



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:51 PM UTC

PDB ID : 5IS7 / pdb_00005is7
Title : Crystal structure of mouse CARM1 in complex with decarboxylated SAH
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 : 2.29 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

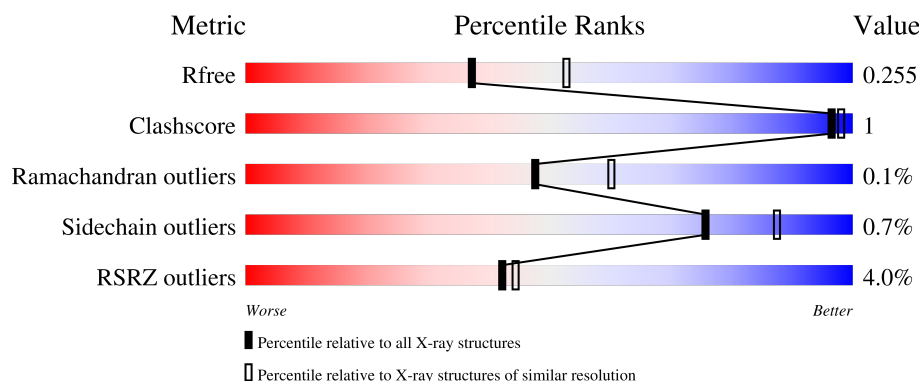
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	361	93% 5%
1	B	361	92% 5%
1	C	361	90% 6%
1	D	361	91% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22214 atoms, of which 10946 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	343	Total	C	H	N	O	S	0	5	0
			5530	1808	2736	458	513	15			
1	B	342	Total	C	H	N	O	S	0	2	0
			5474	1786	2710	455	508	15			
1	C	341	Total	C	H	N	O	S	0	0	0
			5425	1769	2687	452	503	14			
1	D	340	Total	C	H	N	O	S	0	0	0
			5405	1760	2679	451	501	14			

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).



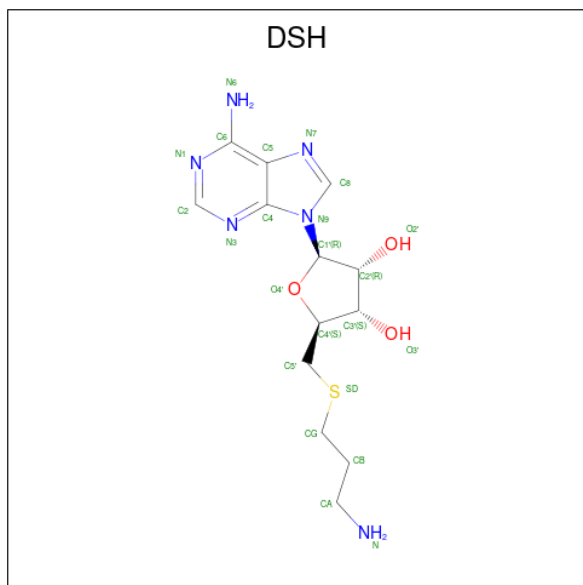
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is 5'-S-(3-aminopropyl)-5'-thioadenosine (CCD ID: DSH) (formula: C₁₃H₂₀N₆O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			44	13	21	6	3	1		
4	B	1	Total	C	H	N	O	S	0	0
			44	13	21	6	3	1		
4	C	1	Total	C	H	N	O	S	0	0
			44	13	21	6	3	1		
4	D	1	Total	C	H	N	O	S	0	0
			44	13	21	6	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	44	Total	O	0	0
			44	44		
5	C	11	Total	O	0	0
			11	11		
5	D	4	Total	O	0	0
			4	4		

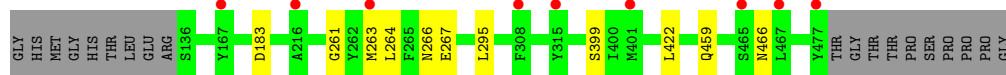
3 Residue-property plots [i](#)

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.

