



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:09 am BST

PDB ID : 3A7K  
Title : Crystal structure of halorhodopsin from Natronomonas pharaonis  
Authors : Kouyama, T.  
Deposited on : 2009-09-27  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

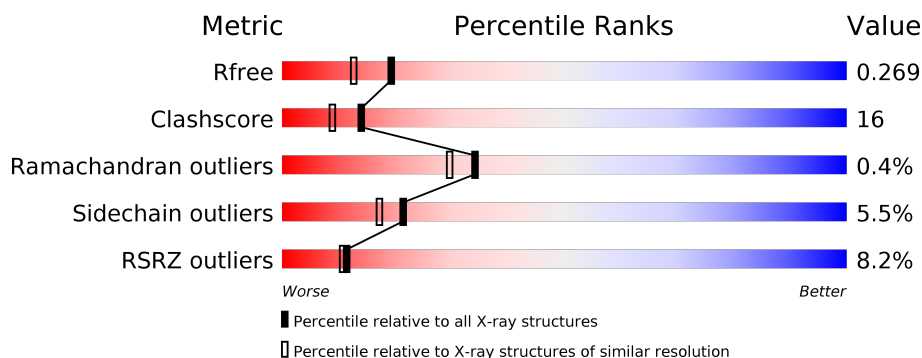
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	291	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	291	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	291	<div> <div>13%</div> <div> <div></div> <div>53%</div> <div>33%</div> <div>•</div> <div>11%</div> </div> </div>

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	22B	D	300	-	-	-	X
4	L1P	A	293	-	-	-	X
4	L1P	B	293	-	-	-	X
4	L1P	B	294	-	-	-	X
5	L2P	A	294	-	-	-	X
5	L2P	A	295	-	-	-	X
5	L2P	B	295	-	-	-	X
5	L2P	B	296	-	-	-	X
5	L2P	D	293	-	-	-	X
5	L2P	D	294	-	-	-	X
6	L3P	A	296	-	-	-	X
6	L3P	A	297	-	-	-	X
6	L3P	A	298	-	-	-	X
6	L3P	A	299	-	-	-	X
6	L3P	A	301	-	-	-	X
6	L3P	A	333	-	-	-	X
6	L3P	B	331	-	-	-	X

## 2 Entry composition [i](#)

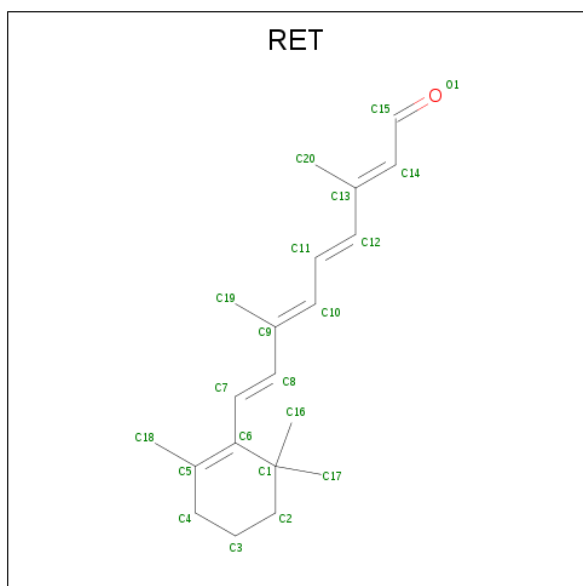
There are 8 unique types of molecules in this entry. The entry contains 6678 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Halorhodopsin.

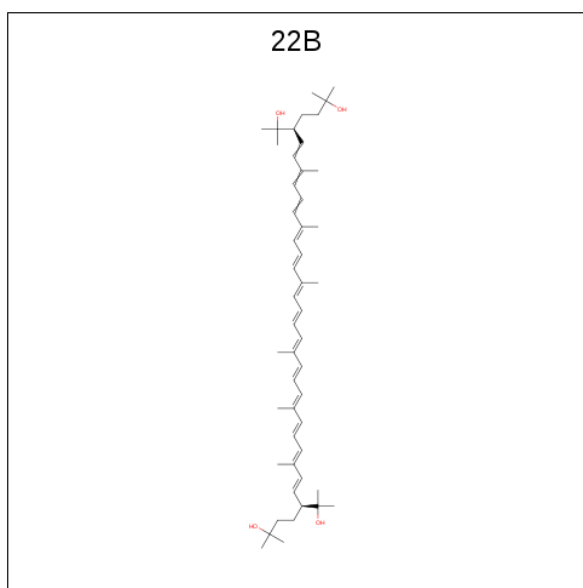
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1958	1299	298	350	11			
1	B	258	Total	C	N	O	S	0	0	0
			1952	1296	297	348	11			
1	D	259	Total	C	N	O	S	0	0	0
			1958	1299	298	350	11			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



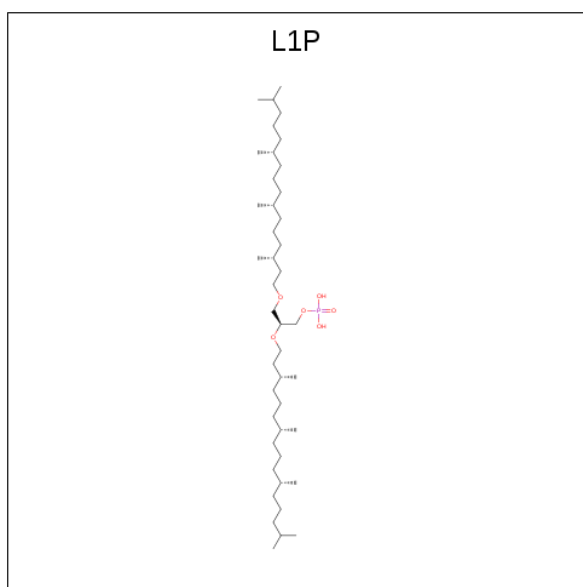
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		
2	D	1	Total	C	0	0
			20	20		

- Molecule 3 is BACTERIORUBERIN (three-letter code: 22B) (formula:  $C_{50}H_{76}O_4$ ).



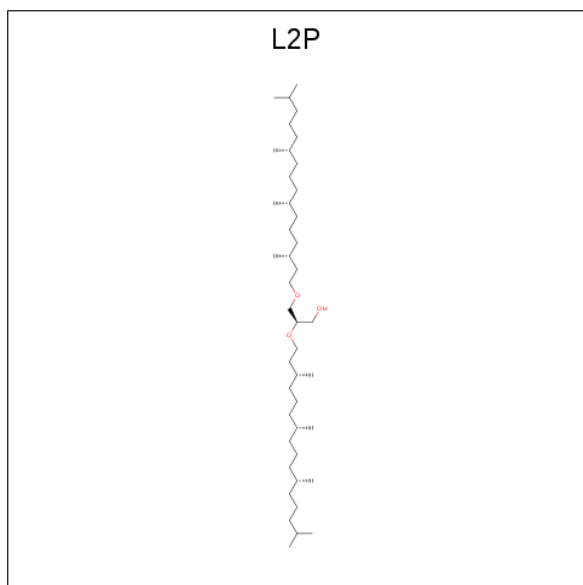
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			54	50	4		
3	B	1	Total	C	O	0	0
			54	50	4		
3	D	1	Total	C	O	0	0
			54	50	4		

- Molecule 4 is 3-PHOSPHORYL-[1,2-DI-PHYTANYL]GLYCEROL (three-letter code: L1P) (formula:  $C_{43}H_{89}O_6P$ ).



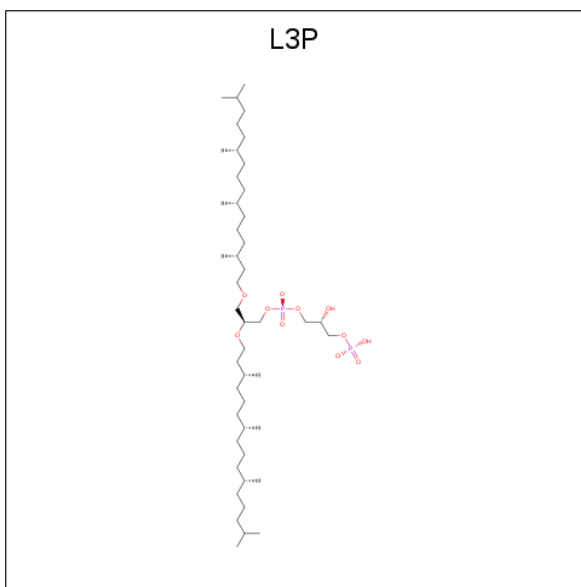
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			46	43	3		
4	B	1	Total	C	O	0	0
			46	43	3		
4	B	1	Total	C	O	0	0
			46	43	3		

- Molecule 5 is 2,3-DI-PHYTANYL-GLYCEROL (three-letter code: L2P) (formula:  $C_{43}H_{88}O_3$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			20	20		
5	A	1	Total	C	0	0
			20	20		
5	B	1	Total	C	0	0
			20	20		
5	B	1	Total	C	0	0
			20	20		
5	D	1	Total	C	0	0
			20	20		
5	D	1	Total	C	0	0
			20	20		

- Molecule 6 is 2,3-DI-O-PHYTANYL-3'-SN-GLYCERO-1-PHOSPHORYL-3'-SN-GLYCEROL-1'-PHOSPHATE (three-letter code: L3P) (formula:  $C_{46}H_{94}O_{11}P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 20 20	0	0
6	A	1	Total C 20 20	0	0
6	A	1	Total C 20 20	0	0
6	A	1	Total C 20 20	0	0
6	A	1	Total C 20 20	0	0
6	A	1	Total C 20 20	0	0
6	A	1	Total C 20 20	0	0
6	B	1	Total C 20 20	0	0
6	D	1	Total C 20 20	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Cl 2 2	0	0
7	A	2	Total Cl 2 2	0	0
7	D	2	Total Cl 2 2	0	0

- Molecule 8 is water.

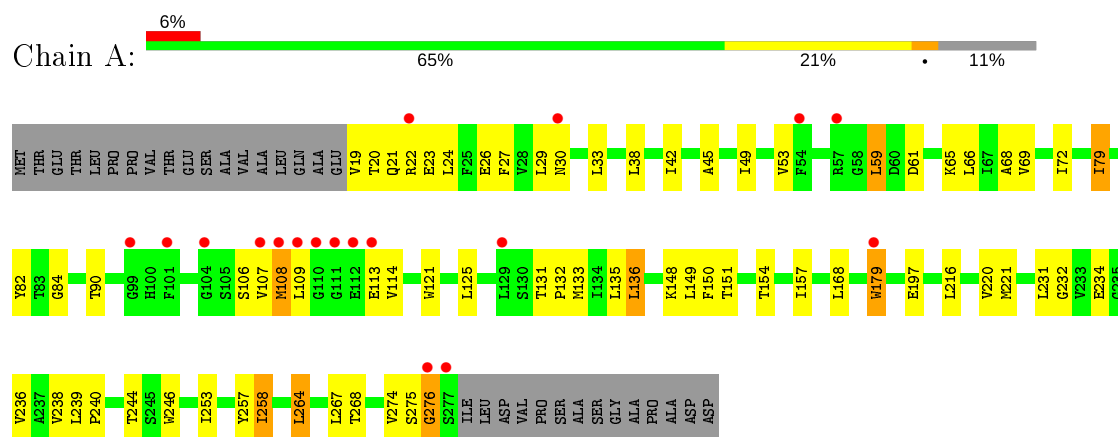
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	51	Total 51	O 51	0	0
8	B	60	Total 60	O 60	0	0
8	D	33	Total 33	O 33	0	0



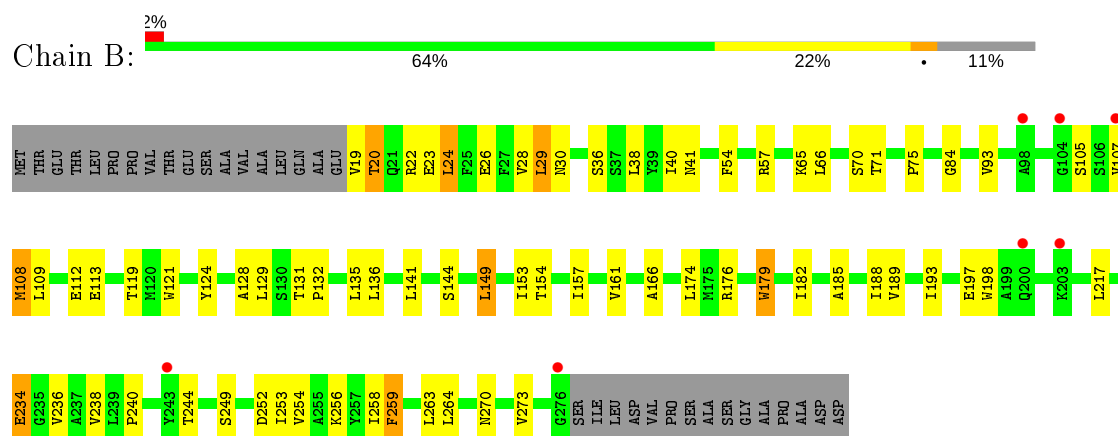
### 3 Residue-property plots [i](#)

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

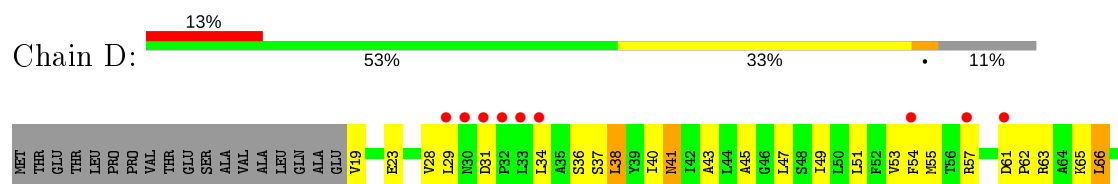
#### • Molecule 1: Halorhodopsin

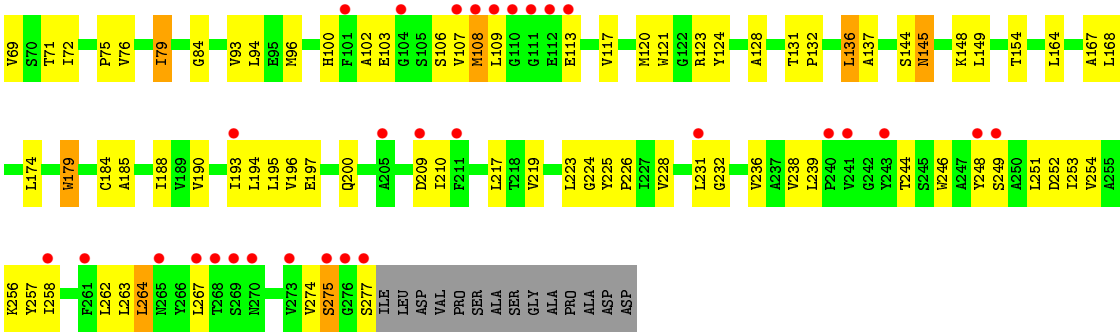


#### • Molecule 1: Halorhodopsin



#### • Molecule 1: Halorhodopsin





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.83Å 99.77Å 99.27Å 90.00° 127.67° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 46.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (15.00-2.00) 99.4 (46.57-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.274 0.243 , 0.269	Depositor DCC
$R_{free}$ test set	3975 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 78.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, L1P, 22B, RET, L2P, L3P

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	0.40	0/2004	0.59	0/2744
1	B	0.37	0/1998	0.57	1/2736 (0.0%)
1	D	0.32	0/2004	0.52	0/2744
All	All	0.37	0/6006	0.56	1/8224 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	29	LEU	N-CA-C	-5.30	96.68	111.00

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	1958	0	2012	58	0
1	B	1952	0	2007	67	0
1	D	1958	0	2012	89	0
2	A	20	0	27	0	0
2	B	20	0	27	1	0
2	D	20	0	27	0	0
3	A	54	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	54	0	76	2	0
3	D	54	0	76	0	0
4	A	46	0	87	3	0
4	B	92	0	174	4	0
5	A	40	0	78	8	0
5	B	40	0	78	7	0
5	D	40	0	78	5	0
6	A	140	0	273	2	0
6	B	20	0	39	0	0
6	D	20	0	39	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	D	2	0	0	0	0
8	A	51	0	0	1	1
8	B	60	0	0	3	0
8	D	33	0	0	3	0
All	All	6678	0	7186	215	1

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 16.

