



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:32 pm BST

PDB ID : 5EGI
Title : Structure of a Trimeric Intracellular Cation channel from *C. elegans* with bound Ca^{2+}
Authors : Yang, H.T.; Hu, M.H.; Liu, Z.F.
Deposited on : 2015-10-27
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

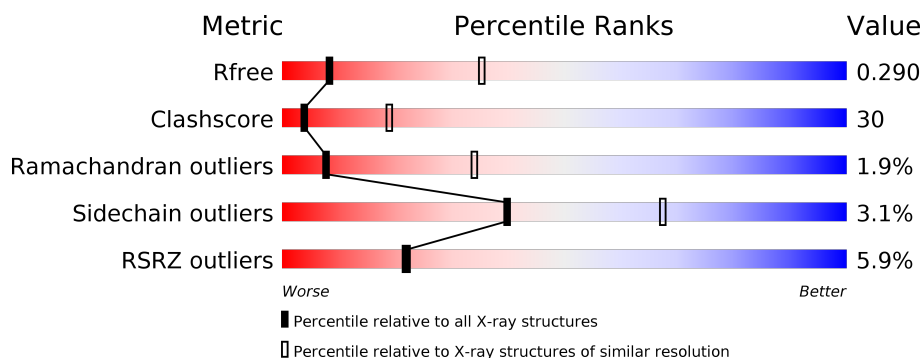
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	<div> <div>7%</div> <div> <div>43%</div> <div>45%</div> <div>10%</div> </div> </div>
1	B	257	<div> <div>4%</div> <div> <div>49%</div> <div>38%</div> <div>9%</div> </div> </div>
1	C	257	<div> <div>5%</div> <div> <div>47%</div> <div>41%</div> <div>10%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5704 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.

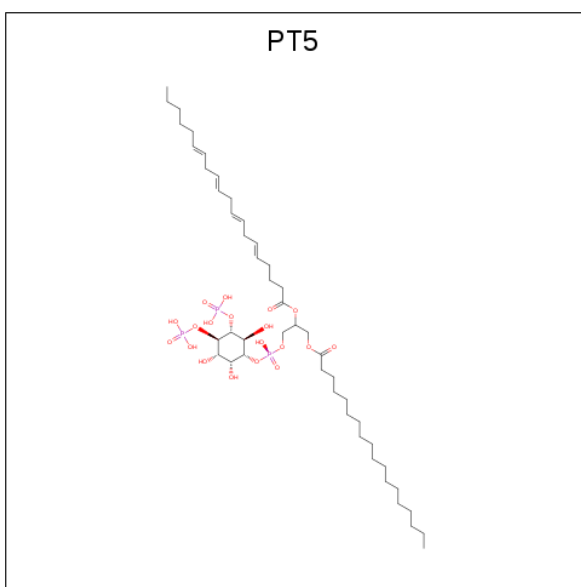
- Molecule 1 is a protein called Uncharacterized protein Y57A10A.10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1825	1209	299	308	9			
1	B	233	Total	C	N	O	S	0	0	0
			1830	1211	299	311	9			
1	C	232	Total	C	N	O	S	0	0	0
			1825	1209	299	308	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	HIS	-	expression tag	UNP Q9NA75
A	253	HIS	-	expression tag	UNP Q9NA75
A	254	HIS	-	expression tag	UNP Q9NA75
A	255	HIS	-	expression tag	UNP Q9NA75
A	256	HIS	-	expression tag	UNP Q9NA75
A	257	HIS	-	expression tag	UNP Q9NA75
B	252	HIS	-	expression tag	UNP Q9NA75
B	253	HIS	-	expression tag	UNP Q9NA75
B	254	HIS	-	expression tag	UNP Q9NA75
B	255	HIS	-	expression tag	UNP Q9NA75
B	256	HIS	-	expression tag	UNP Q9NA75
B	257	HIS	-	expression tag	UNP Q9NA75
C	252	HIS	-	expression tag	UNP Q9NA75
C	253	HIS	-	expression tag	UNP Q9NA75
C	254	HIS	-	expression tag	UNP Q9NA75
C	255	HIS	-	expression tag	UNP Q9NA75
C	256	HIS	-	expression tag	UNP Q9NA75
C	257	HIS	-	expression tag	UNP Q9NA75

