

wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2024 – 11:25 am BST

PDB ID : 80W6

Title: PERIDININ-CHLOROPHYLL-PROTEIN OF HETEROCAPSA PYG-

MAEA, 100K

Authors: Hofmann, E.; Schulte, T.

Deposited on : 2023-04-27

Resolution : 1.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36.2

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

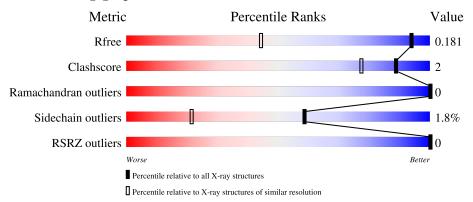
Validation Pipeline (wwPDB-VP) : 2.36.2

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 1.20 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 <=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	149	98%	
1	С	149	96%	
2	В	149	94%	6%
2	D	149	93%	7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	A	601	X	-	-	-
3	CLA	В	601	X	-	-	-
3	CLA	С	601	X	-	-	-
3	CLA	D	601	X	-	-	-
4	PID	D	613	X	-	-	-



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12518 atoms, of which 5917 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 Peridinin-chl a protein.

Mol	Chain	Residues		${f Atoms}$					ZeroOcc	AltConf	Trace
1	A	149	10001	C 701		N 180	O 219	S 7	0	3	0
1	С	149	Total 2228	_	H 1112	N 182	O 220	S 7	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

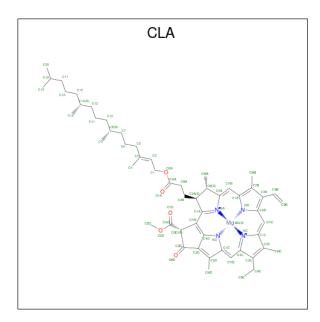
Chain	Residue	Modelled	Actual	Comment	Reference
A	108	ALA	VAL	$\operatorname{conflict}$	UNP Q9FEY4
С	108	ALA	VAL	conflict	UNP Q9FEY4

• Molecule 2 is a protein called Peridinin-chl a protein.

Mol	Chain	Residues			Atom	ıs			ZeroOcc	AltConf	Trace
2	В	149	Total 2322	_	H 1165	N 187	O 231	S 7	0	15	0
2	D	149		_	H 1142		O 223	S 7	0	7	0

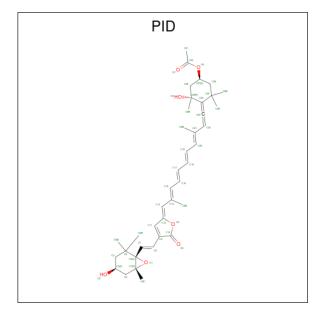
• Molecule 3 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	
3	Λ	1	Total	С	Н	Mg	N	О	0	0	
)	A	1	137	55	72	1	4	5	<u> </u>	0	
3	В	1	Total	С	Н	Mg	N	О	0	0	
)	Ъ	1	137	55	72	1	4	5	0	0	
3	С	1	Total	С	Н	Mg	N	О	0	0	
)		1	137	55	72	1	4	5	U	0	
3	D	1	Total	С	Н	Mg	N	О	0	0	
3	ע	1	137	55	72	1	4	5	U	U	

• Molecule 4 is PERIDININ (three-letter code: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).

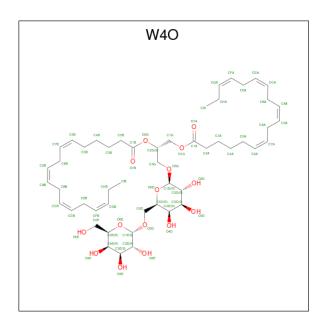




Mol	Chain	Residues	I	Aton	ns		ZeroOcc	AltConf
4	۸	1	Total	С	Н	О	0	0
4	A	1	96	39	50	7	0	0
4	۸	1	Total	С	Н	О	0	0
4	A	1	96	39	50	7	U	0
4	A	1	Total	С	Н	О	0	0
4	A	1	96	39	50	7	0	0
4	A	1	Total	С	Н	О	0	0
4	A	1	96	39	50	7	0	0
4	В	1	Total	С	Н	О	0	0
4	Ъ	1	96	39	50	7		
4	В	1	Total	С	Η	Ο	0	0
4	D	1	96	39	50	7	0	U
4	В	1	Total	С	Н	Ο	0	0
4	D	1	96	39	50	7	0	U
4	В	1	Total	С	Η	Ο	0	0
-1	D	1	96	39	50	7	U	0
4	$^{\rm C}$	1	Total	С	Н	О	0	0
-1	C	1	96	39	50	7	0	U
4	С	1	Total	С	Н	О	0	0
	C	1	96	39	50	7	0	0
4	$^{\rm C}$	1	Total	С	Н	Ο	0	0
	C	1	96	39	50	7	0	
4	C	1	Total	С	Η	Ο	0	0
1	C	1	96	39	50	7	Ů	
4	D	1	Total	С	Н	Ο	0	0
1	D	1	96	39	50	7	0	
4	D	1	Total	С	Н	Ο	0	0
1	D	1	96	39	50	7	0	
4	D	1	Total	С	Η	Ο	0	0
1	D	1	96	39	50	7		
4	D	1	Total	С	Н	Ο	0	0
	ر ا	1	96	39	50	7		

• Molecule 5 is [(2 {S})-3-[(2 {R},3 {R},4 {S},5 {R},6 {R})-6-[[(2 {S},3 {R},4 {S},5 {R},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-2-[(6 {Z},9 {Z},12 {Z},15 {Z})-octadeca-6,9,12,15-tetraenoyl]oxy-propyl] (6 {Z},9 {Z},12 {Z},15 {Z})-octadeca-6,9,12,15-tetraenoate (three-letter code: W4O) (formula: $C_{51}H_{80}O_{15}$) (labeled as "Ligand of Interest" by depositor).





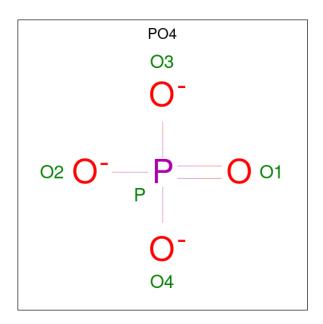
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	С	Н	О	0	0	
	Λ	1	144	51	78	15	0	0	
5	D	1	Total	С	Н	О	0	0	
9	Ъ	1	144	51	78	15	0		
5	C	1	Total	С	Н	О	0	0	
9		1	144	51	78	15	0	U	
5	D	1	Total	С	Н	О	0	0	
9	ש	1	144	51	78	15	0		

• Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	В	1	Total K 1 1	0	0

 \bullet Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 5	O 4	P 1	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	Total Cl 1 1	0	0

• Molecule 9 is water.

