



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 12:11 AM EDT

PDB ID : 5TBJ
Title : Crystal structure of mouse CARM1 in complex with inhibitor LH1452
Authors : Cura, V.; Marechal, N.; Troffer-Charlier, N.; Halby, L.; Arimondo, P.; Bonnefond, L.; Cavarelli, J.
Deposited on : 2016-09-12
Resolution : 2.32 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

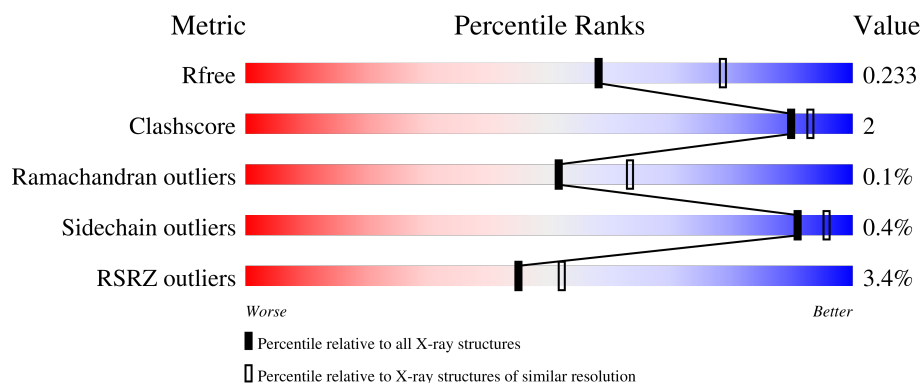
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

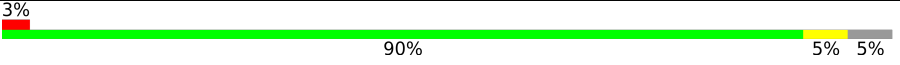
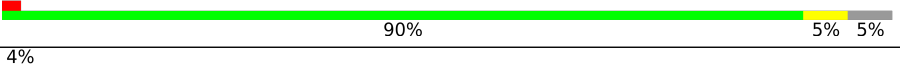
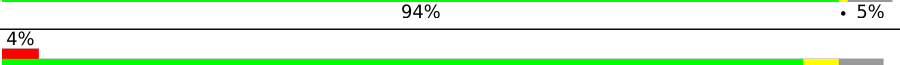

The reported resolution of this entry is 2.32 Å.

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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	 3% 90% 5% 5%
1	B	361	 2% 90% 5% 5%
1	C	361	 4% 94% 5% 5%
1	D	361	 4% 90% 5% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23041 atoms, of which 11054 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.

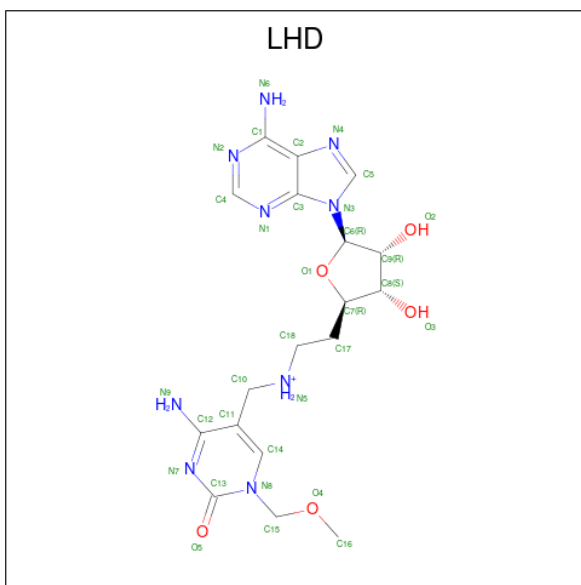
- Molecule 1 is a protein called Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	0	0
			5450	1776	2699	454	507	14			
1	B	343	Total	C	H	N	O	S	0	2	0
			5478	1783	2714	459	508	14			
1	C	343	Total	C	H	N	O	S	0	0	0
			5450	1776	2699	454	507	14			
1	D	342	Total	C	H	N	O	S	0	0	0
			5439	1769	2696	456	504	14			

There are 12 discrepancies between the modelled and reference sequences:

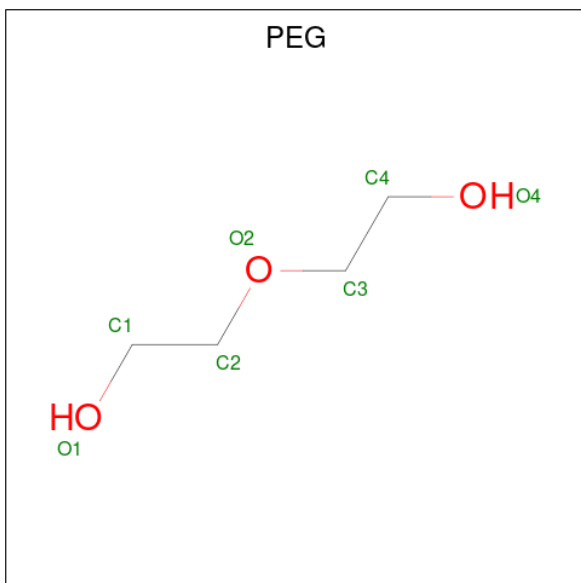
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	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 2-[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]ethyl-[[4-azanyl-1-(methoxymethyl)-2-oxidanylidene-pyrimidin-5-yl]methyl]azanium (three-letter code: LHD) (formula: C₁₈H₂₆N₉O₅).