All (215) 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:A:238:VAL:HG23	1:A:239:LEU:HD13	1.51	0.92
1:A:45:ALA:HB3	1:A:79:ILE:HG23	1.60	0.83
1:A:238:VAL:HG23	1:A:239:LEU:CD1	2.14	0.78
1:A:108:MET:HA	1:A:113:GLU:HA	1.64	0.77
1:D:108:MET:HB2	1:D:113:GLU:HG3	1.68	0.76
1:D:254:VAL:HA	1:D:258:ILE:HG22	1.68	0.75
1:D:45:ALA:HB3	1:D:79:ILE:HG23	1.72	0.71
1:D:185:ALA:O	1:D:188:ILE:HG12	1.91	0.71
1:D:154:THR:HG22	5:D:294:L2P:H262	1.71	0.71
1:A:234:GLU:HG3	8:A:507:HOH:O	1.91	0.70
1:B:179:TRP:HH2	1:D:84:GLY:HA2	1.56	0.70
1:D:131:THR:OG1	1:D:132:PRO:HD3	1.92	0.70
1:D:190:VAL:O	1:D:193:ILE:HG13	1.92	0.69
1:B:254:VAL:HA	1:B:258:ILE:HG12	1.74	0.69
1:B:136:LEU:HG	5:B:295:L2P:H212	1.75	0.69
1:A:22:ARG:HG3	1:A:23:GLU:N	2.07	0.68
1:B:29:LEU:O	1:B:30:ASN:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HB3	1:B:273:VAL:HG12	1.73	0.68
1:B:236:VAL:HG13	1:B:238:VAL:HG13	1.76	0.67
1:A:253:ILE:O	1:A:258:ILE:HG23	1.95	0.67
5:A:294:L2P:H201	5:B:295:L2P:H251	1.75	0.67
1:B:270:ASN:HB3	1:B:273:VAL:CG1	2.25	0.67
1:B:20:THR:HG22	1:B:23:GLU:H	1.59	0.66
1:A:150:PHE:HD2	5:A:294:L2P:H152	1.58	0.66
1:A:29:LEU:O	1:A:30:ASN:HB2	1.95	0.66
1:D:108:MET:HA	1:D:113:GLU:HA	1.80	0.64
1:B:19:VAL:HG21	1:B:93:VAL:HG11	1.79	0.63
1:D:238:VAL:HG23	1:D:239:LEU:HD13	1.81	0.63
1:B:108:MET:HA	1:B:113:GLU:HA	1.81	0.62
1:D:149:LEU:HG	5:D:294:L2P:H151	1.80	0.62
1:D:145:ASN:C	1:D:145:ASN:HD22	2.03	0.62
1:B:270:ASN:O	1:B:273:VAL:HG12	1.99	0.62
1:D:167:ALA:HB2	8:D:519:HOH:O	1.99	0.62
1:A:236:VAL:HG13	1:A:238:VAL:HG13	1.83	0.61
1:D:43:ALA:O	1:D:47:LEU:HD13	2.00	0.61
1:A:20:THR:HG22	1:A:22:ARG:H	1.65	0.61
1:D:36:SER:O	1:D:40:ILE:HG12	2.00	0.60
1:A:84:GLY:HA2	1:D:179:TRP:HH2	1.64	0.60
1:D:123:ARG:HD2	8:D:506:HOH:O	2.01	0.60
1:D:164:LEU:O	1:D:168:LEU:HD23	2.02	0.59
1:D:253:ILE:HA	1:D:257:TYR:CD2	2.37	0.59
1:D:195:LEU:HD21	1:D:219:VAL:HG21	1.84	0.59
1:B:254:VAL:HG13	1:B:258:ILE:HD11	1.84	0.59
1:D:254:VAL:HA	1:D:258:ILE:CG2	2.33	0.59
1:A:121:TRP:HZ3	1:A:125:LEU:HD22	1.67	0.59
1:A:157:ILE:HG21	5:A:294:L2P:H241	1.84	0.59
1:A:179:TRP:HH2	1:B:84:GLY:HA2	1.67	0.59
1:A:133:MET:HE1	5:A:295:L2P:H251	1.85	0.59
1:B:179:TRP:CH2	1:D:84:GLY:HA2	2.37	0.58
1:A:20:THR:CG2	1:A:22:ARG:HG2	2.33	0.58
1:A:151:THR:HG21	3:B:300:22B:H243	1.85	0.58
1:A:264:LEU:O	1:A:268:THR:HG22	2.04	0.58
1:D:23:GLU:HB3	1:D:109:LEU:HB3	1.84	0.58
1:D:51:LEU:O	1:D:55:MET:HG3	2.03	0.58
1:B:20:THR:HG21	8:B:535:HOH:O	2.04	0.58
1:B:36:SER:O	1:B:40:ILE:HG12	2.04	0.58
1:D:66:LEU:HD11	5:D:293:L2P:H192	1.85	0.57
1:D:217:LEU:HD11	1:D:254:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ILE:HG13	1:B:259:PHE:N	2.20	0.56
1:D:193:ILE:HD12	1:D:194:LEU:N	2.21	0.56
1:A:22:ARG:HG3	1:A:23:GLU:H	1.69	0.56
1:A:20:THR:HG22	1:A:21:GLN:N	2.19	0.55
1:A:26:GLU:O	1:A:29:LEU:O	2.25	0.55
1:D:19:VAL:HG21	1:D:93:VAL:HG11	1.88	0.55
1:D:71:THR:HG21	1:D:264:LEU:HD13	1.89	0.55
1:D:29:LEU:C	1:D:31:ASP:H	2.10	0.55
4:A:293:L1P:H493	1:D:164:LEU:HD21	1.89	0.55
1:A:84:GLY:HA2	1:D:179:TRP:CH2	2.42	0.55
1:B:144:SER:OG	1:B:149:LEU:HD22	2.07	0.55
1:B:166:ALA:HB2	1:B:179:TRP:HB3	1.88	0.55
1:B:185:ALA:O	1:B:188:ILE:HG12	2.06	0.54
1:D:100:HIS:CD2	1:D:102:ALA:H	2.25	0.54
1:D:106:SER:HB3	1:D:113:GLU:HG2	1.88	0.54
1:D:28:VAL:HG13	1:D:34:LEU:HD12	1.90	0.54
1:A:33:LEU:HD22	1:A:246:TRP:HD1	1.73	0.54
1:D:54:PHE:HB3	1:D:57:ARG:NH1	2.23	0.54
1:D:65:LYS:O	1:D:69:VAL:HG23	2.08	0.53
1:B:70:SER:OG	1:B:136:LEU:HD12	2.09	0.53
1:D:196:VAL:O	1:D:200:GLN:HG2	2.08	0.53
1:A:20:THR:HG21	1:A:22:ARG:HG2	1.91	0.52
1:D:63:ARG:HH11	1:D:63:ARG:HG2	1.75	0.52
1:A:133:MET:HE1	5:A:295:L2P:H271	1.92	0.52
1:A:136:LEU:HD21	5:A:295:L2P:H201	1.92	0.52
1:B:240:PRO:O	1:B:244:THR:HG22	2.10	0.51
1:B:54:PHE:O	1:B:57:ARG:HG2	2.09	0.51
1:D:128:ALA:O	1:D:132:PRO:HG2	2.10	0.51
1:D:148:LYS:HE2	1:D:197:GLU:OE1	2.11	0.51
1:B:129:LEU:HA	5:B:295:L2P:H293	1.92	0.51
1:A:275:SER:O	1:A:276:GLY:C	2.49	0.51
1:D:38:LEU:HD11	1:D:120:MET:HE1	1.91	0.51
1:D:154:THR:HG22	5:D:294:L2P:C26	2.39	0.51
1:A:20:THR:HG21	1:A:22:ARG:NH1	2.25	0.50
1:D:145:ASN:ND2	1:D:148:LYS:H	2.09	0.50
1:B:93:VAL:HG13	1:B:93:VAL:O	2.10	0.50
1:B:29:LEU:O	1:B:30:ASN:CB	2.59	0.50
1:B:109:LEU:N	1:B:109:LEU:HD22	2.26	0.50
1:D:144:SER:HB3	1:D:149:LEU:CD2	2.41	0.50
1:D:49:ILE:O	1:D:53:VAL:HG23	2.12	0.50
1:B:182:ILE:HG13	8:D:532:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ASP:OD2	1:D:275:SER:HA	2.12	0.50
1:D:238:VAL:HG23	1:D:239:LEU:CD1	2.42	0.49
1:D:29:LEU:C	1:D:31:ASP:N	2.66	0.49
1:B:19:VAL:CG2	1:B:93:VAL:HG11	2.43	0.49
1:D:232:GLY:CA	1:D:244:THR:HG21	2.43	0.49
1:A:240:PRO:O	1:A:244:THR:HG23	2.13	0.49
1:A:107:VAL:HG12	1:A:114:VAL:O	2.13	0.49
1:D:232:GLY:HA2	1:D:244:THR:HG21	1.94	0.49
1:B:108:MET:HA	1:B:112:GLU:O	2.13	0.48
1:B:141:LEU:HD22	1:B:263:LEU:HD13	1.96	0.48
1:A:20:THR:CG2	1:A:21:GLN:N	2.76	0.48
6:A:298:L3P:H222	1:D:174:LEU:HD23	1.96	0.48
1:A:29:LEU:O	1:A:30:ASN:CB	2.59	0.48
1:D:108:MET:HB2	1:D:113:GLU:CG	2.42	0.48
1:D:76:VAL:O	1:D:79:ILE:HG13	2.14	0.48
1:A:49:ILE:O	1:A:53:VAL:HG23	2.14	0.48
1:B:249:SER:O	1:B:253:ILE:HG13	2.14	0.47
1:D:109:LEU:N	1:D:109:LEU:HD22	2.29	0.47
1:D:62:PRO:HG2	1:D:277:SER:HB3	1.96	0.47
1:D:121:TRP:HA	1:D:124:TYR:CD2	2.49	0.47
1:D:184:CYS:O	1:D:188:ILE:HG23	2.14	0.47
1:A:231:LEU:HD22	1:A:238:VAL:HG21	1.97	0.47
1:B:217:LEU:C	1:B:217:LEU:HD23	2.35	0.47
1:A:19:VAL:HG23	1:A:19:VAL:O	2.15	0.47
1:B:26:GLU:O	1:B:29:LEU:O	2.33	0.47
1:B:193:ILE:HA	1:B:197:GLU:HG2	1.97	0.46
1:B:254:VAL:HG13	1:B:258:ILE:CD1	2.46	0.46
1:D:100:HIS:O	1:D:103:GLU:HB3	2.16	0.46
1:B:107:VAL:O	1:B:108:MET:HB2	2.15	0.46
1:A:231:LEU:O	1:A:238:VAL:HG22	2.15	0.46
1:A:65:LYS:O	1:A:69:VAL:HG23	2.16	0.46
1:B:153:ILE:HG21	5:B:295:L2P:H243	1.97	0.46
1:A:131:THR:N	1:A:132:PRO:CD	2.79	0.46
1:B:131:THR:N	1:B:132:PRO:CD	2.79	0.46
1:D:45:ALA:O	1:D:49:ILE:HG13	2.16	0.46
1:B:157:ILE:HG21	5:B:296:L2P:H241	1.97	0.45
2:B:292:RET:H181	2:B:292:RET:H7	1.81	0.45
1:D:258:ILE:O	1:D:262:LEU:HG	2.17	0.45
1:A:45:ALA:CB	1:A:79:ILE:HG23	2.40	0.45
1:D:239:LEU:HB3	1:D:244:THR:HG23	1.98	0.45
1:D:41:ASN:HA	1:D:41:ASN:HD22	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LYS:HD3	3:B:300:22B:H253	1.99	0.45
1:D:219:VAL:O	1:D:223:LEU:HG	2.16	0.45
1:B:188:ILE:HG13	1:B:189:VAL:N	2.31	0.45
1:D:136:LEU:HD21	5:D:293:L2P:H191	1.99	0.45
1:A:33:LEU:HD22	1:A:246:TRP:CD1	2.51	0.45
1:B:20:THR:CG2	1:B:22:ARG:H	2.31	0.44
1:B:144:SER:HB2	1:B:198:TRP:NE1	2.32	0.44
4:A:293:L1P:H571	4:A:293:L1P:H543	1.99	0.44
1:B:28:VAL:C	1:B:29:LEU:O	2.53	0.44
1:D:107:VAL:HG13	1:D:108:MET:N	2.32	0.44
1:D:225:TYR:N	1:D:226:PRO:HD2	2.33	0.44
1:D:267:LEU:CD1	1:D:274:VAL:HG21	2.48	0.44
1:A:59:LEU:HB3	1:A:65:LYS:HG2	1.98	0.44
1:B:154:THR:HG22	5:B:296:L2P:H202	2.00	0.44
1:D:224:GLY:O	1:D:228:VAL:HG23	2.18	0.44
1:D:61:ASP:OD1	1:D:277:SER:HB2	2.17	0.44
1:A:267:LEU:CD1	1:A:274:VAL:HG21	2.48	0.44
4:B:294:L1P:H543	4:B:294:L1P:H571	1.98	0.44
1:D:93:VAL:HA	1:D:117:VAL:O	2.18	0.44
1:D:145:ASN:C	1:D:145:ASN:ND2	2.70	0.44
1:D:28:VAL:HG13	1:D:34:LEU:CD1	2.48	0.44
1:D:37:SER:HB3	1:D:246:TRP:CD1	2.53	0.44
1:D:267:LEU:HD11	1:D:274:VAL:HG21	2.00	0.43
1:B:193:ILE:HA	1:B:197:GLU:CG	2.47	0.43
1:D:94:LEU:HD11	1:D:168:LEU:HD13	2.00	0.43
1:D:193:ILE:C	1:D:193:ILE:HD12	2.39	0.43
1:A:27:PHE:HB2	1:A:109:LEU:HD12	1.99	0.43
1:B:176:ARG:HH22	1:B:234:GLU:HG3	1.82	0.43
1:D:100:HIS:CD2	1:D:102:ALA:HB3	2.54	0.43
1:B:119:THR:HG23	1:B:234:GLU:OE1	2.19	0.43
1:D:145:ASN:HD21	1:D:148:LYS:HG3	1.84	0.43
4:B:293:L1P:H451	4:B:293:L1P:H18	2.01	0.43
1:A:232:GLY:HA2	1:A:239:LEU:HB2	2.01	0.42
1:B:128:ALA:O	1:B:132:PRO:HG2	2.19	0.42
1:B:144:SER:HG	1:B:149:LEU:HD22	1.84	0.42
4:B:293:L1P:H521	4:B:293:L1P:H23	2.01	0.42
1:D:209:ASP:CG	1:D:210:ILE:H	2.22	0.42
1:A:179:TRP:CH2	1:B:84:GLY:HA2	2.50	0.42
1:A:154:THR:HG22	5:A:294:L2P:H202	2.01	0.42
1:A:33:LEU:HD23	6:A:333:L3P:H152	2.01	0.42
1:B:71:THR:HG23	8:B:521:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:TRP:HA	1:B:124:TYR:CD2	2.54	0.42
1:D:252:ASP:O	1:D:256:LYS:HB2	2.20	0.42
1:A:61:ASP:O	1:A:65:LYS:HG3	2.20	0.42
1:D:249:SER:O	1:D:253:ILE:HG13	2.19	0.42
1:D:63:ARG:NH1	1:D:63:ARG:HG2	2.35	0.42
1:D:75:PRO:O	1:D:79:ILE:HG12	2.19	0.42
1:A:79:ILE:H	1:A:79:ILE:HG13	1.58	0.41
1:B:109:LEU:O	1:B:112:GLU:HG2	2.20	0.41
1:B:252:ASP:O	1:B:256:LYS:HB2	2.20	0.41
1:D:248:TYR:HA	1:D:251:LEU:HD12	2.01	0.41
1:D:137:ALA:HB1	1:D:263:LEU:HD21	2.02	0.41
1:A:42:ILE:HG13	1:A:82:TYR:HB3	2.02	0.41
1:D:231:LEU:HA	1:D:236:VAL:HG12	2.01	0.41
1:B:193:ILE:C	1:B:193:ILE:HD12	2.41	0.41
1:B:20:THR:HG23	1:B:22:ARG:H	1.86	0.41
1:B:259:PHE:C	1:B:259:PHE:CD1	2.93	0.41
1:B:41:ASN:HD22	1:B:41:ASN:HA	1.63	0.41
1:D:96:MET:HG3	1:D:100:HIS:CD2	2.56	0.41
1:A:220:VAL:HG12	1:A:221:MET:CE	2.51	0.41
1:A:148:LYS:HD3	1:A:197:GLU:HB3	2.02	0.41
1:A:68:ALA:O	1:A:72:ILE:HG13	2.21	0.41
1:B:20:THR:HG22	1:B:22:ARG:N	2.36	0.41
1:A:106:SER:HB3	1:A:113:GLU:CG	2.51	0.41
1:A:253:ILE:HA	1:A:257:TYR:CD2	2.56	0.40
1:A:133:MET:CE	5:A:295:L2P:H271	2.51	0.40
1:B:105:SER:HB3	8:B:525:HOH:O	2.20	0.40
1:B:270:ASN:HB3	1:B:273:VAL:HG11	2.03	0.40
1:B:71:THR:O	1:B:75:PRO:HD2	2.20	0.40
1:D:72:ILE:O	1:D:76:VAL:HG23	2.21	0.40
5:B:295:L2P:H242	5:B:296:L2P:H143	2.03	0.40
1:A:90:THR:HG21	4:A:293:L1P:H242	2.03	0.40
1:B:236:VAL:HG22	1:B:236:VAL:O	2.22	0.40
1:B:24:LEU:HD12	1:B:24:LEU:HA	1.82	0.40
1:B:161:VAL:HG11	4:B:294:L1P:H292	2.03	0.40

All (1) 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)
8:A:600:HOH:O	8:A:600:HOH:O 2_656	1.13	1.07

## 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	257/291 (88%)	247 (96%)	9 (4%)	1 (0%)	34	30
1	B	256/291 (88%)	249 (97%)	7 (3%)	0	100	100
1	D	257/291 (88%)	245 (95%)	10 (4%)	2 (1%)	19	13
All	All	770/873 (88%)	741 (96%)	26 (3%)	3 (0%)	34	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	275	SER
1	A	276	GLY
1	D	108	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	208/233 (89%)	194 (93%)	14 (7%)	16	11
1	B	207/233 (89%)	195 (94%)	12 (6%)	20	15
1	D	208/233 (89%)	200 (96%)	8 (4%)	33	31
All	All	623/699 (89%)	589 (94%)	34 (6%)	21	17

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	38	LEU
1	A	59	LEU
1	A	66	LEU
1	A	79	ILE
1	A	108	MET
1	A	135	LEU
1	A	136	LEU
1	A	149	LEU
1	A	168	LEU
1	A	179	TRP
1	A	216	LEU
1	A	258	ILE
1	A	264	LEU
1	B	20	THR
1	B	24	LEU
1	B	38	LEU
1	B	66	LEU
1	B	108	MET
1	B	135	LEU
1	B	149	LEU
1	B	174	LEU
1	B	179	TRP
1	B	234	GLU
1	B	259	PHE
1	B	264	LEU
1	D	38	LEU
1	D	41	ASN
1	D	66	LEU
1	D	79	ILE
1	D	136	LEU
1	D	145	ASN
1	D	179	TRP
1	D	264	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	B	41	ASN
1	B	265	ASN
1	D	41	ASN
1	D	100	HIS

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Mol	Chain	Res	Type
1	D	145	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	L1P	A	293	-	45,45,49	1.83	15 (33%)	51,53,60	1.30	6 (11%)
5	L2P	B	295	-	19,19,45	1.86	7 (36%)	22,22,53	0.87	1 (4%)
6	L3P	A	299	-	19,19,58	1.97	8 (42%)	22,22,73	1.32	3 (13%)
5	L2P	D	293	-	19,19,45	1.92	7 (36%)	22,22,53	0.92	1 (4%)
5	L2P	A	295	-	19,19,45	1.93	7 (36%)	22,22,53	0.87	2 (9%)
5	L2P	D	294	-	19,19,45	1.92	7 (36%)	22,22,53	0.91	0
2	RET	D	292	1	20,20,21	2.26	5 (25%)	27,27,28	1.82	10 (37%)
4	L1P	B	294	-	45,45,49	1.82	15 (33%)	51,53,60	1.31	6 (11%)
5	L2P	A	294	-	19,19,45	1.89	7 (36%)	22,22,53	0.98	1 (4%)
4	L1P	B	293	-	45,45,49	1.80	13 (28%)	51,53,60	1.36	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	L3P	A	298	-	19,19,58	1.94	8 (42%)	22,22,73	1.20	3 (13%)
3	22B	D	300	-	51,53,53	2.99	19 (37%)	62,72,72	2.08	19 (30%)
6	L3P	B	331	-	19,19,58	1.95	8 (42%)	22,22,73	1.23	3 (13%)
6	L3P	A	331	-	19,19,58	1.98	8 (42%)	22,22,73	1.23	3 (13%)
6	L3P	A	333	-	19,19,58	1.93	8 (42%)	22,22,73	1.18	1 (4%)
2	RET	A	292	1	20,20,21	2.21	5 (25%)	27,27,28	1.62	7 (25%)
6	L3P	D	330	-	19,19,58	1.95	8 (42%)	22,22,73	1.17	2 (9%)
6	L3P	A	301	-	19,19,58	1.95	8 (42%)	22,22,73	1.22	3 (13%)
3	22B	B	300	-	51,53,53	3.22	20 (39%)	62,72,72	1.98	19 (30%)
2	RET	B	292	1	20,20,21	2.23	5 (25%)	27,27,28	1.69	5 (18%)
5	L2P	B	296	-	19,19,45	1.90	7 (36%)	22,22,53	0.96	1 (4%)
6	L3P	A	296	-	19,19,58	1.94	8 (42%)	22,22,73	1.21	3 (13%)
6	L3P	A	297	-	19,19,58	2.02	8 (42%)	22,22,73	1.27	3 (13%)
3	22B	A	300	-	51,53,53	3.12	19 (37%)	62,72,72	2.06	21 (33%)

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	L1P	A	293	-	-	17/51/51/55	-
5	L2P	B	295	-	-	3/20/20/51	-
6	L3P	A	299	-	-	6/20/20/67	-
5	L2P	D	293	-	-	2/20/20/51	-
5	L2P	A	295	-	-	0/20/20/51	-
5	L2P	D	294	-	-	3/20/20/51	-
2	RET	D	292	1	-	0/13/30/31	0/1/1/1
4	L1P	B	294	-	-	19/51/51/55	-
5	L2P	A	294	-	-	1/20/20/51	-
4	L1P	B	293	-	-	21/51/51/55	-
6	L3P	A	298	-	-	10/20/20/67	-
3	22B	D	300	-	-	14/65/65/65	-
6	L3P	B	331	-	-	6/20/20/67	-
6	L3P	A	331	-	-	9/20/20/67	-
6	L3P	A	333	-	-	6/20/20/67	-
2	RET	A	292	1	-	0/13/30/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	L3P	D	330	-	-	8/20/20/67	-
6	L3P	A	301	-	-	7/20/20/67	-
3	22B	B	300	-	-	6/65/65/65	-
2	RET	B	292	1	-	0/13/30/31	0/1/1/1
5	L2P	B	296	-	-	3/20/20/51	-
6	L3P	A	296	-	-	6/20/20/67	-
6	L3P	A	297	-	-	3/20/20/67	-
3	22B	A	300	-	-	9/65/65/65	-