- Molecule 2 is (1S)-2-[[[(R)-hydroxy{[(1R,2R,3S,4R,5R,6S)-2,3,6-trihydroxy-4,5-bis(phosphonoxy)cyclohexyl]oxy}phosphoryl]oxy}-1-[(octadecanoyloxy)methyl]ethyl (8E,11E)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: C₄₇H₈₅O₁₉P₃).

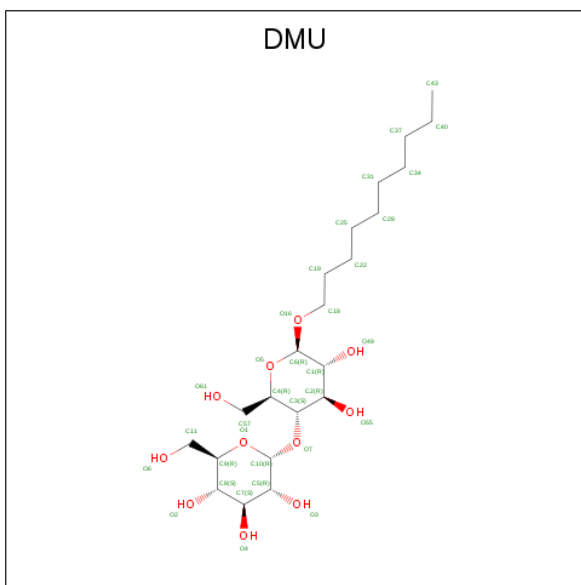


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			61	39	19	3		
2	B	1	Total	C	O	P	0	0
			61	39	19	3		
2	C	1	Total	C	O	P	0	0
			61	39	19	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			33	22	11		

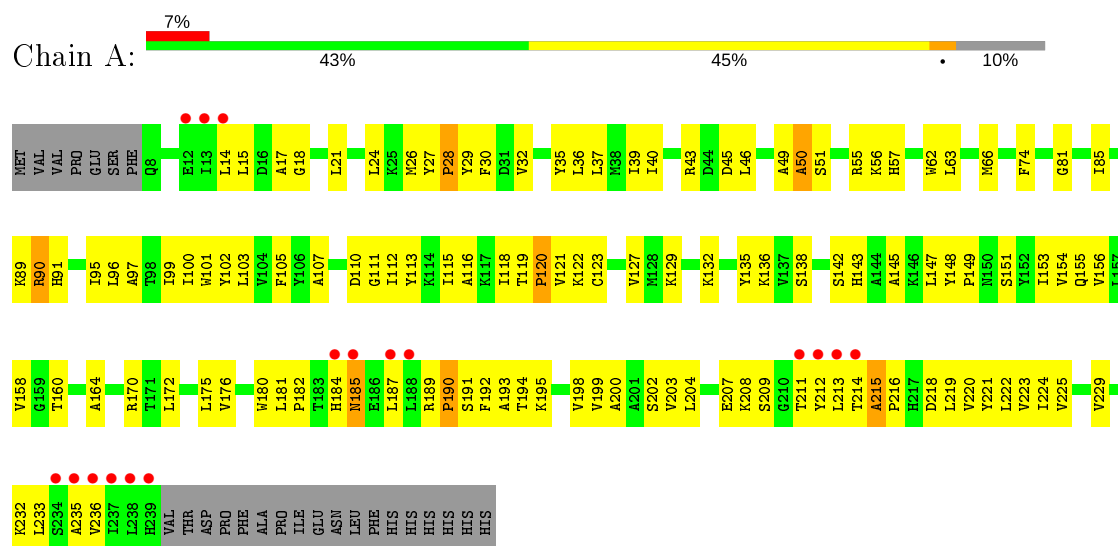
- Molecule 5 is water.

