	EDO	B	504	4/4	0.54	0.44	59,60,62,62	0
2	EDO	A	502	4/4	0.60	0.56	52,57,64,67	0
2	EDO	A	501	4/4	0.65	0.26	54,65,70,70	0
2	EDO	C	504	4/4	0.71	0.18	59,60,63,65	0
4	DXE	C	505	6/6	0.75	0.18	59,71,78,78	0
6	B3P	A	507	19/19	0.80	0.24	38,53,77,79	0
2	EDO	B	503	4/4	0.80	0.19	54,54,56,57	0
2	EDO	A	503	4/4	0.80	0.27	57,59,62,65	0
6	B3P	D	503	19/19	0.81	0.17	42,57,73,73	0
2	EDO	C	503	4/4	0.83	0.23	57,58,60,62	0
6	B3P	B	506	19/19	0.85	0.18	30,47,58,61	0
3	PEG	A	504	7/7	0.85	0.24	52,62,68,68	0
5	M2M	A	506	9/9	0.86	0.26	41,52,62,62	0
2	EDO	B	501	4/4	0.86	0.13	53,64,66,69	0
3	PEG	D	502	7/7	0.87	0.23	53,64,70,71	0
2	EDO	B	502	4/4	0.87	0.15	57,69,71,71	0
2	EDO	C	502	4/4	0.88	0.21	65,78,80,80	0
2	EDO	D	501	4/4	0.88	0.23	60,61,61,62	0
2	EDO	B	505	4/4	0.89	0.64	57,58,58,61	0
7	6L7	C	506	29/29	0.89	0.17	45,62,77,78	0
4	DXE	A	505	6/6	0.90	0.19	43,53,64,64	0
2	EDO	C	501	4/4	0.91	0.23	54,65,66,67	0
7	6L7	B	507	29/29	0.93	0.13	24,37,56,58	0
7	6L7	D	504	29/29	0.93	0.14	30,45,66,71	0
7	6L7	A	508	29/29	0.93	0.16	25,39,62,70	0

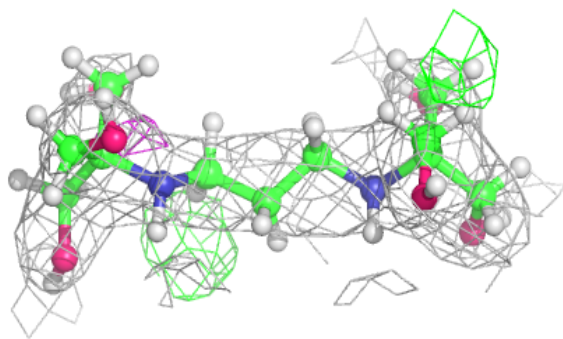
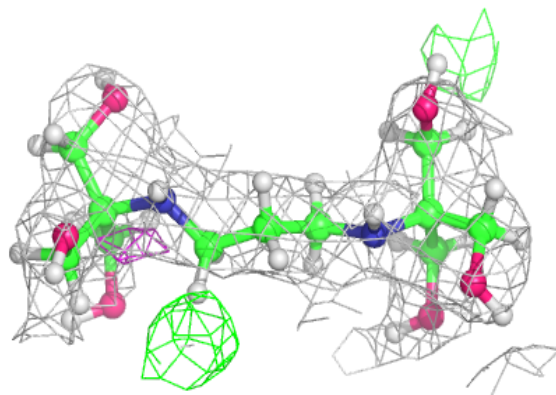
The following is a graphical depiction of the model fit to experimental electron density of all

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.