All (230) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	22B	C2-C3	12.23	1.63	1.49
3	B	300	22B	C2-C3	12.20	1.63	1.49
3	D	300	22B	C2-C3	12.00	1.63	1.49
3	B	300	22B	C33-C32	10.35	1.61	1.49
3	A	300	22B	C33-C32	9.22	1.60	1.49
3	D	300	22B	C33-C32	8.93	1.59	1.49
3	B	300	22B	C34-C33	7.30	1.63	1.53
3	A	300	22B	C34-C33	7.09	1.63	1.53
2	D	292	RET	C1-C6	6.09	1.62	1.53
2	A	292	RET	C1-C6	5.86	1.61	1.53
2	B	292	RET	C1-C6	5.81	1.61	1.53
3	D	300	22B	C34-C33	4.97	1.60	1.53
3	A	300	22B	C21-C2	4.61	1.59	1.53
3	D	300	22B	C21-C2	4.54	1.59	1.53
2	B	292	RET	C14-C13	4.50	1.37	1.33
3	B	300	22B	C49-C47	4.43	1.59	1.52
3	D	300	22B	C49-C47	4.42	1.59	1.52
3	A	300	22B	C49-C47	4.34	1.59	1.52
2	D	292	RET	C5-C6	4.29	1.41	1.34
2	D	292	RET	C14-C13	4.27	1.37	1.33
2	A	292	RET	C5-C6	4.26	1.41	1.34
3	B	300	22B	C21-C2	4.21	1.59	1.53
3	B	300	22B	C16-C1	4.08	1.59	1.52
3	A	300	22B	C16-C1	3.99	1.59	1.52
3	A	300	22B	O27-C23	3.92	1.54	1.44
3	D	300	22B	O27-C23	3.88	1.54	1.44
3	B	300	22B	O27-C23	3.86	1.54	1.44
2	B	292	RET	C5-C6	3.83	1.41	1.34
3	D	300	22B	C16-C1	3.82	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	292	RET	C14-C13	3.82	1.36	1.33
4	A	293	L1P	C3-C2	3.79	1.60	1.51
4	B	294	L1P	C3-C2	3.78	1.60	1.51
4	B	293	L1P	C3-C2	3.68	1.60	1.51
3	B	300	22B	C19-C9	3.68	1.58	1.50
3	A	300	22B	C19-C9	3.62	1.58	1.50
3	D	300	22B	C19-C9	3.61	1.58	1.50
3	B	300	22B	C48-C47	3.53	1.58	1.52
3	A	300	22B	C48-C47	3.50	1.58	1.52
3	D	300	22B	C48-C47	3.47	1.58	1.52
3	A	300	22B	C30-C29	3.22	1.57	1.50
3	A	300	22B	C17-C1	3.20	1.57	1.52
3	B	300	22B	C30-C29	3.19	1.57	1.50
4	B	293	L1P	C12-C11	3.15	1.61	1.50
4	B	294	L1P	C12-C11	3.13	1.61	1.50
3	D	300	22B	C30-C29	3.13	1.57	1.50
3	D	300	22B	C17-C1	3.12	1.57	1.52
3	B	300	22B	C26-C39	3.10	1.57	1.50
4	A	293	L1P	C12-C11	3.06	1.61	1.50
3	A	300	22B	C26-C39	3.05	1.57	1.50
2	B	292	RET	C7-C6	3.04	1.55	1.45
5	D	293	L2P	C15-C13	3.03	1.68	1.52
3	B	300	22B	C17-C1	3.03	1.57	1.52
5	B	295	L2P	C15-C13	2.98	1.68	1.52
6	A	331	L3P	C15-C13	2.98	1.68	1.52
6	B	331	L3P	C15-C13	2.97	1.68	1.52
5	A	295	L2P	C15-C13	2.95	1.68	1.52
6	A	297	L3P	C26-C27	2.95	1.64	1.52
3	D	300	22B	C26-C39	2.95	1.57	1.50
6	A	299	L3P	C15-C13	2.94	1.68	1.52
6	A	301	L3P	C15-C13	2.93	1.68	1.52
6	A	297	L3P	C15-C13	2.93	1.68	1.52
3	A	300	22B	C22-C21	2.93	1.61	1.53
3	B	300	22B	C20-C13	2.92	1.56	1.50
5	D	294	L2P	C15-C13	2.92	1.67	1.52
6	D	330	L3P	C15-C13	2.92	1.67	1.52
6	A	296	L3P	C15-C13	2.92	1.67	1.52
3	A	300	22B	C20-C13	2.91	1.56	1.50
6	A	298	L3P	C15-C13	2.90	1.67	1.52
5	B	296	L2P	C15-C13	2.89	1.67	1.52
4	A	293	L1P	C56-C55	2.88	1.64	1.52
2	D	292	RET	C7-C6	2.87	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	294	L1P	C55-C53	2.86	1.67	1.52
6	A	333	L3P	C15-C13	2.86	1.67	1.52
4	A	293	L1P	C55-C53	2.86	1.67	1.52
5	D	293	L2P	C14-C13	2.85	1.61	1.52
5	A	294	L2P	C14-C13	2.85	1.61	1.52
3	D	300	22B	C20-C13	2.84	1.56	1.50
3	D	300	22B	C22-C21	2.84	1.61	1.53
3	B	300	22B	C22-C21	2.83	1.61	1.53
5	A	295	L2P	C26-C27	2.83	1.64	1.52
5	A	294	L2P	C15-C13	2.82	1.67	1.52
4	B	294	L1P	C56-C55	2.81	1.64	1.52
5	A	295	L2P	C14-C13	2.80	1.61	1.52
4	B	294	L1P	C54-C53	2.80	1.61	1.52
4	B	293	L1P	C25-C23	2.78	1.67	1.52
5	D	294	L2P	C14-C13	2.78	1.61	1.52
6	A	299	L3P	C26-C27	2.78	1.64	1.52
4	B	294	L1P	C25-C23	2.78	1.67	1.52
6	A	299	L3P	C25-C23	2.78	1.67	1.52
4	B	293	L1P	C55-C53	2.76	1.67	1.52
3	B	300	22B	C28-C29	2.76	1.39	1.35
5	B	296	L2P	C14-C13	2.76	1.61	1.52
5	B	295	L2P	C14-C13	2.75	1.61	1.52
6	A	297	L3P	C19-C18	2.75	1.61	1.52
2	A	292	RET	C2-C3	-2.74	1.45	1.52
4	A	293	L1P	C54-C53	2.72	1.61	1.52
3	B	300	22B	C50-C43	2.71	1.56	1.50
4	B	293	L1P	C56-C55	2.71	1.63	1.52
6	A	297	L3P	C25-C23	2.70	1.66	1.52
3	D	300	22B	C50-C43	2.70	1.56	1.50
3	D	300	22B	C18-C5	2.70	1.56	1.50
6	A	333	L3P	C26-C27	2.68	1.63	1.52
4	B	293	L1P	C15-C13	2.68	1.66	1.52
4	A	293	L1P	C15-C13	2.68	1.66	1.52
6	A	301	L3P	C26-C27	2.66	1.63	1.52
3	A	300	22B	C50-C43	2.66	1.56	1.50
4	A	293	L1P	C25-C23	2.66	1.66	1.52
6	A	331	L3P	C26-C27	2.65	1.63	1.52
2	A	292	RET	C7-C6	2.65	1.54	1.45
6	D	330	L3P	C25-C23	2.65	1.66	1.52
6	A	331	L3P	C14-C13	2.65	1.61	1.52
6	D	330	L3P	C26-C27	2.65	1.63	1.52
6	A	301	L3P	C25-C23	2.64	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	331	L3P	C26-C27	2.64	1.63	1.52
6	A	298	L3P	C26-C27	2.64	1.63	1.52
6	A	296	L3P	C14-C13	2.63	1.61	1.52
6	A	331	L3P	C25-C23	2.63	1.66	1.52
4	B	294	L1P	C14-C13	2.63	1.61	1.52
6	A	299	L3P	C14-C13	2.62	1.61	1.52
5	D	294	L2P	C26-C27	2.62	1.63	1.52
6	A	298	L3P	C25-C23	2.62	1.66	1.52
6	A	331	L3P	C19-C18	2.62	1.61	1.52
6	B	331	L3P	C25-C23	2.62	1.66	1.52
4	B	293	L1P	C14-C13	2.61	1.61	1.52
4	B	294	L1P	C15-C13	2.61	1.66	1.52
6	A	333	L3P	C25-C23	2.61	1.66	1.52
6	A	301	L3P	C14-C13	2.61	1.61	1.52
6	A	301	L3P	C19-C18	2.61	1.61	1.52
6	B	331	L3P	C19-C18	2.60	1.61	1.52
6	D	330	L3P	C14-C13	2.60	1.61	1.52
6	A	296	L3P	C25-C23	2.59	1.66	1.52
6	A	333	L3P	C19-C18	2.59	1.61	1.52
4	B	294	L1P	C26-C27	2.59	1.63	1.52
2	B	292	RET	C2-C3	-2.59	1.46	1.52
6	A	298	L3P	C14-C13	2.59	1.61	1.52
6	A	296	L3P	C26-C27	2.58	1.63	1.52
6	A	333	L3P	C17-C18	2.58	1.66	1.52
6	B	331	L3P	C17-C18	2.58	1.66	1.52
3	A	300	22B	C18-C5	2.58	1.56	1.50
6	A	331	L3P	C17-C18	2.57	1.66	1.52
6	D	330	L3P	C19-C18	2.56	1.60	1.52
6	A	297	L3P	C17-C18	2.56	1.66	1.52
5	D	294	L2P	C25-C23	2.56	1.66	1.52
4	B	293	L1P	C19-C18	2.56	1.60	1.52
4	A	293	L1P	C14-C13	2.55	1.60	1.52
5	B	296	L2P	C26-C27	2.55	1.63	1.52
4	B	294	L1P	C19-C18	2.55	1.60	1.52
4	B	293	L1P	C26-C27	2.55	1.63	1.52
4	A	293	L1P	C19-C18	2.54	1.60	1.52
2	D	292	RET	C2-C3	-2.54	1.46	1.52
5	D	294	L2P	C26-C25	2.54	1.63	1.52
6	A	298	L3P	C19-C18	2.54	1.60	1.52
4	A	293	L1P	C26-C27	2.54	1.63	1.52
5	D	293	L2P	C25-C23	2.53	1.65	1.52
4	B	294	L1P	C26-C25	2.53	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	296	L3P	C17-C18	2.53	1.65	1.52
6	A	333	L3P	C14-C13	2.52	1.60	1.52
4	B	293	L1P	C54-C53	2.52	1.60	1.52
5	A	295	L2P	C25-C23	2.52	1.65	1.52
5	B	296	L2P	C25-C23	2.52	1.65	1.52
6	B	331	L3P	C14-C13	2.52	1.60	1.52
4	B	294	L1P	O1-C11	2.51	1.52	1.42
6	A	296	L3P	C19-C18	2.51	1.60	1.52
6	A	299	L3P	C26-C25	2.51	1.62	1.52
6	D	330	L3P	C17-C18	2.51	1.65	1.52
6	A	297	L3P	C14-C13	2.51	1.60	1.52
4	B	293	L1P	O1-C11	2.50	1.52	1.42
4	B	293	L1P	C26-C25	2.50	1.62	1.52
5	A	294	L2P	C25-C23	2.48	1.65	1.52
6	A	297	L3P	C26-C25	2.46	1.62	1.52
4	A	293	L1P	C17-C18	2.45	1.65	1.52
6	A	299	L3P	C19-C18	2.45	1.60	1.52
5	B	296	L2P	C17-C18	2.45	1.65	1.52
4	B	293	L1P	C17-C18	2.45	1.65	1.52
4	A	293	L1P	O1-C11	2.45	1.52	1.42
6	A	301	L3P	C17-C18	2.45	1.65	1.52
5	B	295	L2P	C26-C27	2.45	1.62	1.52
5	A	294	L2P	C26-C27	2.44	1.62	1.52
6	A	298	L3P	C17-C18	2.44	1.65	1.52
5	A	295	L2P	C26-C25	2.44	1.62	1.52
4	B	294	L1P	C17-C18	2.43	1.65	1.52
6	A	331	L3P	C26-C25	2.43	1.62	1.52
5	D	293	L2P	C26-C27	2.42	1.62	1.52
6	D	330	L3P	C26-C25	2.41	1.62	1.52
6	A	333	L3P	C26-C25	2.41	1.62	1.52
5	D	293	L2P	C19-C18	2.41	1.60	1.52
4	A	293	L1P	C26-C25	2.41	1.62	1.52
5	A	295	L2P	C19-C18	2.41	1.60	1.52
5	D	294	L2P	C19-C18	2.40	1.60	1.52
5	D	293	L2P	C17-C18	2.40	1.65	1.52
6	A	301	L3P	C26-C25	2.39	1.62	1.52
5	D	294	L2P	C17-C18	2.38	1.65	1.52
5	A	294	L2P	C17-C18	2.38	1.65	1.52
6	A	299	L3P	C17-C18	2.38	1.65	1.52
6	A	298	L3P	C26-C25	2.37	1.62	1.52
5	A	295	L2P	C17-C18	2.36	1.64	1.52
5	B	295	L2P	C25-C23	2.34	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	331	L3P	C26-C25	2.33	1.62	1.52
5	B	295	L2P	C17-C18	2.33	1.64	1.52
5	B	296	L2P	C26-C25	2.33	1.62	1.52
6	A	296	L3P	C26-C25	2.33	1.62	1.52
5	B	295	L2P	C19-C18	2.32	1.60	1.52
5	D	293	L2P	C26-C25	2.32	1.62	1.52
5	A	294	L2P	C19-C18	2.31	1.60	1.52
5	B	295	L2P	C26-C25	2.30	1.62	1.52
3	B	300	22B	C18-C5	2.30	1.55	1.50
3	B	300	22B	C38-C39	2.24	1.50	1.45
5	A	294	L2P	C26-C25	2.24	1.61	1.52
3	D	300	22B	C28-C29	2.24	1.38	1.35
5	B	296	L2P	C19-C18	2.19	1.59	1.52
4	A	293	L1P	O2-C41	2.19	1.49	1.43
3	D	300	22B	O1-C36	-2.18	1.39	1.44
6	B	331	L3P	C16-C15	2.14	1.61	1.52
6	A	298	L3P	C16-C15	2.14	1.61	1.52
3	A	300	22B	C35-C34	2.12	1.59	1.53
6	A	333	L3P	C16-C15	2.12	1.61	1.52
6	A	331	L3P	C16-C15	2.11	1.61	1.52
3	A	300	22B	C4-C3	2.09	1.37	1.32
6	D	330	L3P	C16-C15	2.09	1.61	1.52
6	A	296	L3P	C16-C15	2.08	1.61	1.52
6	A	301	L3P	C16-C15	2.08	1.61	1.52
6	A	297	L3P	C16-C15	2.08	1.61	1.52
3	D	300	22B	C38-C39	2.07	1.50	1.45
3	A	300	22B	O1-C36	-2.06	1.39	1.44
6	A	299	L3P	C16-C15	2.06	1.61	1.52
3	B	300	22B	O1-C36	-2.05	1.39	1.44
4	B	294	L1P	O2-C41	2.05	1.48	1.43
4	B	294	L1P	C1-C2	2.02	1.56	1.50
4	A	293	L1P	C1-C2	2.01	1.56	1.50
3	B	300	22B	C35-C34	2.01	1.58	1.53

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	300	22B	C2-C3-C4	5.96	134.85	125.15
3	D	300	22B	C12-C13-C14	-5.43	110.60	118.94
4	B	294	L1P	O1-C1-C2	5.26	121.80	109.44
3	A	300	22B	C2-C3-C4	5.24	133.67	125.15
4	A	293	L1P	O1-C1-C2	5.22	121.71	109.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	293	L1P	O1-C1-C2	5.19	121.64	109.44
3	D	300	22B	C2-C3-C4	5.17	133.55	125.15
3	D	300	22B	C15-C14-C13	5.16	134.68	127.31
3	A	300	22B	C12-C13-C14	-5.10	111.11	118.94
3	A	300	22B	C15-C14-C13	4.31	133.46	127.31
3	A	300	22B	C20-C13-C12	4.27	124.80	118.08
3	B	300	22B	C12-C13-C14	-4.22	112.46	118.94
3	D	300	22B	C20-C13-C12	4.22	124.72	118.08
3	A	300	22B	C42-C43-C44	-4.16	112.56	118.94
3	B	300	22B	C21-C22-C23	4.15	124.38	116.39
3	D	300	22B	C42-C43-C44	-4.14	112.58	118.94
3	B	300	22B	C16-C1-C2	3.99	117.47	111.72
3	A	300	22B	C21-C22-C23	3.98	124.05	116.39
6	A	299	L3P	C26-C25-C23	3.88	128.46	115.92
6	A	297	L3P	C26-C25-C23	3.81	128.24	115.92
3	B	300	22B	C20-C13-C12	3.71	123.93	118.08
3	B	300	22B	C15-C14-C13	3.70	132.58	127.31
6	A	333	L3P	C26-C25-C23	3.67	127.77	115.92
6	B	331	L3P	C26-C25-C23	3.66	127.76	115.92
6	A	301	L3P	C26-C25-C23	3.60	127.57	115.92
2	D	292	RET	C1-C6-C7	3.57	125.88	115.78
6	A	298	L3P	C26-C25-C23	3.53	127.33	115.92
6	A	331	L3P	C26-C25-C23	3.53	127.33	115.92
3	D	300	22B	C21-C22-C23	3.51	123.15	116.39
3	D	300	22B	C4-C5-C6	-3.49	113.58	118.94
3	B	300	22B	C4-C5-C6	-3.47	113.62	118.94
3	D	300	22B	C17-C1-C16	-3.45	105.63	110.56
3	A	300	22B	C4-C5-C6	-3.45	113.65	118.94
6	D	330	L3P	C26-C25-C23	3.43	127.02	115.92
6	A	296	L3P	C26-C25-C23	3.41	126.93	115.92
4	A	293	L1P	C21-C20-C18	3.40	126.90	115.92
3	A	300	22B	C50-C43-C42	3.34	123.34	118.08
3	B	300	22B	C42-C43-C44	-3.33	113.83	118.94
3	D	300	22B	C18-C5-C4	3.32	123.31	118.08
2	B	292	RET	C1-C6-C7	3.31	125.16	115.78
4	B	294	L1P	C21-C20-C18	3.30	126.58	115.92
3	A	300	22B	C17-C1-C16	-3.29	105.86	110.56
3	D	300	22B	C50-C43-C42	3.26	123.22	118.08
3	B	300	22B	C17-C1-C16	-3.26	105.90	110.56
3	A	300	22B	C18-C5-C4	3.24	123.18	118.08
3	A	300	22B	C16-C1-C2	3.24	116.39	111.72
4	B	293	L1P	C21-C20-C18	3.22	126.34	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	300	22B	C16-C1-C2	3.18	116.31	111.72
2	B	292	RET	C1-C6-C5	-3.15	118.17	122.61
3	A	300	22B	C31-C29-C28	-3.13	114.14	118.94
3	B	300	22B	C18-C5-C4	3.05	122.89	118.08
4	B	293	L1P	C56-C55-C53	3.03	125.72	115.92
2	A	292	RET	C1-C6-C7	3.00	124.26	115.78
2	D	292	RET	C1-C6-C5	-2.99	118.39	122.61
3	A	300	22B	C49-C47-C48	-2.99	106.29	110.56
3	D	300	22B	C31-C29-C28	-2.98	114.36	118.94
2	A	292	RET	C8-C9-C10	-2.94	114.43	118.94
3	D	300	22B	C26-C39-C38	2.94	122.71	118.08
2	B	292	RET	C2-C1-C6	2.92	114.97	110.48
3	B	300	22B	C50-C43-C42	2.92	122.67	118.08
2	A	292	RET	C1-C6-C5	-2.91	118.51	122.61
4	A	293	L1P	C16-C17-C18	2.90	125.28	115.92
3	A	300	22B	C26-C39-C38	2.86	122.58	118.08
3	B	300	22B	C49-C47-C48	-2.86	106.47	110.56
3	B	300	22B	C31-C29-C28	-2.79	114.65	118.94
4	B	294	L1P	C16-C17-C18	2.78	124.91	115.92
2	D	292	RET	C19-C9-C8	2.72	122.36	118.08
2	A	292	RET	C19-C9-C8	2.71	122.34	118.08
3	D	300	22B	C45-C44-C43	2.68	131.14	127.31
5	A	294	L2P	C21-C20-C18	2.64	124.46	115.92
3	A	300	22B	C45-C44-C43	2.64	131.07	127.31
3	B	300	22B	C26-C39-C38	2.62	122.21	118.08
4	B	293	L1P	C47-C46-C45	-2.62	101.19	113.24
2	A	292	RET	C2-C1-C6	2.61	114.50	110.48
2	B	292	RET	C19-C9-C8	2.60	122.17	118.08
4	B	293	L1P	C16-C17-C18	2.58	124.27	115.92
6	A	299	L3P	C21-C20-C18	2.57	124.24	115.92
4	B	294	L1P	C47-C46-C45	-2.57	101.44	113.24
3	D	300	22B	C49-C47-C48	-2.54	106.93	110.56
2	D	292	RET	C16-C1-C6	2.47	114.31	110.30
2	B	292	RET	C8-C9-C10	-2.46	115.16	118.94
2	D	292	RET	C2-C1-C6	2.44	114.24	110.48
3	A	300	22B	C30-C29-C31	2.42	121.89	118.08
4	A	293	L1P	C47-C46-C45	-2.41	102.16	113.24
5	B	296	L2P	C21-C20-C18	2.40	123.66	115.92
6	A	297	L3P	C16-C17-C18	2.37	123.59	115.92
2	D	292	RET	C7-C6-C5	-2.37	115.73	121.46
5	A	295	L2P	C17-C16-C15	2.35	124.05	113.24
3	D	300	22B	C38-C39-C40	-2.33	115.37	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	22B	C38-C39-C40	-2.30	115.41	118.94
3	D	300	22B	C30-C29-C31	2.30	121.70	118.08
6	A	331	L3P	C16-C17-C18	2.29	123.32	115.92
3	B	300	22B	C30-C29-C31	2.27	121.66	118.08
3	D	300	22B	C8-C9-C10	-2.27	115.46	118.94
2	D	292	RET	C8-C9-C10	-2.27	115.46	118.94
2	D	292	RET	C20-C13-C12	2.26	121.64	118.08
4	A	293	L1P	C56-C55-C53	2.25	123.20	115.92
6	A	297	L3P	C21-C20-C18	2.24	123.17	115.92
6	A	299	L3P	C16-C17-C18	2.24	123.16	115.92
3	A	300	22B	C25-C23-C22	2.23	118.31	111.42
3	B	300	22B	C25-C23-C22	2.21	118.24	111.42
2	A	292	RET	C17-C1-C6	2.20	113.87	110.30
6	B	331	L3P	C21-C20-C18	2.18	122.96	115.92
4	B	294	L1P	C56-C55-C53	2.15	122.88	115.92
6	A	296	L3P	C16-C17-C18	2.15	122.88	115.92
6	B	331	L3P	C16-C17-C18	2.15	122.86	115.92
6	A	296	L3P	C21-C20-C18	2.15	122.86	115.92
5	B	295	L2P	C17-C16-C15	2.14	123.08	113.24
4	A	293	L1P	O3-C3-C2	-2.14	106.11	111.78
6	A	301	L3P	C16-C17-C18	2.14	122.84	115.92
3	D	300	22B	C25-C23-C22	2.14	118.02	111.42
4	B	294	L1P	O3-C3-C2	-2.14	106.11	111.78
4	B	293	L1P	O3-C3-C2	-2.13	106.12	111.78
2	D	292	RET	C2-C3-C4	2.10	116.06	111.38
3	B	300	22B	C11-C10-C9	-2.10	124.32	127.31
3	B	300	22B	C8-C9-C10	-2.10	115.72	118.94
3	B	300	22B	C19-C9-C8	2.09	121.37	118.08
2	D	292	RET	C17-C1-C6	2.09	113.69	110.30
3	A	300	22B	C15-C45-C44	-2.09	119.20	123.47
6	A	301	L3P	C21-C20-C18	2.07	122.60	115.92
3	A	300	22B	C19-C9-C8	2.05	121.30	118.08
5	D	293	L2P	C17-C16-C15	2.04	122.63	113.24
5	A	295	L2P	C16-C15-C13	-2.04	109.33	115.92
6	A	331	L3P	C21-C20-C18	2.04	122.51	115.92
2	A	292	RET	C20-C13-C12	2.03	121.28	118.08
6	D	330	L3P	C16-C17-C18	2.03	122.49	115.92
6	A	298	L3P	C21-C20-C18	2.03	122.48	115.92
6	A	298	L3P	C16-C17-C18	2.01	122.42	115.92
3	A	300	22B	C8-C9-C10	-2.01	115.86	118.94