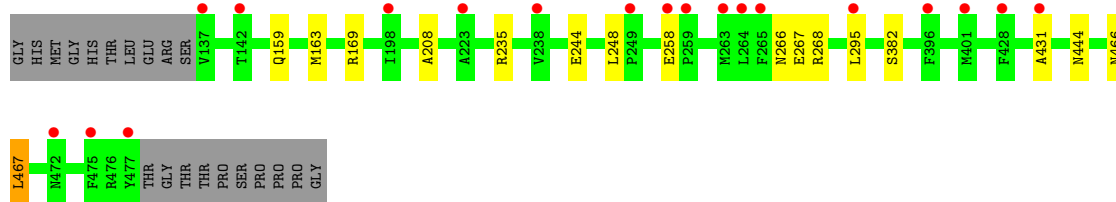
- Molecule 1: Histone-arginine methyltransferase CARM1



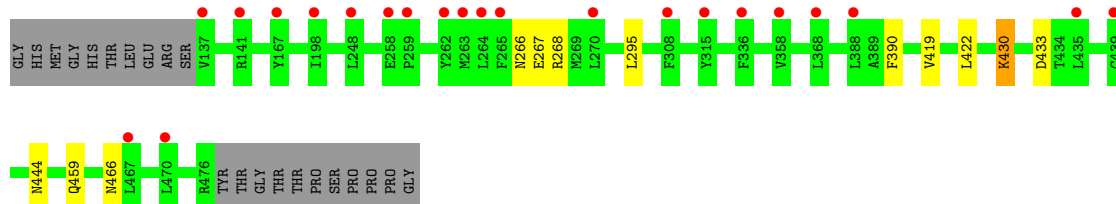
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	74.53Å 98.94Å 206.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.29 48.11 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.11-2.29) 99.7 (48.11-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_1980	Depositor
R, R_{free}	0.209 , 0.247 0.219 , 0.255	Depositor DCC
R_{free} test set	3434 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22214	wwPDB-VP
Average B, all atoms (Å ²)	91.0	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 75.46 % 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 1.2590e-06. 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: DSH, EDO, 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	0.29	0/2876	0.57	0/3897
1	B	0.27	0/2835	0.56	0/3841
1	C	0.26	0/2808	0.56	0/3805
1	D	0.26	0/2795	0.56	0/3787
All	All	0.27	0/11314	0.56	0/15330

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	2794	2736	2726	3	0
1	B	2764	2710	2708	6	0
1	C	2738	2687	2687	7	0
1	D	2726	2679	2678	6	0
2	A	4	6	6	0	0
2	B	8	12	12	0	0
2	C	4	6	6	0	0
2	D	4	6	6	0	0
3	A	14	20	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	23	21	20	0	0
4	B	23	21	20	0	0
4	C	23	21	20	0	0
4	D	23	21	20	0	0
5	A	61	0	0	0	0
5	B	44	0	0	0	0
5	C	11	0	0	0	0
5	D	4	0	0	0	0
All	All	11268	10946	10929	22	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 1.

All (22) 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:169:ARG:NH2	1:C:258:GLU:OE2	2.43	0.52
1:D:430:LYS:NZ	1:D:433:ASP:OD1	2.42	0.52
1:C:466:ASN:OD1	1:C:467:LEU:N	2.42	0.51
1:A:208:ALA:O	1:A:235:ARG:NH2	2.40	0.50
1:B:183:ASP:OD1	1:B:399:SER:OG	2.27	0.50
1:C:208:ALA:O	1:C:235:ARG:NH1	2.39	0.50
1:B:459:GLN:OE1	1:B:459:GLN:N	2.46	0.49
1:C:268:ARG:NH1	1:C:444:ASN:O	2.46	0.48
1:D:268:ARG:NH1	1:D:444:ASN:O	2.44	0.47
1:C:382:SER:OG	1:C:431:ALA:N	2.48	0.46
1:B:263:MET:O	1:B:264:LEU:HB3	2.15	0.46
1:D:459:GLN:OE1	1:D:459:GLN:N	2.49	0.46
1:A:265:PHE:HB3	1:A:449:TYR:CE1	2.52	0.45
1:D:390:PHE:N	1:D:419:VAL:O	2.43	0.45
1:A:266:ASN:O	1:A:267:GLU:HB2	2.17	0.45
1:B:266:ASN:O	1:B:267:GLU:HB2	2.18	0.44
1:D:422:LEU:O	1:D:466:ASN:ND2	2.49	0.43
1:C:266:ASN:O	1:C:267:GLU:HB2	2.18	0.43
1:C:159:GLN:NE2	1:C:163:MET:HE3	2.34	0.42
1:D:266:ASN:O	1:D:267:GLU:HB2	2.20	0.41
1:B:422:LEU:O	1:B:466:ASN:ND2	2.45	0.41
1:B:261:GLY:O	1:B:264:LEU:N	2.51	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	346/361 (96%)	335 (97%)	10 (3%)	1 (0%)	36	46
1	B	342/361 (95%)	332 (97%)	10 (3%)	0	100	100
1	C	339/361 (94%)	323 (95%)	16 (5%)	0	100	100
1	D	338/361 (94%)	326 (96%)	12 (4%)	0	100	100
All	All	1365/1444 (94%)	1316 (96%)	48 (4%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	MET