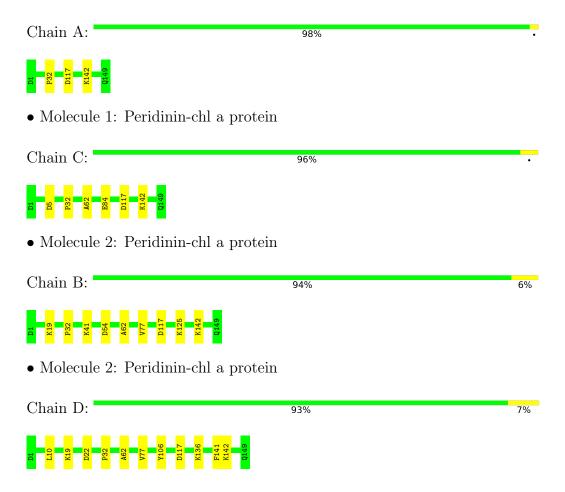
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	240	Total O 240 240	0	0
9	В	233	Total O 233 233	0	0
9	С	181	Total O 181 181	0	0
9	D	165	Total O 165 165	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Peridinin-chl a protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants	90.61Å 90.61Å 155.61Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.50 - 1.20	Depositor
resolution (A)	43.50 - 1.20	EDS
% Data completeness	99.9 (43.50-1.20)	Depositor
(in resolution range)	96.3 (43.50-1.20)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.17 (at 1.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.149 , 0.171	Depositor
it, it _{free}	0.159 , 0.181	DCC
R_{free} test set	2139 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å ²)	9.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.42, 35.8	EDS
L-test for twinning ²	$< L > = 0.41, < L^2> = 0.23$	Xtriage
Estimated twinning fraction	0.368 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12518	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: K, HYP, W4O, CLA, PO4, CL, PID

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	0.58	0/1135	0.54	0/1522	
1	С	0.57	0/1145	0.55	0/1536	
2	В	0.58	0/1228	0.54	0/1644	
2	D	0.53	0/1165	0.54	0/1560	
All	All	0.56	0/4673	0.54	0/6262	

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	1107	1098	1073	0	0
1	С	1116	1112	1089	4	0
2	В	1157	1165	1103	6	0
2	D	1134	1142	1115	6	0
3	A	65	72	72	0	0
3	В	65	72	72	0	0
3	С	65	72	72	0	0
3	D	65	72	72	0	0
4	A	184	200	200	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	184	200	200	2	0
4	С	184	200	200	4	0
4	D	184	200	200	2	0
5	A	66	78	0	0	0
5	В	66	78	0	0	0
5	С	66	78	0	0	0
5	D	66	78	0	0	0
6	A	1	0	0	0	0
6	В	1	0	0	0	1
7	A	5	0	0	0	0
8	В	1	0	0	0	0
9	A	240	0	0	0	10
9	В	233	0	0	3	6
9	С	181	0	0	2	2
9	D	165	0	0	2	1
All	All	6601	5917	5468	22	12

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.

The worst 5 of 22 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:B:125:LYS:NZ	9:B:722:HOH:O	1.96	0.93
4:C:613:PID:H311	2:D:62:ALA:HB2	1.60	0.84
4:C:613:PID:C31	2:D:62:ALA:HB2	2.19	0.73
2:D:106:TYR:OH	9:D:738:HOH:O	2.00	0.69
4:A:613:PID:H311	2:B:62:ALA:HB2	1.74	0.69

The worst 5 of 12 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
6:B:607:K:K	6:B:607:K:K[4_555]	1.31	0.89
9:A:856:HOH:O	9:C:775:HOH:O[3_555]	1.81	0.39
9:A:838:HOH:O	9:B:847:HOH:O[2_445]	1.89	0.31
9:A:828:HOH:O	9:B:910:HOH:O[3_555]	1.94	0.26
9:A:777:HOH:O	9:B:836:HOH:O[3_555]	1.95	0.25



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	Perce	ntiles
1	A	$148/149\ (99\%)$	146 (99%)	2 (1%)	0	100	100
1	\mathbf{C}	150/149 (101%)	148 (99%)	2 (1%)	0	100	100
2	В	160/149~(107%)	158 (99%)	2 (1%)	0	100	100
2	D	153/149 (103%)	151 (99%)	2 (1%)	0	100	100
All	All	$611/596 \ (102\%)$	603 (99%)	8 (1%)	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	Perce	ntiles
1	A	111/108 (103%)	109 (98%)	2 (2%)	59	21
1	С	111/108 (103%)	110 (99%)	1 (1%)	78	50
2	В	123/109 (113%)	121 (98%)	2 (2%)	62	27
2	D	115/109 (106%)	111 (96%)	4 (4%)	36	5
All	All	460/434 (106%)	451 (98%)	9 (2%)	59	17

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	136[B]	LYS
2	D	142	LYS
2	В	142	LYS

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Mol	Chain	Res	Type
1	С	117	ASP
2	D	117	ASP

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	Res	Link	Bond lengths			Bond angles		
Mol Type Chain	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
1	HYP	С	32	1	6,8,9	1.17	1 (16%)	5,10,12	2.21	2 (40%)
1	HYP	A	32	1	6,8,9	1.41	1 (16%)	5,10,12	2.51	2 (40%)
2	HYP	В	32	2	6,8,9	1.19	1 (16%)	5,10,12	2.99	4 (80%)
2	HYP	D	32	2	6,8,9	1.00	0	5,10,12	2.72	3 (60%)

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
1	HYP	С	32	1	-	0/0/11/13	0/1/1/1
1	HYP	A	32	1	-	0/0/11/13	0/1/1/1
2	HYP	В	32	2	-	0/0/11/13	0/1/1/1
2	HYP	D	32	2	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
1	A	32	HYP	OD1-CG	-2.77	1.35	1.43
1	С	32	HYP	OD1-CG	-2.41	1.36	1.43
2	В	32	HYP	OD1-CG	-2.34	1.36	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	32	HYP	CB-CG-CD	-5.39	96.66	103.27
2	D	32	HYP	CB-CG-CD	-4.67	97.54	103.27
1	A	32	HYP	CB-CG-CD	-4.36	97.92	103.27
1	С	32	HYP	CB-CG-CD	-3.60	98.86	103.27
2	D	32	HYP	OD1-CG-CB	2.64	116.57	110.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 for Mogul analysis.