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	294	L1P	C11-C12-C13-C14
4	B	294	L1P	C41-C42-C43-C44
4	B	293	L1P	C11-C12-C13-C14
4	B	293	L1P	C41-C42-C43-C44
3	D	300	22B	C1-C2-C3-C4
3	D	300	22B	C2-C3-C4-C5
3	D	300	22B	C7-C8-C9-C10
3	D	300	22B	C7-C8-C9-C19
3	D	300	22B	C21-C22-C23-C25
3	D	300	22B	C21-C22-C23-O27
3	D	300	22B	C31-C32-C33-C47
3	D	300	22B	C32-C33-C34-C35
3	B	300	22B	C1-C2-C3-C4
3	B	300	22B	C21-C22-C23-C25
3	B	300	22B	C21-C22-C23-O27
3	A	300	22B	C1-C2-C3-C4
3	A	300	22B	C2-C3-C4-C5
3	A	300	22B	C21-C22-C23-C25
3	A	300	22B	C21-C22-C23-O27
4	A	293	L1P	C53-C55-C56-C57
6	A	299	L3P	C15-C16-C17-C18
4	B	294	L1P	C53-C55-C56-C57
4	B	293	L1P	C53-C55-C56-C57
6	A	298	L3P	C15-C16-C17-C18
6	B	331	L3P	C15-C16-C17-C18
6	A	331	L3P	C15-C16-C17-C18
6	A	333	L3P	C15-C16-C17-C18
6	D	330	L3P	C15-C16-C17-C18
6	A	301	L3P	C15-C16-C17-C18
6	A	296	L3P	C15-C16-C17-C18
6	A	297	L3P	C15-C16-C17-C18
6	A	297	L3P	C19-C18-C20-C21
6	B	331	L3P	C18-C20-C21-C22
4	A	293	L1P	C20-C21-C22-C23
6	A	333	L3P	C25-C26-C27-C28
6	A	301	L3P	C25-C26-C27-C28
4	B	294	L1P	C25-C26-C27-C28
5	B	296	L2P	C18-C20-C21-C22
4	B	293	L1P	C23-C25-C26-C27
6	A	298	L3P	C13-C15-C16-C17
6	B	331	L3P	C16-C17-C18-C20
6	A	331	L3P	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
3	D	300	22B	C9-C10-C11-C12
6	A	297	L3P	C18-C20-C21-C22
4	B	294	L1P	C23-C25-C26-C27
6	A	299	L3P	C18-C20-C21-C22
3	D	300	22B	C21-C22-C23-C24
3	B	300	22B	C21-C22-C23-C24
3	A	300	22B	C21-C22-C23-C24
6	A	298	L3P	C25-C26-C27-C28
6	A	296	L3P	C26-C27-C28-C30
4	B	293	L1P	C26-C27-C28-C29
6	A	296	L3P	C26-C27-C28-C29
3	D	300	22B	C2-C21-C22-C23
5	D	294	L2P	C26-C27-C28-C29
5	D	294	L2P	C26-C27-C28-C30
5	A	294	L2P	C18-C20-C21-C22
4	B	293	L1P	C26-C27-C28-C30
6	A	298	L3P	C18-C20-C21-C22
6	A	298	L3P	C22-C23-C25-C26
4	A	293	L1P	C26-C27-C28-C30
6	A	298	L3P	C24-C23-C25-C26
6	B	331	L3P	C16-C17-C18-C19
6	A	331	L3P	C24-C23-C25-C26
4	A	293	L1P	C26-C27-C28-C29
6	B	331	L3P	C26-C27-C28-C29
6	A	331	L3P	C26-C27-C28-C29
6	A	333	L3P	C26-C27-C28-C30
4	B	293	L1P	C25-C26-C27-C28
6	A	296	L3P	C25-C26-C27-C28
6	A	331	L3P	C25-C26-C27-C28
3	D	300	22B	C21-C2-C3-C4
3	B	300	22B	C21-C2-C3-C4
3	A	300	22B	C21-C2-C3-C4
4	A	293	L1P	O1-C1-C2-C3
6	B	331	L3P	C26-C27-C28-C30
6	A	331	L3P	C26-C27-C28-C30
5	D	293	L2P	C26-C27-C28-C30
6	A	298	L3P	C26-C27-C28-C30
6	D	330	L3P	C26-C27-C28-C29
5	B	295	L2P	C18-C20-C21-C22
4	B	293	L1P	O1-C1-C2-O2
4	A	293	L1P	C48-C50-C51-C52
4	B	294	L1P	C50-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
6	A	299	L3P	C17-C18-C20-C21
4	B	294	L1P	C12-C13-C15-C16
6	D	330	L3P	C16-C17-C18-C20
6	D	330	L3P	C17-C18-C20-C21
6	A	301	L3P	C17-C18-C20-C21
6	A	296	L3P	C16-C17-C18-C20
6	A	299	L3P	C19-C18-C20-C21
4	B	294	L1P	C14-C13-C15-C16
5	D	294	L2P	C18-C20-C21-C22
6	A	301	L3P	C18-C20-C21-C22
4	B	293	L1P	C11-C12-C13-C15
4	B	293	L1P	C41-C42-C43-C45
3	B	300	22B	C32-C33-C34-C35
3	A	300	22B	C32-C33-C34-C35
6	A	333	L3P	C26-C27-C28-C29
4	A	293	L1P	O1-C1-C2-O2
4	B	293	L1P	C14-C13-C15-C16
4	B	293	L1P	C49-C48-C50-C51
6	D	330	L3P	C19-C18-C20-C21
6	A	331	L3P	C13-C15-C16-C17
6	D	330	L3P	C18-C20-C21-C22
5	D	293	L2P	C26-C27-C28-C29
6	A	298	L3P	C26-C27-C28-C29
6	D	330	L3P	C26-C27-C28-C30
4	A	293	L1P	C12-C13-C15-C16
4	A	293	L1P	C21-C22-C23-C25
4	A	293	L1P	C22-C23-C25-C26
4	B	294	L1P	C46-C47-C48-C50
4	B	293	L1P	C12-C13-C15-C16
4	B	293	L1P	C46-C47-C48-C50
6	A	333	L3P	C17-C18-C20-C21
5	B	296	L2P	C26-C27-C28-C30
4	B	294	L1P	C41-C42-C43-C45
4	A	293	L1P	C14-C13-C15-C16
4	B	293	L1P	C46-C47-C48-C49
4	B	294	L1P	C21-C22-C23-C25
4	B	294	L1P	C47-C48-C50-C51
4	B	293	L1P	C47-C48-C50-C51
3	D	300	22B	C47-C33-C34-C35
5	B	296	L2P	C26-C27-C28-C29
4	B	294	L1P	O1-C1-C2-O2
4	A	293	L1P	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	A	293	L1P	C24-C23-C25-C26
6	A	299	L3P	C24-C23-C25-C26
4	B	294	L1P	C46-C47-C48-C49
4	B	294	L1P	C49-C48-C50-C51
4	B	293	L1P	C12-C11-O1-C1
5	B	295	L2P	C11-C12-C13-C14
4	B	293	L1P	O1-C1-C2-C3
4	B	294	L1P	C21-C22-C23-C24
6	D	330	L3P	C16-C17-C18-C19
6	A	301	L3P	C19-C18-C20-C21
6	A	296	L3P	C16-C17-C18-C19
4	B	293	L1P	C20-C21-C22-C23
4	A	293	L1P	C56-C57-C58-C60
6	A	301	L3P	C26-C27-C28-C30
4	B	294	L1P	C56-C57-C58-C60
3	A	300	22B	C9-C10-C11-C12
4	B	293	L1P	C2-C1-O1-C11
3	D	300	22B	C31-C32-C33-C34
4	B	294	L1P	C11-C12-C13-C15
4	B	294	L1P	O1-C1-C2-C3
5	B	295	L2P	C26-C27-C28-C29
4	A	293	L1P	C56-C57-C58-C59
6	A	299	L3P	C16-C17-C18-C20
6	A	331	L3P	C16-C17-C18-C20
4	A	293	L1P	C46-C47-C48-C49
6	A	298	L3P	C16-C17-C18-C19
4	A	293	L1P	C41-C42-C43-C45
6	A	301	L3P	C26-C27-C28-C29
6	A	331	L3P	C16-C17-C18-C19
6	A	333	L3P	C19-C18-C20-C21
6	A	298	L3P	C16-C17-C18-C20
3	A	300	22B	C47-C33-C34-C35
4	B	293	L1P	C15-C16-C17-C18

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	293	L1P	3	0
5	B	295	L2P	5	0
5	D	293	L2P	2	0
5	A	295	L2P	4	0

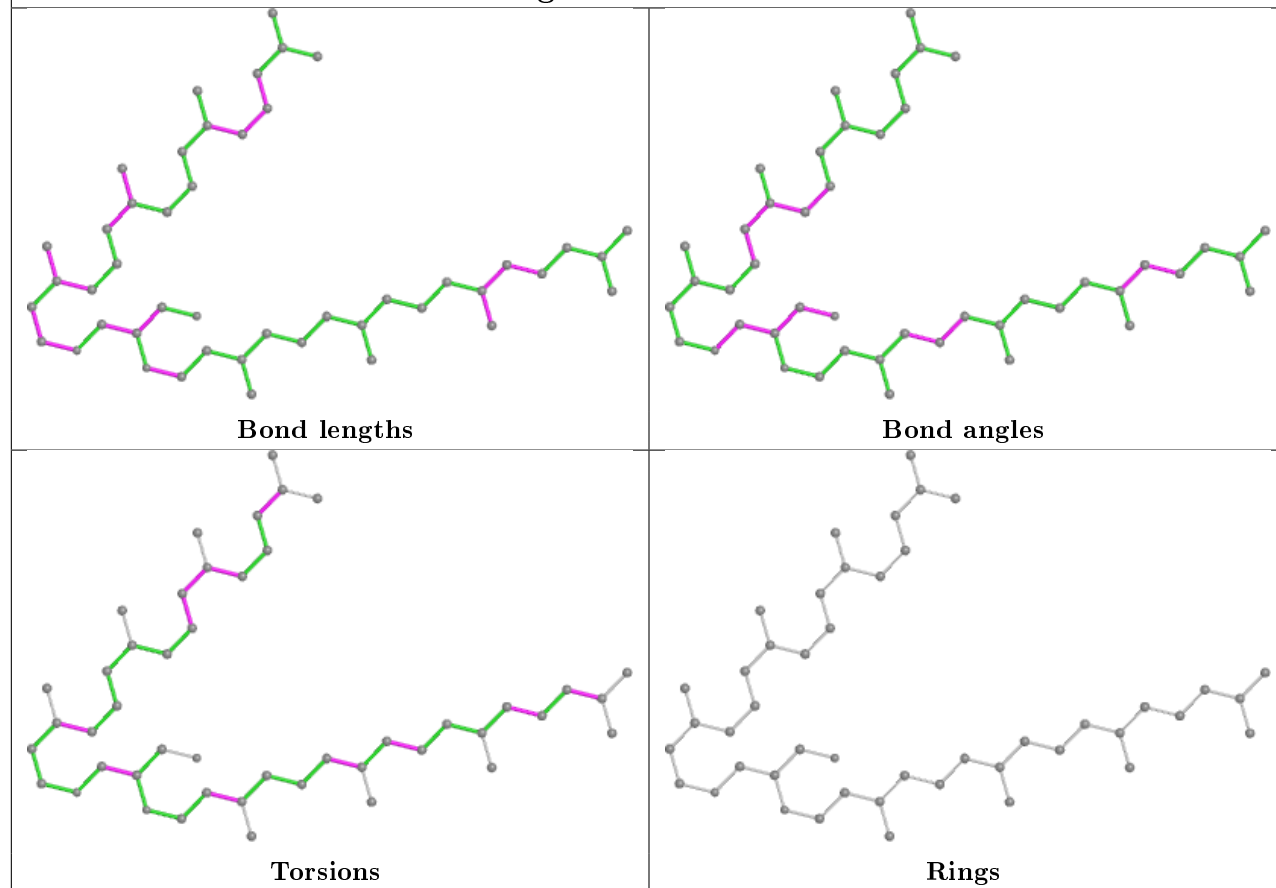
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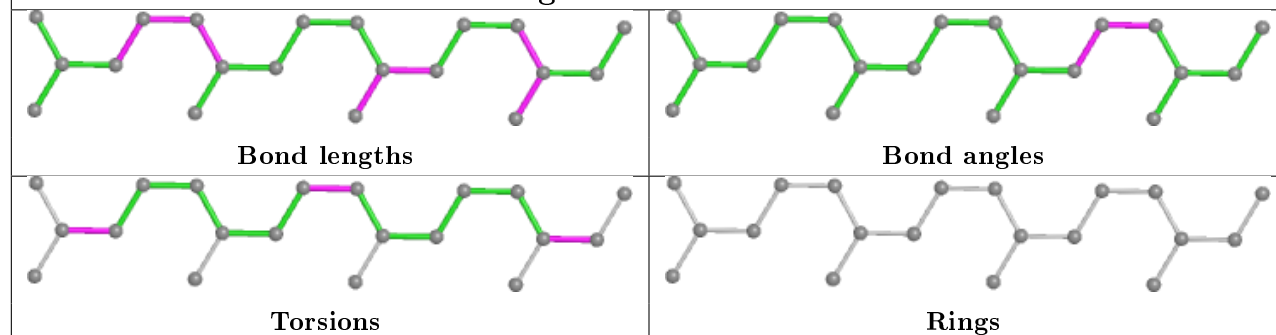
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	294	L2P	3	0
4	B	294	L1P	2	0
5	A	294	L2P	4	0
4	B	293	L1P	2	0
6	A	298	L3P	1	0
6	A	333	L3P	1	0
3	B	300	22B	2	0
2	B	292	RET	1	0
5	B	296	L2P	3	0

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.