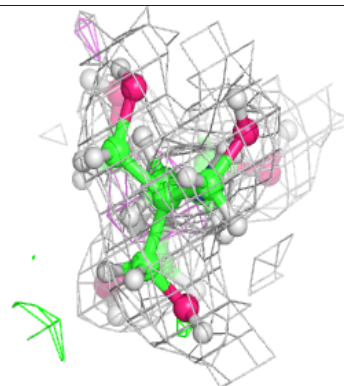
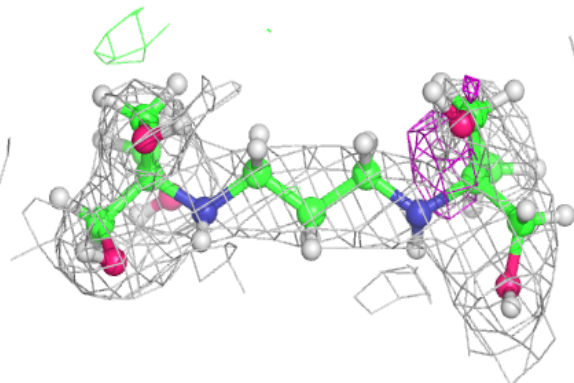
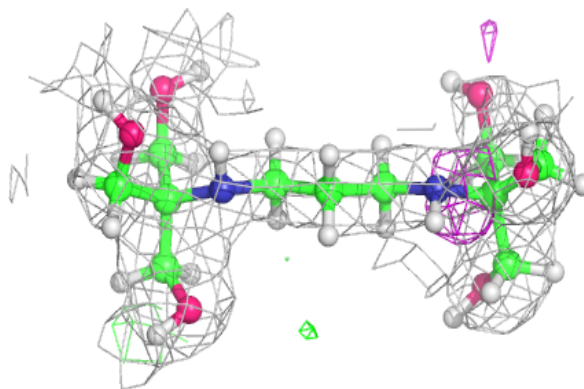


Electron density around B3P D 503:

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

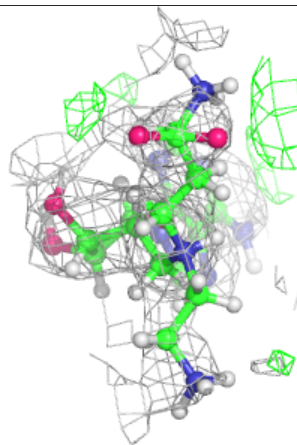
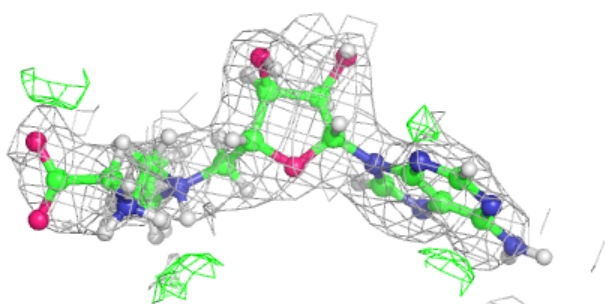
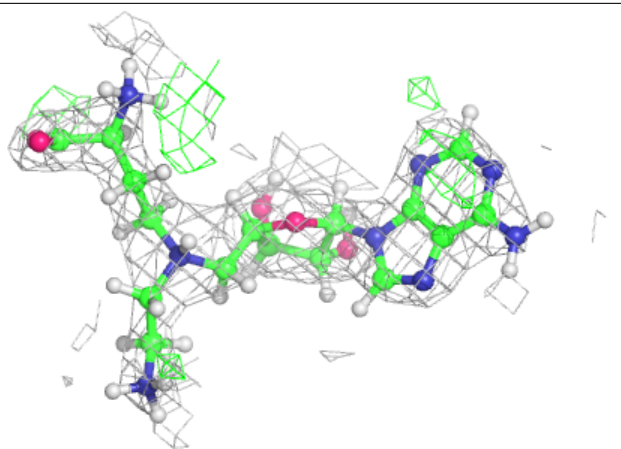
**Electron density around B3P B 506:**