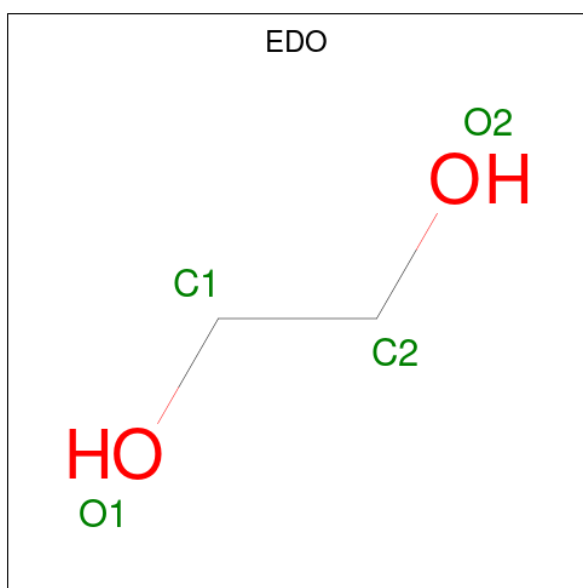
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			58	18	26	9	5		
2	B	1	Total	C	H	N	O	0	0
			58	18	26	9	5		
2	C	1	Total	C	H	N	O	0	0
			58	18	26	9	5		
2	D	1	Total	C	H	N	O	0	0
			58	18	26	9	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



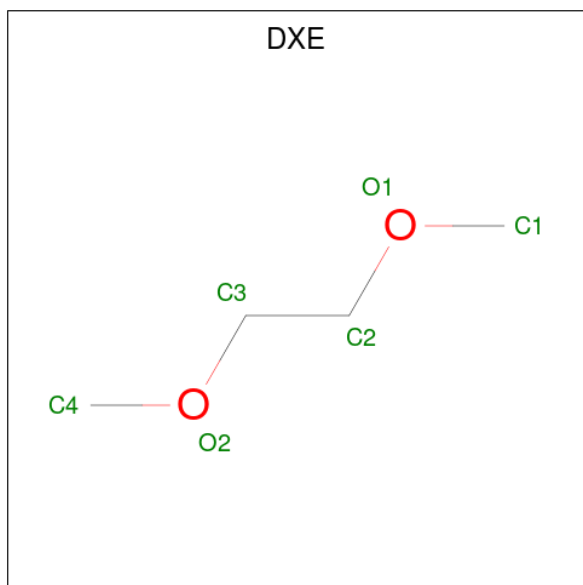
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0

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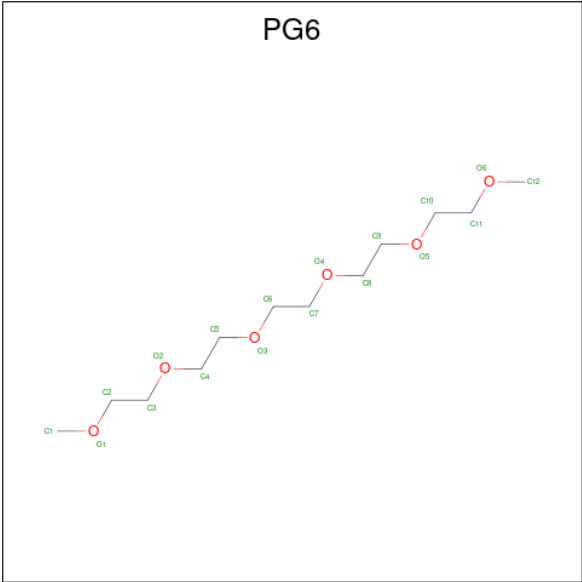
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: C₄H₁₀O₂).



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

- Molecule 6 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (three-letter code: PG6) (formula: C₁₂H₂₆O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			44	12	26	6		

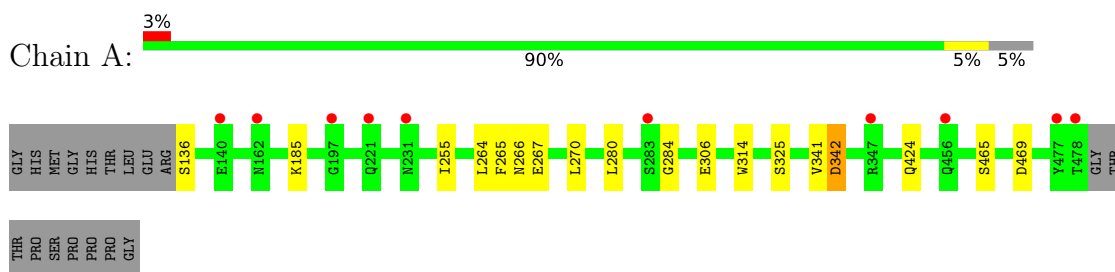
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total	O	0	0
			211	211		
7	B	190	Total	O	0	0
			190	190		
7	C	190	Total	O	0	0
			190	190		
7	D	163	Total	O	0	0
			163	163		

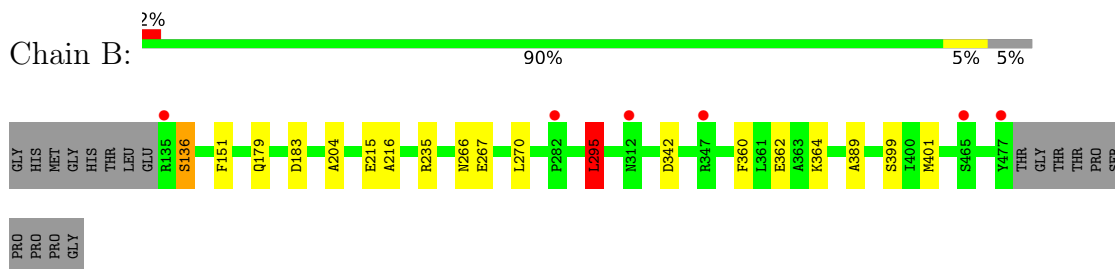
3 Residue-property plots [i](#)

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.

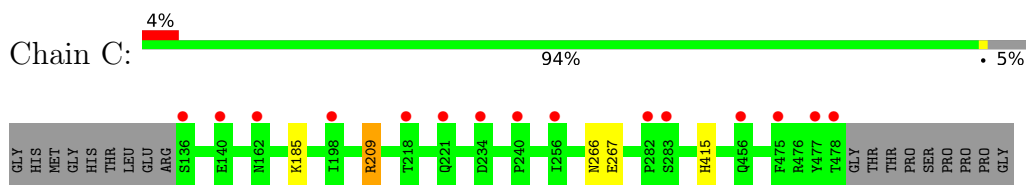
- Molecule 1: Histone-arginine methyltransferase CARM1