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	304/313 (97%)	302 (99%)	2 (1%)	76	87
1	B	300/313 (96%)	299 (100%)	1 (0%)	86	93
1	C	297/313 (95%)	293 (99%)	4 (1%)	61	77
1	D	296/313 (95%)	294 (99%)	2 (1%)	76	87
All	All	1197/1252 (96%)	1188 (99%)	9 (1%)	76	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305[A]	MET
1	A	305[B]	MET
1	B	295	LEU
1	C	244	GLU
1	C	248	LEU
1	C	295	LEU
1	C	467	LEU
1	D	295	LEU
1	D	430	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	GLN
1	A	369	HIS
1	A	381	HIS
1	B	302	GLN
1	B	381	HIS
1	B	424	GLN
1	B	472	ASN
1	C	302	GLN
1	C	381	HIS
1	D	165	GLN
1	D	307	GLN
1	D	381	HIS
1	D	424	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 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	C	501	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	B	501	-	3,3,3	0.44	0	2,2,2	0.38	0
3	PEG	A	503	-	6,6,6	0.51	0	5,5,5	0.44	0
3	PEG	A	502	-	6,6,6	0.49	0	5,5,5	0.46	0
2	EDO	D	501	-	3,3,3	0.44	0	2,2,2	0.39	0
2	EDO	A	501	-	3,3,3	0.44	0	2,2,2	0.38	0
4	DSH	A	504	-	25,25,25	0.13	0	34,35,35	0.50	0
4	DSH	B	503	-	25,25,25	0.11	0	34,35,35	0.44	0
4	DSH	C	502	-	25,25,25	0.11	0	34,35,35	0.54	1 (2%)
4	DSH	D	502	-	25,25,25	0.13	0	34,35,35	0.34	0
2	EDO	B	502	-	3,3,3	0.43	0	2,2,2	0.38	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	C	501	-	-	1/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-
3	PEG	A	503	-	-	1/4/4/4	-
3	PEG	A	502	-	-	1/4/4/4	-
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
4	DSH	A	504	-	-	3/10/26/26	0/3/3/3
4	DSH	B	503	-	-	3/10/26/26	0/3/3/3
4	DSH	C	502	-	-	4/10/26/26	0/3/3/3
4	DSH	D	502	-	-	4/10/26/26	0/3/3/3
2	EDO	B	502	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	DSH	C5'-C4'-C3'	-2.14	109.70	115.06

There are no chirality outliers.

All (19) torsion outliers are listed below:

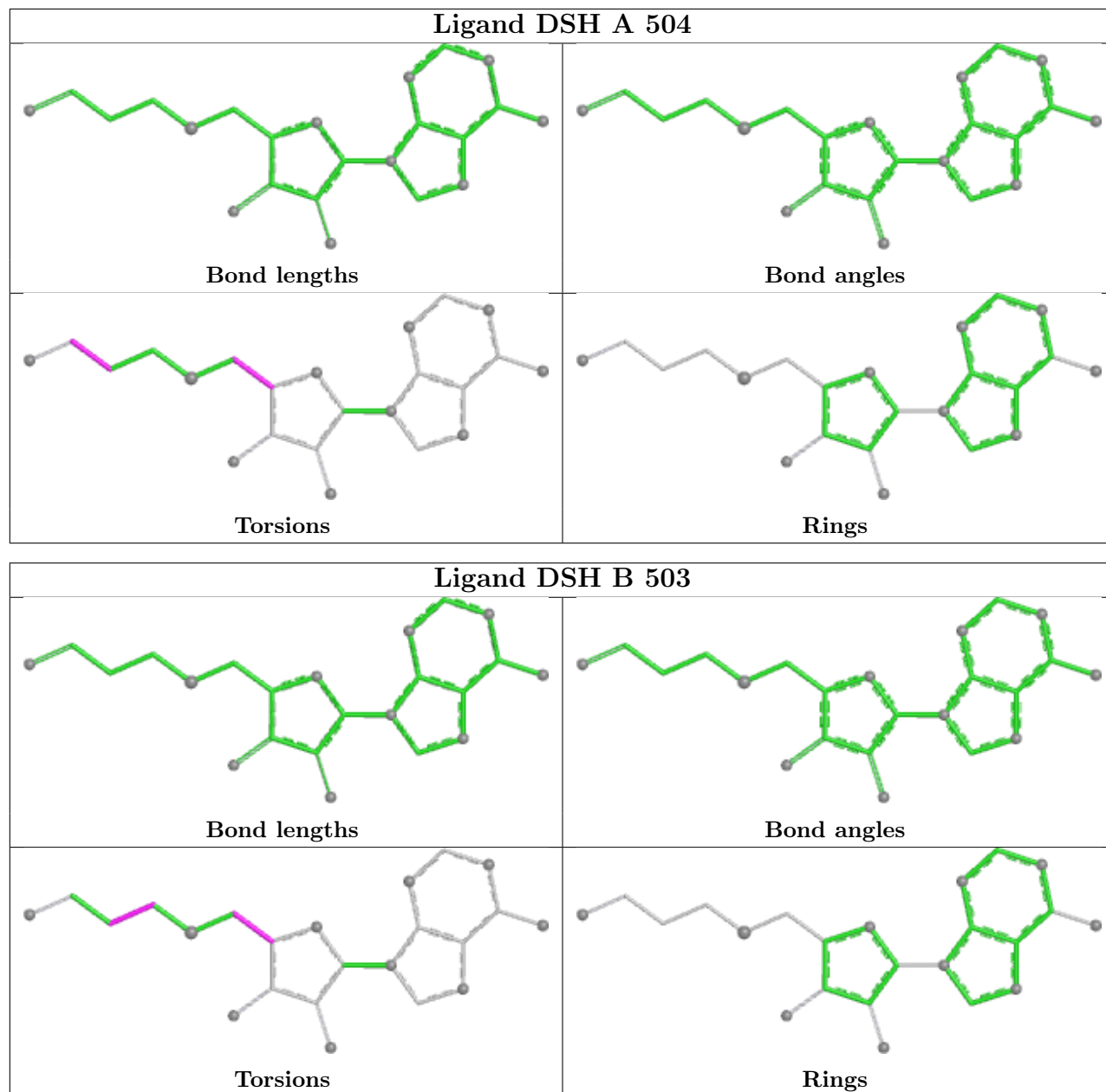
Mol	Chain	Res	Type	Atoms
4	A	504	DSH	C3'-C4'-C5'-SD
4	A	504	DSH	O4'-C4'-C5'-SD
4	B	503	DSH	C3'-C4'-C5'-SD
4	B	503	DSH	O4'-C4'-C5'-SD
4	C	502	DSH	C3'-C4'-C5'-SD
4	C	502	DSH	O4'-C4'-C5'-SD
3	A	503	PEG	O2-C3-C4-O4
4	B	503	DSH	CA-CB-CG-SD
4	C	502	DSH	CA-CB-CG-SD
3	A	502	PEG	O1-C1-C2-O2
4	D	502	DSH	N-CA-CB-CG
2	C	501	EDO	O1-C1-C2-O2
4	D	502	DSH	C2'-C1'-N9-C8
4	D	502	DSH	CA-CB-CG-SD
2	D	501	EDO	O1-C1-C2-O2
4	C	502	DSH	CB-CG-SD-C5'
2	A	501	EDO	O1-C1-C2-O2
4	D	502	DSH	O4'-C1'-N9-C8
4	A	504	DSH	N-CA-CB-CG