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

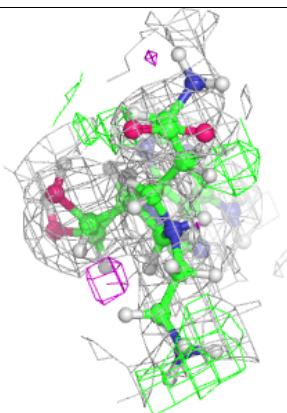
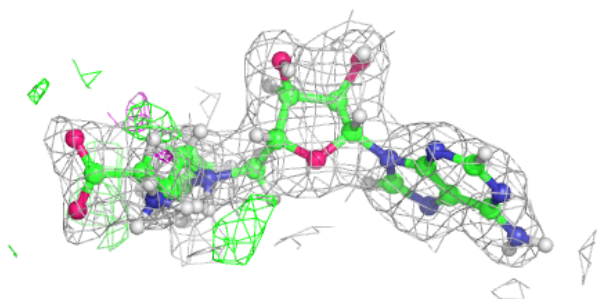
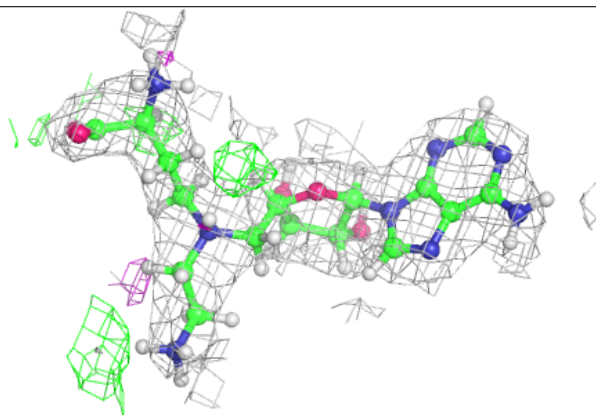


Electron density around 6L7 C 506:

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

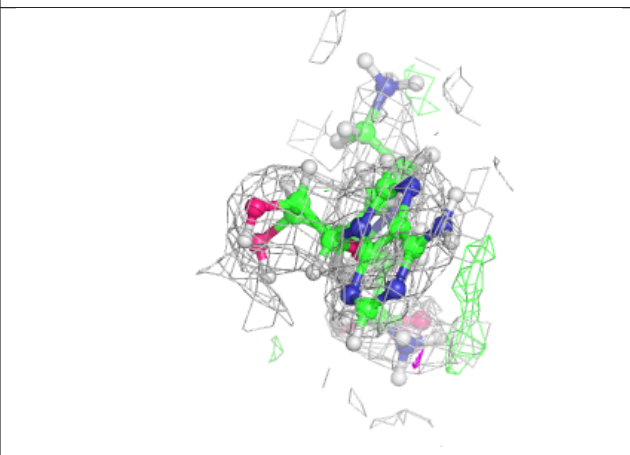
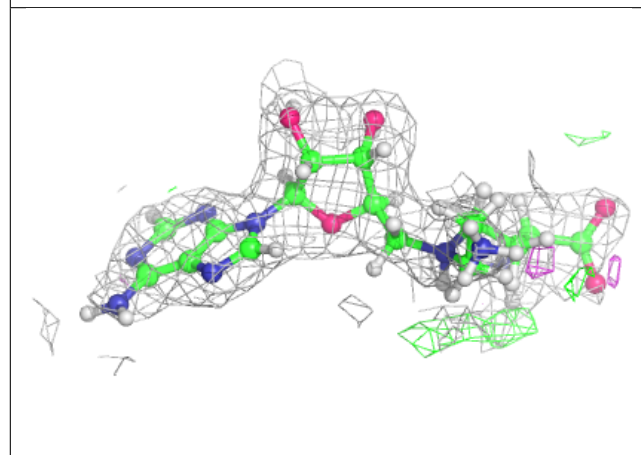
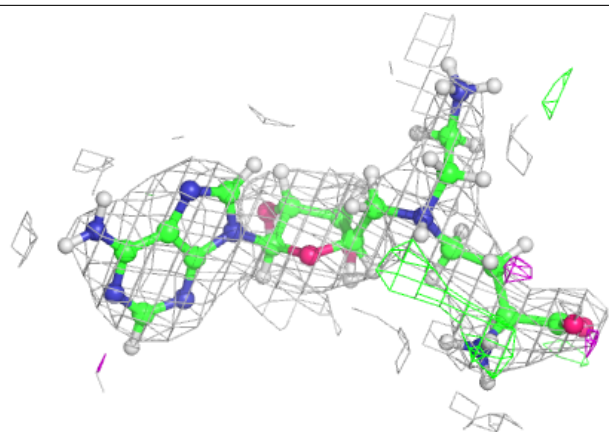
**Electron density around 6L7 B 507:**

