



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:31 AM UTC

PDB ID : 5NTC / pdb_00005ntc
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 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

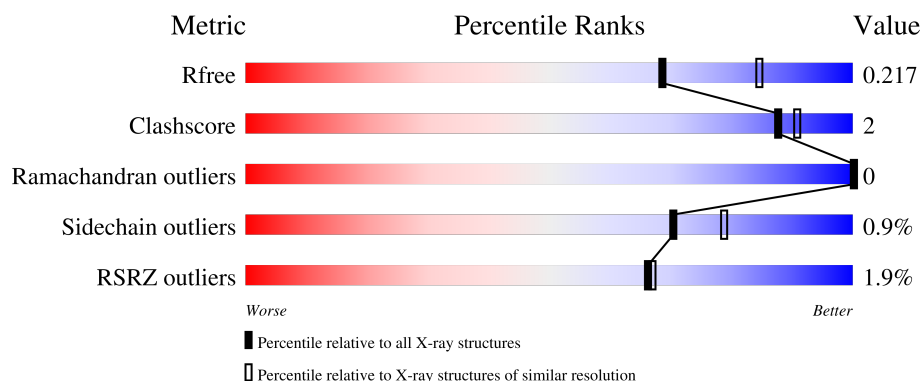
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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	371	89% 5% 6%
1	B	371	86% 10%
1	C	371	3% 87% 6% 6%
1	D	371	2% 84% 5% 10%

2 Entry composition

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

There are 12 discrepancies between the modelled and reference sequences:

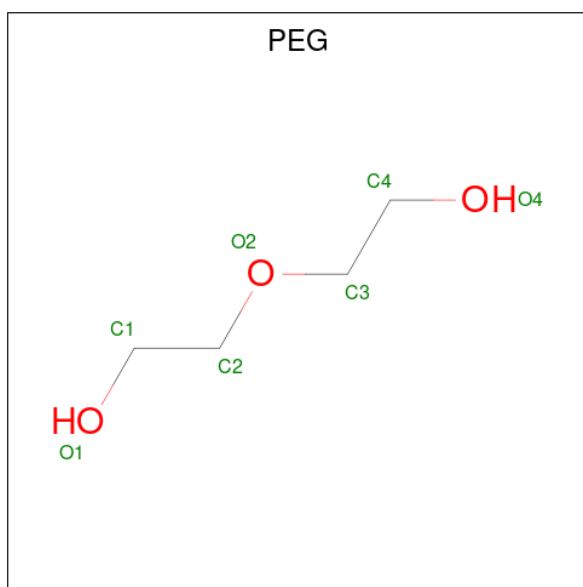
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	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 (CCD ID: EDO) (formula: C₂H₆O₂).



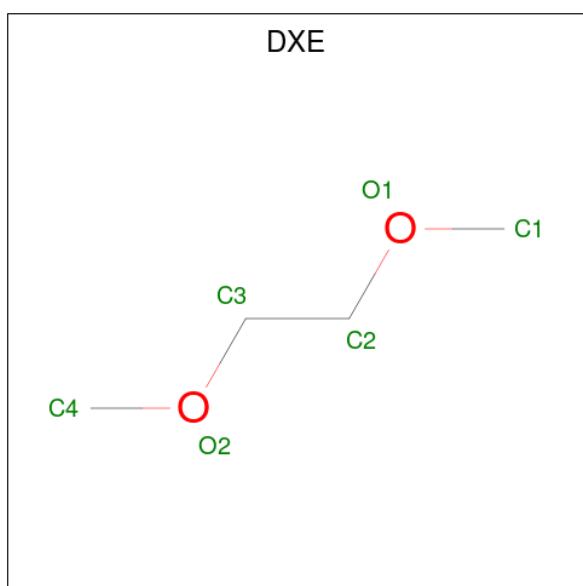
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C H O 10 2 6 2	0	0
2	C	1	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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



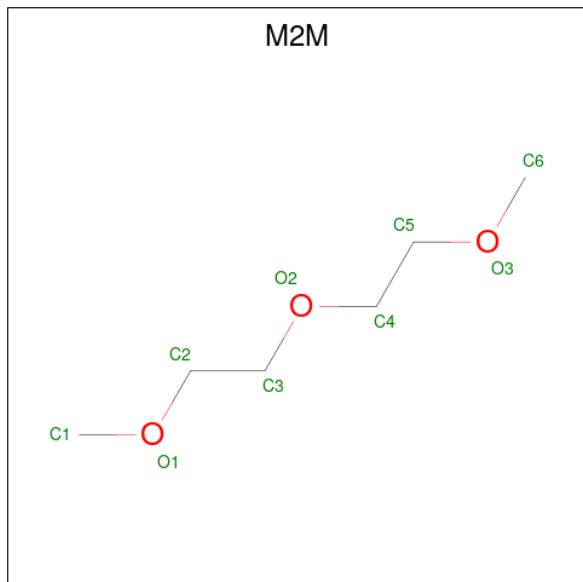
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		

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



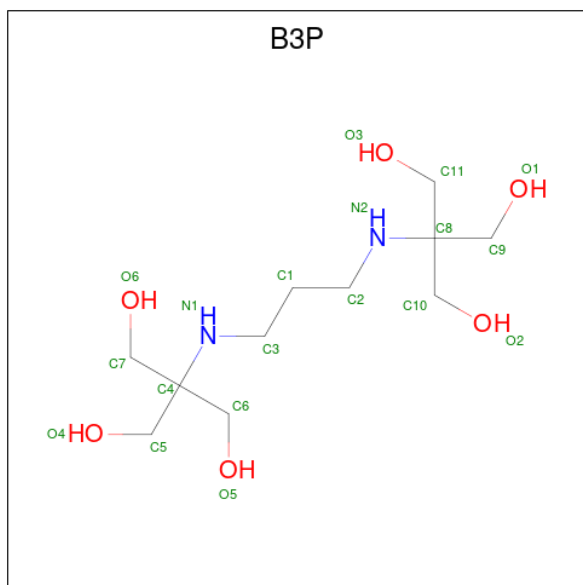
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			16	4	10	2		
4	C	1	Total	C	H	O	0	0
			16	4	10	2		

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



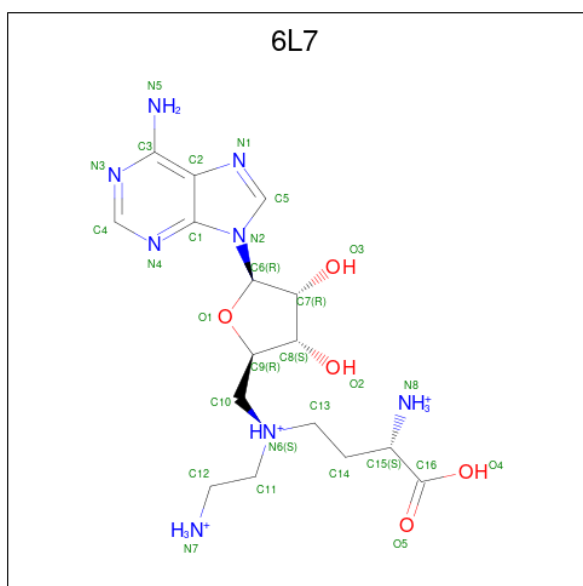
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	23	6	14	3	0	0

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: 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 (CCD ID: 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 216 216	0	0
8	B	164	Total O 164 164	0	0

Continued on next page...