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	Trus	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	В	601	9	65,73,73	1.39	12 (18%)	76,113,113	1.10	5 (6%)
4	PID	С	612	-	41,49,49	1.68	11 (26%)	49,76,76	1.12	5 (10%)
4	PID	A	613	-	41,49,49	1.65	7 (17%)	49,76,76	0.93	2 (4%)
4	PID	A	614	-	41,49,49	1.15	4 (9%)	49,76,76	0.77	1 (2%)



Mol	Type	Chain	Dec	Link	В	ond leng	$\overline{ ext{gths}}$	Во	ond angl	Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
4	PID	D	613	-	41,49,49	1.66	7 (17%)	49,76,76	0.88	2 (4%)		
4	PID	С	611	-	41,49,49	1.46	8 (19%)	49,76,76	0.81	1 (2%)		
4	PID	D	614	-	41,49,49	1.19	3 (7%)	49,76,76	0.93	2 (4%)		
5	W4O	С	615	-	67,67,67	1.33	8 (11%)	79,81,81	1.27	10 (12%)		
4	PID	D	612	-	41,49,49	1.37	9 (21%)	49,76,76	1.01	3 (6%)		
5	W4O	В	615	-	67,67,67	1.37	8 (11%)	79,81,81	1.25	9 (11%)		
4	PID	A	612	-	41,49,49	1.53	6 (14%)	49,76,76	1.02	5 (10%)		
4	PID	В	613	-	41,49,49	1.28	4 (9%)	49,76,76	1.08	5 (10%)		
4	PID	D	611	-	41,49,49	1.27	6 (14%)	49,76,76	0.84	2 (4%)		
3	CLA	С	601	9	65,73,73	1.45	10 (15%)	76,113,113	1.29	4 (5%)		
4	PID	В	614	-	41,49,49	1.39	4 (9%)	49,76,76	0.86	1 (2%)		
4	PID	A	611	-	41,49,49	1.61	5 (12%)	49,76,76	0.91	2 (4%)		
3	CLA	D	601	9	65,73,73	1.43	11 (16%)	76,113,113	1.16	7 (9%)		
4	PID	В	612	-	41,49,49	1.43	8 (19%)	49,76,76	1.06	4 (8%)		
3	CLA	A	601	9	65,73,73	1.53	9 (13%)	76,113,113	1.44	9 (11%)		
5	W4O	D	615	-	67,67,67	1.29	7 (10%)	79,81,81	1.23	8 (10%)		
5	W4O	A	615	-	67,67,67	1.28	9 (13%)	79,81,81	1.25	9 (11%)		
7	PO4	A	608	6	4,4,4	0.97	0	6,6,6	0.32	0		
4	PID	С	613	-	41,49,49	1.70	11 (26%)	49,76,76	0.91	1 (2%)		
4	PID	В	611	-	41,49,49	1.47	4 (9%)	49,76,76	0.83	1 (2%)		
4	PID	С	614	-	41,49,49	1.42	10 (24%)	49,76,76	1.13	4 (8%)		

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
3	CLA	В	601	9	1/1/20/20	1/37/115/115	-
4	PID	С	612	-	-	0/24/93/93	0/4/4/4
4	PID	A	613	_	-	0/24/93/93	0/4/4/4
4	PID	A	614	-	-	0/24/93/93	0/4/4/4
4	PID	D	613	_	1/1/25/25	0/24/93/93	0/4/4/4
4	PID	С	611	-	-	0/24/93/93	0/4/4/4
4	PID	D	614	-	-	0/24/93/93	0/4/4/4
5	W4O	С	615	_	-	11/55/95/95	0/2/2/2
4	PID	D	612	-	-	0/24/93/93	0/4/4/4
5	W4O	В	615	_	-	9/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PID	A	612	-	-	0/24/93/93	0/4/4/4
4	PID	В	613	-	-	0/24/93/93	0/4/4/4
4	PID	D	611	_	-	0/24/93/93	0/4/4/4
3	CLA	С	601	9	1/1/20/20	2/37/115/115	-
4	PID	В	614	-	-	0/24/93/93	0/4/4/4
4	PID	A	611	_	-	0/24/93/93	0/4/4/4
3	CLA	D	601	9	1/1/20/20	1/37/115/115	-
4	PID	В	612	_	-	0/24/93/93	0/4/4/4
3	CLA	A	601	9	1/1/20/20	5/37/115/115	-
5	W4O	D	615	-	-	8/55/95/95	0/2/2/2
5	W4O	A	615	-	-	11/55/95/95	0/2/2/2
4	PID	С	613	-	-	0/24/93/93	0/4/4/4
4	PID	В	611	-	-	0/24/93/93	0/4/4/4
4	PID	С	614	-	-	0/24/93/93	0/4/4/4

The worst 5 of 181 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
3	A	601	CLA	C4B-NB	7.22	1.41	1.35
3	С	601	CLA	C4B-NB	5.70	1.40	1.35
4	A	612	PID	C4-C3	-5.40	1.44	1.52
3	D	601	CLA	C4B-NB	4.85	1.39	1.35
4	A	611	PID	C2-C3	-4.56	1.45	1.52

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
3	A	601	CLA	C4A-NA-C1A	7.86	110.24	106.71
3	С	601	CLA	C4A-NA-C1A	6.75	109.74	106.71
3	D	601	CLA	C4A-NA-C1A	4.95	108.93	106.71
5	A	615	W4O	O5D-C1E-C2E	4.61	115.50	108.30
5	D	615	W4O	C4A-C3A-C2A	4.37	128.89	113.19

All (5) chirality outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atom
3	A	601	CLA	ND
3	В	601	CLA	ND
3	С	601	CLA	ND
3	D	601	CLA	ND
4	D	613	PID	C6



5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	615	W4O	CFA-CGA-CHA-CIA
5	В	615	W4O	CFB-CGB-CHB-CIB
5	D	615	W4O	CFA-CGA-CHA-CIA
5	A	615	W4O	C2A-C3A-C4A-C5A
5	В	615	W4O	C2A-C3A-C4A-C5A

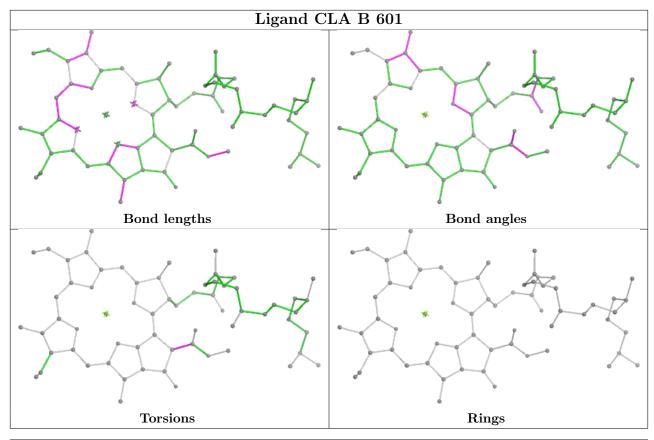
There are no ring outliers.