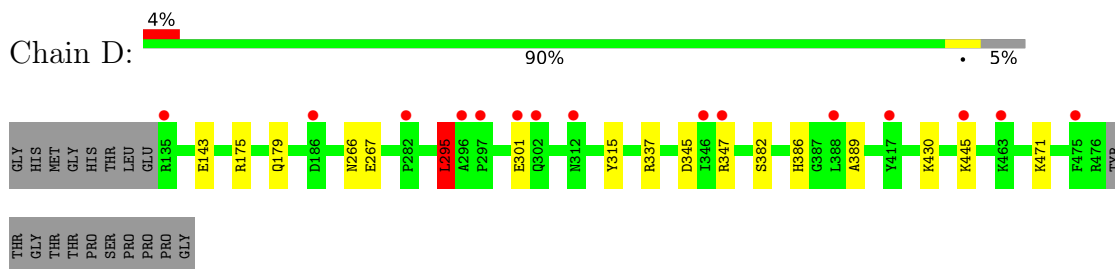
- Molecule 1: Histone-arginine methyltransferase CARM1



- 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	74.84Å 99.20Å 207.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.32 19.97 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.97-2.32) 98.6 (19.97-2.32)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.33Å)	Xtriage
Refinement program	PHENIX dev_1980	Depositor
R, R_{free}	0.202 , 0.237 0.195 , 0.233	Depositor DCC
R_{free} test set	3296 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23041	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 34.71 % 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 6.5344e-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: LHD, DXE, PG6, 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	0.28	0/2821	0.47	0/3823
1	B	0.27	0/2845	0.46	1/3854 (0.0%)
1	C	0.27	0/2821	0.46	0/3823
1	D	0.27	0/2812	0.45	1/3809 (0.0%)
All	All	0.27	0/11299	0.46	2/15309 (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	B	295	LEU	CA-CB-CG	6.18	129.51	115.30
1	D	295	LEU	CA-CB-CG	5.45	127.84	115.30

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	2751	2699	2699	12	0
1	B	2764	2714	2706	12	0
1	C	2751	2699	2699	4	0
1	D	2743	2696	2696	10	0
2	A	32	26	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	32	26	0	1	0
2	C	32	26	0	0	0
2	D	32	26	0	0	0
3	A	7	10	10	0	0
3	B	7	10	10	0	0
3	C	14	20	20	1	0
4	A	8	12	12	0	0
4	B	16	24	24	1	0
4	C	8	12	12	0	0
4	D	12	18	18	0	0
5	A	6	10	10	0	0
6	B	18	26	26	1	0
7	A	211	0	0	5	2
7	B	190	0	0	1	1
7	C	190	0	0	2	0
7	D	163	0	0	2	0
All	All	11987	11054	10942	39	2

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 (39) 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)
2:A:501:LHD:O3	7:A:601:HOH:O	2.11	0.69
1:B:179:GLN:NE2	1:B:401:MET:SD	2.67	0.67
1:D:471:LYS:NZ	7:D:601:HOH:O	2.33	0.60
1:A:469:ASP:OD1	7:A:602:HOH:O	2.16	0.59
1:B:364:LYS:NZ	7:B:608:HOH:O	2.38	0.56
1:A:136:SER:N	7:A:609:HOH:O	2.39	0.55
1:A:306:GLU:OE2	7:A:603:HOH:O	2.19	0.51
1:B:136:SER:HB2	6:B:505:PG6:H41	1.92	0.51
1:D:337:ARG:NE	7:D:609:HOH:O	2.40	0.51
1:D:301:GLU:OE1	1:D:386:HIS:NE2	2.43	0.49
1:A:266:ASN:O	1:A:267:GLU:HB2	2.13	0.48
1:A:185:LYS:NZ	7:A:613:HOH:O	2.43	0.48
1:C:266:ASN:O	1:C:267:GLU:HB2	2.14	0.48
1:D:295:LEU:HD13	1:D:295:LEU:N	2.29	0.47
1:A:314:TRP:O	1:A:325:SER:HA	2.14	0.47
1:B:215:GLU:OE2	2:B:501:LHD:O2	2.33	0.47
1:B:266:ASN:O	1:B:267:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ASP:OD2	1:D:347:ARG:NH2	2.49	0.46
1:D:143:GLU:HG3	1:D:445:LYS:HB3	1.98	0.46
1:C:415:HIS:NE2	3:C:502:PEG:H22	2.31	0.45
1:C:209:ARG:NH2	7:C:620:HOH:O	2.50	0.45
1:D:175:ARG:HG2	1:D:179:GLN:OE1	2.17	0.45
1:B:295:LEU:HA	1:B:389:ALA:O	2.18	0.44
1:B:183:ASP:OD1	1:B:399:SER:OG	2.23	0.44
1:D:266:ASN:O	1:D:267:GLU:HB2	2.18	0.43
1:B:204:ALA:O	1:B:235:ARG:NH2	2.52	0.42
1:A:424:GLN:HG3	1:A:465:SER:O	2.19	0.42
1:C:185:LYS:NZ	7:C:622:HOH:O	2.52	0.42
1:B:295:LEU:CD1	1:B:295:LEU:N	2.83	0.42
1:A:341:VAL:O	1:A:342:ASP:HB3	2.20	0.41
1:D:382:SER:HA	1:D:430:LYS:HA	2.02	0.41
1:B:362:GLU:HG3	4:B:504:EDO:C2	2.50	0.41
1:A:265:PHE:HD1	1:A:270:LEU:HD12	1.86	0.41
1:A:280:LEU:HD11	1:A:284:GLY:HA3	2.03	0.41
1:B:270:LEU:HD22	1:B:360:PHE:CE1	2.56	0.41
1:B:151:PHE:CE1	1:B:216:ALA:HB3	2.55	0.40
1:A:255:ILE:HG13	1:A:280:LEU:HD13	2.03	0.40
1:D:295:LEU:HA	1:D:389:ALA:O	2.22	0.40
1:A:264:LEU:HG	1:A:270:LEU:HD11	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:682:HOH:O	7:A:760:HOH:O[2_655]	2.03	0.17
7:A:732:HOH:O	7:B:755:HOH:O[2_665]	2.13	0.07

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	341/361 (94%)	333 (98%)	7 (2%)	1 (0%)	41	50
1	B	343/361 (95%)	334 (97%)	8 (2%)	1 (0%)	41	50
1	C	341/361 (94%)	331 (97%)	10 (3%)	0	100	100
1	D	340/361 (94%)	331 (97%)	9 (3%)	0	100	100
All	All	1365/1444 (94%)	1329 (97%)	34 (2%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	ASP
1	B	342	ASP