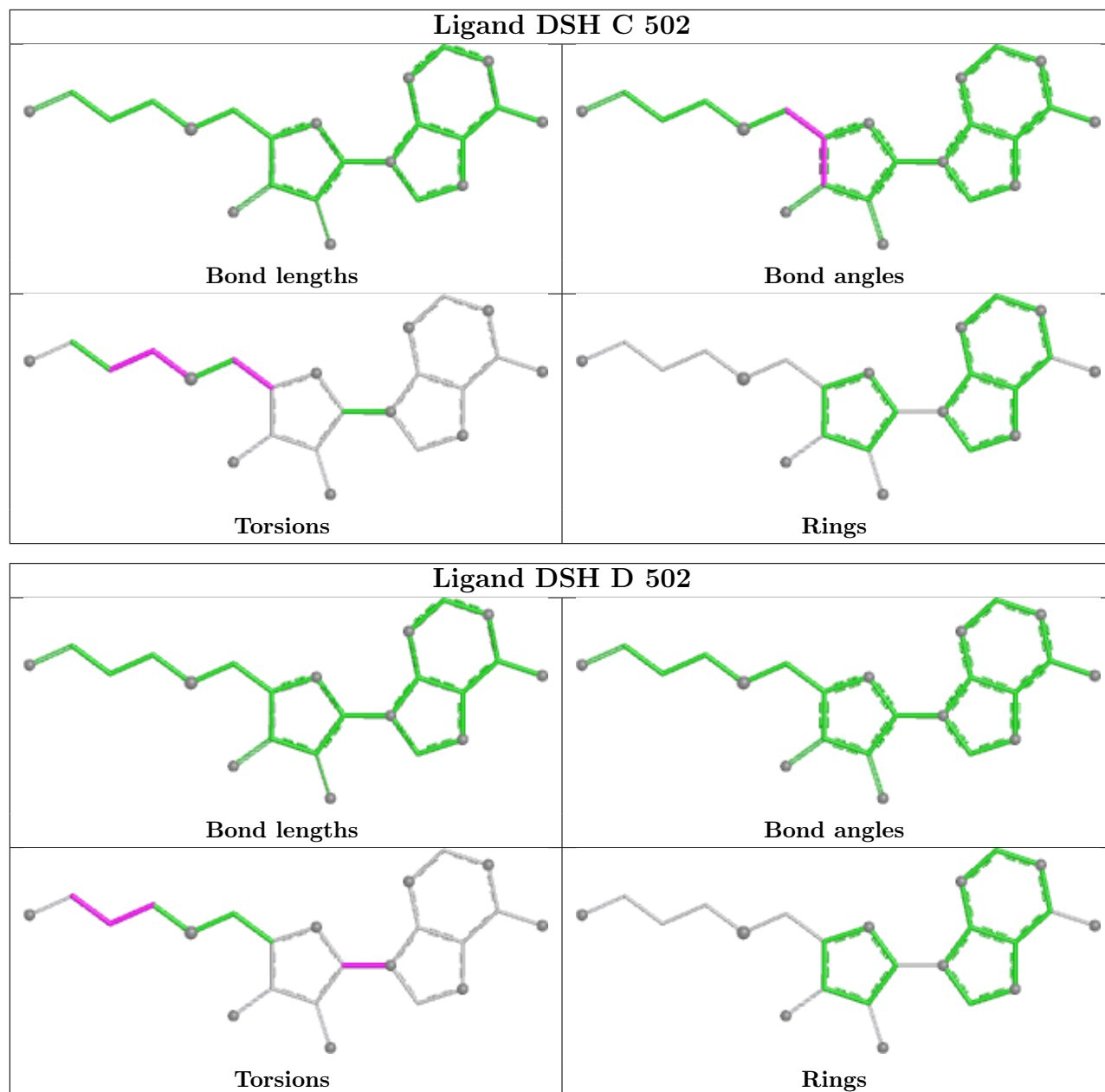
There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.17	5 (1%) 72 73	25, 68, 101, 150	4 (1%)
1	B	342/361 (94%)	0.35	9 (2%) 57 59	35, 76, 112, 135	2 (0%)
1	C	341/361 (94%)	0.72	19 (5%) 30 32	69, 104, 147, 177	0
1	D	340/361 (94%)	0.84	22 (6%) 25 27	72, 110, 140, 199	0
All	All	1366/1444 (94%)	0.52	55 (4%) 42 44	25, 91, 136, 199	6 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167[A]	TYR	6.0
1	B	401[A]	MET	5.4
1	B	167[A]	TYR	4.9
1	D	263	MET	4.1
1	C	477	TYR	3.6
1	A	137	VAL	3.6
1	D	137	VAL	3.5
1	A	478	THR	3.3
1	C	265	PHE	3.3
1	C	475	PHE	3.3
1	B	263	MET	3.2
1	D	265	PHE	3.2
1	D	467	LEU	3.2
1	B	315	TYR	3.0
1	C	258	GLU	2.9
1	D	368	LEU	2.9
1	B	477	TYR	2.9
1	D	198	ILE	2.9
1	A	305[A]	MET	2.8
1	C	263	MET	2.8
1	D	259	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	401	MET	2.7
1	C	137	VAL	2.7
1	D	439	CYS	2.7
1	D	141	ARG	2.6
1	C	472	ASN	2.5
1	C	142	THR	2.5
1	C	249	PRO	2.5
1	D	470	LEU	2.4
1	C	259	PRO	2.4
1	B	465	SER	2.4
1	C	198	ILE	2.4
1	D	258	GLU	2.4
1	A	142	THR	2.3
1	D	308	PHE	2.3
1	B	216	ALA	2.3
1	B	467	LEU	2.3
1	C	295	LEU	2.3
1	D	358	VAL	2.3
1	D	435	LEU	2.2
1	D	167	TYR	2.2
1	D	262	TYR	2.2
1	D	315	TYR	2.2
1	C	428	PHE	2.2
1	D	270	LEU	2.1
1	B	308	PHE	2.1
1	D	388	LEU	2.1
1	C	396	PHE	2.1
1	C	223	ALA	2.1
1	D	336	PHE	2.1
1	C	264	LEU	2.1
1	D	248	LEU	2.1
1	C	238	VAL	2.1
1	C	431	ALA	2.0
1	D	264	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

