



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:49 am BST

PDB ID : 5ISB
Title : Crystal structure of mouse CARM1 in complex with inhibitor SA0435
Authors : Cura, V.; Marechal, N.; Mailliot, J.; Troffer-Charlier, N.; Hassenboehler, P.;
Wurtz, J.M.; Bonnefond, L.; Cavarelli, J.
Deposited on : 2016-03-15
Resolution : 2.00 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 : 2.11
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) : 2.11

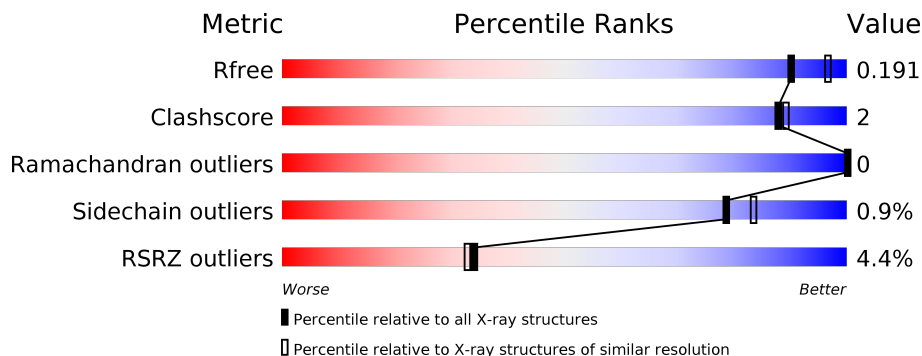
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	361	 3% 91% 5%
1	B	361	 5% 89% 6% 5%
1	C	361	 4% 93% 5%
1	D	361	 4% 90% 5%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 23368 atoms, of which 11059 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	343	Total	C	H	N	O	S	0	4	0
			5515	1796	2730	460	513	16			
1	B	343	Total	C	H	N	O	S	0	4	0
			5502	1792	2723	458	511	18			
1	C	343	Total	C	H	N	O	S	0	3	0
			5498	1793	2722	457	511	15			
1	D	342	Total	C	H	N	O	S	0	2	0
			5464	1782	2704	455	507	16			

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 5'-{[(3S)-3-amino-3-carboxypropyl][(1H-imidazol-4-yl)methyl]amino}-5'-deoxy adenosine (three-letter code: 6CX) (formula: C₁₈H₂₅N₉O₅).

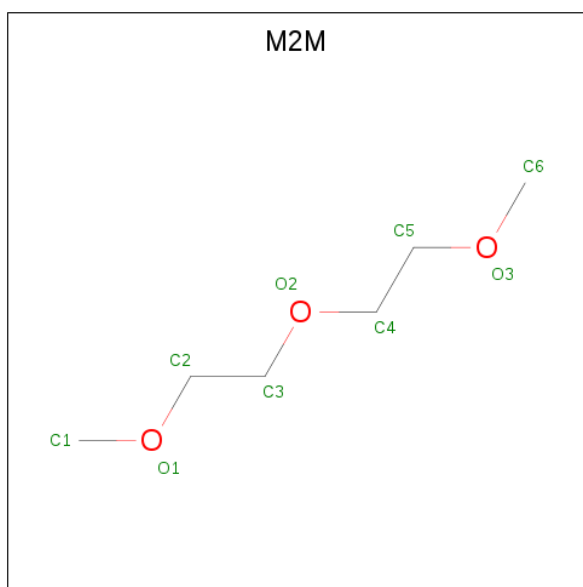
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



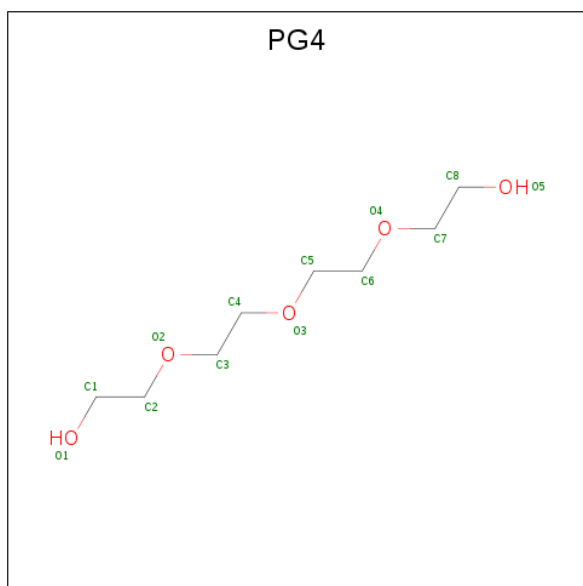
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	17	4	10	3	0	0
4	A	1	17	4	10	3	0	0
4	A	1	17	4	10	3	0	0
4	B	1	17	4	10	3	0	0
4	B	1	17	4	10	3	0	0
4	C	1	17	4	10	3	0	0
4	D	1	17	4	10	3	0	0

- Molecule 5 is 1-METHOXY-2-(2-METHOXYETHOXY)ETHANE (three-letter code: M2M) (formula: C₆H₁₄O₃).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	C	1	13	8	5	0	0

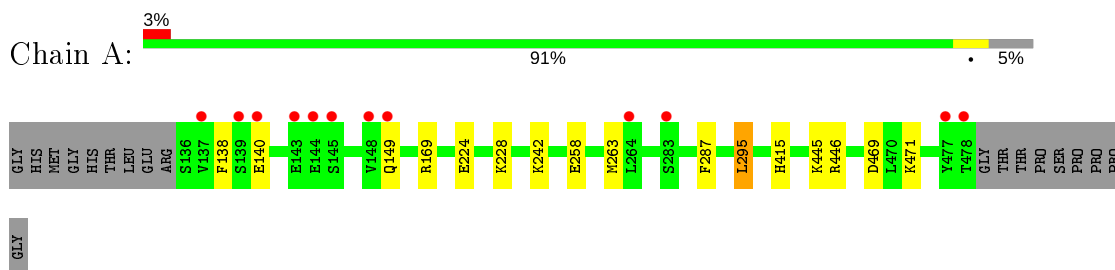
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	263	Total 264	O 264	0	1
7	B	211	Total 212	O 212	0	1
7	C	254	Total 254	O 254	0	0
7	D	215	Total 216	O 216	0	1