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

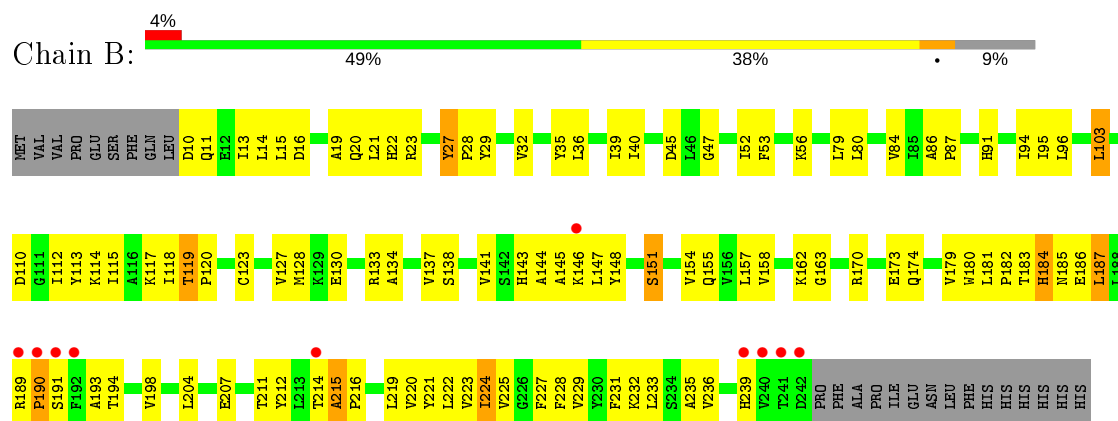
3 Residue-property plots [i](#)

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.

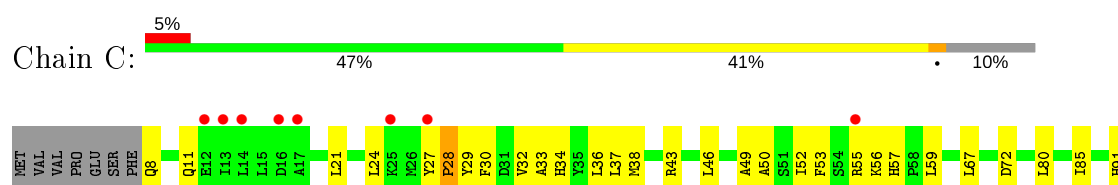
• Molecule 1: Uncharacterized protein Y57A10A.10

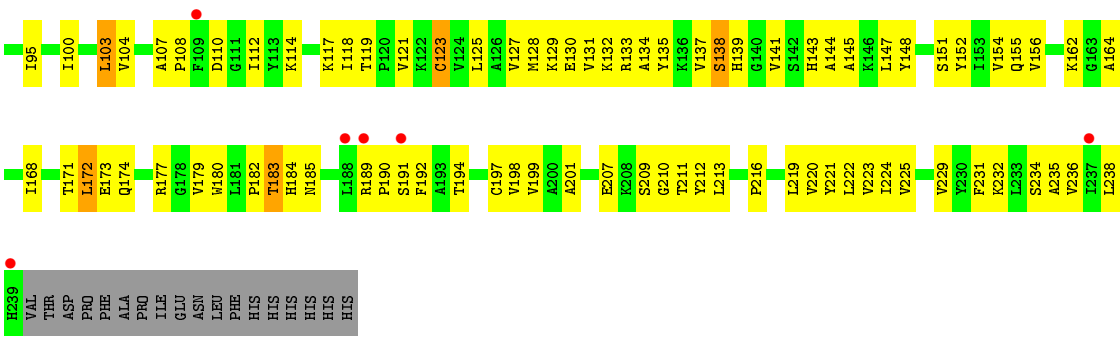


• Molecule 1: Uncharacterized protein Y57A10A.10



• Molecule 1: Uncharacterized protein Y57A10A.10





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.05Å 102.05Å 279.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 95.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.30) 99.5 (95.88-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.263 , 0.272 0.257 , 0.290	Depositor DCC
R_{free} test set	1146 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	108.6	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5704	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PT5, CA, DMU