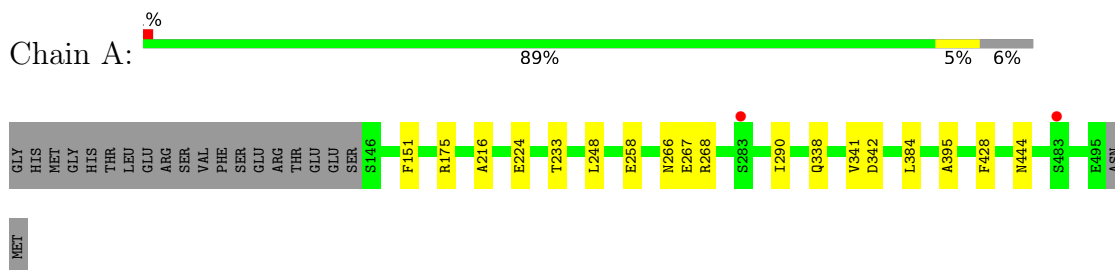
Continued from previous page...

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

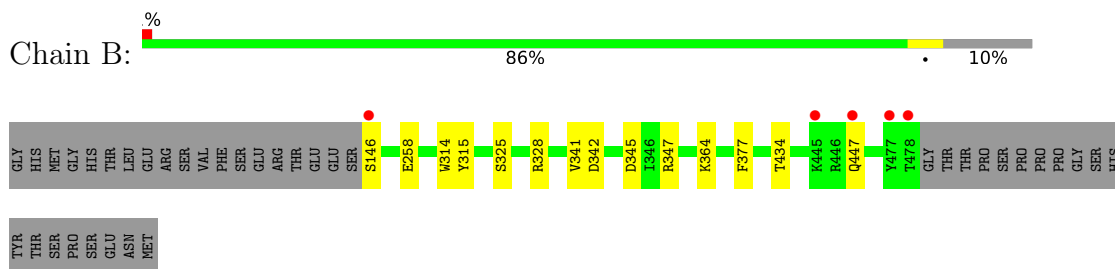
3 Residue-property plots [i](#)

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.

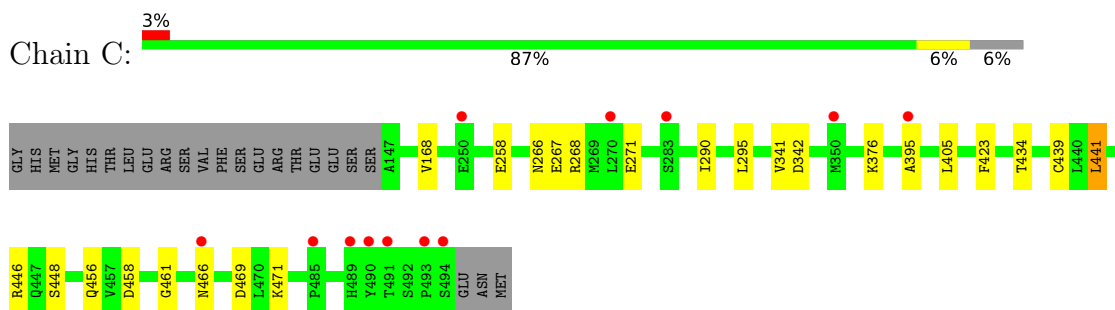
- Molecule 1: Histone-arginine methyltransferase CARM1



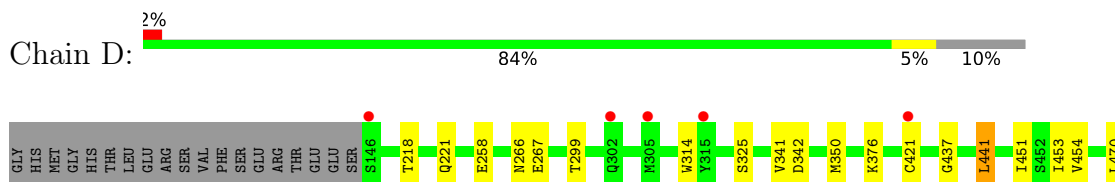
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



Y477	GLY
Y478	THR
	PRO
	SER
	PRO
	PRO
	GLY
	SER
	HIS
	TYR
	THR
	SER
	PRO
	SER
	GLU
	ASN
	MET

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) 99.2 (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)	Xtriage
Refinement program	PHENIX dev_1951	Depositor
R, R_{free}	0.178 , 0.216 0.179 , 0.217	Depositor DCC
R_{free} test set	3640 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22816	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

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

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	0.37	0/2892	0.72	2/3928 (0.1%)
1	B	0.38	0/2758	0.71	0/3739
1	C	0.38	0/2877	0.72	0/3908
1	D	0.38	0/2756	0.72	0/3736
All	All	0.38	0/11283	0.72	2/15311 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	GLN	CA-C-N	-5.00	114.61	119.76
1	A	338	GLN	C-N-CA	-5.00	114.61	119.76

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	14	0
1	D	2686	2640	2638	12	0
2	A	12	6	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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:B:345:ASP:CG	1:B:347:ARG:HE	2.19	0.50
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ASN:O	1:C:267:GLU:HB2	2.14	0.47
1:D:218:THR:O	1:D:221:GLN:HG2	2.14	0.47
1:D:477:TYR:O	1:D:478:THR:C	2.57	0.47
1:B:315:TYR:CD1	1:B:328:ARG:HD2	2.49	0.46
1:A:341:VAL:O	1:A:342:ASP:HB3	2.16	0.45
1:A:268:ARG:NH1	1:A:444:ASN:O	2.49	0.45
1:D:299:THR:HG22	1:D:350:MET:HE3	1.99	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: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: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:B:341:VAL:O	1:B:342:ASP:HB3	2.19	0.41
1:D:266:ASN:O	1:D:267:GLU:HB2	2.21	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:437:GLY:HA3	1:D:454:VAL:O	2.21	0.40
1:D:441:LEU:N	1:D:441:LEU:HD12	2.35	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	303 (99%)	3 (1%)	68	77
1	B	291/323 (90%)	290 (100%)	1 (0%)	86	90
1	C	304/323 (94%)	300 (99%)	4 (1%)	61	72
1	D	291/323 (90%)	288 (99%)	3 (1%)	68	77
All	All	1192/1292 (92%)	1181 (99%)	11 (1%)	70	79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	THR
1	A	248	LEU
1	A	258	GLU
1	B	258	GLU
1	C	258	GLU
1	C	295	LEU
1	C	376	LYS
1	C	441	LEU
1	D	258	GLU
1	D	376	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	441	LEU