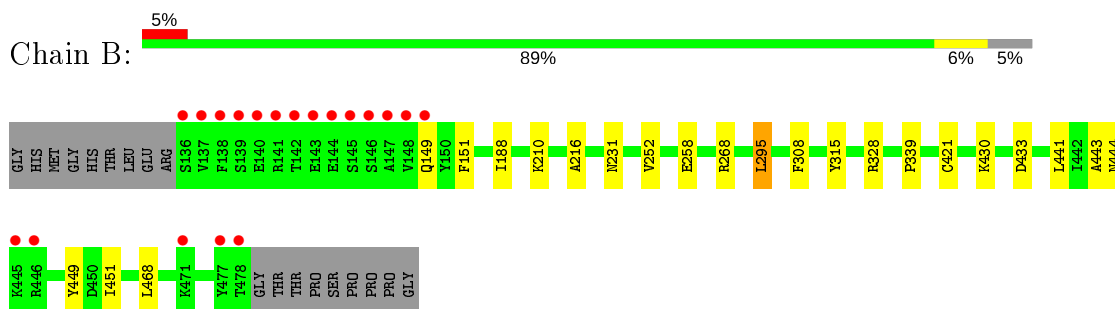
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

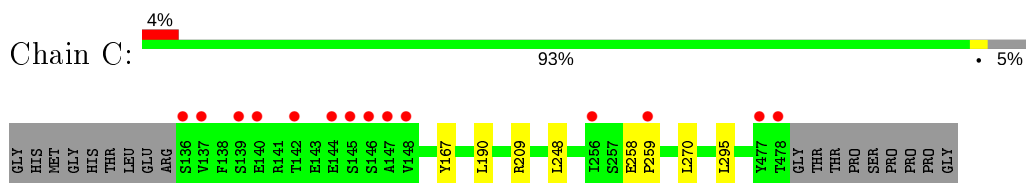
- Molecule 1: Histone-arginine methyltransferase CARM1



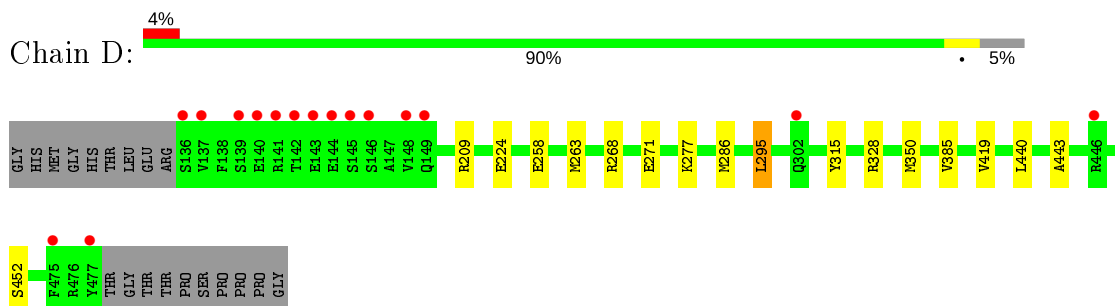
- Molecule 1: Histone-arginine methyltransferase CARM1



- 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	74.43Å 98.08Å 205.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.65 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.00) 99.4 (29.65-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.00Å)	Xtrriage
Refinement program	PHENIX dev_1839	Depositor
R, R_{free}	0.154 , 0.190 0.155 , 0.191	Depositor DCC
R_{free} test set	5117 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.2	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	0.97	EDS
Total number of atoms	23368	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 25.44 % 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 3.1726e-03. 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: 6CX, M2M, PG4, PEG, EDO

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	0.62	0/2856	0.66	1/3869 (0.0%)
1	B	0.57	0/2849	0.64	0/3859
1	C	0.56	0/2847	0.64	0/3857
1	D	0.56	0/2830	0.64	1/3833 (0.0%)
All	All	0.58	0/11382	0.64	2/15418 (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	D	295	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	263	MET	CA-CB-CG	5.42	122.52	113.30