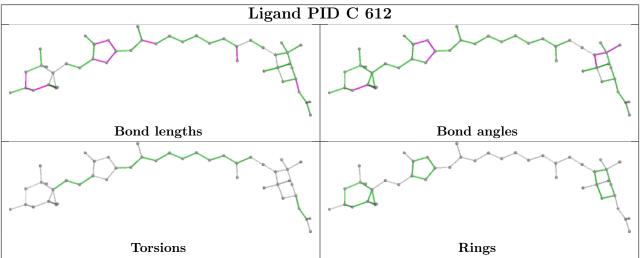
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	613	PID	4	0
4	A	614	PID	2	0
4	D	613	PID	2	0
4	D	614	PID	1	0
4	В	613	PID	1	0
4	В	614	PID	1	0
4	В	612	PID	1	0
4	С	613	PID	3	0
4	С	614	PID	2	0

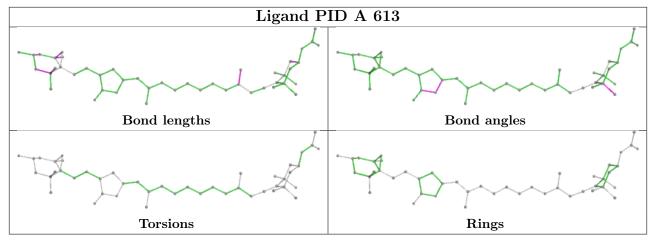
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