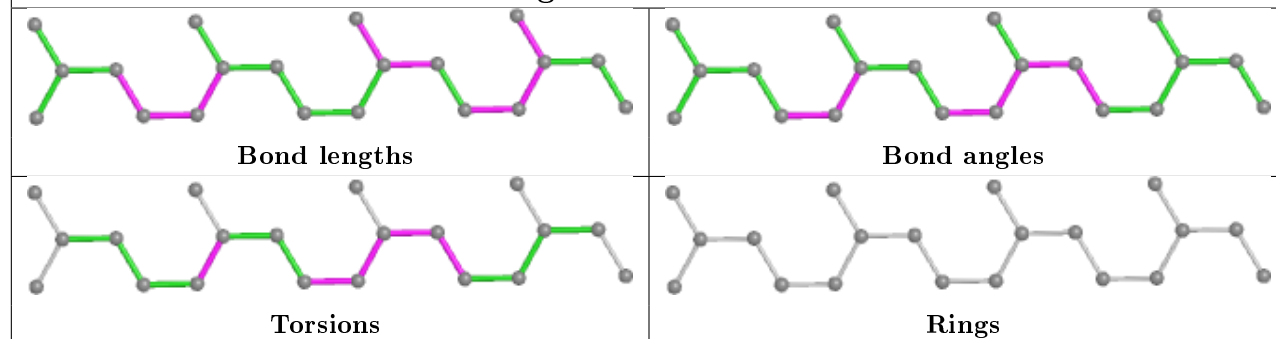
## Ligand L1P A 293

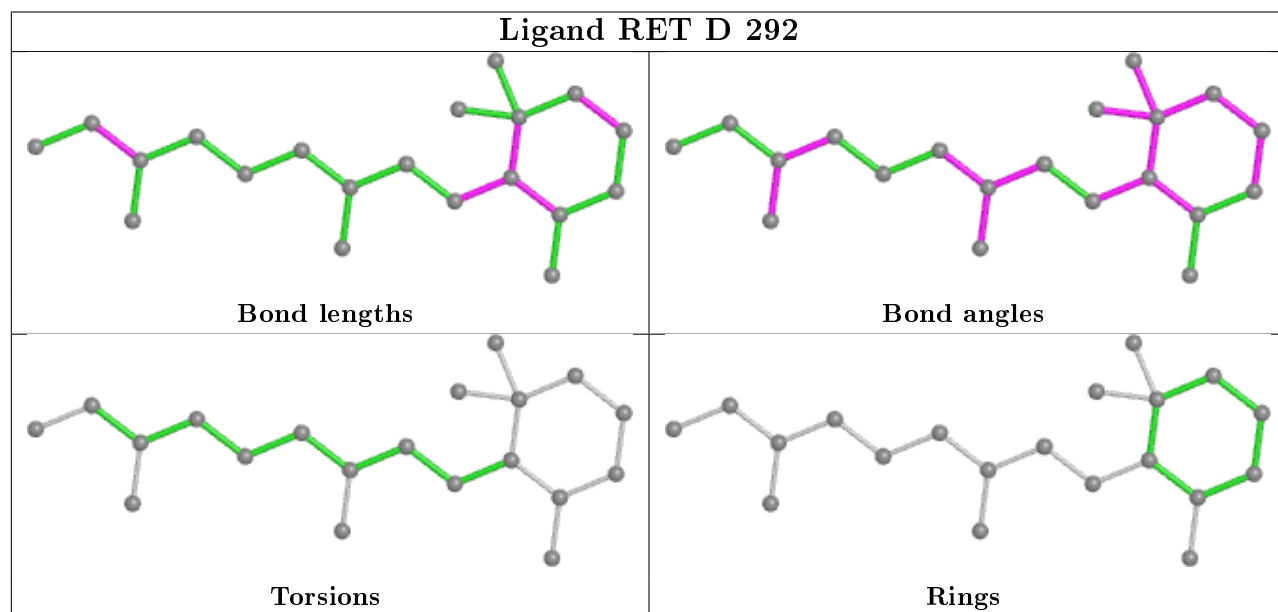
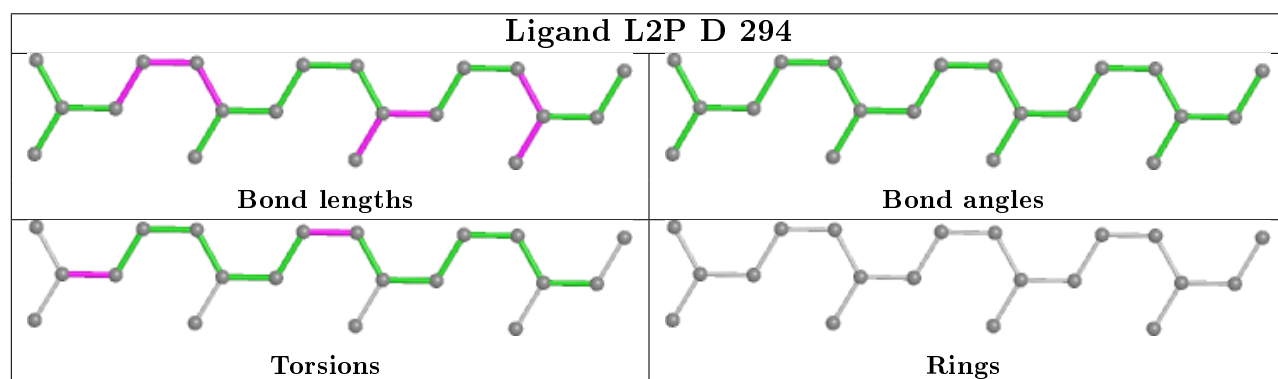
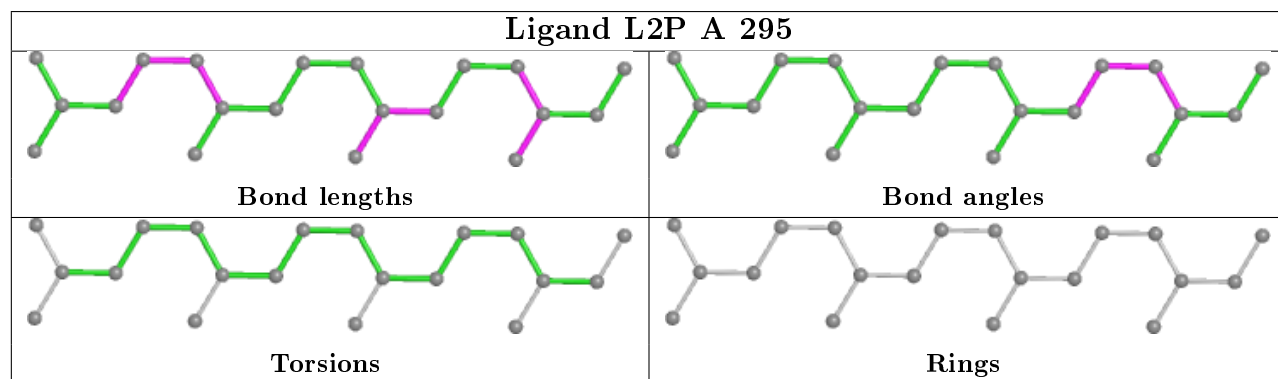
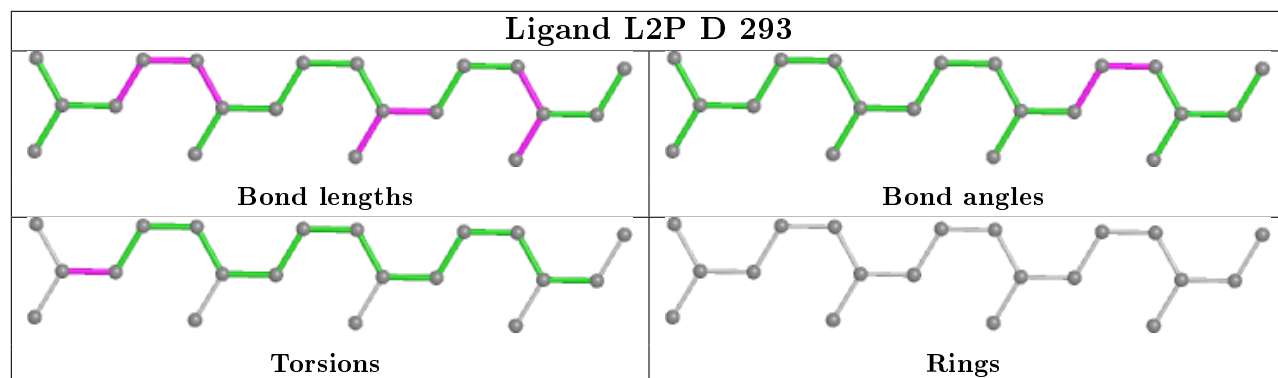


## Ligand L2P B 295

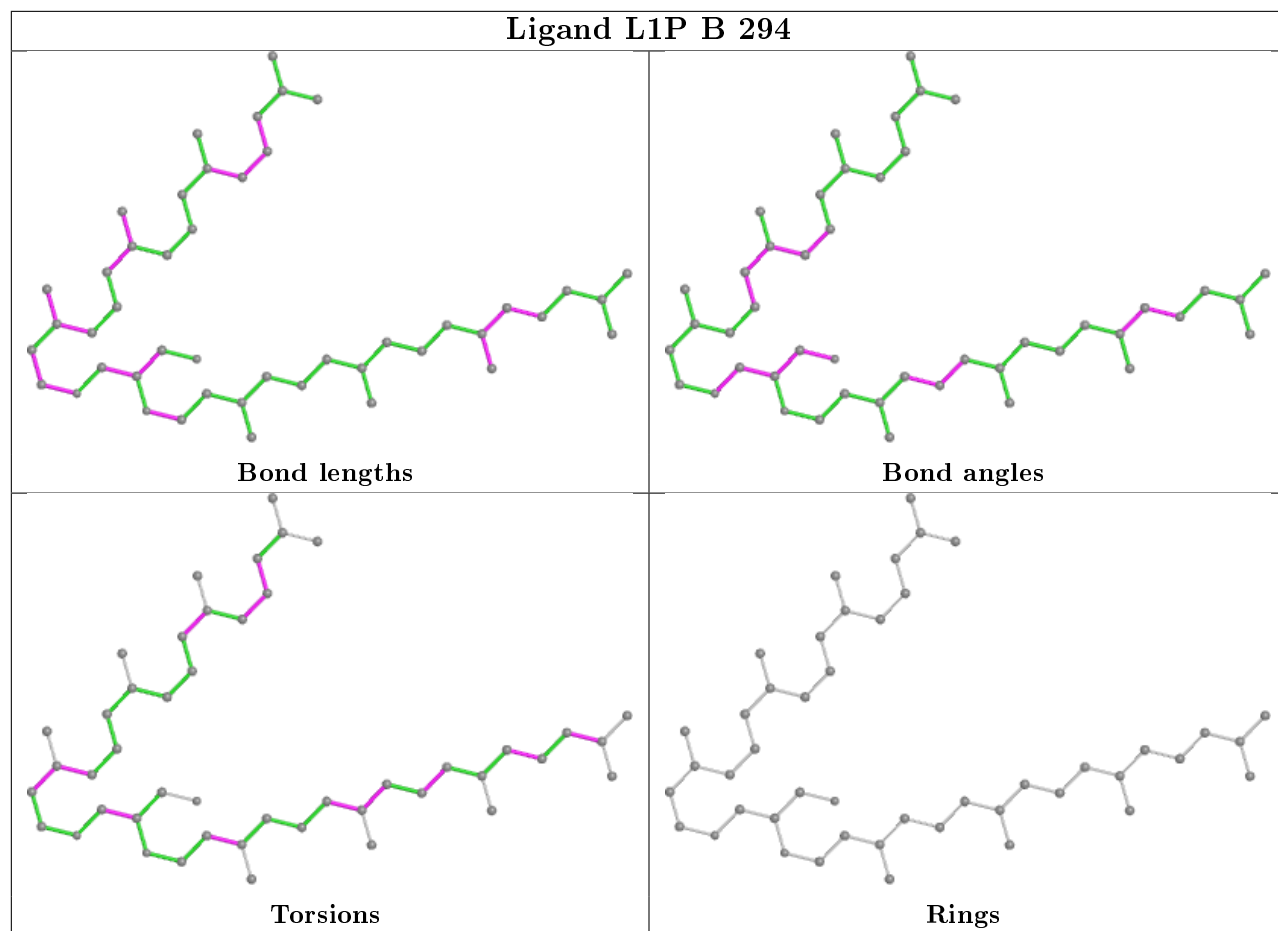


## Ligand L3P A 299

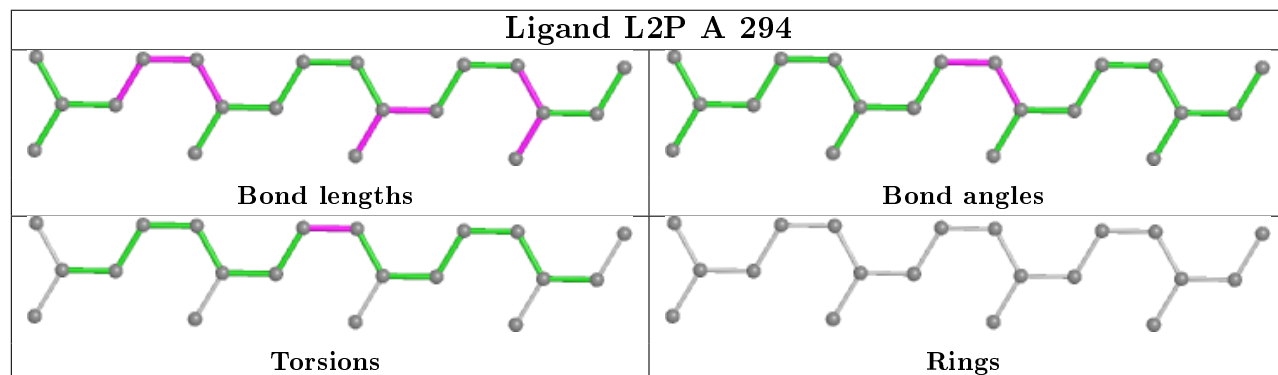




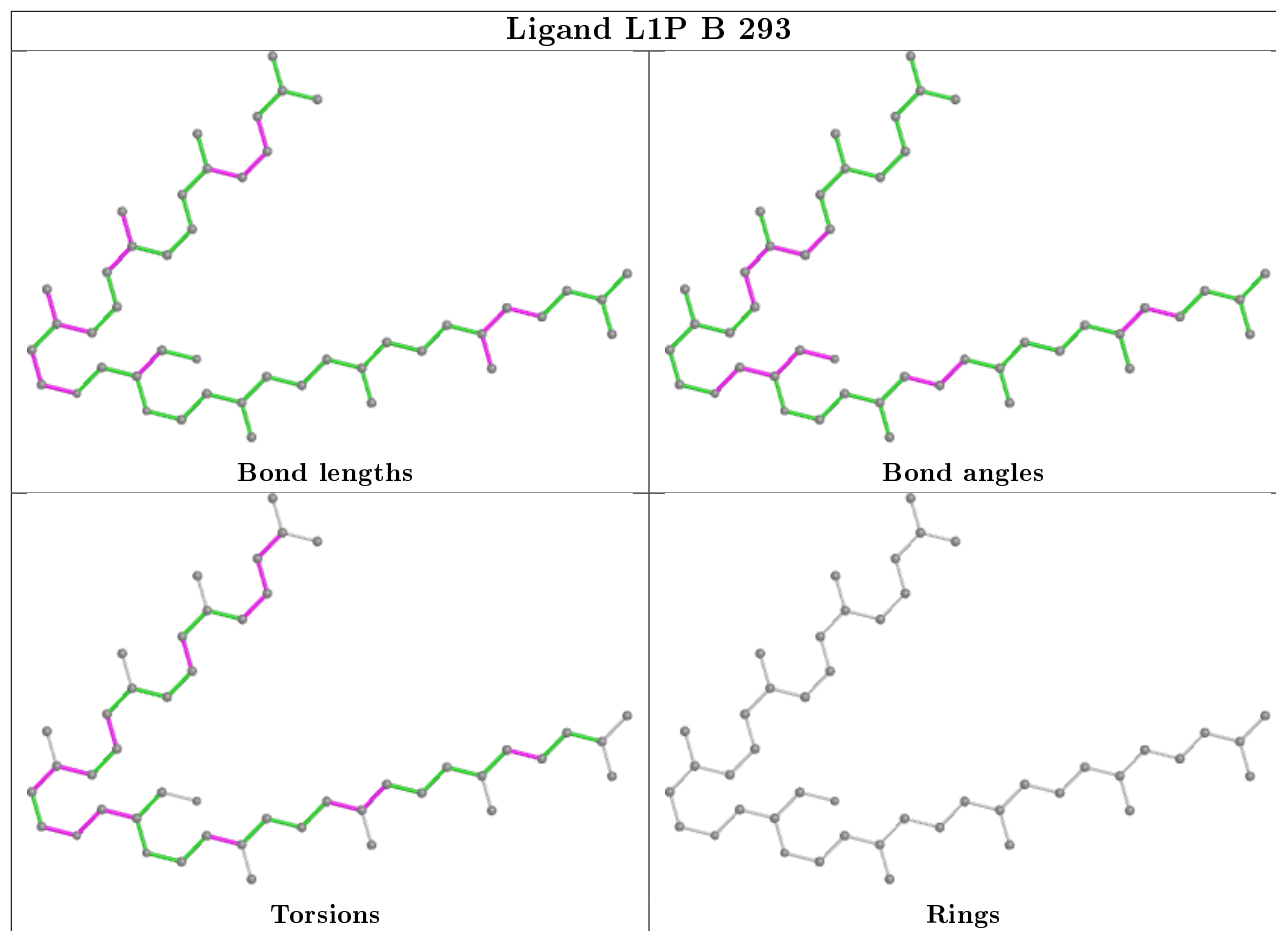
## Ligand L1P B 294



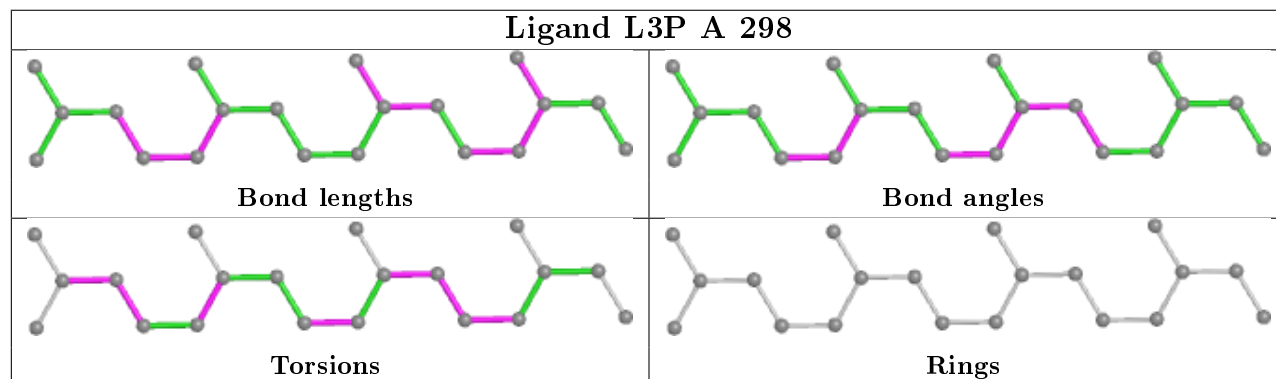
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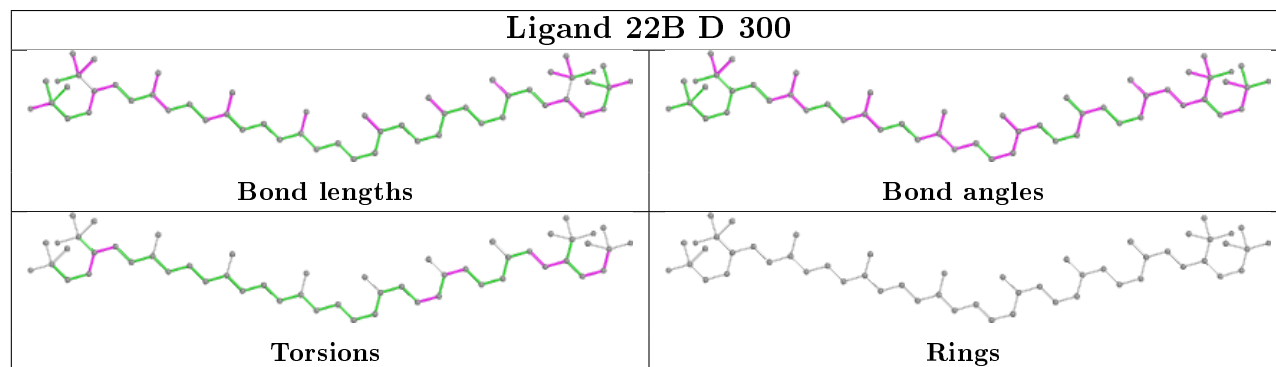
## Ligand L1P B 293