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	0.44	0/1873	0.66	0/2548
1	B	0.46	0/1878	0.71	1/2556 (0.0%)
1	C	0.46	0/1873	0.66	0/2548
All	All	0.45	0/5624	0.68	1/7652 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	LEU	N-CA-C	-6.27	94.07	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	TYR	Sidechain

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	1825	0	1889	130	0
1	B	1830	0	1890	110	0
1	C	1825	0	1889	124	0
2	A	61	0	58	2	0
2	B	61	0	58	5	0
2	C	61	0	58	4	0
3	B	1	0	0	0	0
4	C	33	0	41	3	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
All	All	5704	0	5883	353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ILE:HD11	1:C:121:VAL:HG23	1.34	1.06
1:B:187:LEU:HB2	1:B:190:PRO:HD3	1.40	1.02
1:A:190:PRO:HB3	2:A:301:PT5:H3	1.45	0.95
1:C:189:ARG:HG3	1:C:235:ALA:HB2	1.52	0.92
1:C:152:TYR:O	1:C:156:VAL:HG23	1.70	0.91
1:A:91:HIS:O	1:A:95:ILE:HG12	1.70	0.91
1:A:37:LEU:HD12	1:A:129:LYS:HD2	1.54	0.90
1:C:123:CYS:SG	1:C:236:VAL:HG11	2.14	0.88
1:C:32:VAL:O	1:C:36:LEU:HB2	1.74	0.87
1:A:221:TYR:O	1:A:225:VAL:HG23	1.74	0.87
1:A:32:VAL:HG12	1:A:96:LEU:HD11	1.57	0.86
1:B:182:PRO:C	1:B:184:HIS:H	1.78	0.85
1:C:220:VAL:O	1:C:223:VAL:HG22	1.77	0.84
1:A:220:VAL:O	1:A:223:VAL:HG22	1.77	0.84
1:B:91:HIS:O	1:B:95:ILE:HG12	1.78	0.83
1:C:59:LEU:HD13	4:C:302:DMU:H17	1.59	0.83
1:B:110:ASP:HB3	1:B:114:LYS:HE2	1.61	0.82
1:C:216:PRO:HG2	1:C:219:LEU:HB3	1.61	0.82
1:C:194:THR:O	1:C:198:VAL:HG23	1.80	0.82
1:A:17:ALA:HB3	1:A:222:LEU:HD22	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HB3	1:B:112:ILE:HG21	1.61	0.81
1:B:27:TYR:CD1	1:B:28:PRO:HB3	2.16	0.80
1:A:103:LEU:HB3	1:A:112:ILE:HG21	1.61	0.80
1:C:207:GLU:OE1	1:C:220:VAL:HG11	1.80	0.80
1:A:123:CYS:O	1:A:127:VAL:HG23	1.82	0.79
1:A:118:ILE:HD11	1:A:121:VAL:HG23	1.62	0.79
1:A:219:LEU:O	1:A:223:VAL:HG13	1.83	0.78
1:C:180:TRP:NE1	1:C:182:PRO:HB3	1.98	0.78
1:B:187:LEU:HB2	1:B:190:PRO:CD	2.12	0.77
1:B:10:ASP:O	1:B:13:ILE:HG22	1.85	0.76
1:A:216:PRO:HG2	1:A:219:LEU:HB2	1.69	0.75
1:B:183:THR:C	1:B:185:ASN:H	1.87	0.75
1:B:23:ARG:HH11	1:B:23:ARG:HG2	1.52	0.75