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	299/313 (96%)	299 (100%)	0	100	100
1	B	301/313 (96%)	299 (99%)	2 (1%)	84	92
1	C	299/313 (96%)	298 (100%)	1 (0%)	92	96
1	D	298/313 (95%)	296 (99%)	2 (1%)	84	92
All	All	1197/1252 (96%)	1192 (100%)	5 (0%)	91	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	136	SER
1	B	295	LEU
1	C	209	ARG
1	D	295	LEU
1	D	315	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 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	$\# Z > 2$
4	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.47	0
4	EDO	A	503	-	3,3,3	0.48	0	2,2,2	0.46	0
4	EDO	B	503	-	3,3,3	0.49	0	2,2,2	0.49	0
4	EDO	B	504	-	3,3,3	0.48	0	2,2,2	0.42	0
4	EDO	D	504	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.41	0
6	PG6	B	505	-	17,17,17	0.51	0	16,16,16	0.49	0
2	LHD	D	501	-	30,35,35	0.55	0	27,50,50	0.63	1 (3%)
2	LHD	B	501	-	30,35,35	0.54	0	27,50,50	0.89	3 (11%)
4	EDO	B	507	-	3,3,3	0.48	0	2,2,2	0.48	0
4	EDO	D	502	-	3,3,3	0.48	0	2,2,2	0.45	0
3	PEG	B	506	-	6,6,6	0.49	0	5,5,5	0.45	0
4	EDO	C	505	-	3,3,3	0.46	0	2,2,2	0.49	0
4	EDO	D	503	-	3,3,3	0.48	0	2,2,2	0.48	0
3	PEG	C	502	-	6,6,6	0.46	0	5,5,5	0.57	0
4	EDO	A	504	-	3,3,3	0.46	0	2,2,2	0.46	0
3	PEG	C	503	-	6,6,6	0.48	0	5,5,5	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DXE	A	505	-	5,5,5	0.41	0	4,4,4	0.19	0
3	PEG	A	502	-	6,6,6	0.49	0	5,5,5	0.43	0
2	LHD	C	501	-	30,35,35	0.55	0	27,50,50	0.63	1 (3%)
2	LHD	A	501	-	30,35,35	0.54	0	27,50,50	0.65	1 (3%)

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
4	EDO	B	502	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
4	EDO	B	503	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	D	504	-	-	1/1/1/1	-
4	EDO	C	504	-	-	1/1/1/1	-
6	PG6	B	505	-	-	10/15/15/15	-
2	LHD	D	501	-	-	4/9/30/30	0/4/4/4
2	LHD	B	501	-	-	6/9/30/30	0/4/4/4
4	EDO	B	507	-	-	1/1/1/1	-
4	EDO	D	502	-	-	1/1/1/1	-
3	PEG	B	506	-	-	1/4/4/4	-
4	EDO	C	505	-	-	1/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
3	PEG	C	502	-	-	2/4/4/4	-
4	EDO	A	504	-	-	0/1/1/1	-
3	PEG	C	503	-	-	3/4/4/4	-
5	DXE	A	505	-	-	1/3/3/3	-
3	PEG	A	502	-	-	1/4/4/4	-
2	LHD	C	501	-	-	3/9/30/30	0/4/4/4
2	LHD	A	501	-	-	6/9/30/30	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	LHD	C2-C1-N6	2.38	123.97	120.35
2	B	501	LHD	C10-C11-C14	-2.36	117.67	121.21
2	B	501	LHD	C2-C1-N6	2.32	123.89	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	LHD	C2-C1-N6	2.31	123.86	120.35
2	A	501	LHD	C2-C1-N6	2.26	123.79	120.35
2	B	501	LHD	C11-C10-N5	-2.05	103.57	111.77

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LHD	C18-C17-C7-O1
2	A	501	LHD	C18-C17-C7-C8
2	A	501	LHD	O4-C15-N8-C13
2	A	501	LHD	N8-C15-O4-C16
2	B	501	LHD	C18-C17-C7-O1
2	B	501	LHD	C18-C17-C7-C8
2	B	501	LHD	C11-C10-N5-C18
2	B	501	LHD	O4-C15-N8-C13
2	B	501	LHD	O4-C15-N8-C14
2	B	501	LHD	N8-C15-O4-C16
2	C	501	LHD	C18-C17-C7-O1
2	C	501	LHD	C18-C17-C7-C8
2	D	501	LHD	C18-C17-C7-O1
2	D	501	LHD	C18-C17-C7-C8
2	D	501	LHD	C11-C10-N5-C18
3	C	503	PEG	C1-C2-O2-C3
5	A	505	DXE	O1-C2-C3-O2
6	B	505	PG6	O2-C4-C5-O3
3	A	502	PEG	O2-C3-C4-O4
3	B	506	PEG	O1-C1-C2-O2
3	C	503	PEG	O2-C3-C4-O4
4	C	504	EDO	O1-C1-C2-O2
4	D	502	EDO	O1-C1-C2-O2
2	D	501	LHD	N8-C15-O4-C16
4	A	503	EDO	O1-C1-C2-O2
4	B	507	EDO	O1-C1-C2-O2
6	B	505	PG6	O1-C2-C3-O2
6	B	505	PG6	O5-C10-C11-O6
4	B	502	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
4	C	505	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2
3	C	502	PEG	C1-C2-O2-C3
6	B	505	PG6	C9-C8-O4-C7

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Mol	Chain	Res	Type	Atoms
6	B	505	PG6	C3-C2-O1-C1
3	C	503	PEG	C4-C3-O2-C2
2	A	501	LHD	C11-C10-N5-C18
2	C	501	LHD	C11-C10-N5-C18
6	B	505	PG6	C8-C9-O5-C10
6	B	505	PG6	C5-C4-O2-C3
4	B	504	EDO	O1-C1-C2-O2
3	C	502	PEG	C4-C3-O2-C2
2	A	501	LHD	O4-C15-N8-C14
6	B	505	PG6	C2-C3-O2-C4
6	B	505	PG6	O4-C8-C9-O5
6	B	505	PG6	C11-C10-O5-C9
4	D	504	EDO	O1-C1-C2-O2

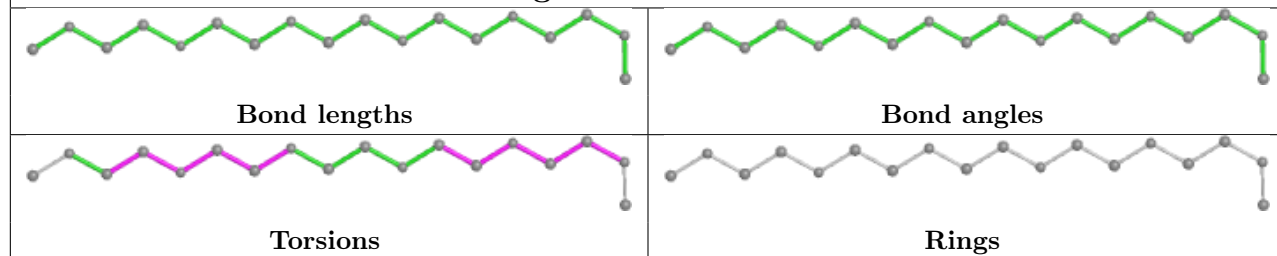
There are no ring outliers.