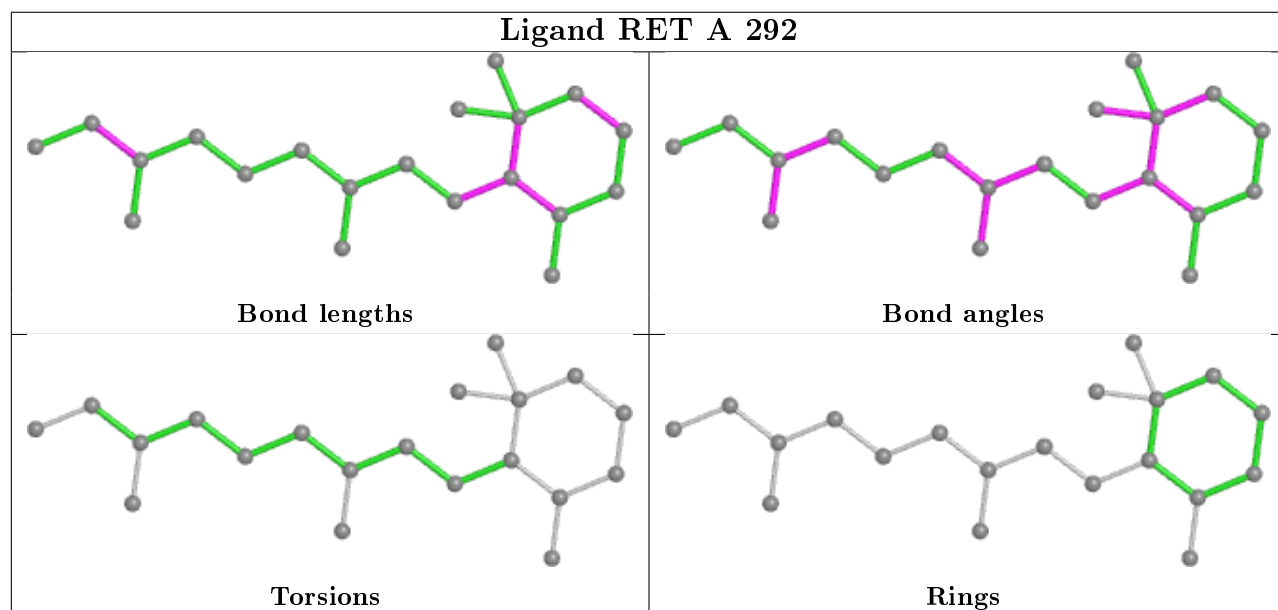
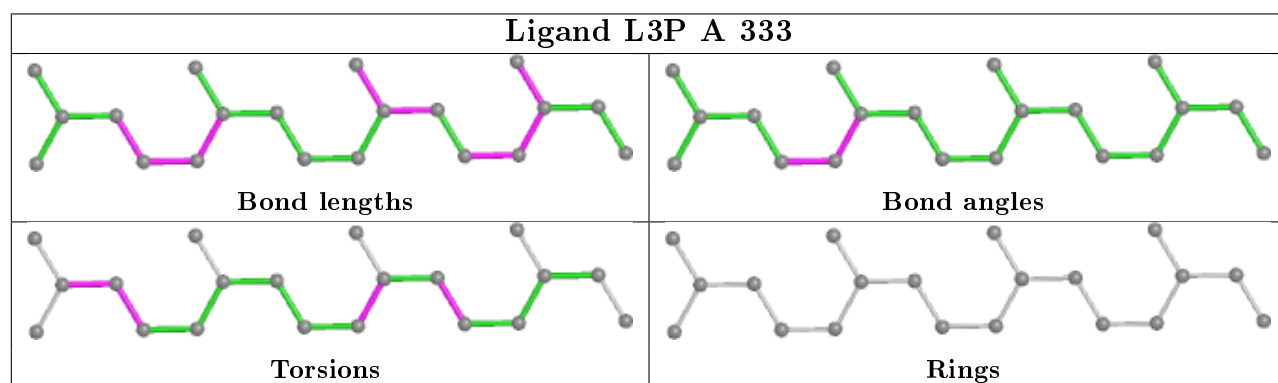
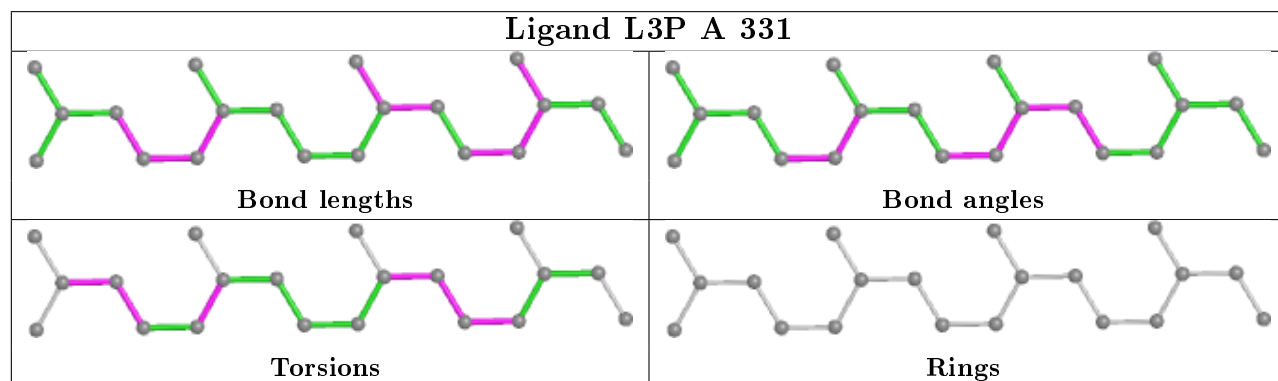
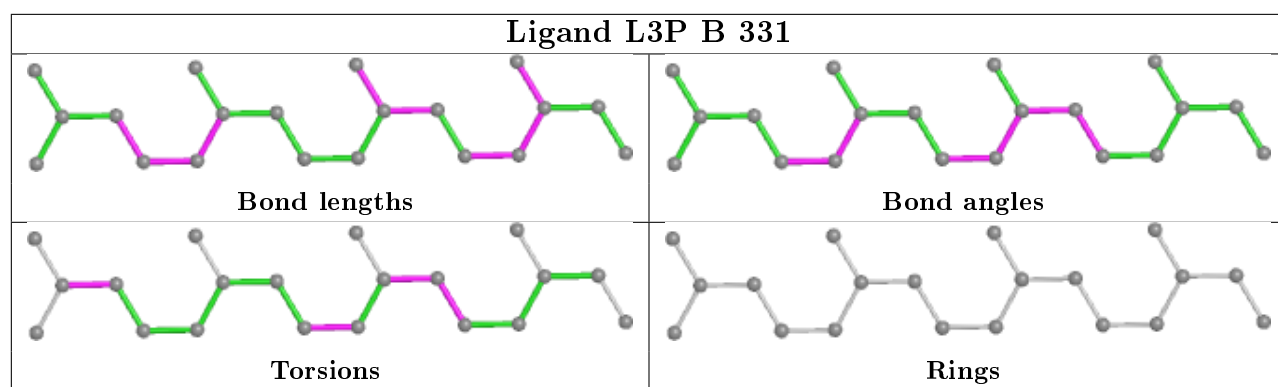
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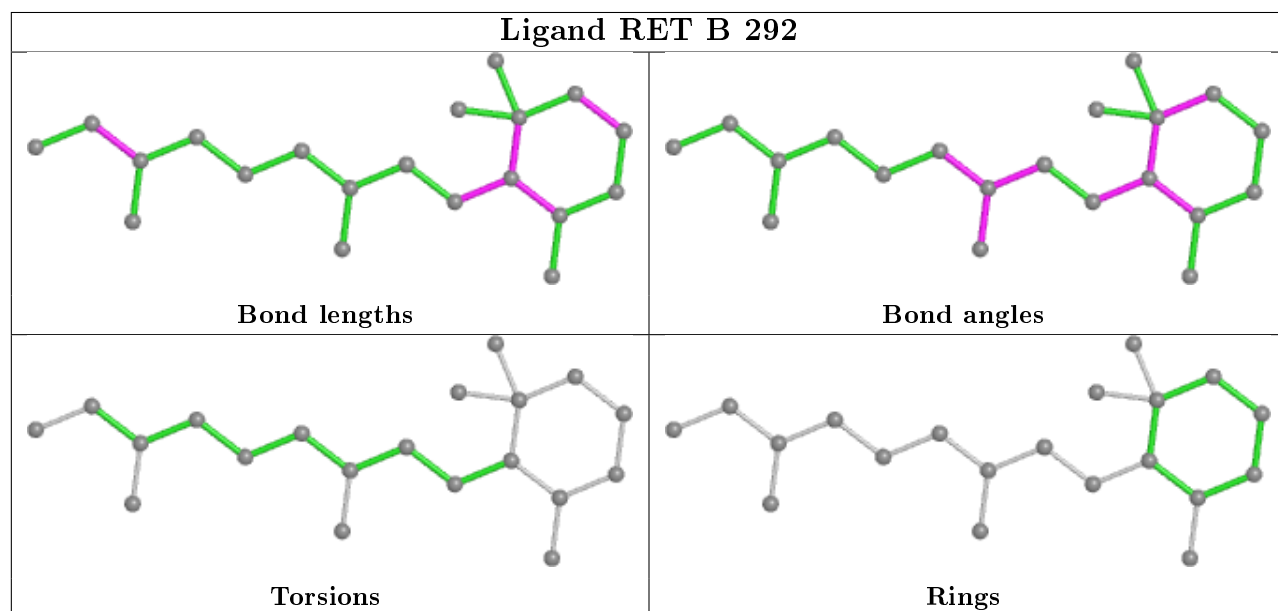
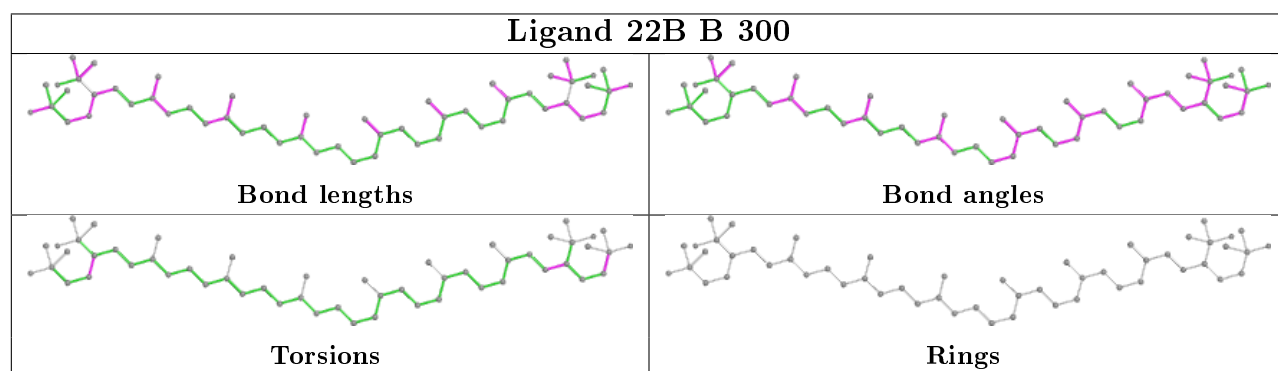
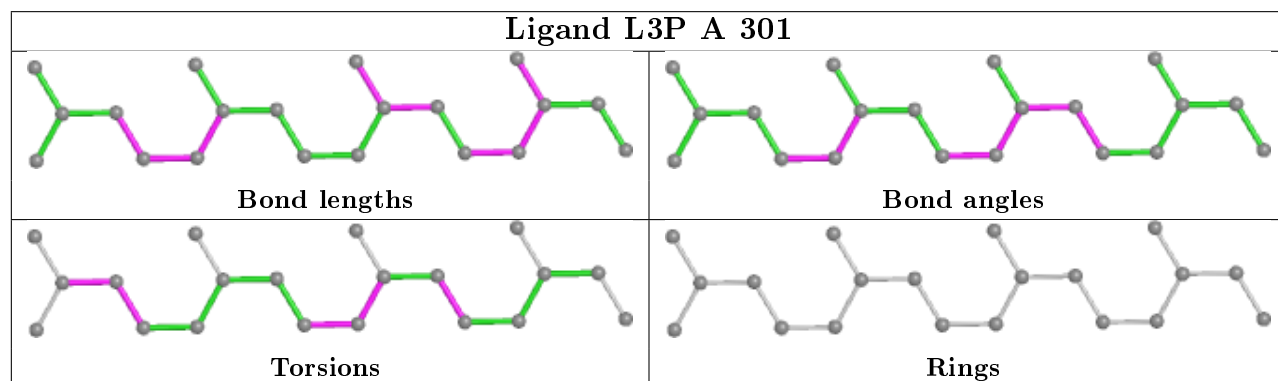
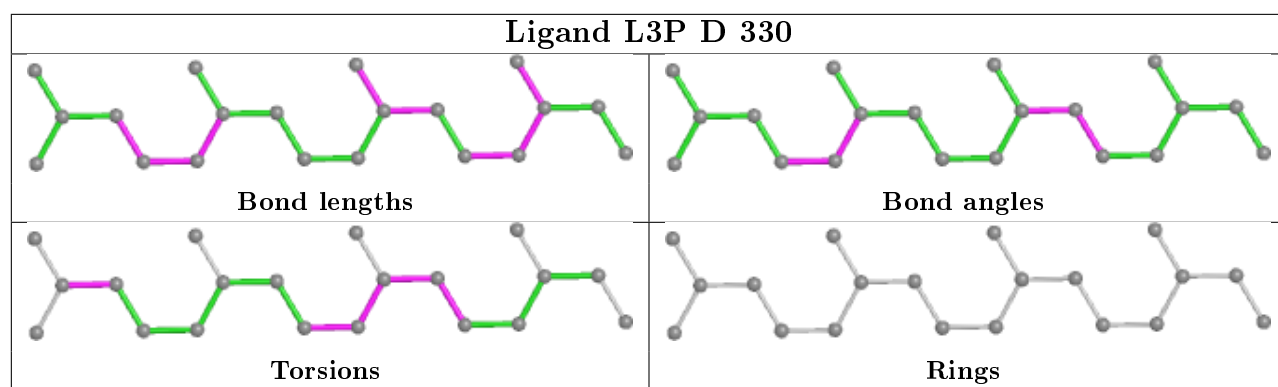


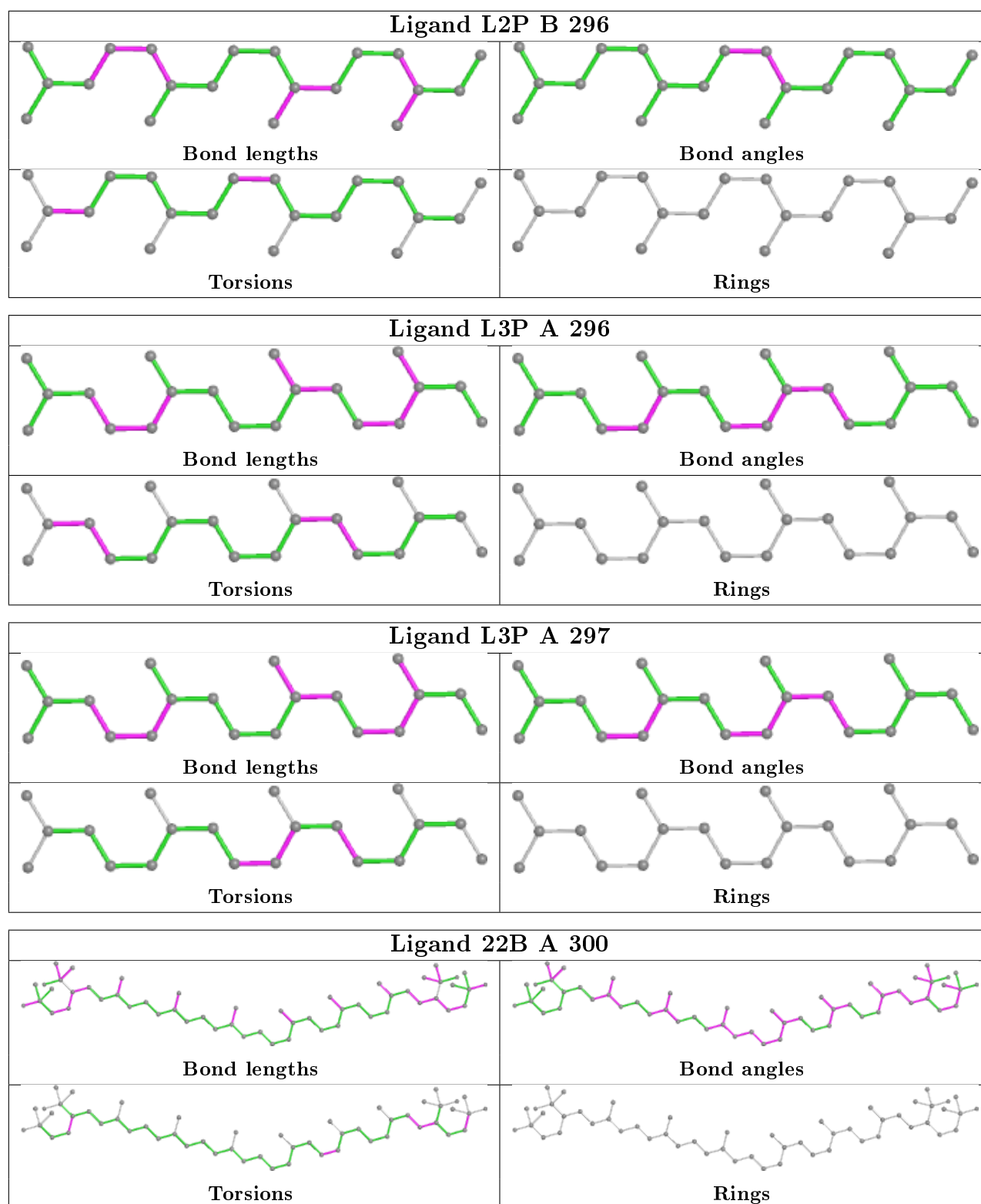
## Ligand 22B D 300











## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	259/291 (89%)	0.21	18 (6%) 16 16	23, 34, 66, 85	0
1	B	258/291 (88%)	0.08	7 (2%) 54 53	26, 39, 55, 67	0
1	D	259/291 (89%)	1.07	39 (15%) 2 1	33, 54, 79, 96	0
All	All	776/873 (88%)	0.45	64 (8%) 11 11	23, 42, 72, 96	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	LEU	8.8
1	D	276	GLY	8.2
1	D	277	SER	7.7
1	A	110	GLY	7.4
1	D	111	GLY	7.2
1	D	112	GLU	6.6
1	D	32	PRO	6.3
1	D	243	TYR	5.6
1	A	107	VAL	5.6
1	A	104	GLY	5.4
1	B	276	GLY	5.3
1	D	110	GLY	5.3
1	D	113	GLU	5.1
1	D	275	SER	4.8
1	A	111	GLY	4.6
1	D	269	SER	4.6
1	B	104	GLY	4.3
1	D	261	PHE	4.2
1	A	109	LEU	4.1
1	D	108	MET	4.1
1	D	249	SER	4.0
1	D	29	LEU	3.9
1	D	240	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	107	VAL	3.6
1	A	30	ASN	3.5
1	D	209	ASP	3.3
1	A	276	GLY	3.3
1	A	54	PHE	3.2
1	D	270	ASN	3.1
1	D	241	VAL	3.1
1	D	54	PHE	3.1
1	D	273	VAL	3.1
1	A	112	GLU	3.1
1	D	211	PHE	3.1
1	B	98	ALA	3.1
1	A	108	MET	3.0
1	D	205	ALA	2.9
1	D	101	PHE	2.8
1	A	99	GLY	2.8
1	D	30	ASN	2.8
1	D	248	TYR	2.7
1	A	113	GLU	2.6
1	A	277	SER	2.6
1	D	33	LEU	2.6
1	D	193	ILE	2.6
1	A	57	ARG	2.6
1	D	265	ASN	2.6
1	B	107	VAL	2.5
1	D	34	LEU	2.5
1	D	267	LEU	2.5
1	D	268	THR	2.4
1	B	200	GLN	2.4
1	D	57	ARG	2.4
1	A	101	PHE	2.3
1	B	243	TYR	2.3
1	A	129	LEU	2.2
1	B	203	LYS	2.2
1	D	258	ILE	2.2
1	D	104	GLY	2.2
1	D	31	ASP	2.2
1	A	22	ARG	2.1
1	D	61	ASP	2.0
1	A	179	TRP	2.0
1	D	231	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 ⓘ

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	L3P	A	331	20/59	0.29	0.40	80,82,83,83	0
6	L3P	A	298	20/59	0.31	0.69	111,112,113,113	0
5	L2P	A	295	20/46	0.34	0.79	114,115,118,118	0
6	L3P	A	296	20/59	0.38	0.49	102,103,104,104	0
4	L1P	B	293	46/50	0.40	0.69	92,103,105,105	0
6	L3P	D	330	20/59	0.44	0.33	96,97,98,98	0
4	L1P	B	294	46/50	0.44	0.67	94,101,105,105	0
6	L3P	A	297	20/59	0.44	0.57	110,112,114,114	0
6	L3P	A	301	20/59	0.45	0.45	90,91,92,92	0
6	L3P	B	331	20/59	0.46	0.46	94,97,99,99	0
3	22B	D	300	54/54	0.46	0.46	111,114,120,120	0
5	L2P	D	293	20/46	0.47	0.61	94,96,98,99	0
6	L3P	A	299	20/59	0.49	0.92	115,116,118,118	0
5	L2P	D	294	20/46	0.50	0.67	88,90,96,97	0
5	L2P	B	295	20/46	0.52	0.61	94,96,97,97	0
4	L1P	A	293	46/50	0.53	0.63	70,96,99,100	0
6	L3P	A	333	20/59	0.56	0.42	60,73,75,77	0
3	22B	A	300	54/54	0.59	0.36	71,82,110,111	0
5	L2P	B	296	20/46	0.64	0.69	85,90,93,93	0
5	L2P	A	294	20/46	0.70	0.65	79,89,96,96	0
3	22B	B	300	54/54	0.82	0.21	36,57,91,91	0
2	RET	D	292	20/21	0.83	0.15	42,44,45,47	0
7	CL	D	402	1/1	0.84	0.24	65,65,65,65	0
7	CL	B	402	1/1	0.95	0.20	62,62,62,62	0
7	CL	D	401	1/1	0.96	0.15	51,51,51,51	0
2	RET	B	292	20/21	0.96	0.12	24,30,35,35	0

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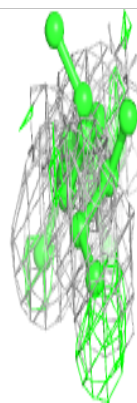
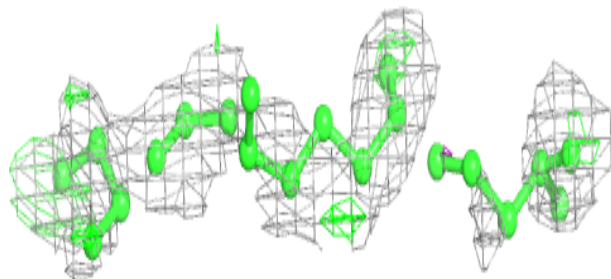
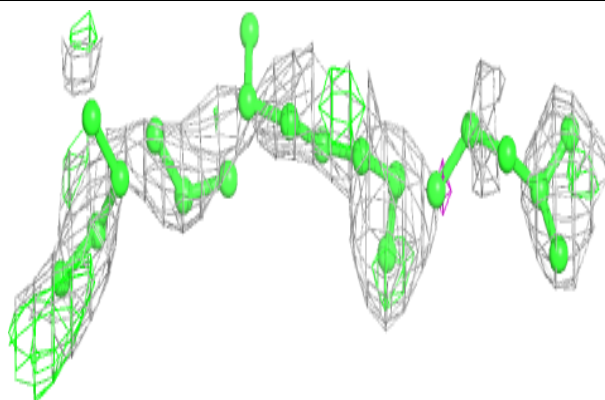
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RET	A	292	20/21	0.96	0.13	19,25,29,29	0
7	CL	A	402	1/1	0.97	0.05	42,42,42,42	0
7	CL	B	401	1/1	0.99	0.09	28,28,28,28	0
7	CL	A	401	1/1	1.00	0.11	26,26,26,26	0