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	251	GLN
1	A	378	HIS
1	A	472	ASN
1	A	489	HIS
1	C	149	GLN
1	C	152	GLN
1	C	159	GLN
1	C	316	GLN
1	C	456	GLN
1	C	472	ASN
1	C	489	HIS
1	D	162	ASN
1	D	165	GLN
1	D	381	HIS
1	D	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 oligosaccharides 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	$\# Z > 2$
2	EDO	A	502	-	3,3,3	0.44	0	2,2,2	0.53	0
4	DXE	A	505	-	5,5,5	0.43	0	4,4,4	0.31	0
7	6L7	C	506	-	30,31,31	0.72	0	39,44,44	0.68	2 (5%)
3	PEG	D	502	-	6,6,6	0.48	0	5,5,5	0.45	0
2	EDO	C	501	-	3,3,3	0.45	0	2,2,2	0.51	0
2	EDO	B	502	-	3,3,3	0.44	0	2,2,2	0.51	0
2	EDO	C	504	-	3,3,3	0.44	0	2,2,2	0.50	0
6	B3P	B	506	-	18,18,18	0.20	0	23,23,23	0.43	0
2	EDO	A	503	-	3,3,3	0.44	0	2,2,2	0.52	0
7	6L7	A	508	-	30,31,31	0.64	0	39,44,44	0.85	2 (5%)
2	EDO	C	503	-	3,3,3	0.44	0	2,2,2	0.51	0
7	6L7	B	507	-	30,31,31	0.67	0	39,44,44	0.91	2 (5%)
2	EDO	B	504	-	3,3,3	0.44	0	2,2,2	0.50	0
6	B3P	A	507	-	18,18,18	0.29	0	23,23,23	0.46	0
6	B3P	D	503	-	18,18,18	0.32	0	23,23,23	0.44	0
2	EDO	A	501	-	3,3,3	0.45	0	2,2,2	0.49	0
2	EDO	B	501	-	3,3,3	0.44	0	2,2,2	0.52	0
5	M2M	A	506	-	8,8,8	0.59	0	7,7,7	0.46	0
2	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.52	0
2	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.50	0
2	EDO	C	502	-	3,3,3	0.45	0	2,2,2	0.57	0
4	DXE	C	505	-	5,5,5	0.45	0	4,4,4	0.26	0
7	6L7	D	504	-	30,31,31	0.65	0	39,44,44	0.64	1 (2%)
2	EDO	D	501	-	3,3,3	0.44	0	2,2,2	0.52	0
3	PEG	A	504	-	6,6,6	0.48	0	5,5,5	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	502	-	-	1/1/1/1	-
4	DXE	A	505	-	-	3/3/3/3	-
7	6L7	C	506	-	-	11/20/36/36	0/3/3/3
3	PEG	D	502	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	B	502	-	-	1/1/1/1	-
2	EDO	C	504	-	-	1/1/1/1	-
6	B3P	B	506	-	-	6/28/28/28	-
2	EDO	A	503	-	-	1/1/1/1	-
7	6L7	A	508	-	-	10/20/36/36	0/3/3/3
2	EDO	C	503	-	-	0/1/1/1	-
7	6L7	B	507	-	-	11/20/36/36	0/3/3/3
2	EDO	B	504	-	-	0/1/1/1	-
6	B3P	A	507	-	-	5/28/28/28	-
6	B3P	D	503	-	-	7/28/28/28	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
5	M2M	A	506	-	-	4/6/6/6	-
2	EDO	B	503	-	-	0/1/1/1	-
2	EDO	B	505	-	-	0/1/1/1	-
2	EDO	C	502	-	-	1/1/1/1	-
4	DXE	C	505	-	-	1/3/3/3	-
7	6L7	D	504	-	-	7/20/36/36	0/3/3/3
2	EDO	D	501	-	-	0/1/1/1	-
3	PEG	A	504	-	-	4/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	507	6L7	C13-N6-C10	3.32	119.65	111.89
7	B	507	6L7	C12-C11-N6	3.02	121.31	113.39
7	A	508	6L7	C13-N6-C10	2.90	118.65	111.89
7	A	508	6L7	C12-C11-N6	2.83	120.81	113.39
7	C	506	6L7	C12-C11-N6	2.57	120.15	113.39
7	D	504	6L7	C13-N6-C10	2.45	117.60	111.89
7	C	506	6L7	C13-N6-C10	2.34	117.35	111.89