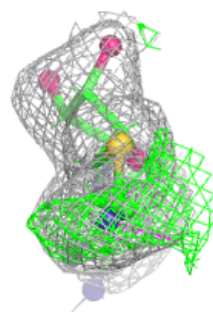
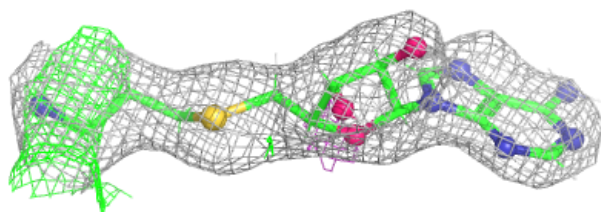
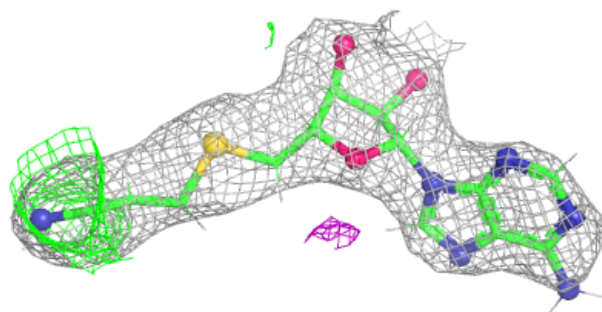
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	501	4/4	0.19	0.39	230,276,276,277	0
2	EDO	D	501	4/4	0.33	0.36	256,307,307,308	0
2	EDO	B	501	4/4	0.76	0.20	77,92,95,97	0
4	DSH	C	502	23/23	0.80	0.16	107,122,146,148	0
4	DSH	D	502	23/23	0.83	0.16	117,126,151,151	0
2	EDO	C	501	4/4	0.87	0.10	88,105,107,109	0
2	EDO	B	502	4/4	0.88	0.11	86,103,106,107	0
4	DSH	A	504	23/23	0.88	0.12	57,73,92,93	0
3	PEG	A	502	7/7	0.89	0.13	85,102,109,109	0
4	DSH	B	503	23/23	0.89	0.12	65,80,102,105	0
3	PEG	A	503	7/7	0.90	0.12	84,101,114,114	0