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	2785	2730	2724	11	0
1	B	2779	2723	2723	16	0
1	C	2776	2722	2719	4	0
1	D	2760	2704	2708	12	0
2	A	32	24	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	32	24	0	0	0
2	C	32	24	0	0	0
2	D	32	24	0	0	0
3	A	12	0	18	0	0
3	B	20	0	30	0	0
3	C	16	0	24	1	0
3	D	16	0	24	0	0
4	A	21	30	30	2	0
4	B	14	20	20	0	0
4	C	7	10	10	0	0
4	D	7	10	10	0	0
5	A	9	14	14	0	0
6	C	13	0	18	1	0
7	A	264	0	0	1	0
7	B	212	0	0	2	0
7	C	254	0	0	3	0
7	D	216	0	0	3	0
All	All	12309	11059	11072	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:B:433:ASP:OD2	7:B:601:HOH:O	2.13	0.66
1:D:268:ARG:HD2	1:D:271:GLU:OE2	1.98	0.64
1:A:140:GLU:O	1:A:445:LYS:NZ	2.32	0.63
1:D:263:MET:CE	1:D:419:VAL:HG11	2.31	0.60
1:D:209:ARG:NH1	7:D:603:HOH:O	2.30	0.59
1:B:421[A]:CYS:SG	1:B:468:LEU:HD22	2.42	0.59
1:B:315:TYR:HD1	1:B:328:ARG:HD2	1.70	0.55
6:C:507:PG4:H72	7:C:747:HOH:O	2.06	0.55
1:A:149:GLN:NE2	1:B:149:GLN:OE1	2.40	0.54
1:D:277:LYS:HD3	1:D:286[A]:MET:SD	2.48	0.54
1:B:339:PRO:HG3	1:B:468:LEU:HG	1.90	0.53
1:D:328:ARG:NH1	7:D:607:HOH:O	2.44	0.50
1:B:315:TYR:CD1	1:B:328:ARG:HD2	2.46	0.50
1:B:451:ILE:HB	1:B:468:LEU:HB3	1.93	0.50
1:D:263:MET:HE3	1:D:419:VAL:HG11	1.94	0.49
1:D:350[A]:MET:SD	1:D:385:VAL:HG22	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HD2	1:A:471:LYS:NZ	2.28	0.48
1:B:295:LEU:HD12	1:B:295:LEU:N	2.29	0.47
1:A:446:ARG:HD2	1:A:471:LYS:HZ3	1.80	0.47
1:B:421[A]:CYS:SG	1:B:468:LEU:CD2	3.02	0.47
1:A:415[B]:HIS:CE1	4:A:507:PEG:H31	2.51	0.46
1:C:209:ARG:NH2	7:C:614:HOH:O	2.48	0.46
1:D:315:TYR:CD1	1:D:328:ARG:HD2	2.52	0.45
1:A:224:GLU:OE1	1:A:228:LYS:HE3	2.17	0.44
1:A:469:ASP:OD1	1:A:471:LYS:HG2	2.18	0.44
1:D:263:MET:HE2	1:D:419:VAL:HG11	1.99	0.44
1:D:224:GLU:OE1	7:D:601:HOH:O	2.21	0.44
1:C:259:PRO:HG2	1:C:270:LEU:HD23	2.00	0.43
1:D:268:ARG:HD3	1:D:443:ALA:HB1	2.00	0.43
1:A:295:LEU:HD23	1:A:295:LEU:N	2.34	0.43
4:A:507:PEG:H41	7:A:784:HOH:O	2.18	0.43
1:A:138:PHE:CD2	1:A:242:LYS:HD3	2.54	0.42
1:B:188:ILE:HG22	1:B:252:VAL:HG12	2.01	0.42
1:B:430:LYS:HD3	1:C:167:TYR:CE2	2.53	0.42
1:C:190:LEU:HD13	1:C:248:LEU:HD21	2.01	0.42
1:A:169:ARG:HD3	1:A:415[A]:HIS:CE1	2.55	0.42
1:B:268:ARG:CZ	1:B:443:ALA:HB1	2.50	0.42
1:A:469:ASP:OD2	1:A:471:LYS:HE2	2.20	0.41
1:B:231:ASN:HB3	7:B:767:HOH:O	2.20	0.41
3:C:503:EDO:H22	7:C:823:HOH:O	2.18	0.41
1:B:441:LEU:HB3	1:B:449:TYR:CD2	2.56	0.41
1:D:440:LEU:HB3	1:D:452:SER:HB3	2.01	0.41
1:B:151:PHE:CE1	1:B:216:ALA:HB3	2.55	0.41
1:B:268:ARG:NH2	1:B:444:ASN:O	2.54	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	345/361 (96%)	335 (97%)	10 (3%)	0	100	100
1	B	345/361 (96%)	335 (97%)	10 (3%)	0	100	100
1	C	344/361 (95%)	334 (97%)	10 (3%)	0	100	100
1	D	342/361 (95%)	331 (97%)	11 (3%)	0	100	100
All	All	1376/1444 (95%)	1335 (97%)	41 (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	303/313 (97%)	300 (99%)	3 (1%)	76	81
1	B	303/313 (97%)	299 (99%)	4 (1%)	69	74
1	C	302/313 (96%)	300 (99%)	2 (1%)	84	88
1	D	300/313 (96%)	298 (99%)	2 (1%)	84	88
All	All	1208/1252 (96%)	1197 (99%)	11 (1%)	78	83

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

Mol	Chain	Res	Type
1	A	258	GLU
1	A	287	PHE
1	A	295	LEU
1	B	210	LYS
1	B	258	GLU
1	B	295	LEU
1	B	308	PHE
1	C	258	GLU
1	C	295	LEU
1	D	258	GLU
1	D	295	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	B	149	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