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 L3P A 331:**

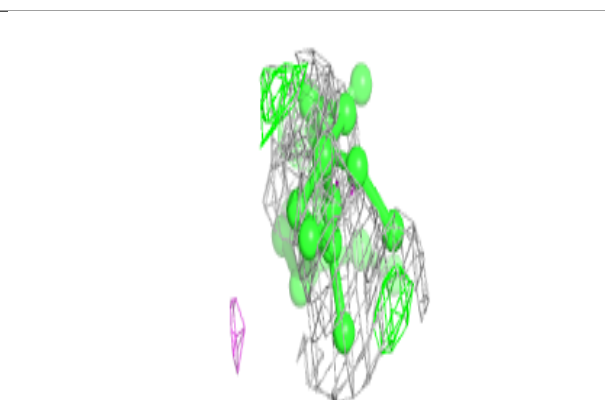
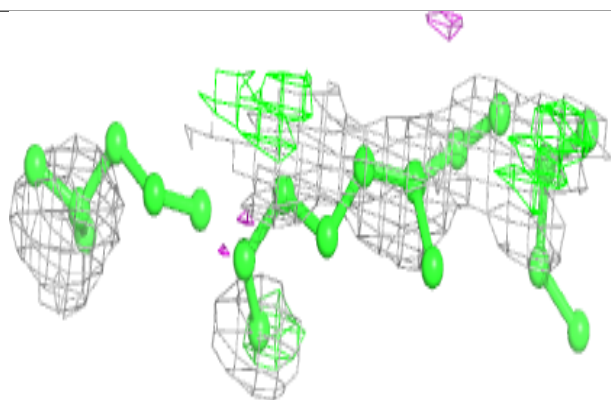
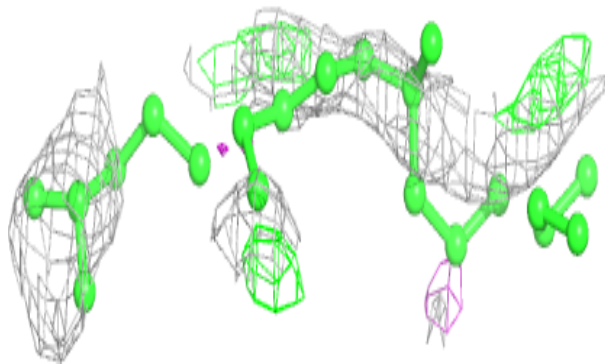
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



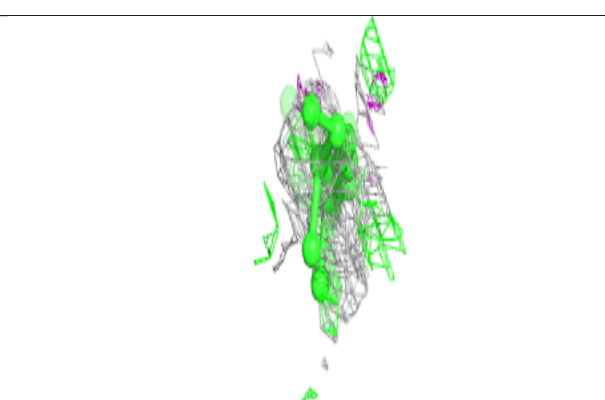
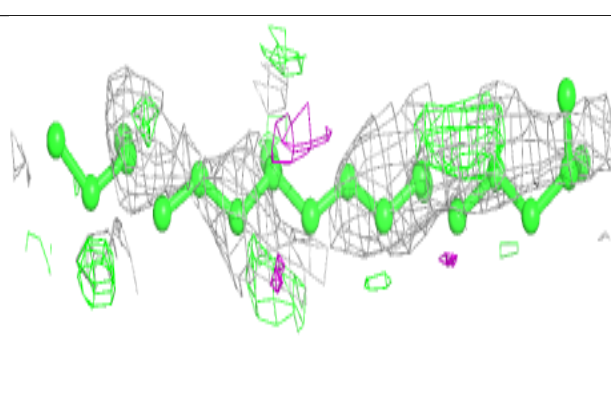
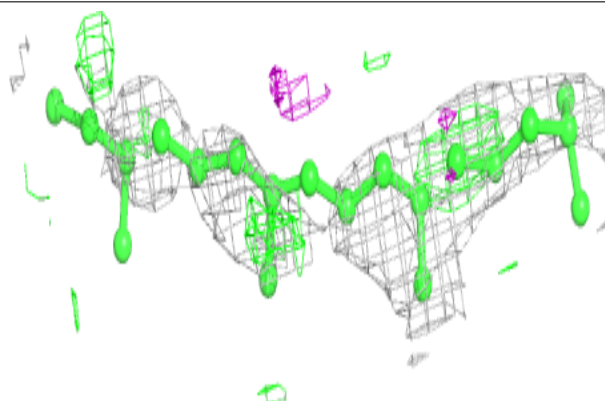


**Electron density around L3P A 298:**

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

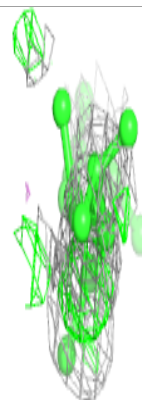
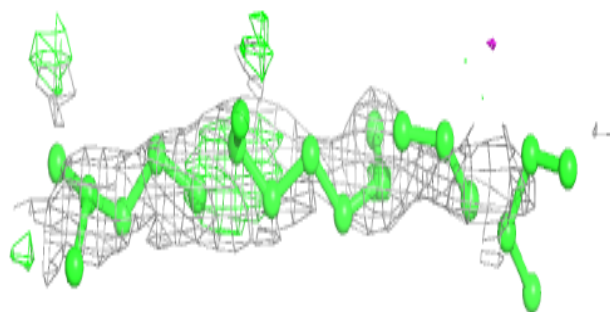
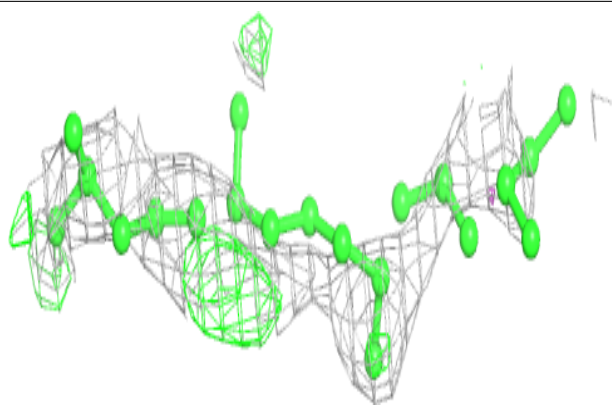
**Electron density around L2P A 295:**

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and green (positive)

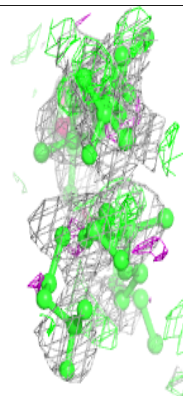
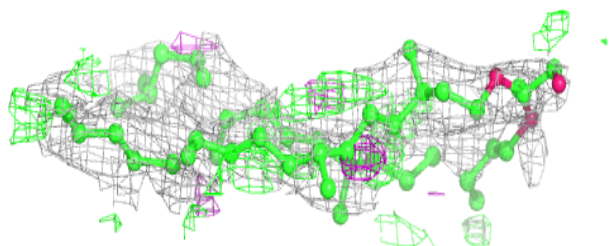
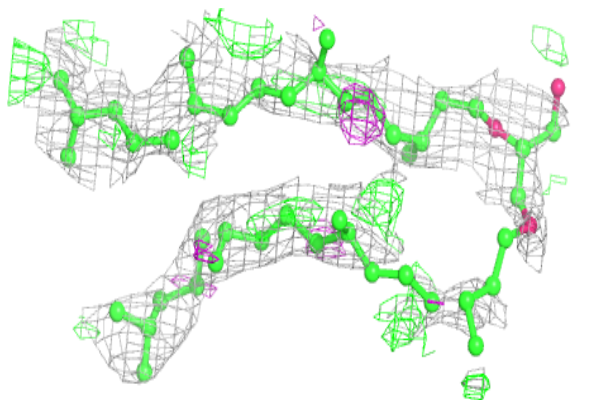


**Electron density around L3P A 296:**

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

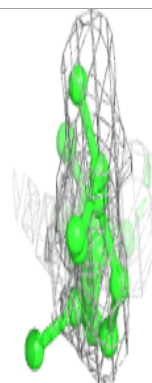
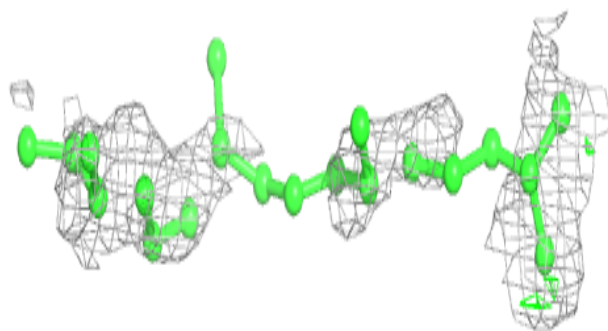
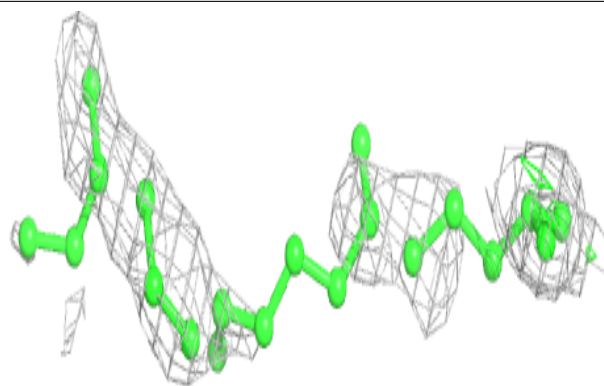
**Electron density around L1P B 293:**

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

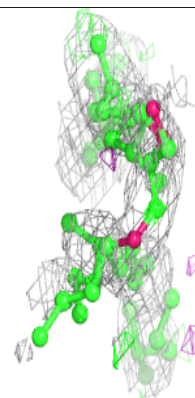
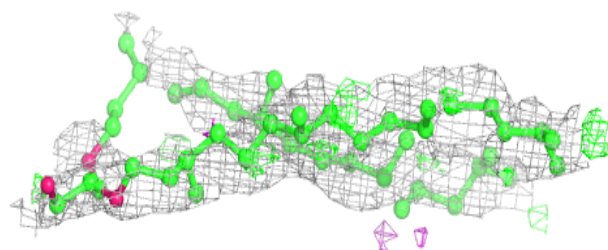
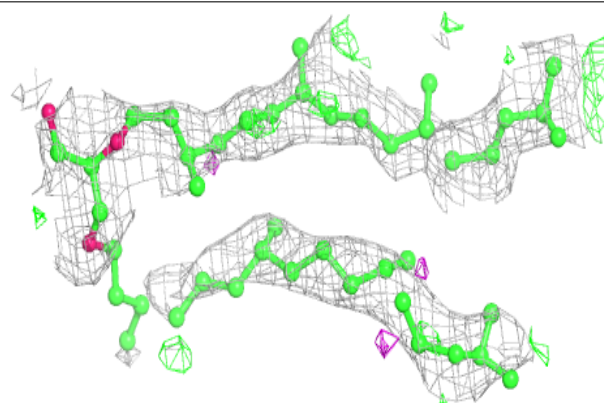


**Electron density around L3P D 330:**

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

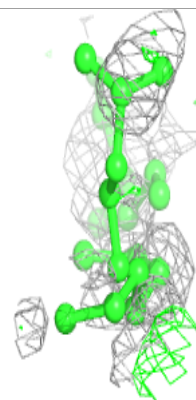
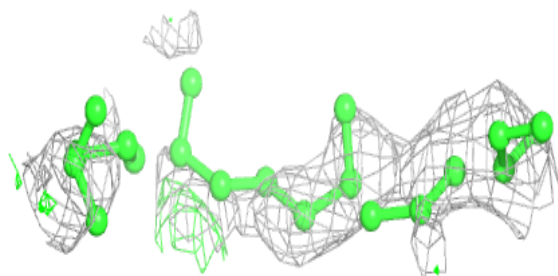
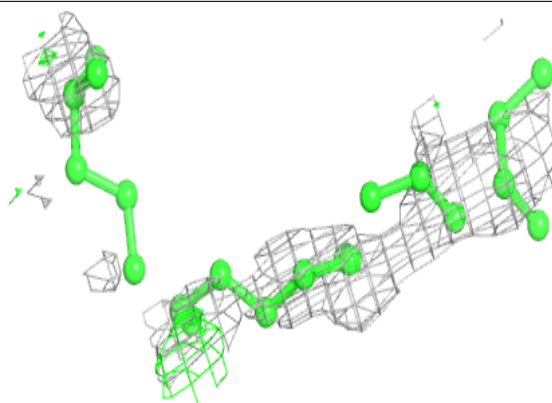
**Electron density around L1P B 294:**

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

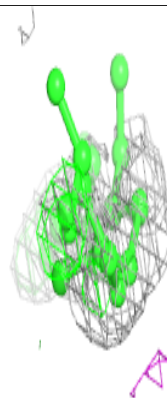
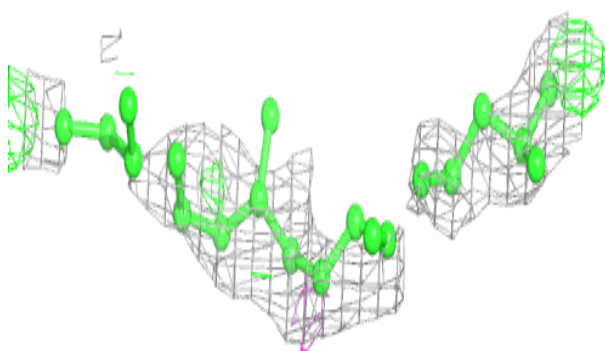
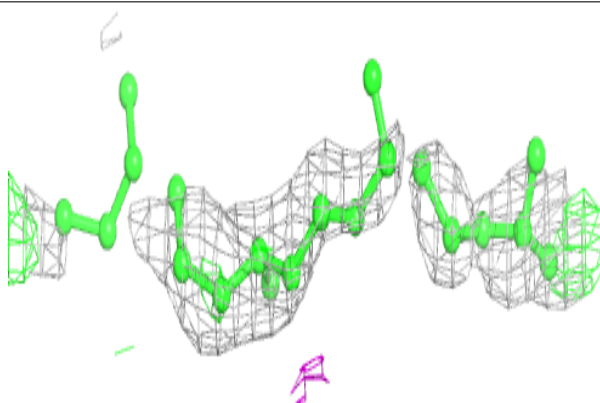


**Electron density around L3P A 297:**

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and green (positive)

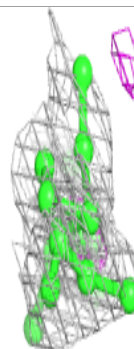
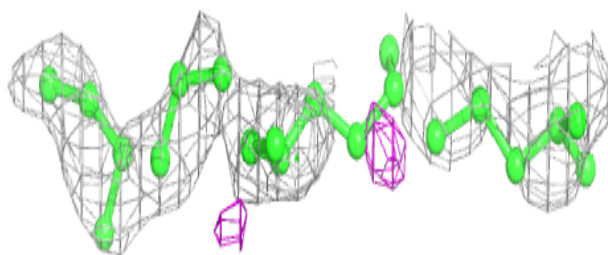
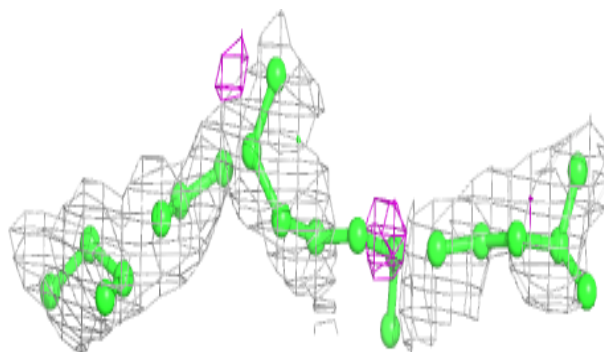
**Electron density around L3P A 301:**

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

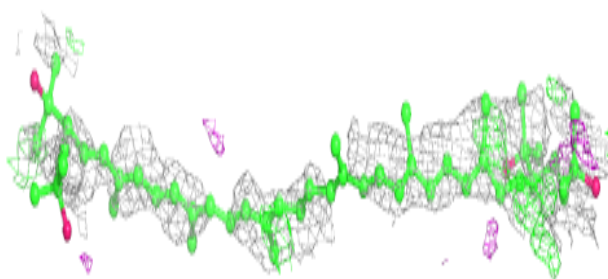
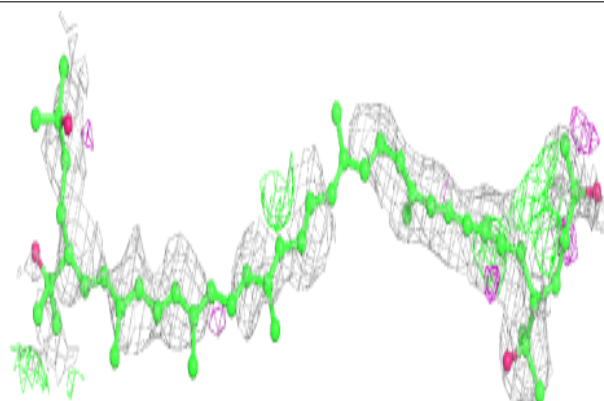


**Electron density around L3P B 331:**

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

**Electron density around 22B D 300:**

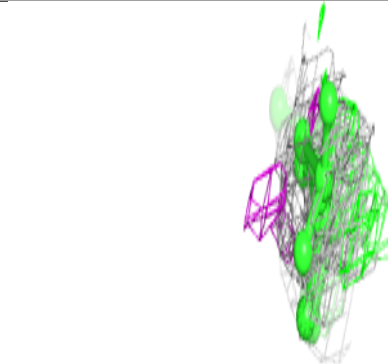
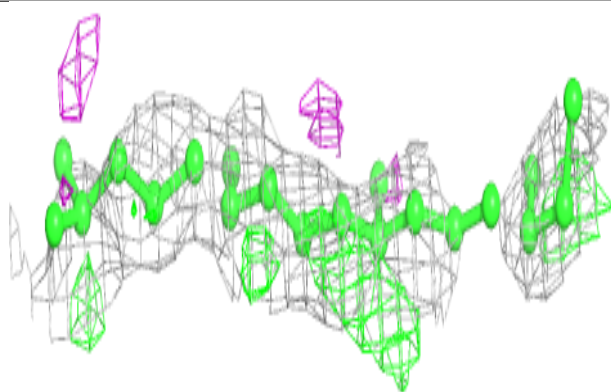
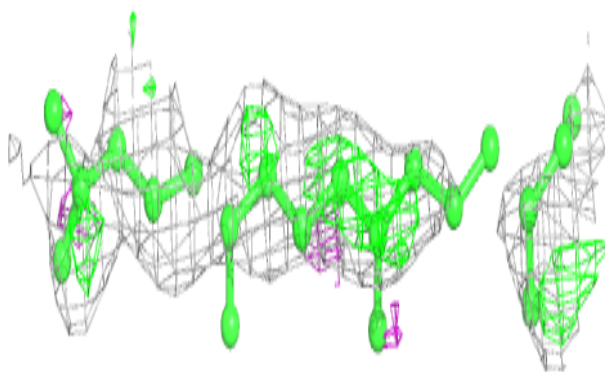
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



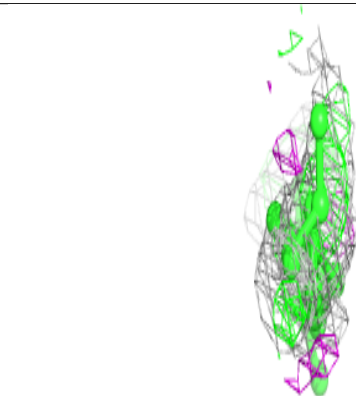
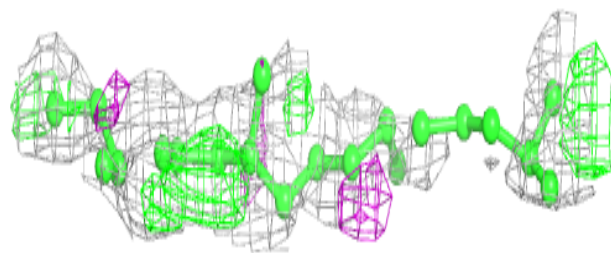
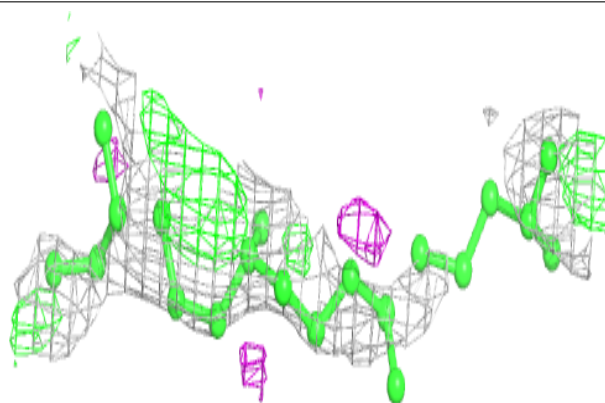