1:C:91:HIS:O	1:C:95:ILE:HG12	1.86	0.75
1:B:11:GLN:HE21	1:B:15:LEU:HD11	1.52	0.74
1:A:232:LYS:O	1:A:236:VAL:HG23	1.87	0.73
1:A:27:TYR:CE1	1:A:28:PRO:HB3	2.23	0.73
1:C:234:SER:O	1:C:238:LEU:HB2	1.88	0.73
1:C:145:ALA:HA	1:C:155:GLN:HE21	1.53	0.73
1:A:194:THR:O	1:A:198:VAL:HG23	1.89	0.72
1:A:164:ALA:HB1	1:A:194:THR:HG22	1.70	0.72
1:A:123:CYS:SG	1:A:236:VAL:HG11	2.29	0.72
1:B:220:VAL:O	1:B:223:VAL:HG22	1.89	0.72
1:C:137:VAL:O	1:C:141:VAL:HG23	1.90	0.71
1:A:143:HIS:O	1:A:147:LEU:HD13	1.89	0.71
1:C:28:PRO:HD2	1:C:29:TYR:CD1	2.25	0.71
1:B:27:TYR:CE1	1:B:28:PRO:HB3	2.25	0.71
1:B:187:LEU:O	1:B:190:PRO:HD2	1.90	0.70
1:B:32:VAL:O	1:B:36:LEU:HB2	1.92	0.70
1:A:32:VAL:O	1:A:36:LEU:HB2	1.92	0.70
1:B:110:ASP:O	1:B:114:LYS:HG3	1.91	0.70
1:B:103:LEU:HB3	1:B:112:ILE:HD13	1.72	0.69
1:C:100:ILE:O	1:C:104:VAL:HG23	1.92	0.69
1:C:143:HIS:O	1:C:147:LEU:HD13	1.93	0.69
1:A:142:SER:HA	1:A:208:LYS:HE2	1.74	0.68
1:B:154:VAL:O	1:B:158:VAL:HG23	1.93	0.68
1:A:21:LEU:O	1:A:24:LEU:HB3	1.94	0.68
1:A:209:SER:OG	1:A:211:THR:HG22	1.93	0.68
1:C:151:SER:O	1:C:155:GLN:HG3	1.94	0.68
1:B:151:SER:HA	1:C:91:HIS:HE1	1.58	0.67
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:HD3	2:B:301:PT5:O51	1.95	0.66
1:C:225:VAL:O	1:C:229:VAL:HG23	1.96	0.66
1:A:132:LYS:HE3	1:A:136:LYS:HE3	1.77	0.66
1:B:21:LEU:HD22	1:B:222:LEU:HD12	1.77	0.66
1:A:107:ALA:HB2	1:A:112:ILE:HG22	1.76	0.66
1:C:180:TRP:O	1:C:182:PRO:HD3	1.96	0.66
1:A:107:ALA:CB	1:A:112:ILE:HG22	2.26	0.65
1:C:72:ASP:OD2	1:C:162:LYS:HE3	1.97	0.65
1:C:168:ILE:O	1:C:172:LEU:HD22	1.96	0.65
1:C:21:LEU:HD21	1:C:225:VAL:HG21	1.79	0.65
1:A:35:TYR:CD2	1:A:97:ALA:HA	2.32	0.65
1:B:157:LEU:HD12	1:C:85:ILE:HD11	1.79	0.64
1:C:127:VAL:HG13	1:C:229:VAL:HG13	1.79	0.64
1:B:144:ALA:CB	1:B:155:GLN:HA	2.28	0.64
1:B:182:PRO:C	1:B:184:HIS:N	2.48	0.64
1:C:119:THR:O	1:C:123:CYS:HB2	1.98	0.64
1:C:189:ARG:CG	1:C:235:ALA:HB2	2.27	0.63
1:A:215:ALA:HB1	1:A:219:LEU:HD23	1.81	0.63
2:B:301:PT5:H33	1:C:67:LEU:CD2	2.29	0.62
1:C:118:ILE:CD1	1:C:121:VAL:HG23	2.22	0.62
1:A:190:PRO:HA	1:A:193:ALA:CB	2.29	0.62
1:B:148:TYR:HB3	1:B:151:SER:OG	1.99	0.62