5 monomers are involved in 5 short contacts:

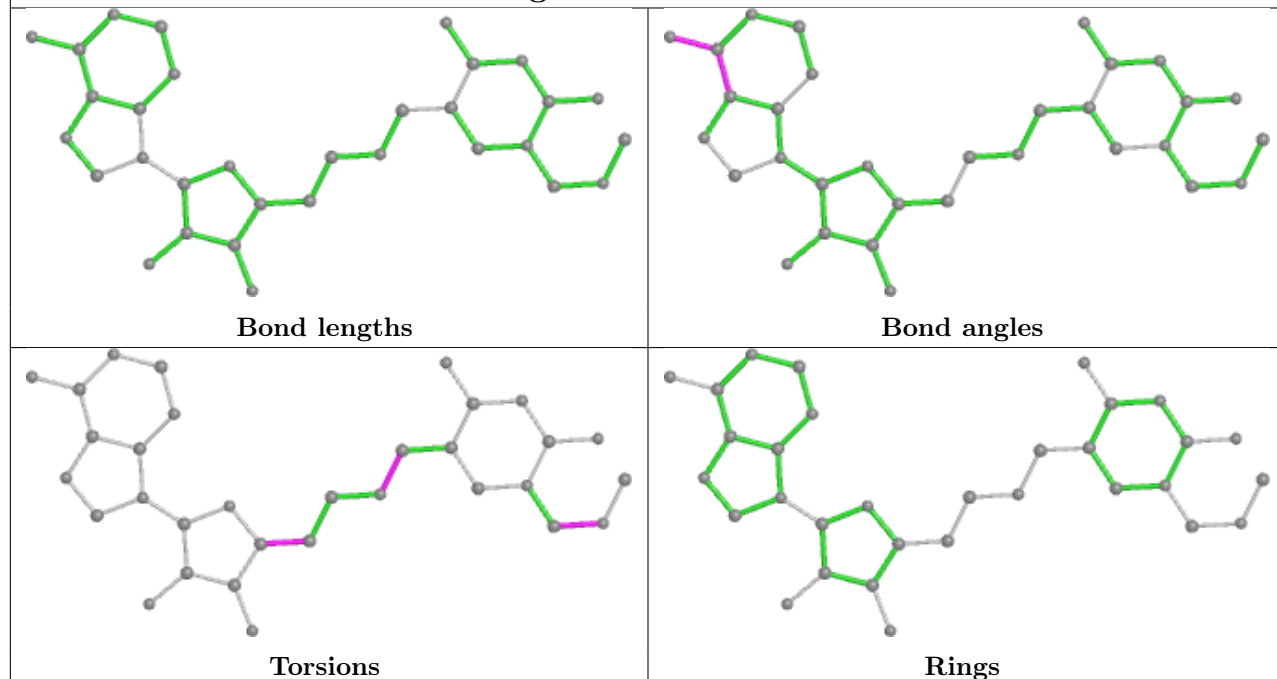
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	EDO	1	0
6	B	505	PG6	1	0
2	B	501	LHD	1	0
3	C	502	PEG	1	0
2	A	501	LHD	1	0

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.