29 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
6	PG4	C	507	-	12,12,12	0.53	0	11,11,11	0.59	0
4	PEG	C	506	-	6,6,6	0.47	0	5,5,5	0.43	0
5	M2M	A	508	-	8,8,8	0.66	0	7,7,7	0.62	0
3	EDO	B	502	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	C	505	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.45	0
3	EDO	B	506	-	3,3,3	0.40	0	2,2,2	0.64	0
4	PEG	A	506	-	6,6,6	0.42	0	5,5,5	0.64	0
2	6CX	D	501	-	24,35,35	1.54	5 (20%)	25,50,50	1.98	7 (28%)
4	PEG	D	506	-	6,6,6	0.37	0	5,5,5	0.53	0
3	EDO	D	505	-	3,3,3	0.49	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	503	-	3,3,3	0.48	0	2,2,2	0.41	0
4	PEG	B	507	-	6,6,6	0.47	0	5,5,5	0.42	0
3	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.62	0
3	EDO	B	504	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	D	503	-	3,3,3	0.48	0	2,2,2	0.29	0
4	PEG	B	508	-	6,6,6	0.46	0	5,5,5	0.51	0
3	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.64	0
3	EDO	C	503	-	3,3,3	0.40	0	2,2,2	0.46	0
2	6CX	C	501	-	24,35,35	1.38	3 (12%)	25,50,50	2.02	8 (32%)
3	EDO	D	502	-	3,3,3	0.46	0	2,2,2	0.54	0
4	PEG	A	507	-	6,6,6	0.48	0	5,5,5	0.51	0
2	6CX	A	501	-	24,35,35	1.30	3 (12%)	25,50,50	2.14	8 (32%)
4	PEG	A	505	-	6,6,6	0.57	0	5,5,5	0.62	0
3	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.52	0
3	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	D	504	-	3,3,3	0.48	0	2,2,2	0.43	0
2	6CX	B	501	-	24,35,35	1.53	3 (12%)	25,50,50	2.16	8 (32%)
3	EDO	A	504	-	3,3,3	0.48	0	2,2,2	0.50	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
6	PG4	C	507	-	-	3/10/10/10	-
4	PEG	C	506	-	-	2/4/4/4	-
5	M2M	A	508	-	-	6/6/6/6	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	C	505	-	-	1/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
4	PEG	A	506	-	-	4/4/4/4	-
2	6CX	D	501	-	-	2/13/37/37	0/4/4/4
4	PEG	D	506	-	-	2/4/4/4	-
3	EDO	D	505	-	-	1/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
4	PEG	B	507	-	-	2/4/4/4	-
3	EDO	C	504	-	-	1/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	503	-	-	1/1/1/1	-
4	PEG	B	508	-	-	2/4/4/4	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
2	6CX	C	501	-	-	2/13/37/37	0/4/4/4
3	EDO	D	502	-	-	1/1/1/1	-
4	PEG	A	507	-	-	3/4/4/4	-
2	6CX	A	501	-	-	3/13/37/37	0/4/4/4
4	PEG	A	505	-	-	1/4/4/4	-
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	D	504	-	-	0/1/1/1	-
2	6CX	B	501	-	-	1/13/37/37	0/4/4/4
3	EDO	A	504	-	-	1/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	6CX	C2'-C1'	-4.74	1.46	1.53
2	C	501	6CX	C2'-C1'	-3.89	1.47	1.53
2	D	501	6CX	C2'-C1'	-3.88	1.47	1.53
2	A	501	6CX	C2'-C3'	-2.85	1.45	1.53
2	A	501	6CX	C2'-C1'	-2.79	1.49	1.53
2	A	501	6CX	O4'-C4'	-2.75	1.38	1.45
2	B	501	6CX	CA-N	-2.74	1.41	1.47
2	D	501	6CX	O4'-C4'	-2.71	1.38	1.45
2	D	501	6CX	O4'-C1'	2.54	1.44	1.41
2	D	501	6CX	C2'-C3'	-2.40	1.46	1.53
2	C	501	6CX	C2'-C3'	-2.35	1.46	1.53
2	B	501	6CX	C2'-C3'	-2.34	1.46	1.53
2	D	501	6CX	CA-N	-2.30	1.41	1.47
2	C	501	6CX	C2-N3	2.26	1.35	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	6CX	N3-C2-N1	-4.87	121.06	128.68
2	A	501	6CX	N3-C2-N1	-4.79	121.18	128.68
2	D	501	6CX	N3-C2-N1	-4.64	121.42	128.68
2	C	501	6CX	N3-C2-N1	-4.55	121.57	128.68
2	A	501	6CX	O4'-C1'-C2'	-4.54	100.29	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	6CX	C10-C51-C52	-4.33	123.23	129.61
2	B	501	6CX	C1'-N9-C4	-4.14	119.38	126.64
2	A	501	6CX	C10-C51-C52	-4.09	123.58	129.61
2	A	501	6CX	C52-N53-C54	-3.76	99.91	105.78
2	D	501	6CX	C51-C10-ND	3.64	120.45	112.78
2	B	501	6CX	C52-N53-C54	-3.53	100.27	105.78
2	B	501	6CX	C10-ND-C5'	-3.40	106.99	110.95
2	C	501	6CX	C52-N53-C54	-3.40	100.47	105.78
2	D	501	6CX	C1'-N9-C4	-3.31	120.82	126.64
2	C	501	6CX	O4'-C1'-C2'	-3.28	102.13	106.93
2	B	501	6CX	C51-C10-ND	3.14	119.40	112.78
2	B	501	6CX	C10-C51-C52	-3.14	124.98	129.61
2	D	501	6CX	C52-N53-C54	-3.14	100.89	105.78
2	B	501	6CX	O4'-C1'-C2'	-3.10	102.40	106.93
2	D	501	6CX	C10-C51-C52	-3.04	125.12	129.61
2	C	501	6CX	C10-ND-C5'	-2.83	107.66	110.95
2	B	501	6CX	C3'-C2'-C1'	2.70	105.04	100.98
2	A	501	6CX	C51-C10-ND	2.64	118.34	112.78
2	A	501	6CX	C1'-N9-C4	-2.58	122.11	126.64
2	D	501	6CX	O4'-C1'-C2'	-2.40	103.42	106.93
2	C	501	6CX	C3'-C2'-C1'	2.38	104.56	100.98
2	C	501	6CX	C51-C10-ND	2.36	117.76	112.78
2	A	501	6CX	C3'-C2'-C1'	2.35	104.52	100.98
2	C	501	6CX	C1'-N9-C4	-2.13	122.91	126.64
2	A	501	6CX	C10-ND-CG	-2.12	106.81	111.29
2	D	501	6CX	O3'-C3'-C4'	-2.01	105.24	111.05

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	6CX	C-CA-CB-CG
2	A	501	6CX	C-CA-CB-CG
5	A	508	M2M	C5-C4-O2-C3
4	D	506	PEG	O2-C3-C4-O4
4	B	507	PEG	O2-C3-C4-O4
4	C	506	PEG	O1-C1-C2-O2
4	D	506	PEG	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	D	505	EDO	O1-C1-C2-O2
3	D	502	EDO	O1-C1-C2-O2
4	B	508	PEG	O2-C3-C4-O4