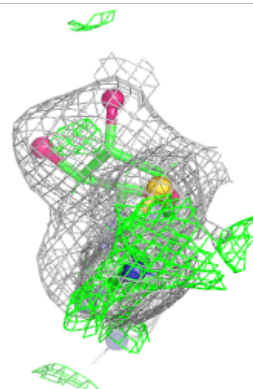
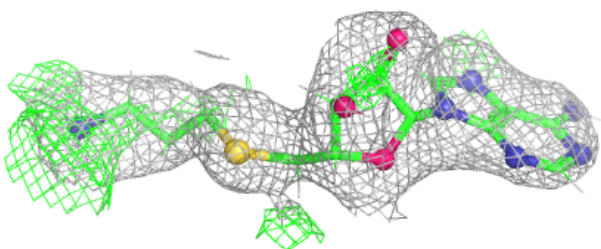
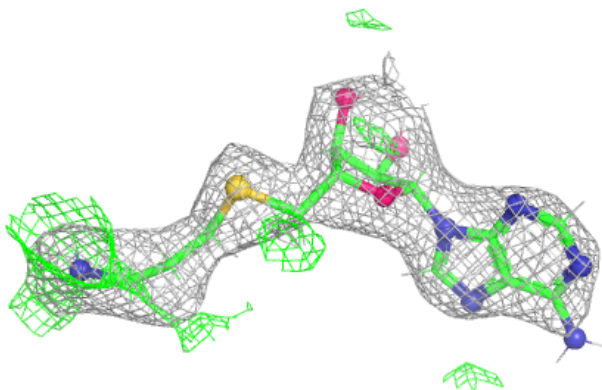
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DSH C 502:

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

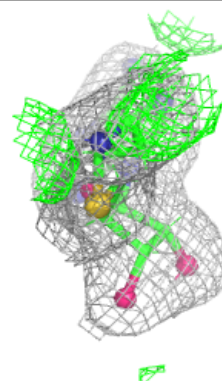
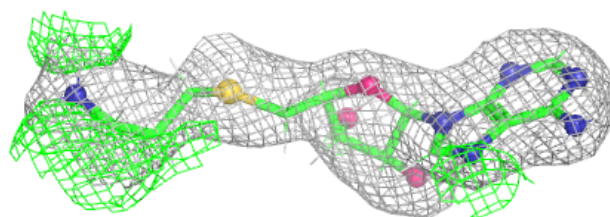
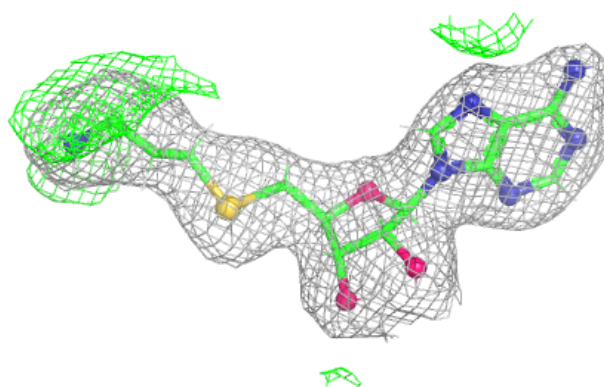
**Electron density around DSH D 502:**

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

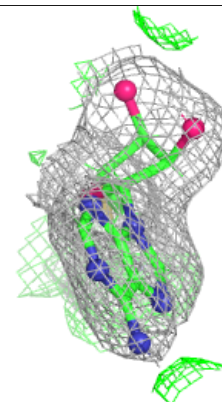
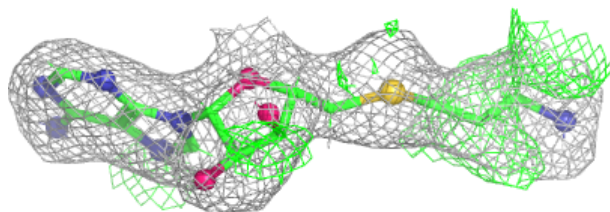
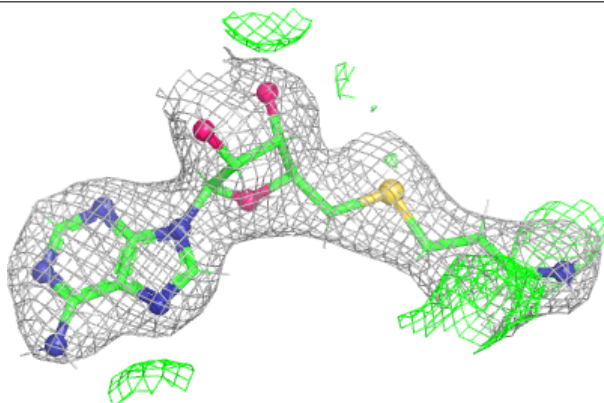


Electron density around DSH A 504:

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

**Electron density around DSH B 503:**

$2mF_o-DF_c$ (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.