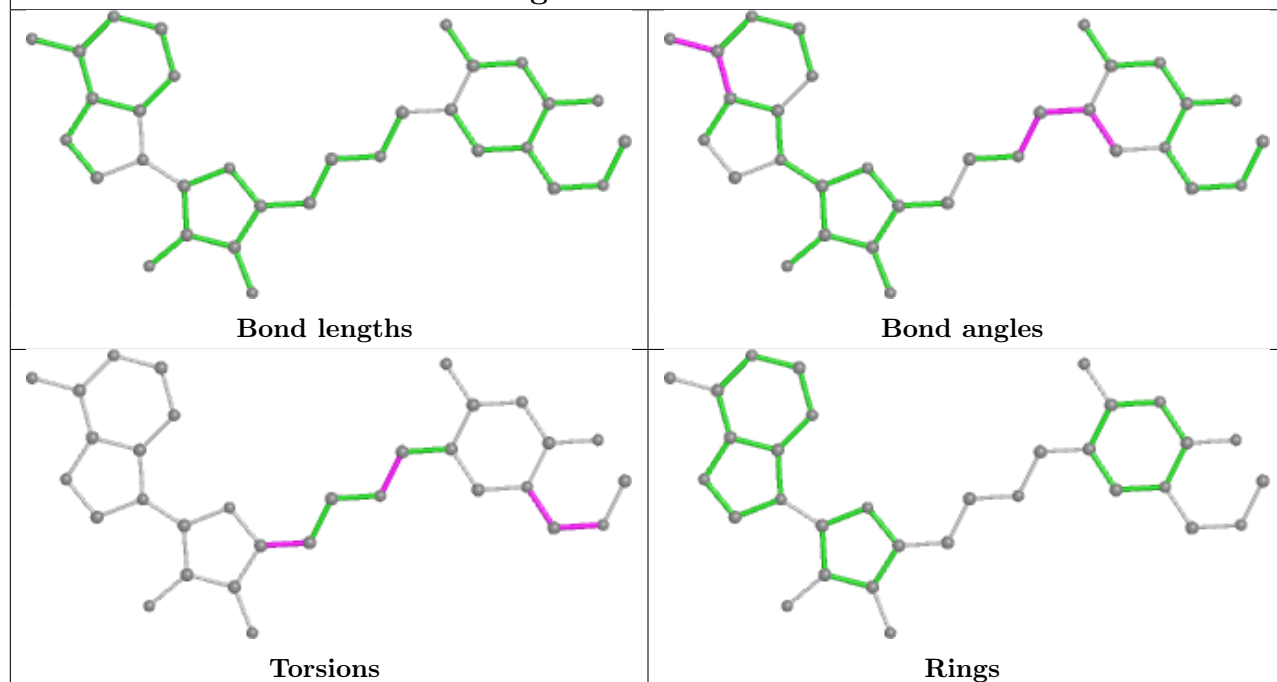
Ligand PG6 B 505

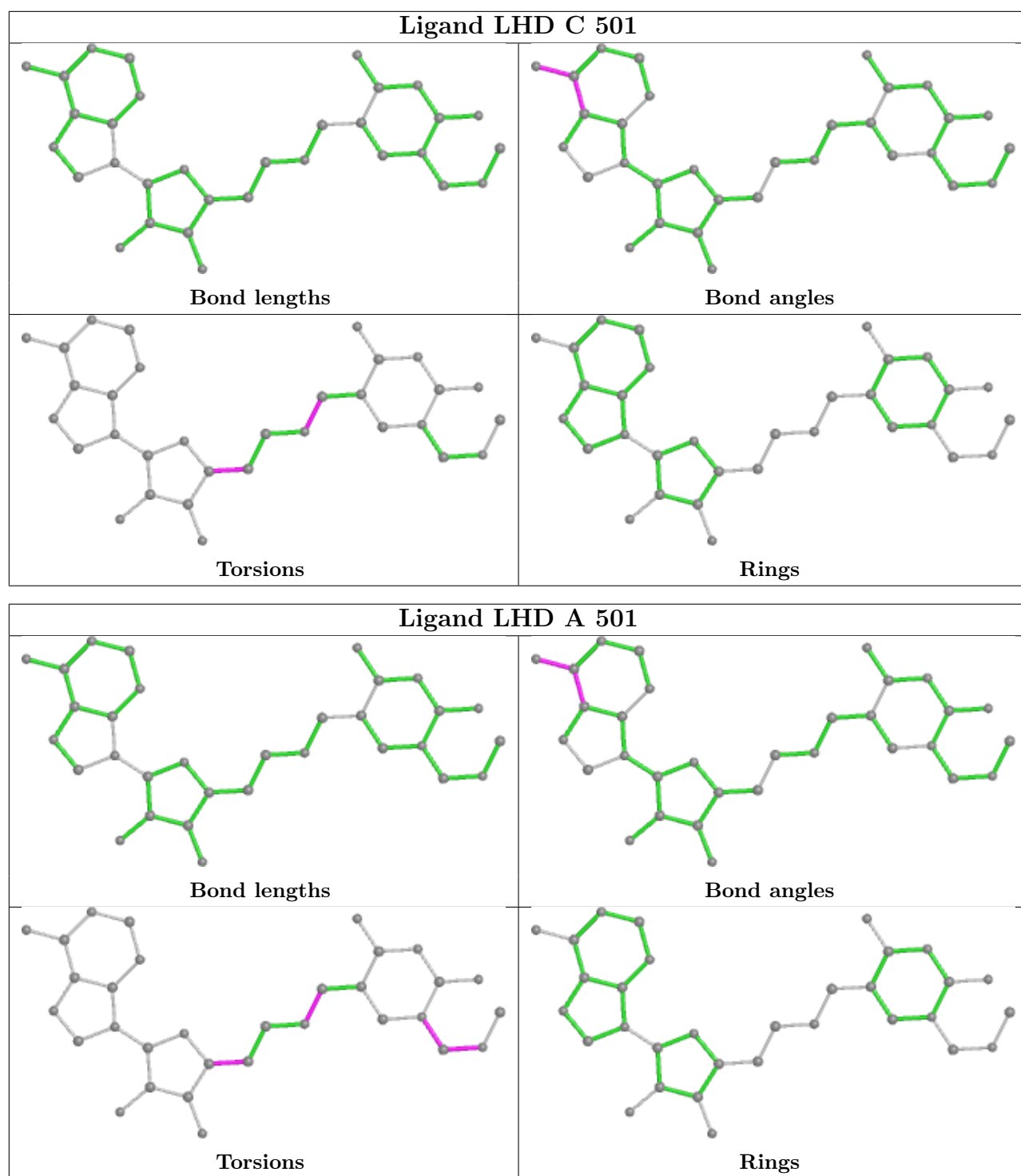


Ligand LHD D 501



Ligand LHD B 501





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	343/361 (95%)	0.15	10 (2%) 51 59	18, 29, 49, 67	0
1	B	343/361 (95%)	0.15	6 (1%) 70 76	20, 33, 52, 82	0
1	C	343/361 (95%)	0.32	15 (4%) 34 41	23, 36, 55, 67	0
1	D	342/361 (94%)	0.29	15 (4%) 34 41	26, 38, 56, 76	0
All	All	1371/1444 (94%)	0.23	46 (3%) 45 52	18, 34, 54, 82	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	478	THR	6.8
1	B	477	TYR	6.8
1	B	135	ARG	5.6
1	A	478	THR	5.4
1	D	135	ARG	5.4
1	B	282	PRO	3.9
1	C	477	TYR	3.9
1	A	283	SER	3.9
1	C	282	PRO	3.7
1	A	347	ARG	3.5
1	C	234	ASP	3.2
1	D	346	ILE	3.1
1	B	347	ARG	3.1
1	D	347	ARG	3.0
1	C	283	SER	2.9
1	C	256	ILE	2.8
1	A	477	TYR	2.8
1	A	456	GLN	2.8
1	C	162	ASN	2.8
1	C	136	SER	2.7
1	C	140	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	465	SER	2.6
1	B	312	ASN	2.6
1	A	140	GLU	2.6
1	D	301	GLU	2.6
1	D	388	LEU	2.5
1	A	221	GLN	2.5
1	D	475	PHE	2.4
1	C	475	PHE	2.4
1	D	312	ASN	2.4
1	D	297	PRO	2.4
1	D	302	GLN	2.4
1	D	282	PRO	2.3
1	D	417	TYR	2.3
1	A	197	GLY	2.3
1	D	445	LYS	2.3
1	D	296	ALA	2.2
1	C	240	PRO	2.2
1	C	198	ILE	2.2
1	A	231	ASN	2.2
1	D	186	ASP	2.2
1	A	162	ASN	2.1
1	D	463	LYS	2.1
1	C	456	GLN	2.0
1	C	221	GLN	2.0
1	C	218	THR	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