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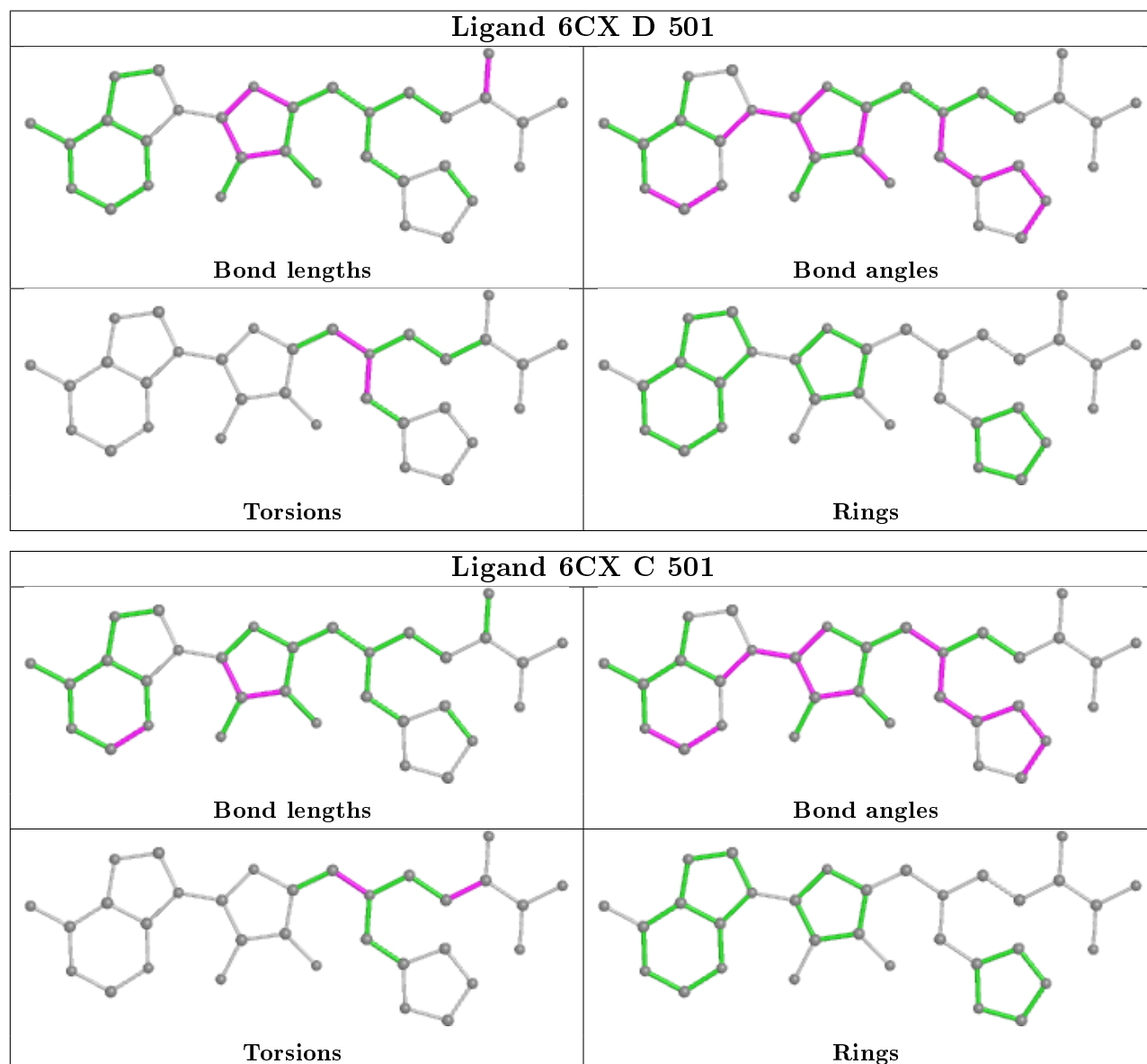
Mol	Chain	Res	Type	Atoms
3	B	505	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
5	A	508	M2M	O1-C2-C3-O2
4	A	505	PEG	O1-C1-C2-O2
2	D	501	6CX	C4'-C5'-ND-CG
2	C	501	6CX	C4'-C5'-ND-CG
2	A	501	6CX	C4'-C5'-ND-CG
3	C	505	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
3	C	504	EDO	O1-C1-C2-O2
2	D	501	6CX	C51-C10-ND-C5'
4	C	506	PEG	C1-C2-O2-C3
4	A	507	PEG	C1-C2-O2-C3
4	B	507	PEG	O1-C1-C2-O2
2	A	501	6CX	N-CA-CB-CG
2	B	501	6CX	C4'-C5'-ND-CG
5	A	508	M2M	C2-C3-O2-C4
4	A	506	PEG	O2-C3-C4-O4
4	A	507	PEG	O1-C1-C2-O2
6	C	507	PG4	C6-C5-O3-C4
4	A	506	PEG	O1-C1-C2-O2
4	A	507	PEG	O2-C3-C4-O4
6	C	507	PG4	C8-C7-O4-C6
5	A	508	M2M	C3-C2-O1-C1
6	C	507	PG4	C3-C4-O3-C5
3	B	502	EDO	O1-C1-C2-O2
5	A	508	M2M	O2-C4-C5-O3
5	A	508	M2M	C4-C5-O3-C6
4	A	506	PEG	C1-C2-O2-C3
4	B	508	PEG	C1-C2-O2-C3
3	D	503	EDO	O1-C1-C2-O2
3	C	502	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
4	A	506	PEG	C4-C3-O2-C2