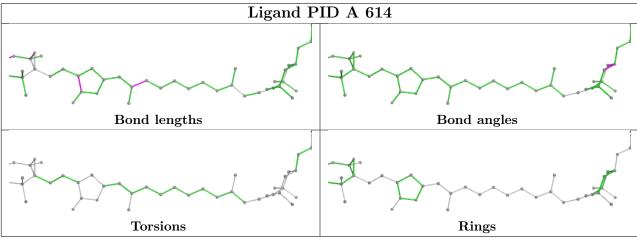


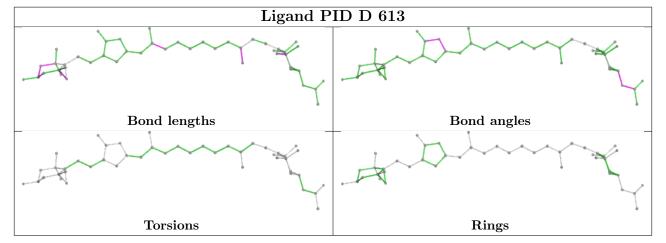




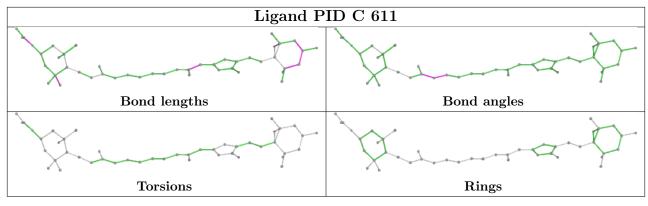


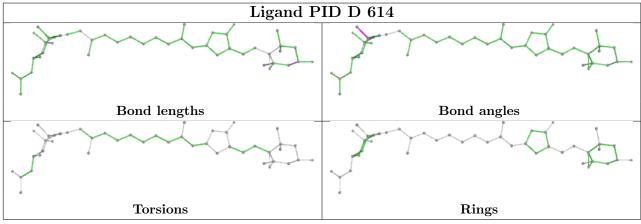


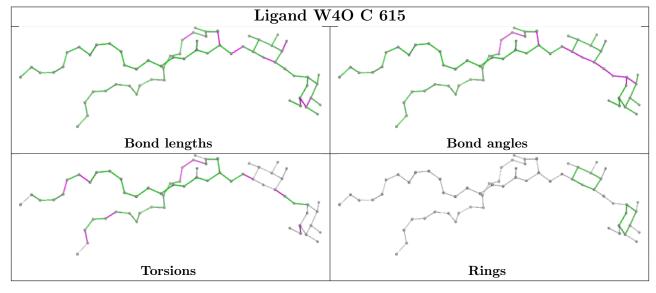




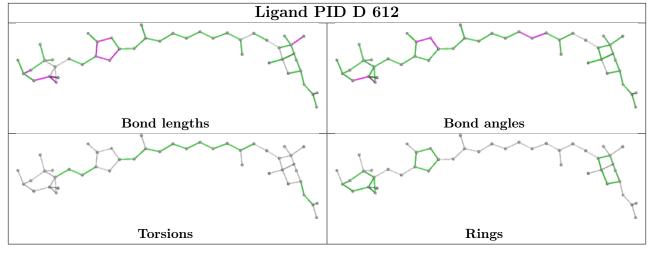


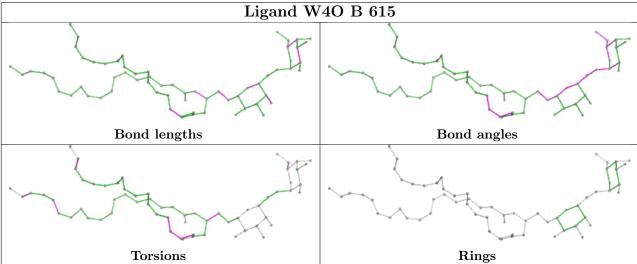


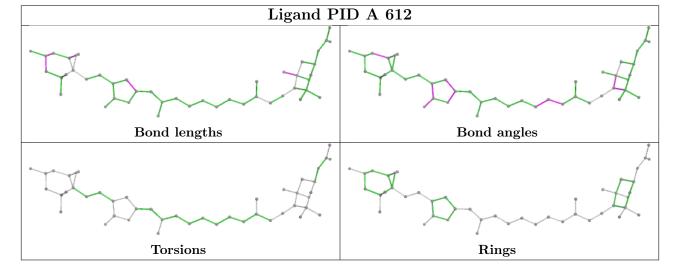




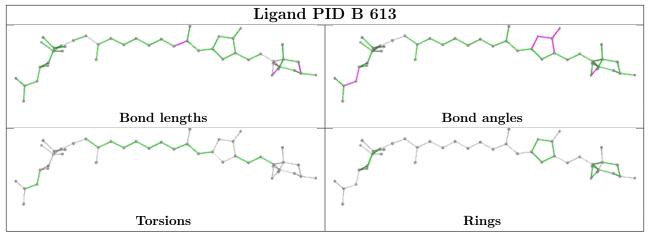


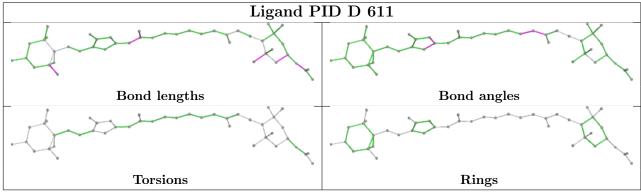


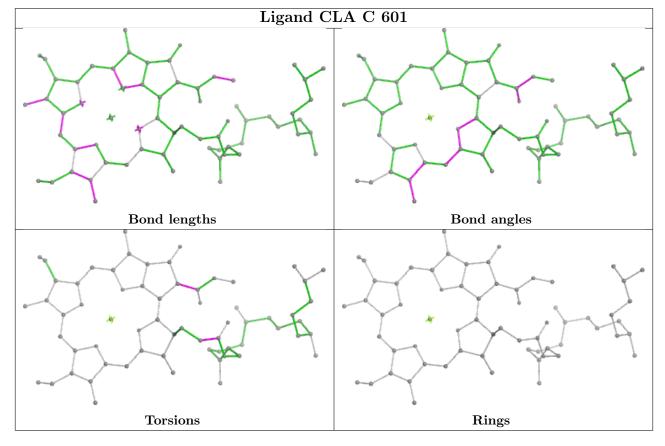




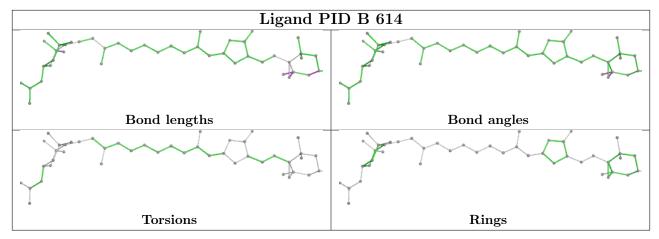


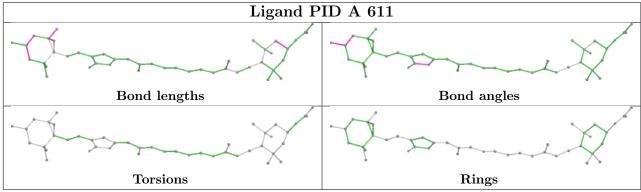


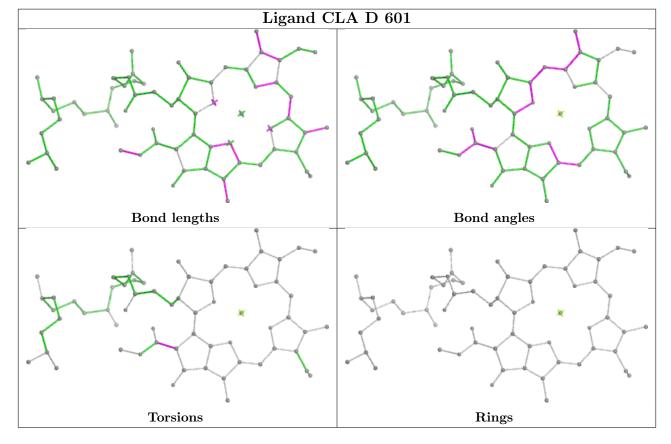




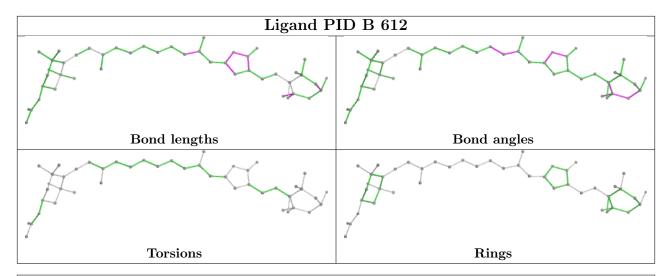


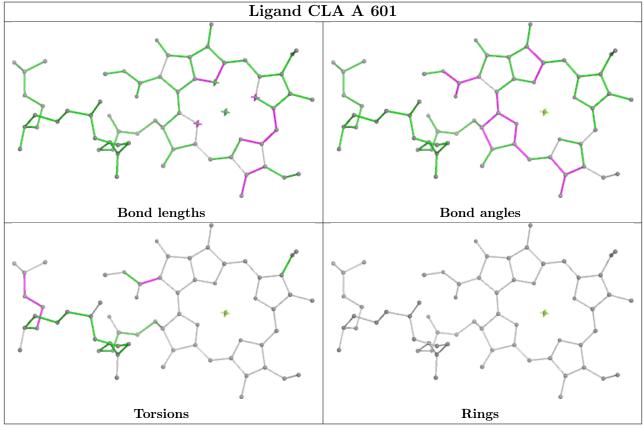




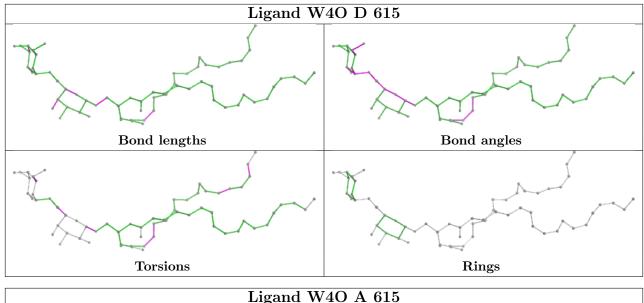


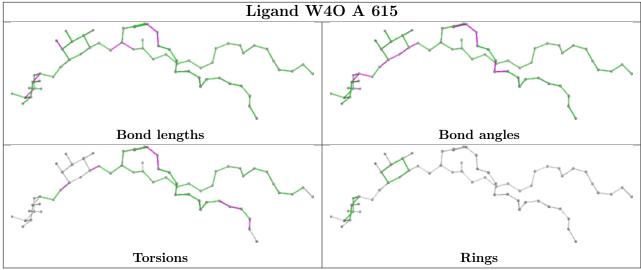


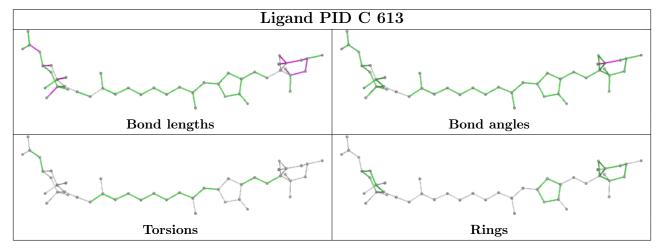




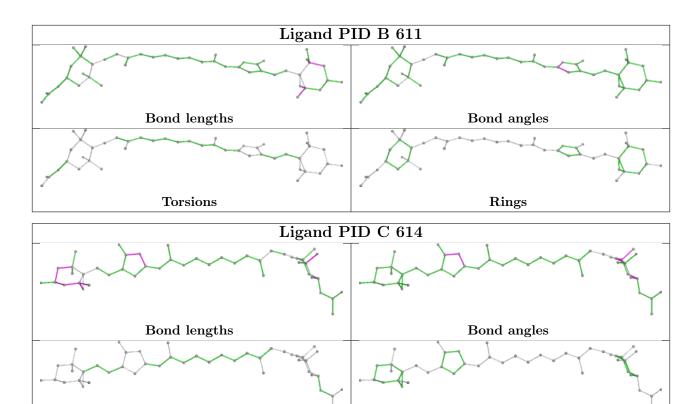












Rings

5.7 Other polymers (i)

There are no such residues in this entry.