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	507	B3P	N1-C4-C7-O6

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

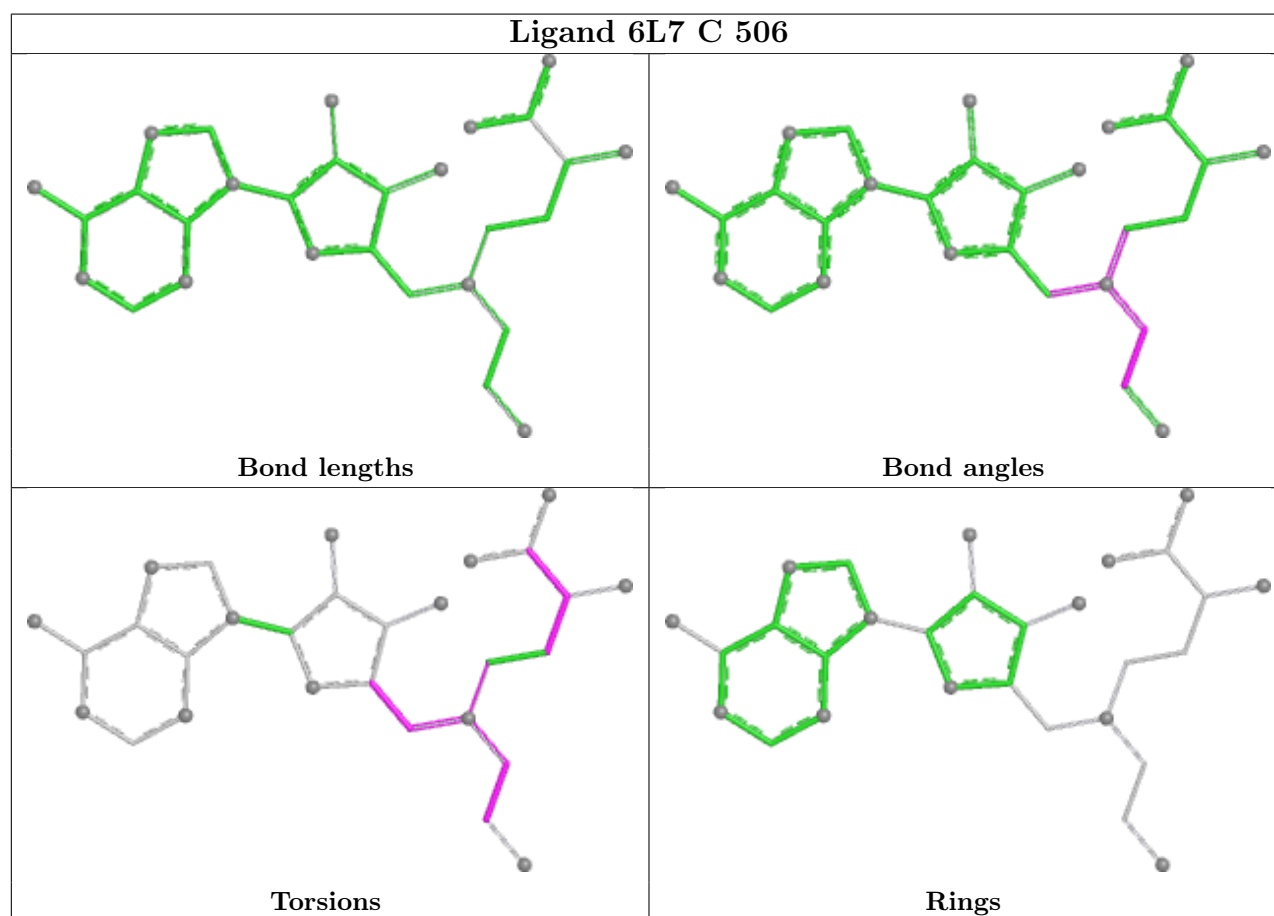
Mol	Chain	Res	Type	Atoms
7	B	507	6L7	C12-C11-N6-C13
7	A	508	6L7	C13-C14-C15-C16
7	C	506	6L7	C13-C14-C15-C16
5	A	506	M2M	C3-C2-O1-C1
6	B	506	B3P	C7-C4-N1-C3
7	D	504	6L7	N6-C13-C14-C15
6	B	506	B3P	C7-C4-C5-O4
6	D	503	B3P	C5-C4-C6-O5
6	D	503	B3P	C11-C8-C9-O1
7	C	506	6L7	C14-C13-N6-C10
3	A	504	PEG	C1-C2-O2-C3
3	A	504	PEG	C4-C3-O2-C2
7	D	504	6L7	N8-C15-C16-O4
6	D	503	B3P	C2-C1-C3-N1
7	C	506	6L7	C12-C11-N6-C13
7	A	508	6L7	C12-C11-N6-C13
7	A	508	6L7	N8-C15-C16-O4
6	B	506	B3P	O3-C11-C8-C10
7	A	508	6L7	N8-C15-C16-O5
6	D	503	B3P	C9-C8-N2-C2
3	A	504	PEG	O1-C1-C2-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
2	B	501	EDO	O1-C1-C2-O2
7	B	507	6L7	N6-C11-C12-N7
7	D	504	6L7	N6-C11-C12-N7
7	A	508	6L7	C13-C14-C15-N8
5	A	506	M2M	O1-C2-C3-O2
4	A	505	DXE	C3-C2-O1-C1
4	A	505	DXE	C2-C3-O2-C4
6	A	507	B3P	C5-C4-N1-C3
7	A	508	6L7	N6-C13-C14-C15
7	D	504	6L7	N8-C15-C16-O5