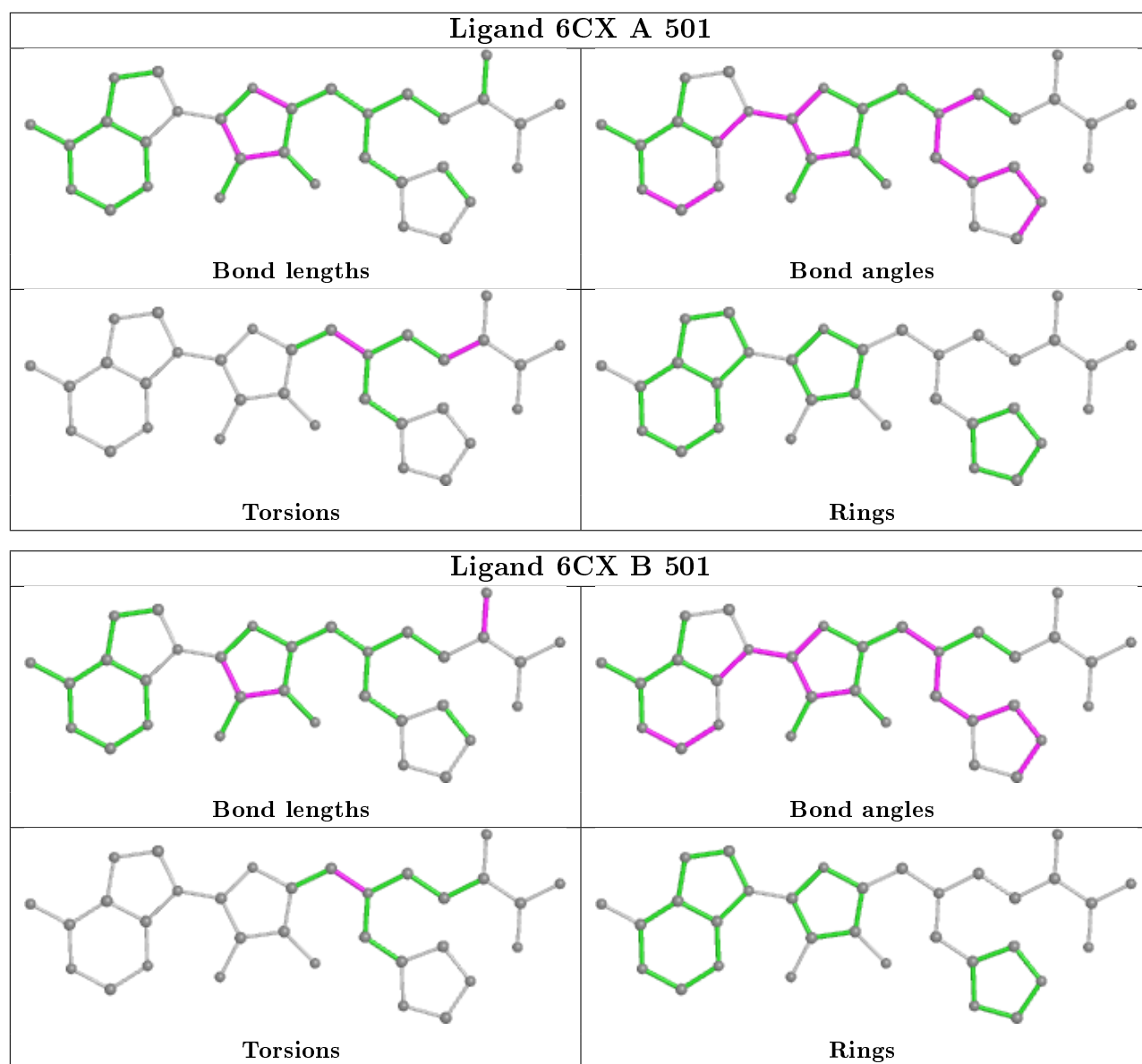
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	507	PG4	1	0
3	C	503	EDO	1	0
4	A	507	PEG	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	343/361 (95%)	-0.16	12 (3%) 44 43	16, 26, 45, 79	0
1	B	343/361 (95%)	-0.15	19 (5%) 25 24	16, 30, 54, 103	0
1	C	343/361 (95%)	-0.10	14 (4%) 37 36	19, 30, 52, 94	0
1	D	342/361 (94%)	-0.15	16 (4%) 31 30	20, 32, 53, 92	0
All	All	1371/1444 (94%)	-0.14	61 (4%) 34 33	16, 29, 52, 103	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	477	TYR	6.9
1	C	478	THR	6.4
1	A	478	THR	6.3
1	B	478	THR	5.9
1	D	136	SER	5.8
1	C	477	TYR	5.7
1	D	139	SER	5.7
1	B	137	VAL	5.3
1	B	136	SER	5.3
1	C	137	VAL	5.1
1	D	148	VAL	5.1
1	C	148	VAL	5.0
1	B	477	TYR	4.7
1	D	137	VAL	4.7
1	B	142	THR	4.4
1	B	148	VAL	4.4
1	A	477	TYR	4.3
1	B	145	SER	4.2
1	D	140	GLU	4.2
1	A	144	GLU	4.1
1	D	142	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	144	GLU	4.1
1	B	139	SER	4.0
1	C	144	GLU	3.8
1	C	136	SER	3.7
1	D	144	GLU	3.7
1	C	145	SER	3.6
1	C	140	GLU	3.6
1	D	146	SER	3.5
1	B	143	GLU	3.4
1	B	446	ARG	3.3
1	D	145	SER	3.2
1	B	140	GLU	3.2
1	C	142	THR	3.1
1	D	143	GLU	2.9
1	A	140	GLU	2.9
1	A	283	SER	2.8
1	B	149	GLN	2.7
1	A	137	VAL	2.6
1	B	146	SER	2.6
1	C	139	SER	2.5
1	A	145	SER	2.5
1	D	141	ARG	2.5
1	D	302	GLN	2.5
1	D	149	GLN	2.5
1	A	148	VAL	2.4
1	A	149	GLN	2.4
1	B	445	LYS	2.4
1	D	475	PHE	2.3
1	C	259	PRO	2.3
1	B	147	ALA	2.3
1	D	446	ARG	2.2
1	A	139	SER	2.2
1	B	138	PHE	2.2
1	C	256	ILE	2.2
1	A	143	GLU	2.1
1	A	264	LEU	2.1
1	B	471	LYS	2.1
1	C	147	ALA	2.1
1	B	141	ARG	2.0
1	C	146	SER	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 carbohydrates 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.