Torsions

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	148/149 (99%)	-0.17	0 100 100	6, 9, 15, 18	0
1	С	148/149 (99%)	-0.13	0 100 100	9, 12, 18, 22	0
2	В	148/149 (99%)	-0.16	0 100 100	7, 9, 14, 19	0
2	D	148/149 (99%)	-0.11	0 100 100	9, 13, 19, 22	0
All	All	592/596 (99%)	-0.14	0 100 100	6, 11, 17, 22	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	${f B\text{-factors}}({f A}^2)$	Q<0.9
1	HYP	С	32	8/9	0.97	0.07	10,12,14,14	0
2	HYP	D	32	8/9	0.97	0.07	11,12,14,14	0
2	HYP	В	32	8/9	0.98	0.06	8,10,10,11	0
1	HYP	A	32	8/9	0.98	0.07	10,11,13,13	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



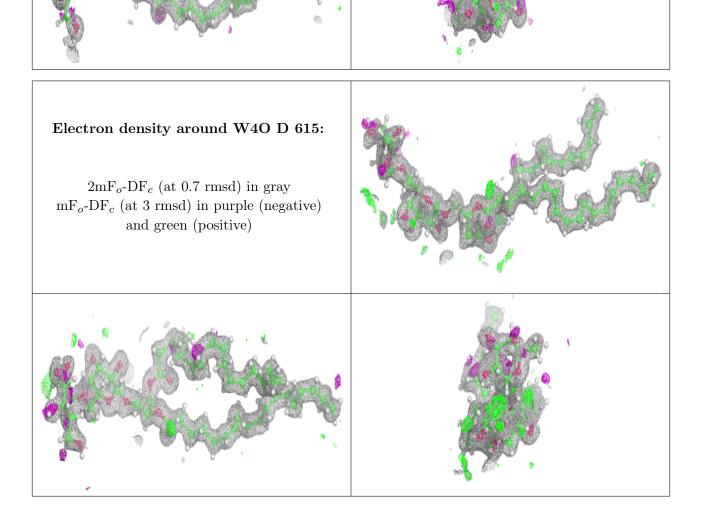
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
8	CL	В	608	1/1	0.84	0.11	33,33,33,33	0
6	K	В	607	1/1	0.93	0.14	13,13,13,13	0
5	W4O	С	615	66/66	0.94	0.10	10,14,46,57	0
5	W4O	D	615	66/66	0.94	0.10	9,14,34,42	0
5	W4O	A	615	66/66	0.95	0.09	9,13,41,49	0
5	W4O	В	615	66/66	0.96	0.09	8,11,29,36	0
4	PID	D	611	46/46	0.97	0.08	8,11,18,21	0
4	PID	D	613	46/46	0.97	0.08	8,12,23,24	0
7	PO4	A	608	5/5	0.97	0.08	13,15,18,18	0
4	PID	D	614	46/46	0.97	0.07	8,11,18,22	0
4	PID	С	611	46/46	0.98	0.07	8,11,15,18	0
4	PID	С	612	46/46	0.98	0.07	7,10,13,14	0
4	PID	С	613	46/46	0.98	0.06	7,10,19,21	0
4	PID	С	614	46/46	0.98	0.07	8,11,13,16	0
3	CLA	A	601	65/65	0.98	0.08	6,8,14,17	0
4	PID	D	612	46/46	0.98	0.06	7,10,15,17	0
3	CLA	С	601	65/65	0.98	0.08	8,10,14,17	0
3	CLA	D	601	65/65	0.98	0.07	7,11,16,17	0
4	PID	A	611	46/46	0.98	0.08	6,8,14,17	0
4	PID	A	613	46/46	0.98	0.07	7,9,14,15	0
4	PID	A	614	46/46	0.98	0.07	6,8,10,12	0
4	PID	В	611	46/46	0.98	0.07	6,9,12,14	0
4	PID	В	612	46/46	0.98	0.08	6,8,12,15	0
4	PID	В	613	46/46	0.98	0.07	6,9,17,19	0
4	PID	В	614	46/46	0.98	0.07	7,8,10,12	0
3	CLA	В	601	65/65	0.99	0.08	6,8,11,13	0
4	PID	A	612	46/46	0.99	0.08	6,8,12,12	0
6	K	A	607	1/1	0.99	0.12	17,17,17,17	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.

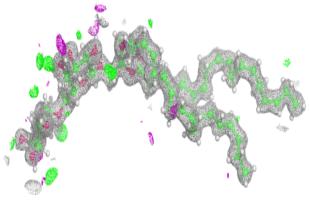


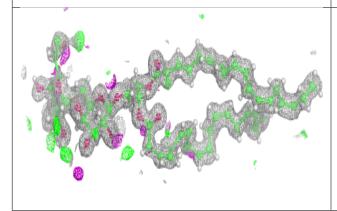


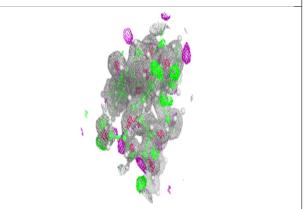


Electron density around W4O A 615:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

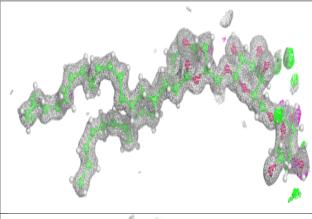


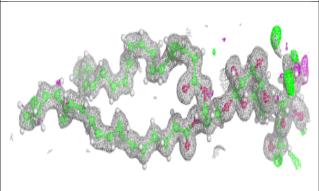


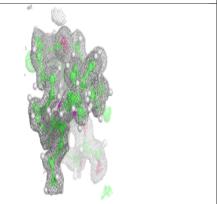


Electron density around W4O B 615:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



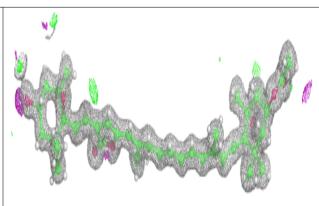


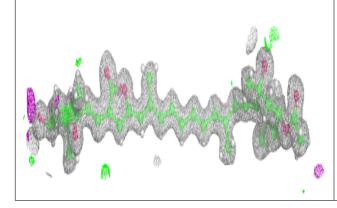


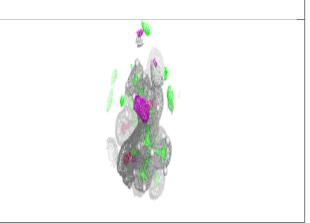


Electron density around PID D 611:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