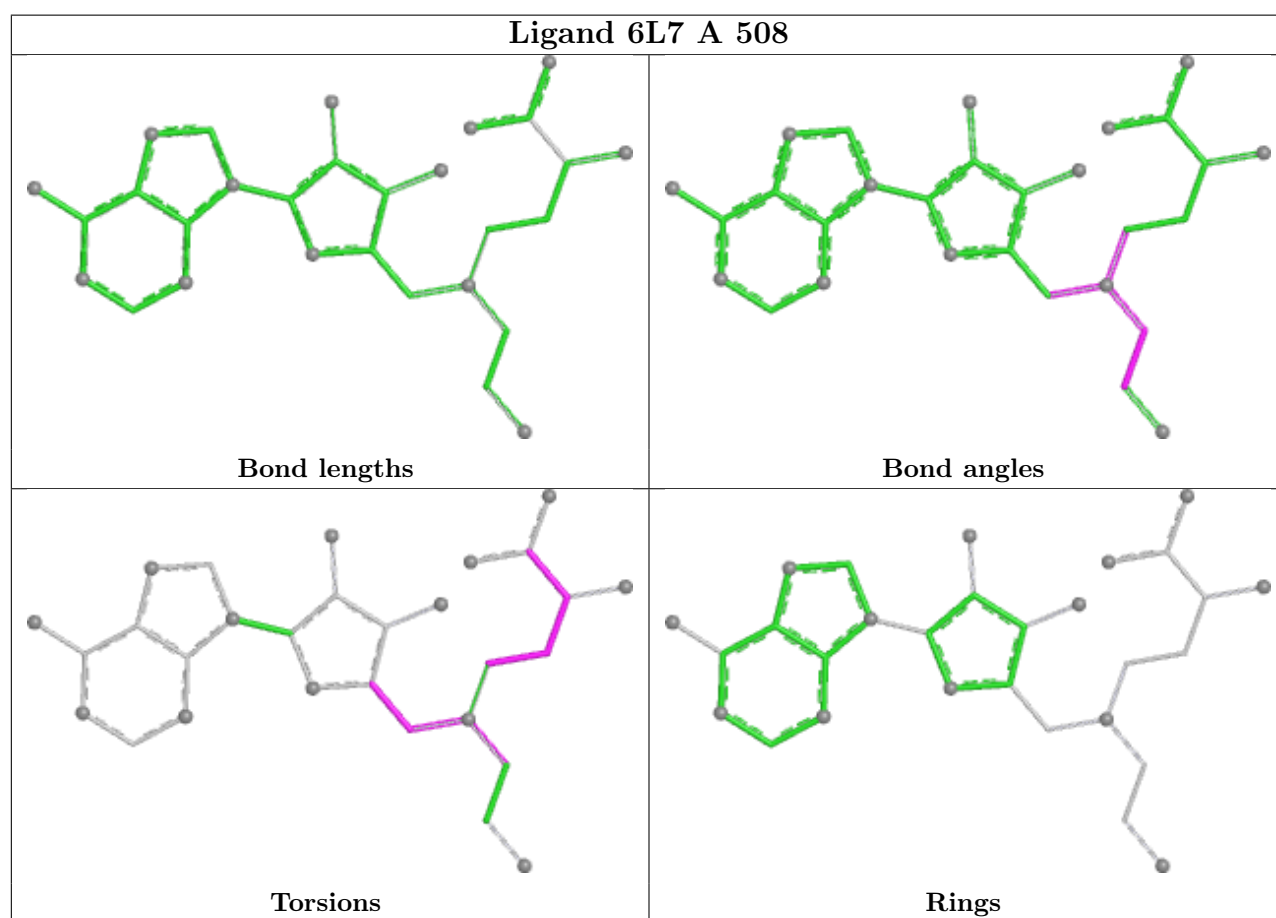
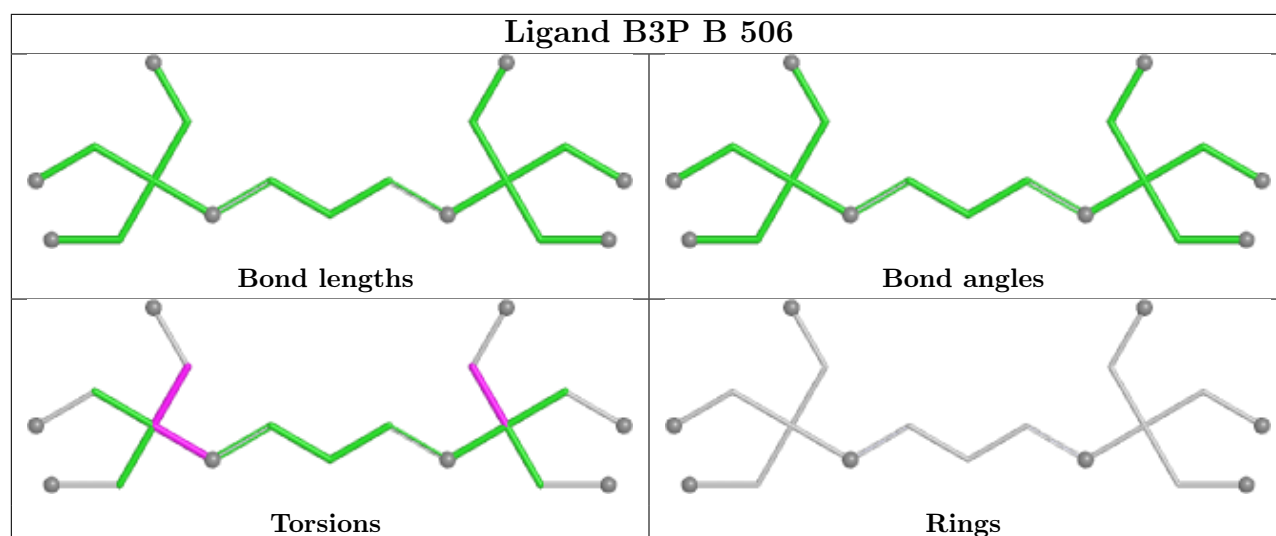
There are no ring outliers.

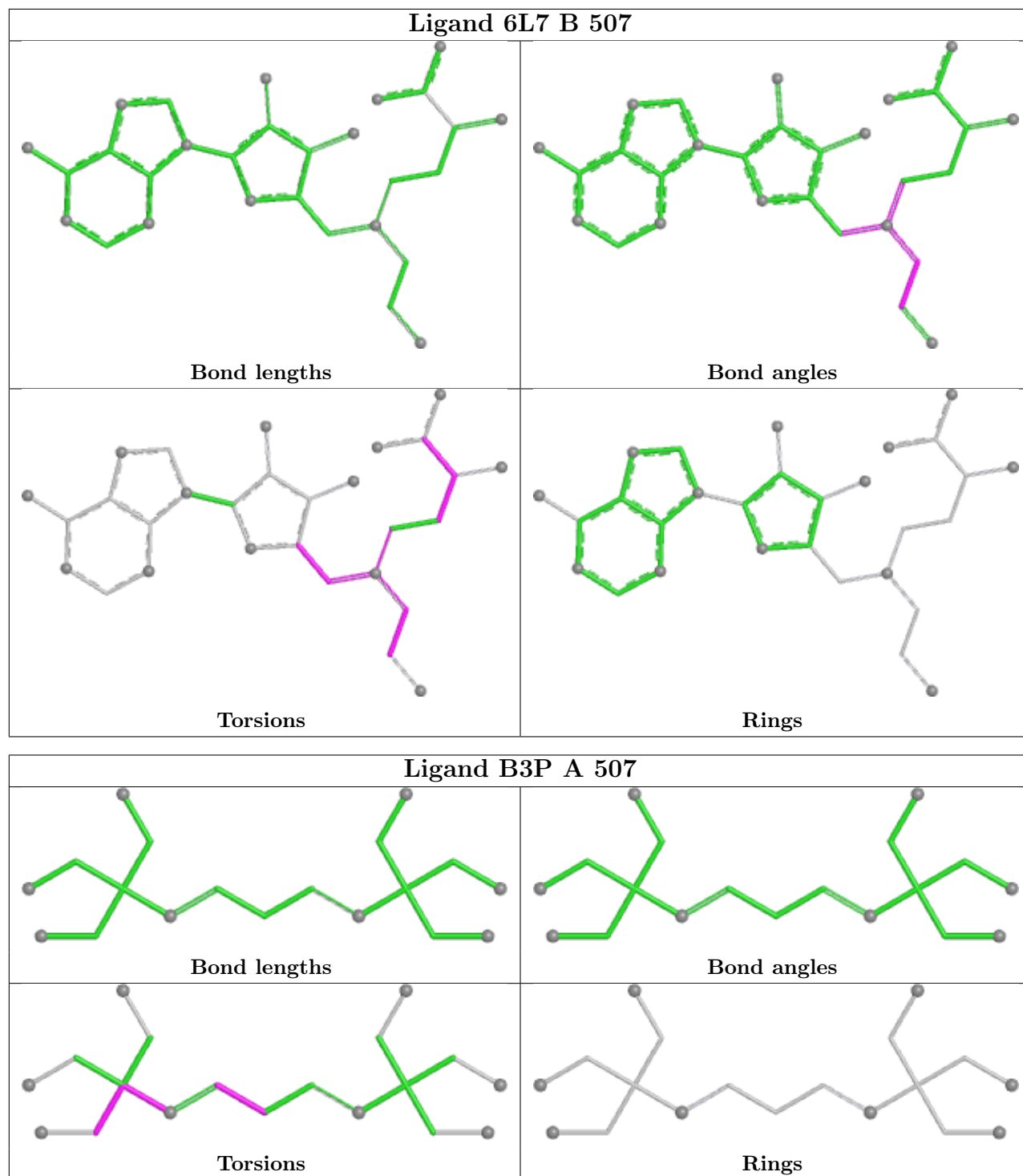
3 monomers are involved in 3 short contacts:

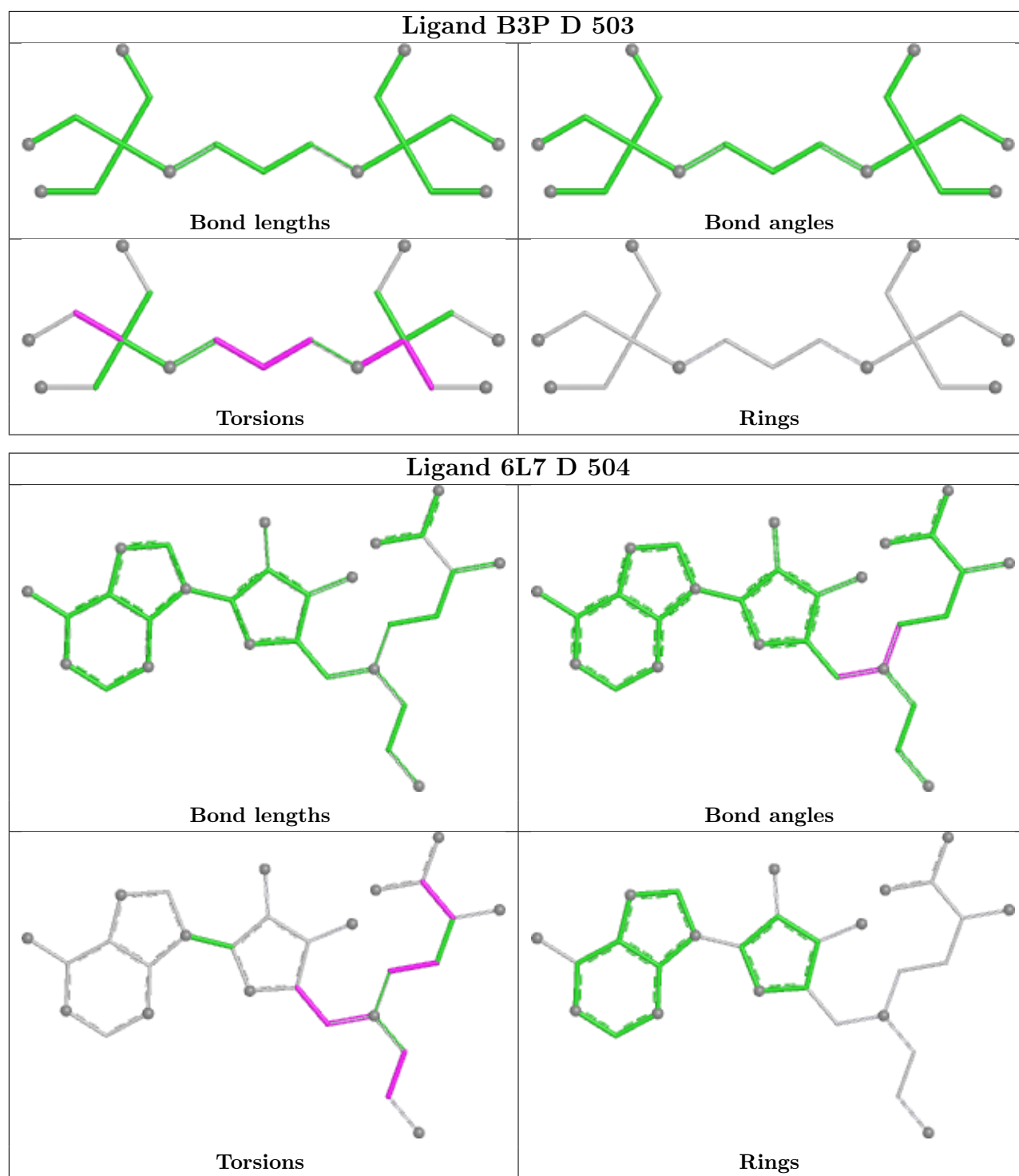
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	504	EDO	1	0
2	B	504	EDO	1	0
6	A	507	B3P	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	350/371 (94%)	-0.34	2 (0%) 85 86	16, 37, 62, 89	1 (0%)
1	B	333/371 (89%)	-0.25	5 (1%) 72 73	20, 39, 67, 88	2 (0%)
1	C	348/371 (93%)	0.26	12 (3%) 48 48	22, 58, 89, 115	1 (0%)
1	D	333/371 (89%)	-0.06	7 (2%) 63 64	20, 50, 76, 104	2 (0%)
All	All	1364/1484 (91%)	-0.10	26 (1%) 66 67	16, 46, 79, 115	6 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	478	THR	3.6
1	D	477	TYR	3.5
1	B	477[A]	TYR	3.2
1	C	490	TYR	3.2
1	C	270	LEU	3.1
1	B	445	LYS	3.1
1	C	466	ASN	3.0
1	C	489	HIS	2.6
1	C	283	SER	2.5
1	D	421	CYS	2.4
1	A	483	SER	2.4
1	C	350	MET	2.4
1	C	493	PRO	2.4
1	B	447	GLN	2.4
1	D	305	MET	2.3
1	B	478	THR	2.3
1	C	491	THR	2.3
1	A	283	SER	2.2
1	C	395	ALA	2.1
1	C	494	SER	2.1
1	C	485	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	146	SER	2.1
1	C	250	GLU	2.0
1	D	315	TYR	2.0
1	B	146	SER	2.0
1	D	302	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	C	502	4/4	0.61	0.15	65,78,80,80	0
2	EDO	C	504	4/4	0.64	0.18	59,60,63,65	0
4	DXE	C	505	6/6	0.64	0.14	59,71,78,78	0
2	EDO	A	502	4/4	0.73	0.15	52,57,64,67	0
2	EDO	B	503	4/4	0.74	0.14	54,54,56,57	0
5	M2M	A	506	9/9	0.74	0.14	41,52,62,62	0
2	EDO	B	505	4/4	0.75	0.14	57,58,58,61	0
2	EDO	D	501	4/4	0.75	0.12	60,61,61,62	0
2	EDO	B	504	4/4	0.76	0.14	59,60,62,62	0
2	EDO	C	503	4/4	0.76	0.15	57,58,60,62	0
2	EDO	A	501	4/4	0.76	0.15	54,65,70,70	0
2	EDO	A	503	4/4	0.77	0.11	57,59,62,65	0
2	EDO	B	501	4/4	0.78	0.12	53,64,66,69	0
4	DXE	A	505	6/6	0.79	0.13	43,53,64,64	0
3	PEG	A	504	7/7	0.81	0.13	52,62,68,68	0
2	EDO	B	502	4/4	0.82	0.10	57,69,71,71	0
6	B3P	A	507	19/19	0.86	0.11	38,53,77,79	0
2	EDO	C	501	4/4	0.87	0.08	54,65,66,67	0