1:C:219:LEU:O	1:C:223:VAL:HG13	1.99	0.62
1:A:91:HIS:CE1	1:C:151:SER:HA	2.35	0.61
1:A:138:SER:HA	1:A:204:LEU:HD13	1.81	0.61
1:A:175:LEU:HD11	1:A:180:TRP:CZ3	2.36	0.61
1:C:103:LEU:HB3	1:C:112:ILE:HG21	1.83	0.61
1:A:190:PRO:HA	1:A:193:ALA:HB3	1.81	0.61
1:A:225:VAL:O	1:A:229:VAL:HG23	1.99	0.61
1:A:96:LEU:HA	1:A:99:ILE:HD12	1.83	0.61
1:B:144:ALA:HB1	1:B:155:GLN:HA	1.81	0.61
1:B:183:THR:C	1:B:185:ASN:N	2.54	0.61
1:C:127:VAL:O	1:C:130:GLU:HB2	2.01	0.61
1:A:32:VAL:CG1	1:A:96:LEU:HD11	2.29	0.60
1:C:182:PRO:HA	1:C:184:HIS:CE1	2.36	0.60
1:B:207:GLU:OE1	1:B:220:VAL:HG11	2.01	0.60
1:A:175:LEU:HD11	1:A:180:TRP:HZ3	1.65	0.60
1:B:189:ARG:O	1:B:191:SER:N	2.34	0.60
1:A:15:LEU:CD2	1:A:216:PRO:HG3	2.31	0.60
1:A:43:ARG:HG3	1:A:105:PHE:CE1	2.37	0.60
1:A:189:ARG:HG3	1:A:235:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ARG:NH1	1:B:193:ALA:HB1	2.16	0.60
1:C:118:ILE:HG13	1:C:121:VAL:H	1.67	0.59
1:A:229:VAL:O	1:A:233:LEU:HG	2.02	0.59
1:B:36:LEU:O	1:B:40:ILE:HG13	2.02	0.59
1:A:216:PRO:HG2	1:A:219:LEU:CB	2.32	0.59
1:C:221:TYR:O	1:C:225:VAL:HG23	2.02	0.59
1:C:190:PRO:HB3	2:C:301:PT5:H3	1.84	0.59
1:B:115:ILE:O	1:B:118:ILE:HG12	2.01	0.59
1:B:183:THR:O	1:B:185:ASN:N	2.35	0.59
1:C:28:PRO:HD2	1:C:29:TYR:HD1	1.66	0.59
1:C:130:GLU:HG3	1:C:232:LYS:HB2	1.84	0.59
1:A:55:ARG:NH1	1:A:55:ARG:HB3	2.17	0.58
1:B:147:LEU:HD12	1:B:147:LEU:N	2.18	0.58
1:A:145:ALA:HA	1:A:155:GLN:NE2	2.19	0.58
1:C:28:PRO:O	1:C:32:VAL:HG13	2.03	0.58
1:C:56:LYS:HG2	1:C:57:HIS:CD2	2.39	0.58
1:A:151:SER:HA	1:B:91:HIS:HE1	1.68	0.58
1:A:18:GLY:HA3	1:A:218:ASP:HB3	1.84	0.58
1:A:170:ARG:HD2	2:A:301:PT5:O51	2.03	0.58
1:A:36:LEU:HD13	1:A:100:ILE:HG23	1.86	0.58
1:C:27:TYR:CD1	1:C:28:PRO:HB3	2.39	0.58
1:A:74:PHE:HB3	2:C:301:PT5:H37	1.84	0.58
1:A:192:PHE:HA	1:A:195:LYS:HD2	1.85	0.58
1:B:103:LEU:CB	1:B:112:ILE:HD13	2.33	0.58
1:C:224:ILE:HG13	1:C:225:VAL:N	2.19	0.58
1:B:151:SER:HA	1:C:91:HIS:CE1	2.39	0.57
1:B:113:TYR:CZ	1:B:117:LYS:HD2	2.40	0.57
1:C:27:TYR:CE1	1:C:28:PRO:HB3	2.39	0.57
1:A:27:TYR:CD1	1:A:28:PRO:HB3	2.40	0.57
2:B:301:PT5:H33	1:C:67:LEU:HD21	1.85	0.57