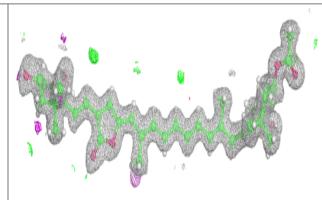


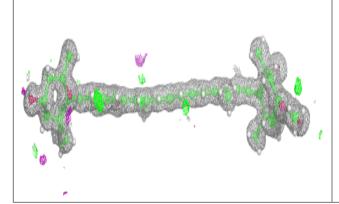


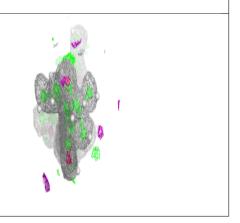


Electron density around PID D 613:

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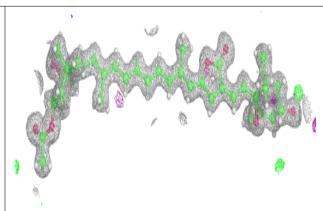


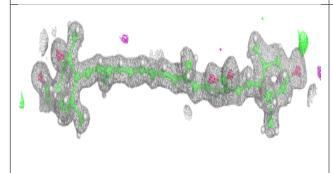


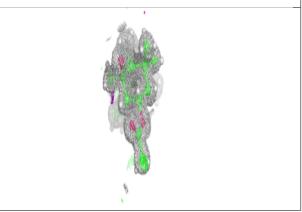


Electron density around PID D 614:

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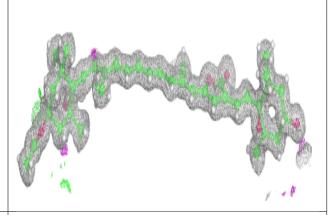


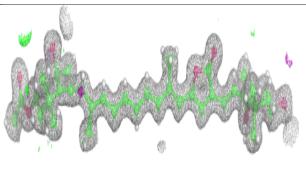


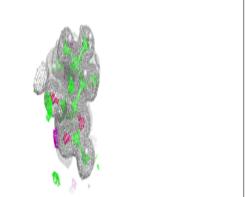


Electron density around PID C 611:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



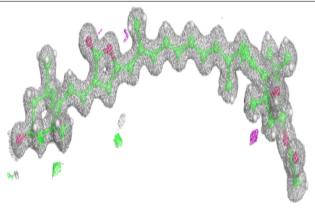


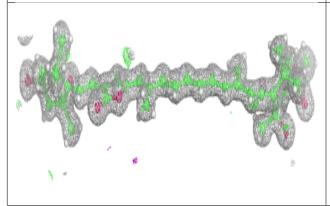


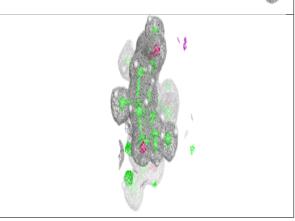


Electron density around PID C 612:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

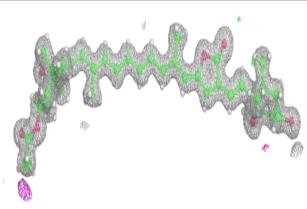


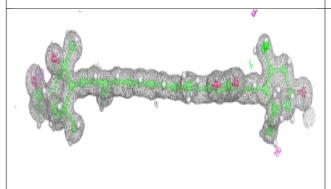


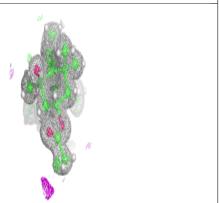


Electron density around PID C 613:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



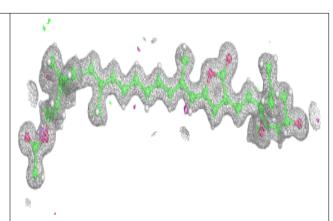


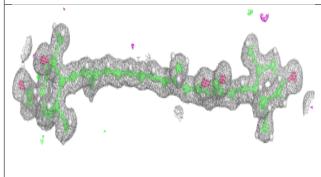


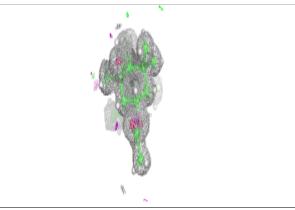


Electron density around PID C 614:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

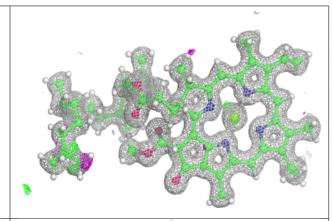


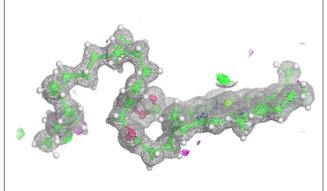


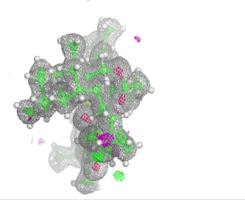


Electron density around CLA A 601:

 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



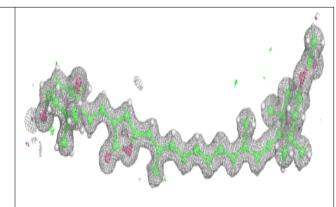


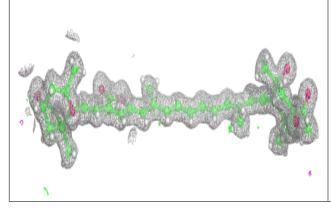


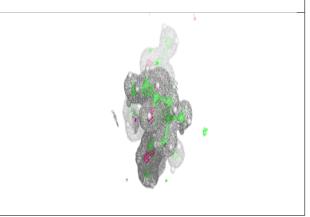


Electron density around PID D 612:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

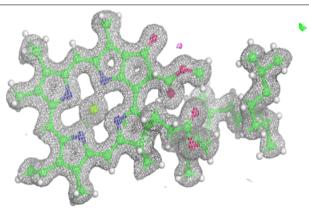


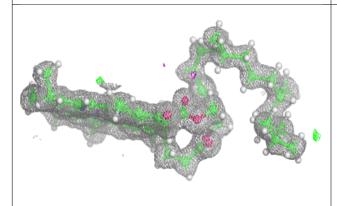


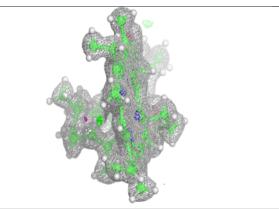


Electron density around CLA C 601:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



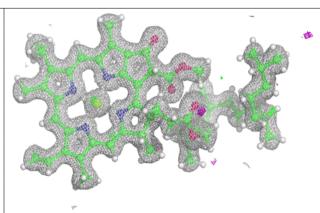


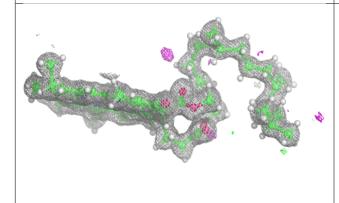


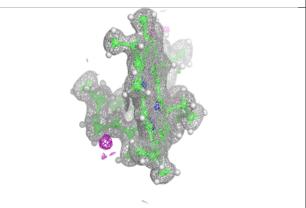


Electron density around CLA D 601:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