Continued on next page...

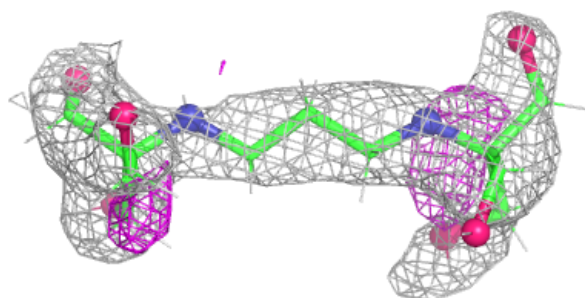
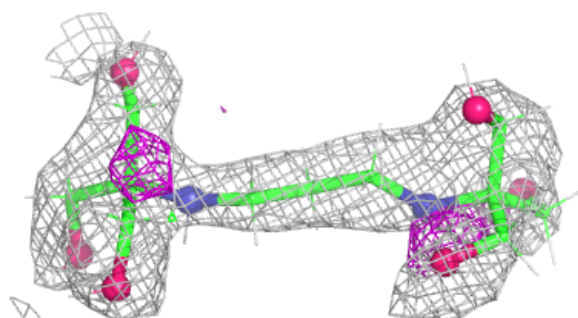
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	D	502	7/7	0.88	0.09	53,64,70,71	0
6	B3P	D	503	19/19	0.89	0.10	42,57,73,73	0
7	6L7	C	506	29/29	0.89	0.10	45,62,77,78	0
7	6L7	D	504	29/29	0.91	0.09	30,45,66,71	0
6	B3P	B	506	19/19	0.92	0.08	30,47,58,61	0
7	6L7	B	507	29/29	0.93	0.07	24,37,56,58	0
7	6L7	A	508	29/29	0.94	0.08	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.

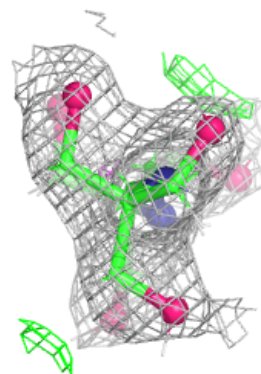
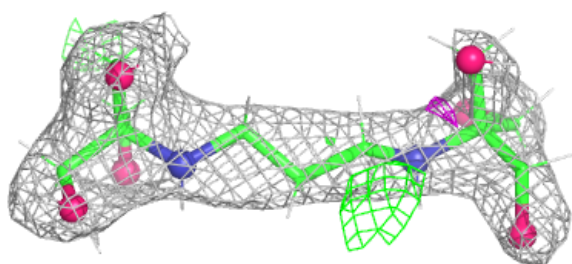
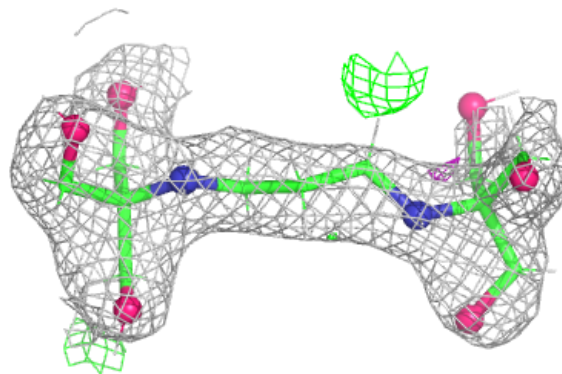
Electron density around B3P A 507:

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

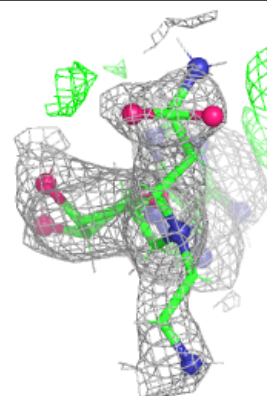
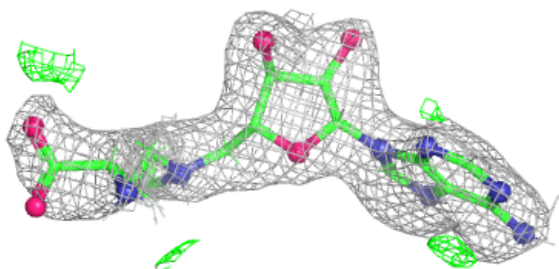
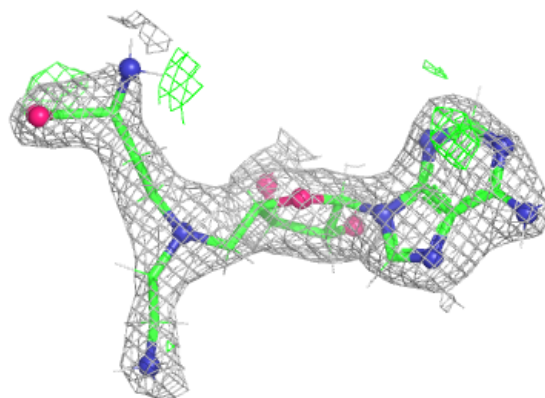


Electron density around B3P D 503:

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

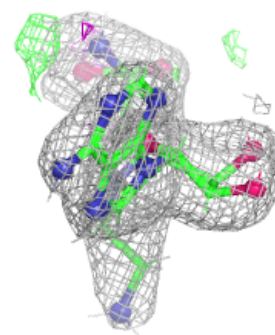
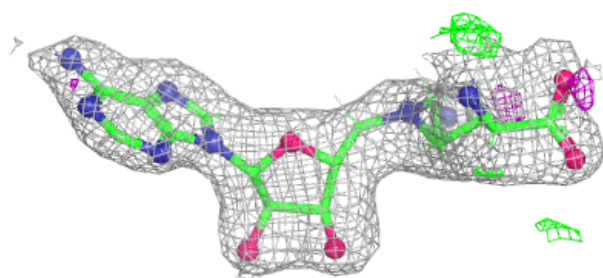
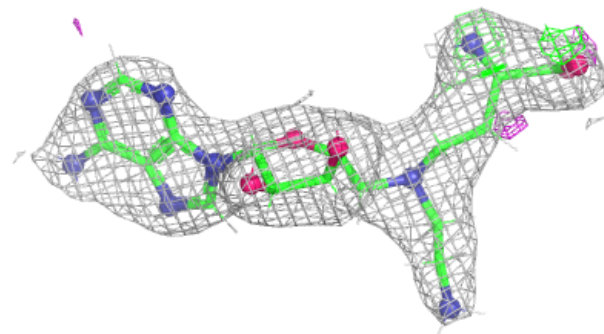
**Electron density around 6L7 C 506:**

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

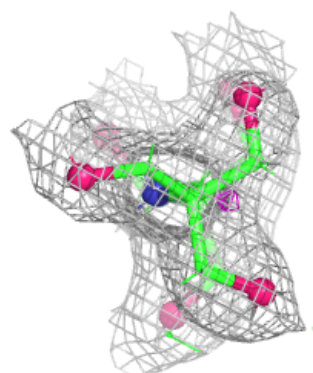
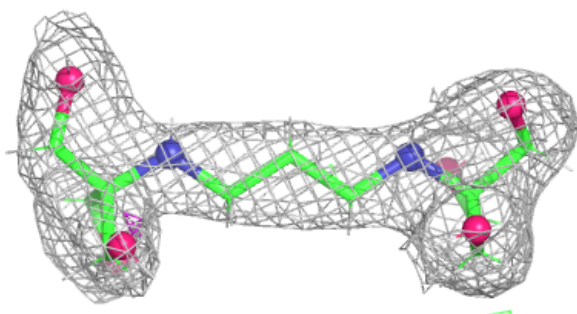
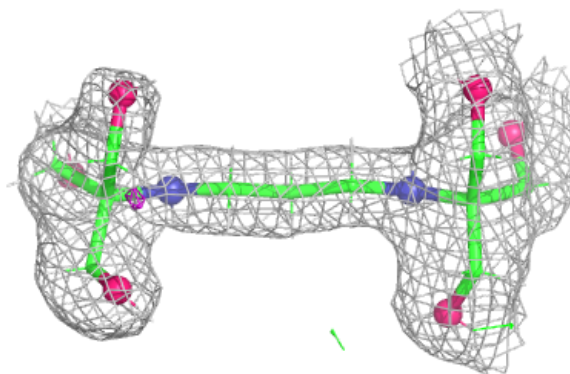


Electron density around 6L7 D 504:

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

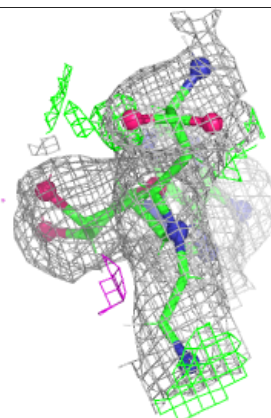
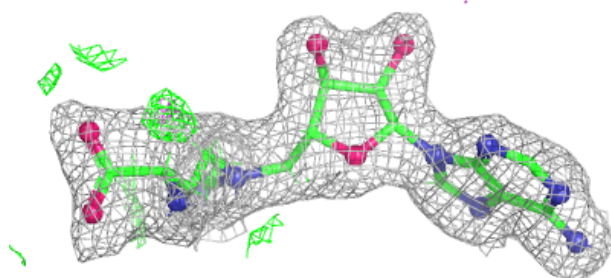
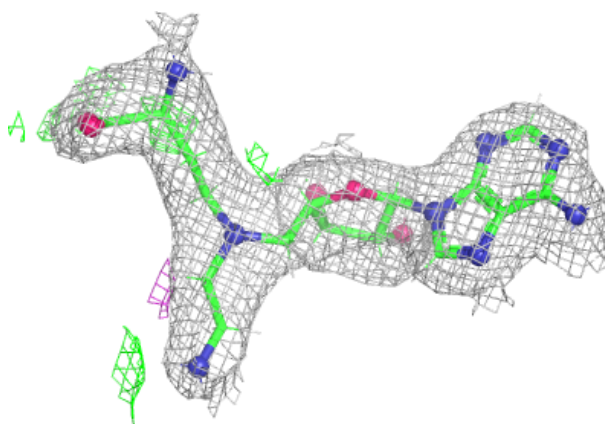
**Electron density around B3P B 506:**

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

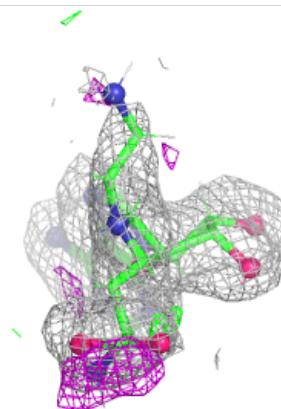
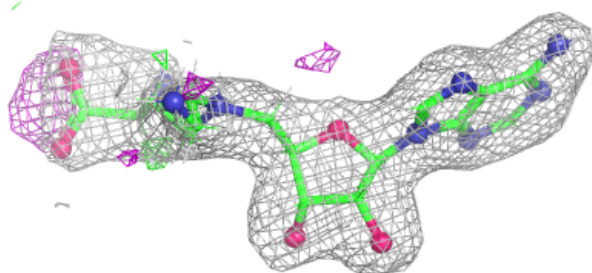
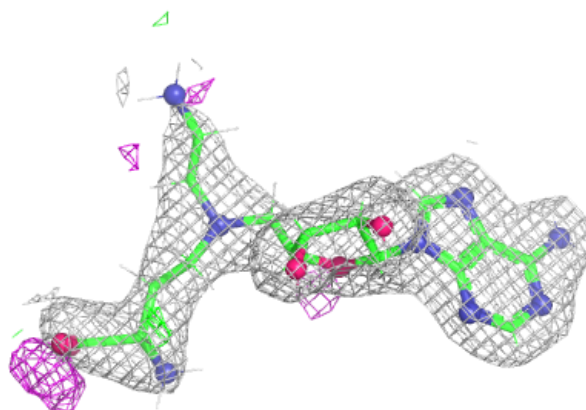


Electron density around 6L7 B 507:

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

**Electron density around 6L7 A 508:**

$2mF_o-DF_c$ (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.