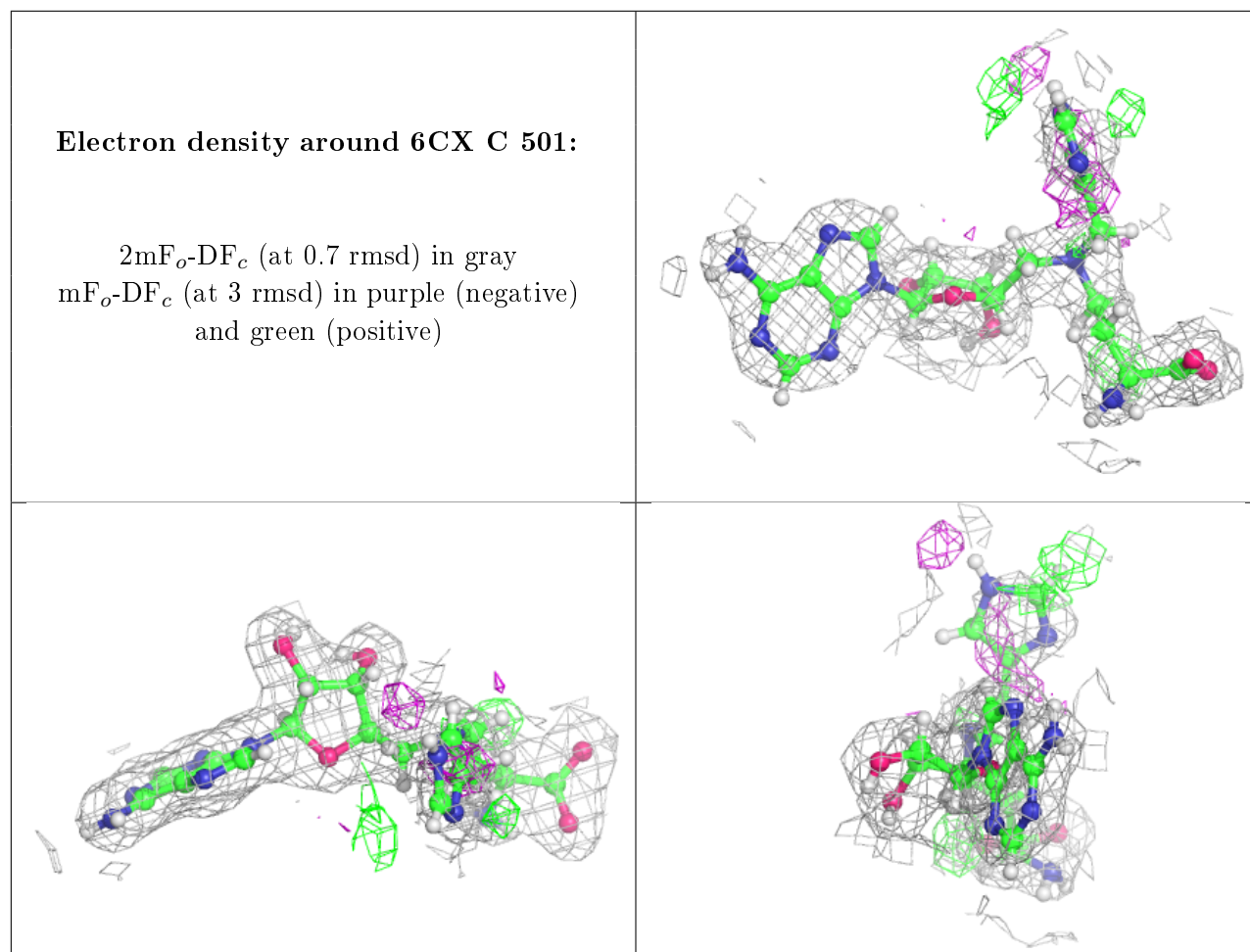
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	D	503	4/4	0.59	0.28	74,78,79,79	0
3	EDO	D	505	4/4	0.64	0.26	62,62,63,64	0
3	EDO	B	505	4/4	0.64	0.15	60,61,62,62	0
3	EDO	A	504	4/4	0.67	0.29	70,72,72,73	0
3	EDO	D	504	4/4	0.71	0.23	67,67,68,68	0
3	EDO	B	504	4/4	0.77	0.36	65,66,66,67	0
5	M2M	A	508	9/9	0.80	0.18	66,79,85,86	0
4	PEG	A	505	7/7	0.80	0.25	54,65,70,70	0
4	PEG	A	507	7/7	0.81	0.20	84,101,113,113	0
4	PEG	B	508	7/7	0.82	0.20	51,61,68,71	0
3	EDO	C	505	4/4	0.83	0.35	33,36,43,45	0
3	EDO	B	502	4/4	0.83	0.26	63,63,64,64	0
4	PEG	C	506	7/7	0.85	0.20	56,67,70,70	0
4	PEG	B	507	7/7	0.85	0.17	72,86,95,96	0
3	EDO	C	504	4/4	0.86	0.17	46,47,48,52	0
6	PG4	C	507	13/13	0.86	0.23	57,61,68,70	0
3	EDO	B	506	4/4	0.86	0.16	33,36,41,42	0
3	EDO	D	502	4/4	0.87	0.11	40,40,41,41	0
3	EDO	A	502	4/4	0.89	0.20	45,46,48,50	0
3	EDO	A	503	4/4	0.90	0.19	48,49,49,49	0
4	PEG	D	506	7/7	0.91	0.34	36,43,49,54	0
3	EDO	C	503	4/4	0.91	0.13	49,49,50,52	0
3	EDO	B	503	4/4	0.93	0.10	48,48,51,53	0
4	PEG	A	506	7/7	0.93	0.14	47,57,70,72	0
3	EDO	C	502	4/4	0.94	0.12	42,43,45,45	0
2	6CX	C	501	32/32	0.95	0.15	20,30,57,69	0
2	6CX	D	501	32/32	0.95	0.12	22,32,54,65	0

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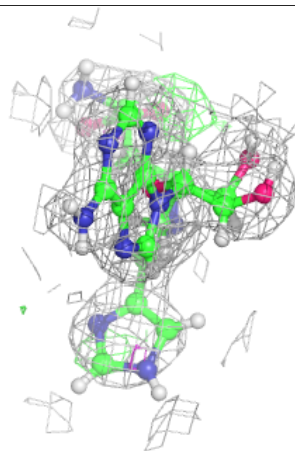
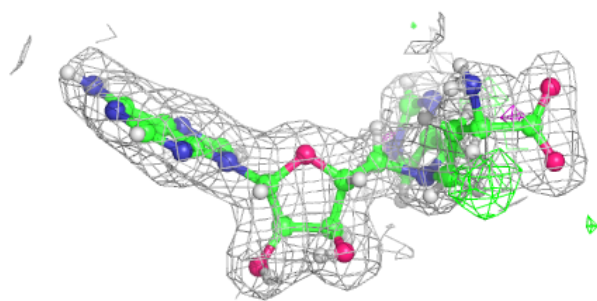
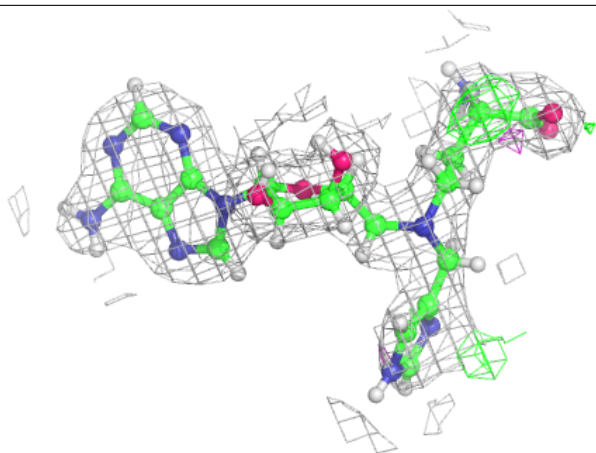
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	6CX	A	501	32/32	0.96	0.16	21,27,54,65	0
2	6CX	B	501	32/32	0.97	0.12	24,31,44,53	0

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.