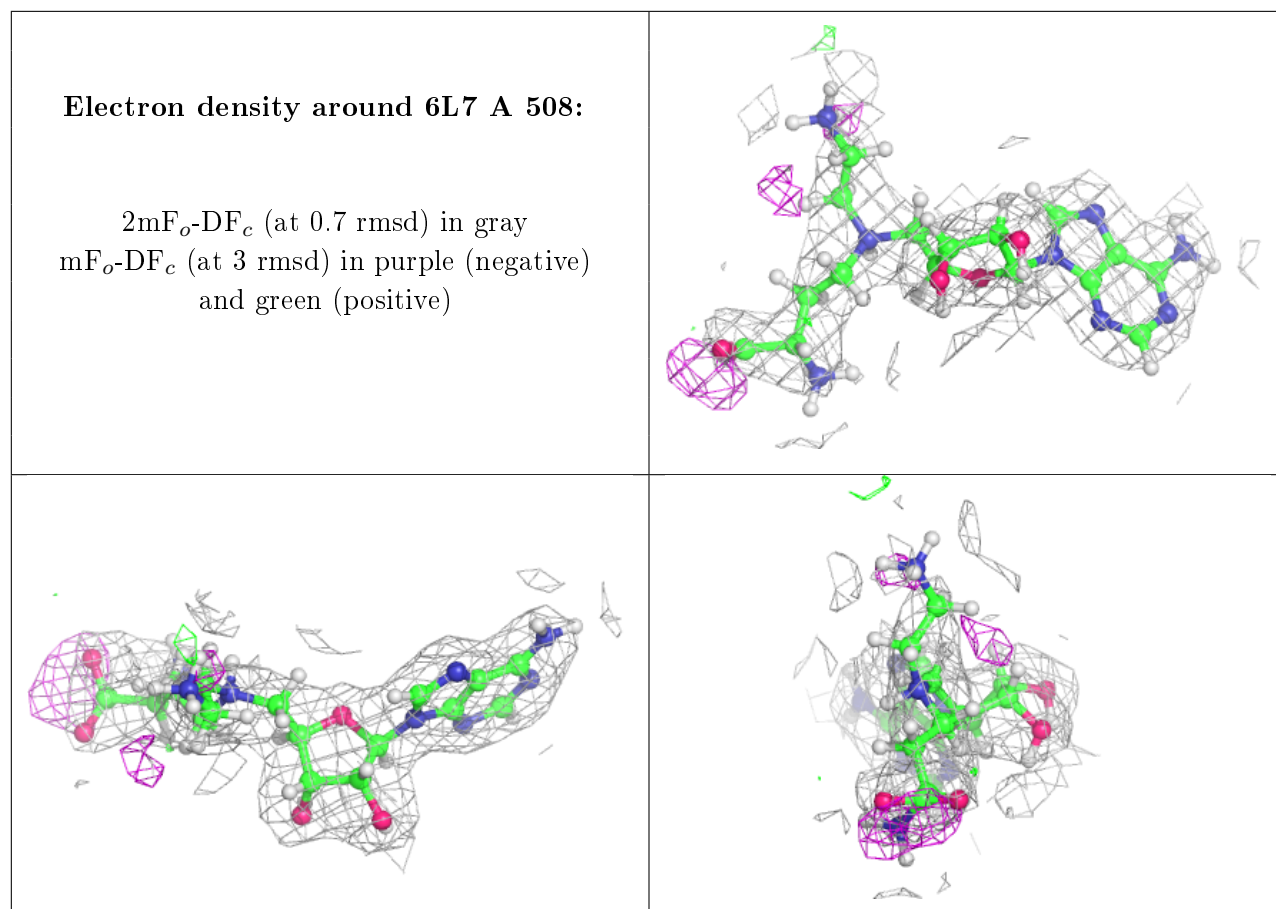
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6L7 D 504:

$2mF_o-DF_c$ (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.