1:B:28:PRO:O	1:B:32:VAL:HG22	2.05	0.56
1:A:189:ARG:N	1:A:190:PRO:CD	2.68	0.56
1:A:190:PRO:O	1:A:194:THR:HG23	2.04	0.56
1:A:15:LEU:HD21	1:A:216:PRO:HG3	1.87	0.56
1:C:145:ALA:HA	1:C:155:GLN:NE2	2.20	0.56
1:A:187:LEU:O	1:A:190:PRO:HD2	2.06	0.55
1:C:168:ILE:HD13	2:C:301:PT5:H62	1.87	0.55
1:B:189:ARG:C	1:B:191:SER:H	2.10	0.55
1:A:195:LYS:O	1:A:199:VAL:HG12	2.07	0.55
1:B:147:LEU:HD12	1:B:147:LEU:H	1.71	0.55
1:C:118:ILE:HD11	1:C:121:VAL:CG2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:VAL:O	1:B:87:PRO:HD2	2.07	0.55
1:C:129:LYS:O	1:C:132:LYS:HB3	2.07	0.55
1:C:133:ARG:HD3	1:C:197:CYS:SG	2.47	0.55
1:C:209:SER:C	1:C:211:THR:H	2.09	0.55
1:A:207:GLU:HA	1:A:213:LEU:HD12	1.89	0.55
1:A:46:LEU:HB3	1:A:50:ALA:HB2	1.89	0.55
1:A:28:PRO:O	1:A:32:VAL:HG13	2.07	0.55
1:A:189:ARG:O	1:A:193:ALA:N	2.37	0.54
1:A:200:ALA:O	1:A:203:VAL:HB	2.07	0.54
1:C:189:ARG:C	1:C:191:SER:H	2.11	0.54
1:C:216:PRO:HG2	1:C:219:LEU:CB	2.36	0.54
1:C:8:GLN:N	1:C:11:GLN:HG3	2.21	0.54
1:A:189:ARG:O	1:A:192:PHE:HB2	2.07	0.54
1:B:187:LEU:HB3	1:B:239:HIS:NE2	2.23	0.54
1:A:132:LYS:O	1:A:135:TYR:HB3	2.08	0.54
1:C:52:ILE:HG23	1:C:53:PHE:N	2.22	0.54
1:A:14:LEU:HB3	1:A:219:LEU:HD13	1.89	0.54
1:B:143:HIS:O	1:B:147:LEU:HD13	2.07	0.54
1:B:216:PRO:HG2	1:B:219:LEU:HB3	1.90	0.54
1:A:160:THR:HG21	1:A:198:VAL:HG22	1.89	0.53
1:B:52:ILE:CG2	1:B:53:PHE:N	2.71	0.53
1:A:116:ALA:HA	1:A:121:VAL:HG11	1.90	0.53
1:C:180:TRP:HE1	1:C:182:PRO:HB3	1.72	0.53
1:B:174:GLN:HB3	1:B:179:VAL:O	2.08	0.53
1:C:91:HIS:O	1:C:95:ILE:CG1	2.56	0.53
1:A:151:SER:O	1:A:155:GLN:HG3	2.08	0.53
1:C:144:ALA:CB	1:C:155:GLN:HA	2.39	0.53
1:C:37:LEU:HD12	1:C:129:LYS:HD3	1.91	0.53
1:C:180:TRP:CE2	1:C:182:PRO:HB3	2.44	0.52
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.74	0.52
1:B:180:TRP:NE1	1:B:182:PRO:CG	2.73	0.52
1:B:79:LEU:O	1:C:85:ILE:HG22	2.09	0.52
1:C:135:TYR:CE1	1:C:139:HIS:CE1	2.98	0.52
1:C:33:ALA:O	1:C:36:LEU:HB3	2.10	0.52
1:C:135:TYR:O	1:C:138:SER:HB3	2.09	0.52
1:A:220:VAL:HA	1:A:223:VAL:HG22	1.90	0.52
1:B:216:PRO:HG2	1:B:219:LEU:CB	2.39	0.51
1:C:46:LEU:HB3	1:C:50:ALA:HA	1.93	0.51