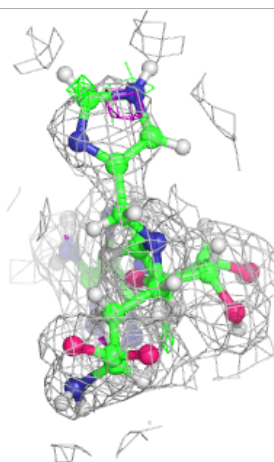
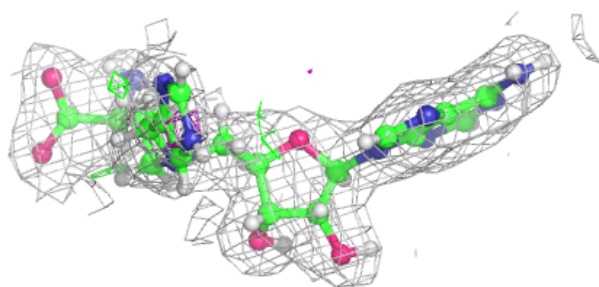
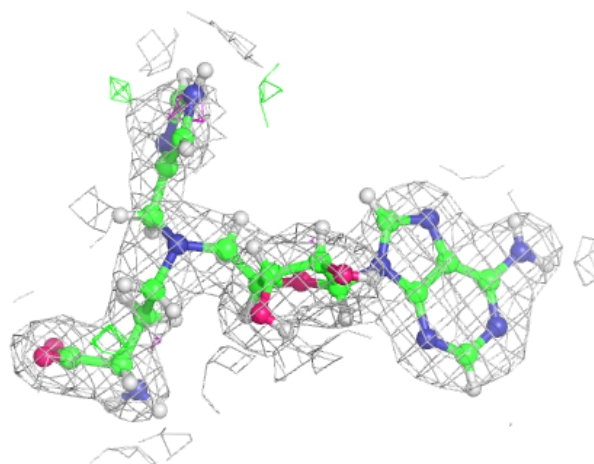
Electron density around 6CX D 501:

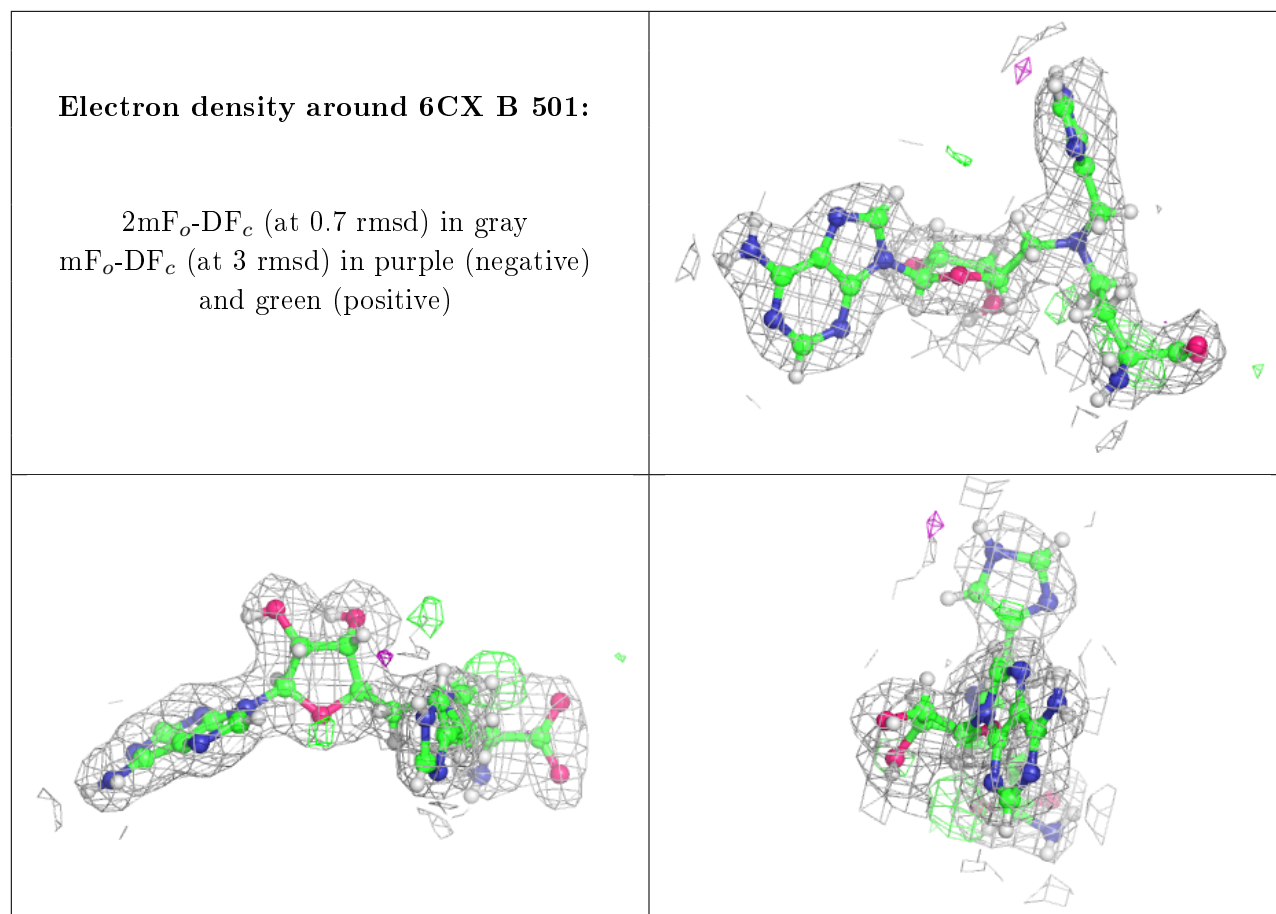
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6CX A 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.