**Electron density around L2P D 293:**

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and green (positive)

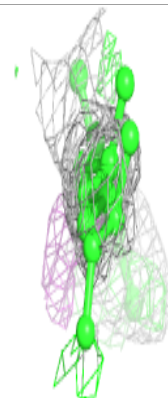
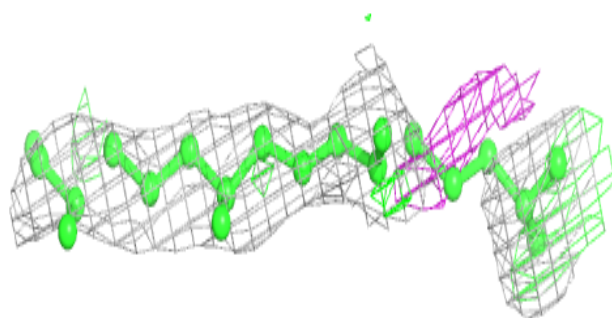
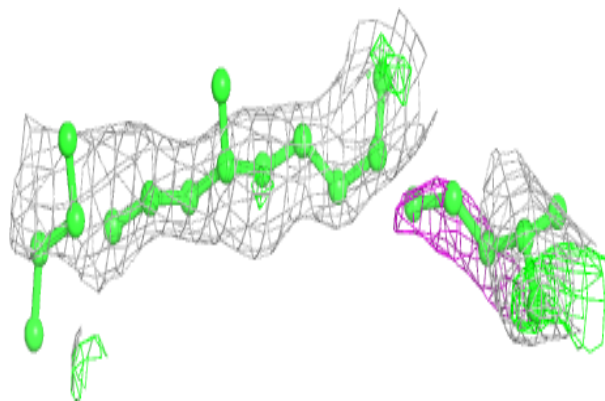
**Electron density around L3P A 299:**

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

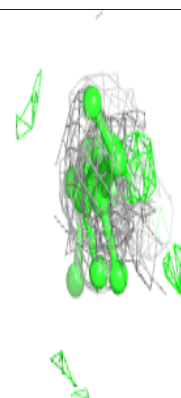
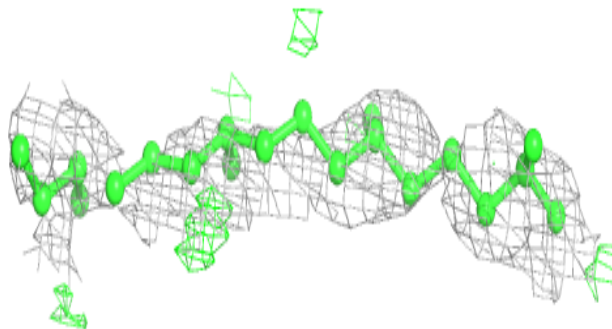
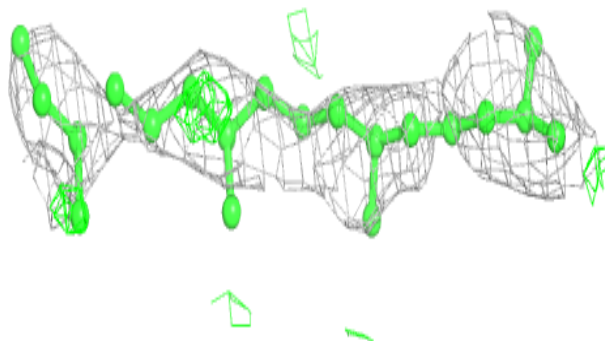


**Electron density around L2P D 294:**

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

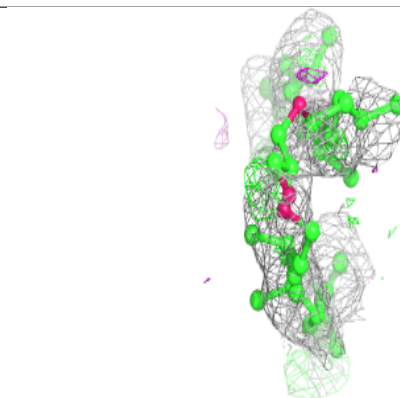
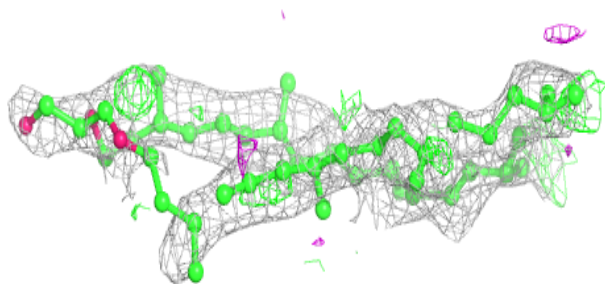
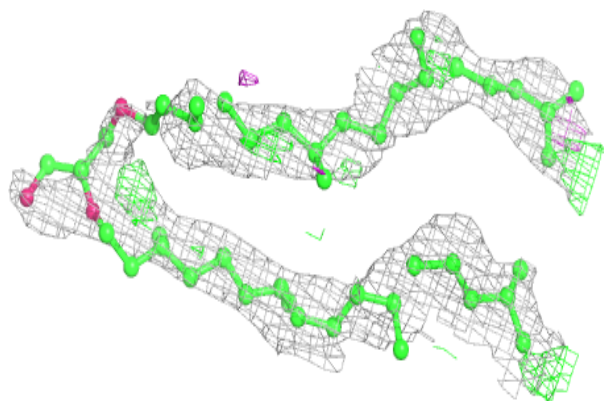
**Electron density around L2P B 295:**

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

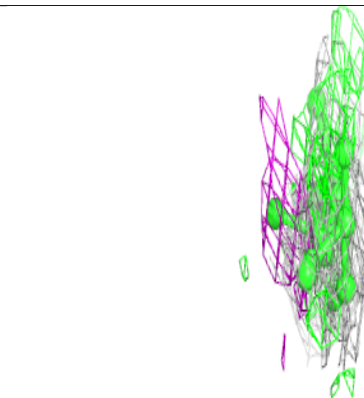
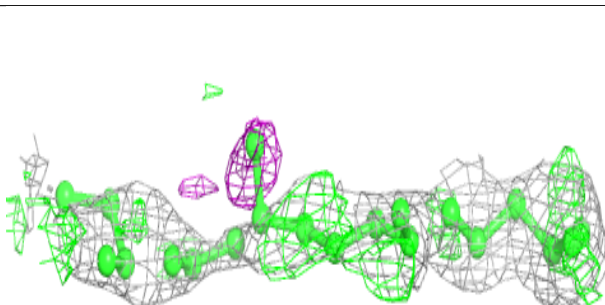
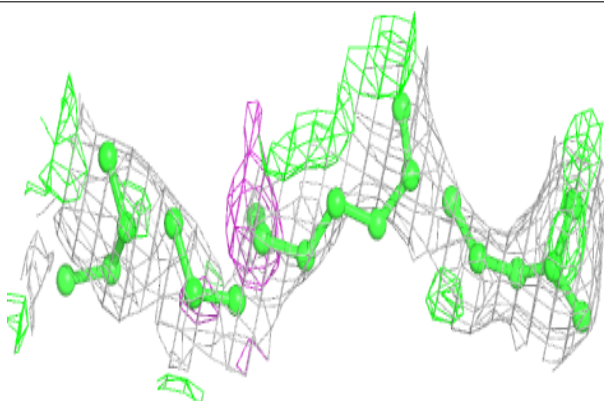


**Electron density around L1P A 293:**

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

**Electron density around L3P A 333:**

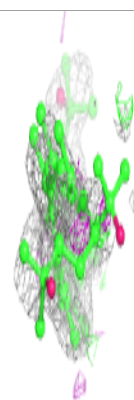
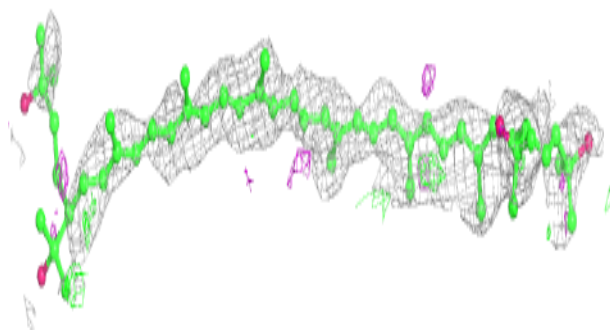
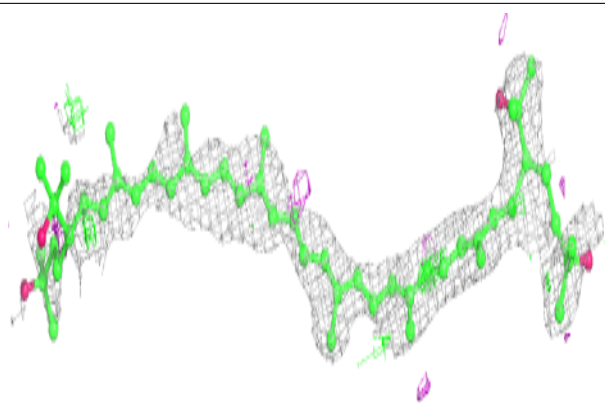
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



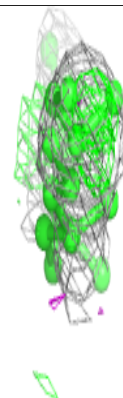
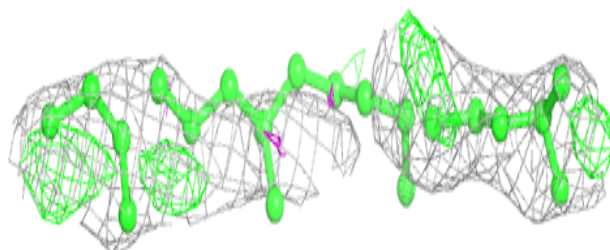
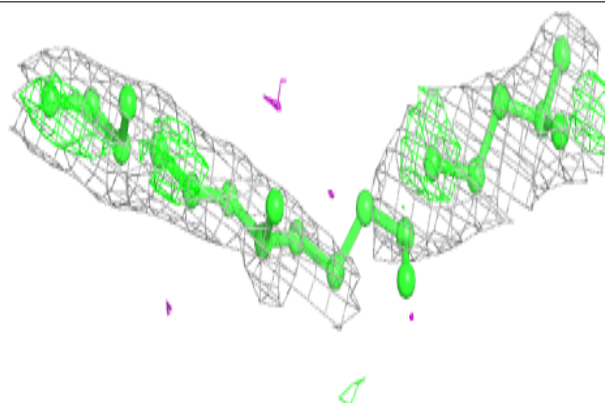


**Electron density around 22B A 300:**

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

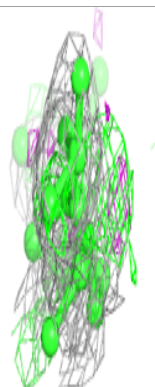
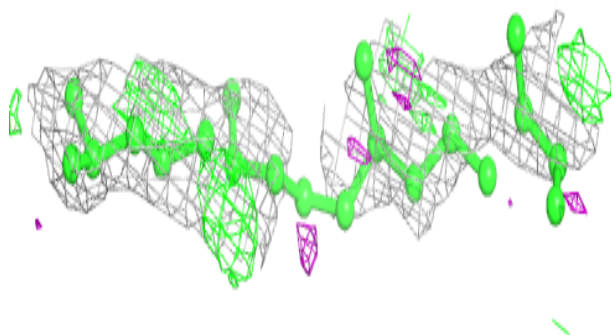
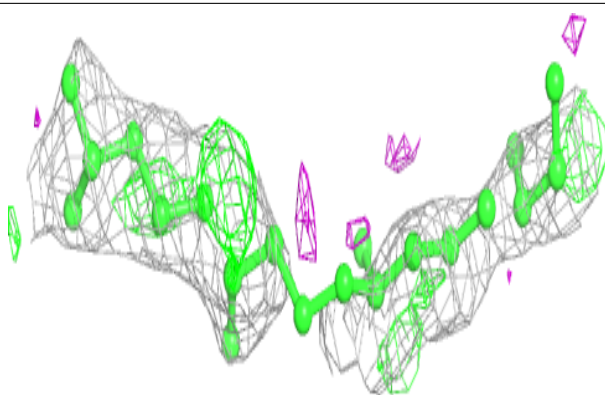
**Electron density around L2P B 296:**

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

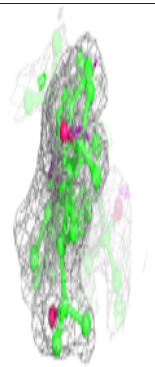
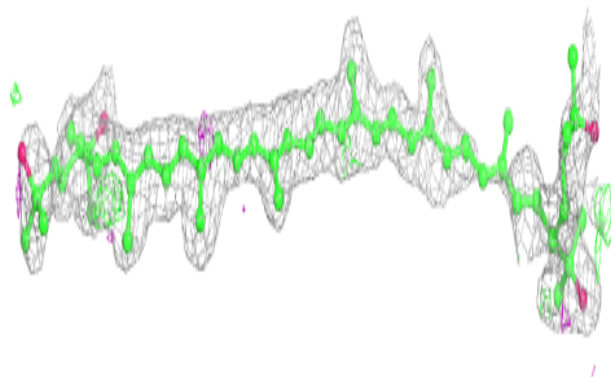
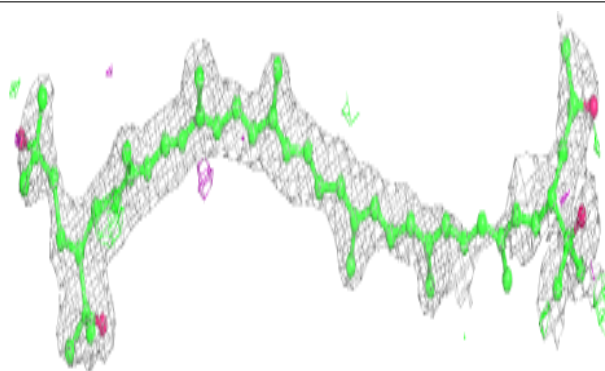


**Electron density around L2P A 294:**

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

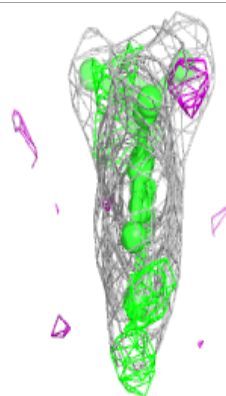
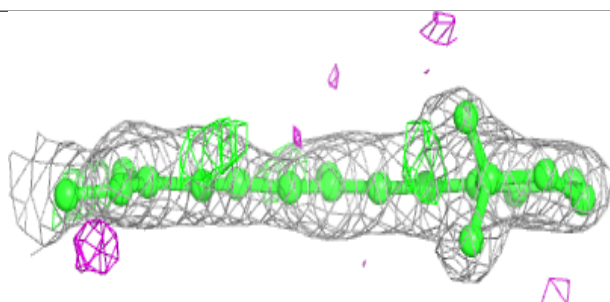
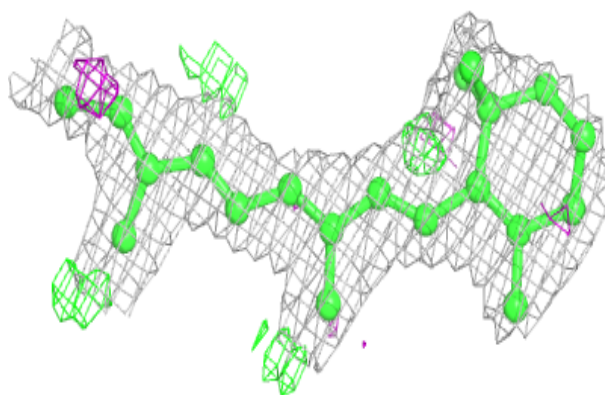
**Electron density around 22B B 300:**

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

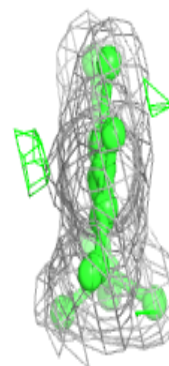
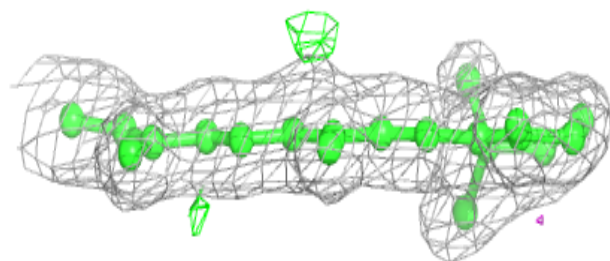
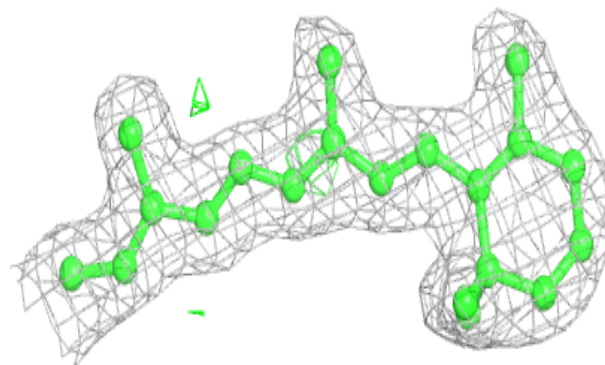


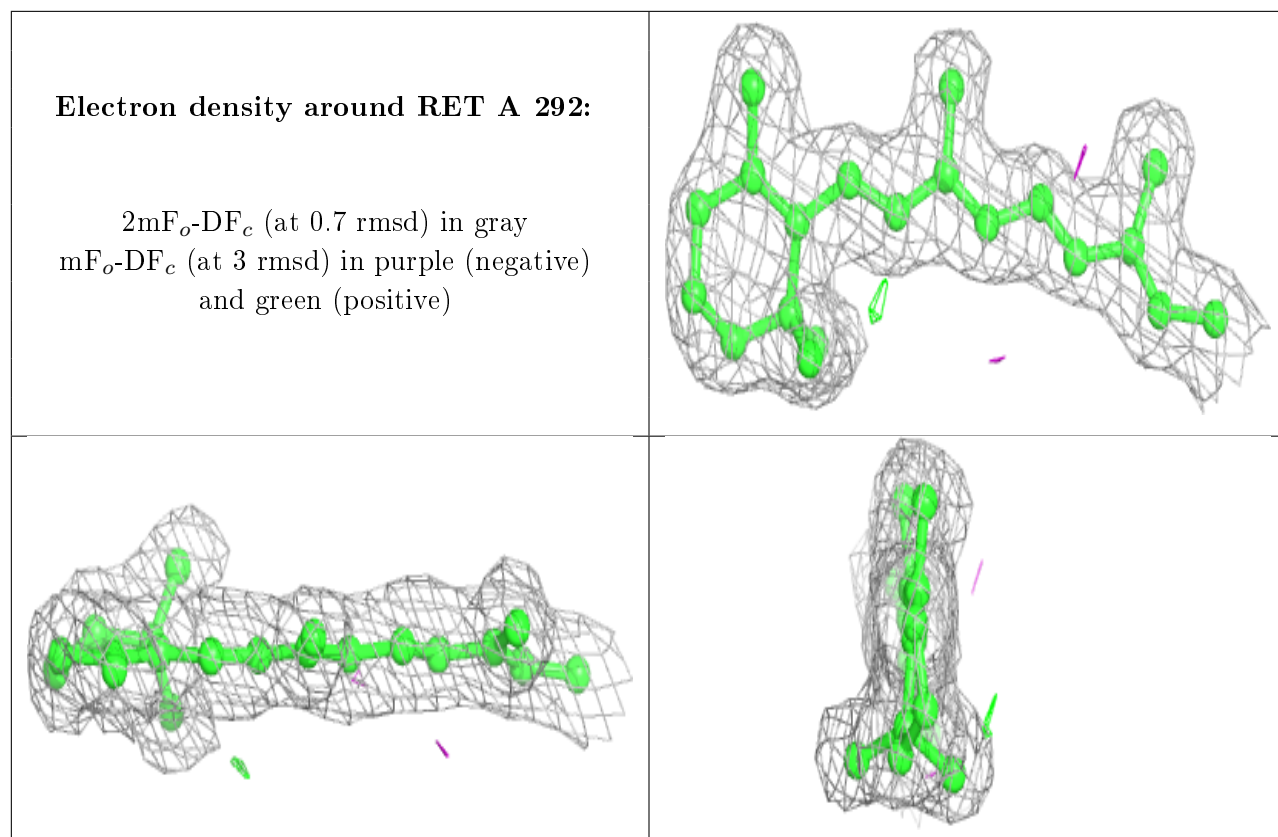
**Electron density around RET D 292:**

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

**Electron density around RET B 292:**

$2mF_o-DF_c$  (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.