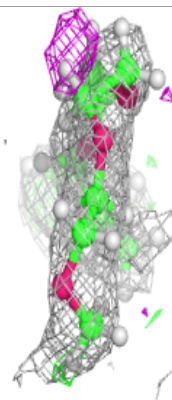
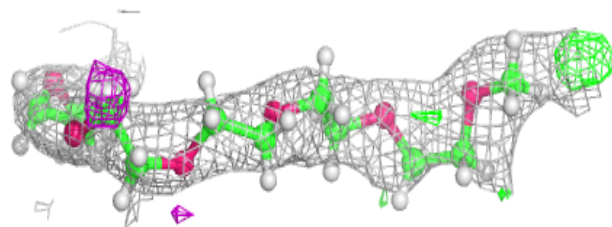
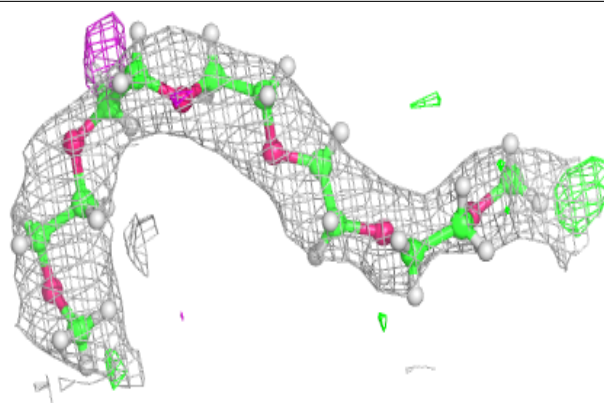
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	C	504	4/4	0.30	0.36	42,57,66,68	0
4	EDO	B	504	4/4	0.46	0.35	55,67,72,73	0
4	EDO	A	503	4/4	0.64	0.28	49,59,64,64	0
4	EDO	D	503	4/4	0.70	0.24	58,70,71,71	0
3	PEG	C	502	7/7	0.73	0.17	46,58,72,72	0
3	PEG	C	503	7/7	0.73	0.30	53,64,75,76	0
4	EDO	B	502	4/4	0.74	0.31	48,58,63,64	0
4	EDO	D	504	4/4	0.79	0.15	38,46,54,55	0
3	PEG	A	502	7/7	0.80	0.14	46,56,60,60	0
4	EDO	B	503	4/4	0.80	0.21	44,53,57,59	0
6	PG6	B	505	18/18	0.82	0.26	39,58,72,73	0
3	PEG	B	506	7/7	0.83	0.23	47,59,71,71	0
4	EDO	A	504	4/4	0.83	0.14	30,39,45,49	0
5	DXE	A	505	6/6	0.83	0.20	45,54,59,59	0
4	EDO	D	502	4/4	0.83	0.18	45,54,58,59	0
2	LHD	A	501	32/32	0.85	0.16	23,38,51,52	0
4	EDO	C	505	4/4	0.87	0.16	47,56,61,61	0
2	LHD	B	501	32/32	0.87	0.17	22,36,50,58	0
2	LHD	D	501	32/32	0.87	0.17	25,38,58,70	0
4	EDO	B	507	4/4	0.91	0.09	37,45,46,46	0
2	LHD	C	501	32/32	0.91	0.15	26,36,48,50	0

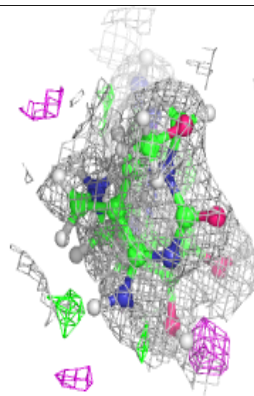
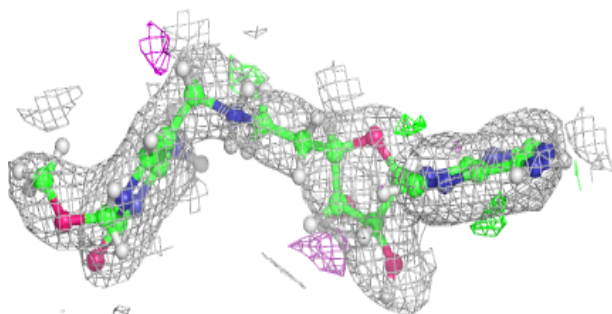
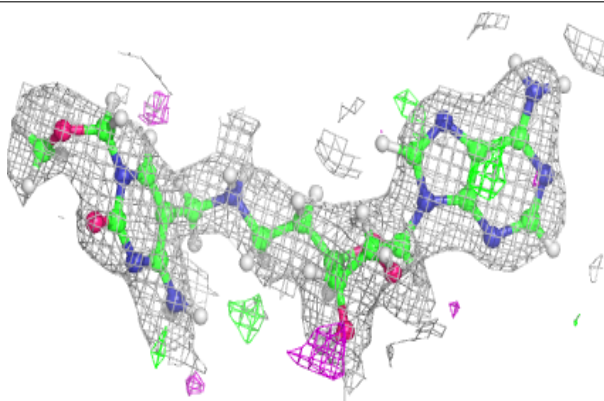
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PG6 B 505:

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

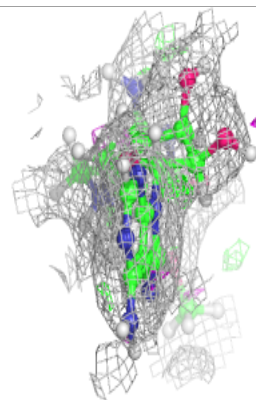
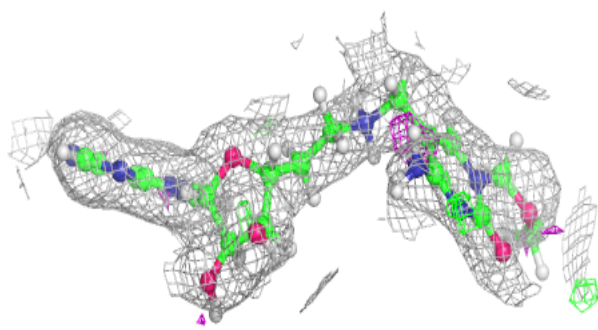
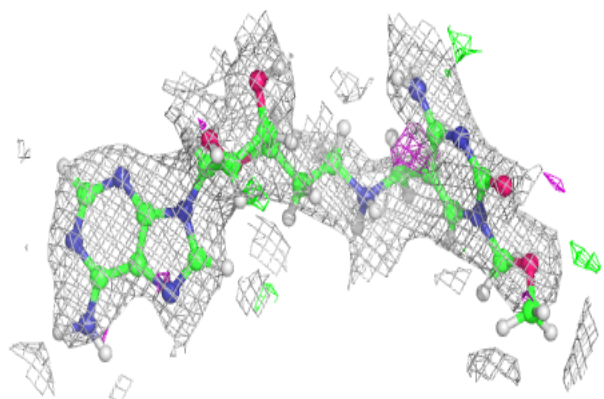
**Electron density around LHD A 501:**