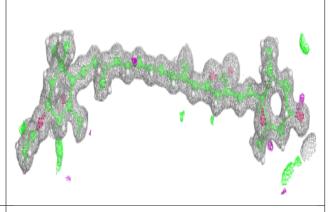


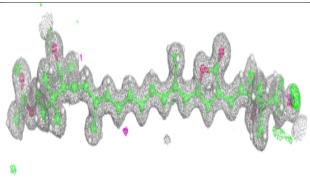


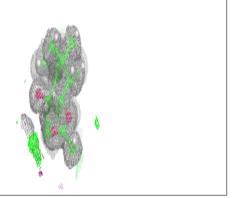


Electron density around PID A 611:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



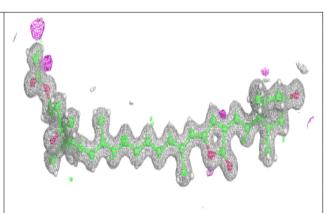


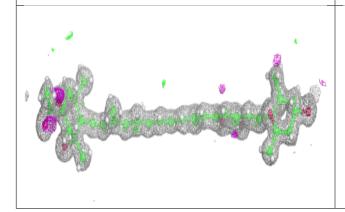


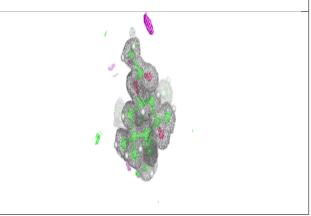


Electron density around PID A 613:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

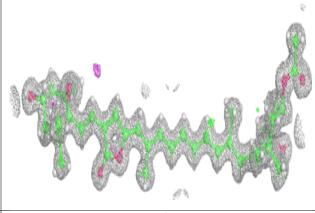


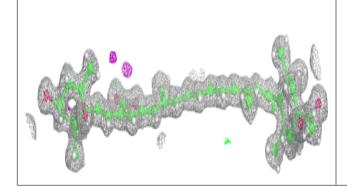


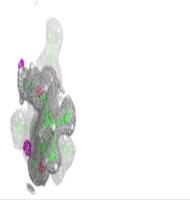


Electron density around PID A 614:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



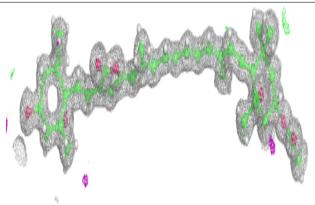


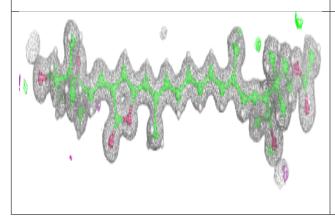


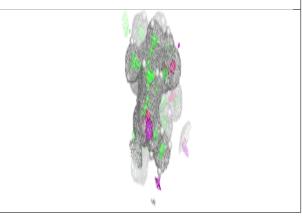


Electron density around PID B 611:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

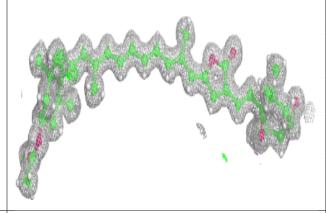


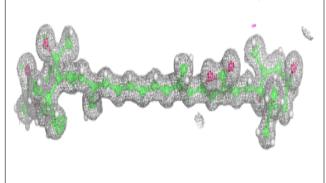


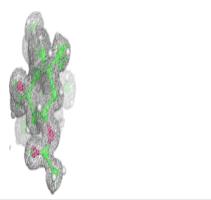


Electron density around PID B 612:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



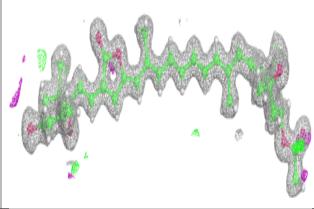


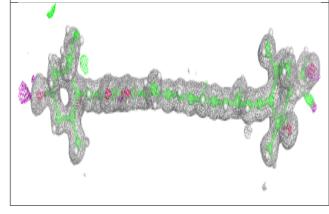


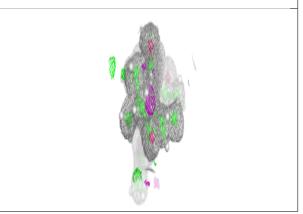


Electron density around PID B 613:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

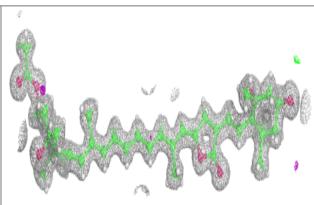


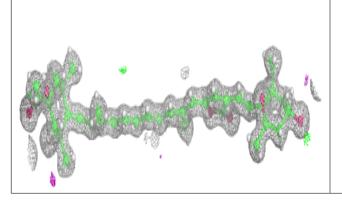


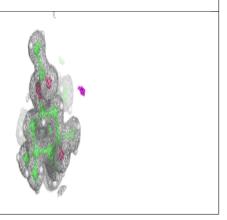


Electron density around PID B 614:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



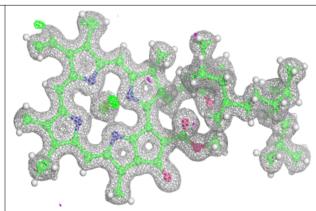


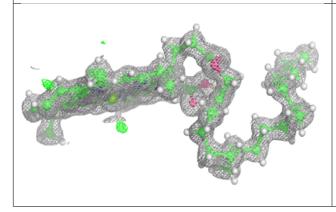


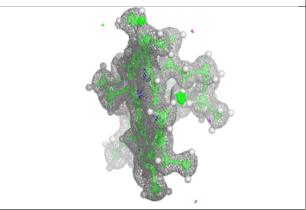


Electron density around CLA B 601:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

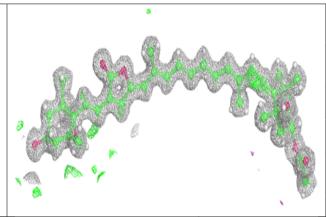


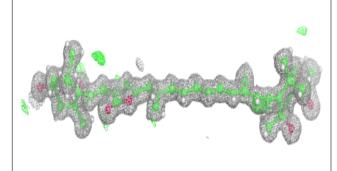


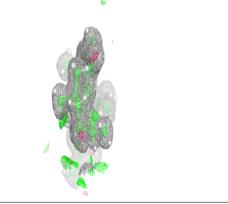


Electron density around PID A 612:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