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

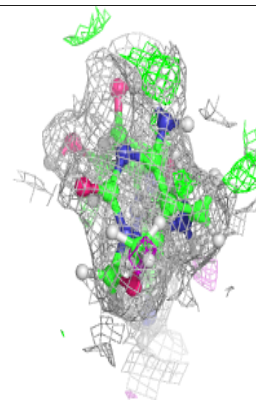
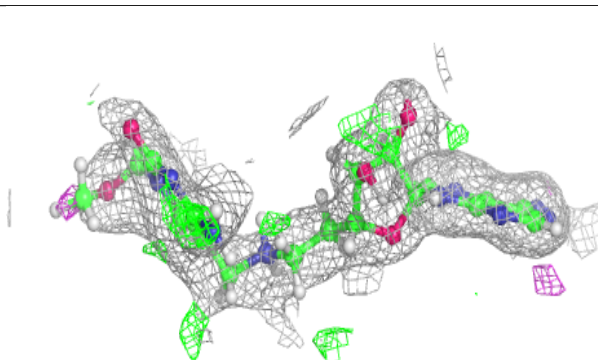
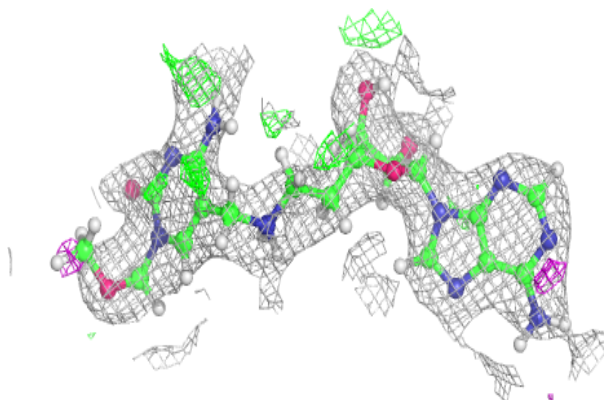


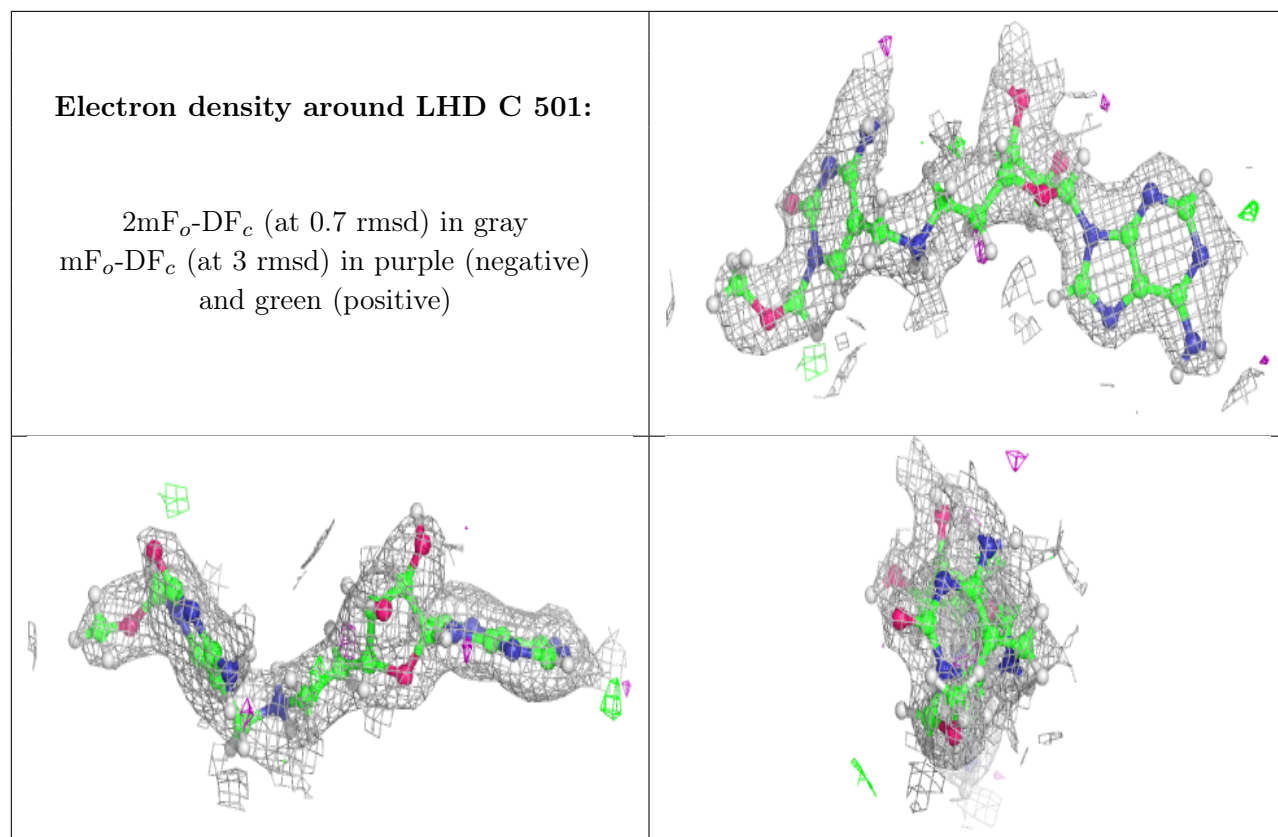
Electron density around LHD B 501:

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

**Electron density around LHD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.