1:C:130:GLU:HG3	1:C:232:LYS:CB	2.40	0.51
1:B:221:TYR:O	1:B:225:VAL:HG23	2.10	0.51
1:A:29:TYR:HA	1:A:32:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:HA	1:C:100:ILE:HG21	1.93	0.51
1:B:134:ALA:CB	1:B:225:VAL:HG22	2.41	0.50
1:A:191:SER:O	1:A:195:LYS:HE3	2.12	0.50
1:A:37:LEU:O	1:A:40:ILE:HB	2.12	0.50
1:C:103:LEU:O	1:C:107:ALA:HB2	2.10	0.50
1:C:56:LYS:O	1:C:57:HIS:HD2	1.95	0.50
1:B:198:VAL:CG2	4:C:302:DMU:H16	2.42	0.50
1:B:27:TYR:HD1	1:B:28:PRO:HB3	1.72	0.50
1:C:30:PHE:HA	1:C:128:MET:HE2	1.93	0.49
1:C:52:ILE:CG2	1:C:53:PHE:N	2.74	0.49
1:A:17:ALA:HB3	1:A:222:LEU:CD2	2.39	0.49
1:B:221:TYR:CE1	1:B:225:VAL:HG21	2.48	0.49
1:B:45:ASP:C	1:B:47:GLY:H	2.15	0.49
1:C:52:ILE:HA	1:C:55:ARG:HH11	1.77	0.49
1:A:185:ASN:HB3	1:A:187:LEU:O	2.13	0.49
1:B:220:VAL:HG13	1:B:221:TYR:N	2.27	0.49
1:A:170:ARG:NH2	1:A:184:HIS:CE1	2.81	0.49
1:C:132:LYS:O	1:C:135:TYR:HB3	2.12	0.49
1:C:182:PRO:C	1:C:184:HIS:H	2.16	0.49
1:B:194:THR:O	1:B:198:VAL:HG23	2.12	0.49
1:A:216:PRO:HD2	1:A:219:LEU:HD23	1.95	0.49
1:A:118:ILE:HG12	1:A:121:VAL:HB	1.96	0.48
1:A:91:HIS:HE1	1:C:151:SER:HA	1.77	0.48
1:B:174:GLN:HE22	1:B:181:LEU:HB3	1.77	0.48
1:C:164:ALA:HB1	1:C:194:THR:HG22	1.95	0.48
1:C:220:VAL:HG13	1:C:221:TYR:N	2.29	0.48
1:A:142:SER:CA	1:A:208:LYS:HE2	2.43	0.48
1:A:199:VAL:O	1:A:203:VAL:HG23	2.14	0.48
1:A:49:ALA:O	1:A:50:ALA:C	2.52	0.48
1:B:130:GLU:HB3	1:B:228:PHE:HB3	1.95	0.48
1:B:52:ILE:HG23	1:B:53:PHE:N	2.29	0.48
1:B:143:HIS:CE1	1:B:147:LEU:HD11	2.48	0.48
1:B:23:ARG:NH1	1:B:23:ARG:HG2	2.21	0.48
1:A:43:ARG:NH1	1:A:113:TYR:CG	2.82	0.48
1:C:36:LEU:HD13	1:C:100:ILE:HG23	1.96	0.48
1:A:89:LYS:O	1:A:91:HIS:N	2.46	0.47
1:B:189:ARG:C	1:B:191:SER:N	2.68	0.47
1:A:18:GLY:HA3	1:A:218:ASP:O	2.14	0.47
1:B:35:TYR:O	1:B:39:ILE:HG13	2.14	0.47
1:C:46:LEU:HB2	1:C:50:ALA:HB2	1.95	0.47
1:A:180:TRP:CD1	1:A:182:PRO:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:C	1:A:218:ASP:HB3	2.35	0.47
1:A:95:ILE:O	1:A:99:ILE:HG13	2.14	0.47
1:A:148:TYR:CD1	1:A:148:TYR:N	2.81	0.47
1:A:216:PRO:HD2	1:A:219:LEU:CD2	2.45	0.47
1:A:147:LEU:C	1:A:149:PRO:HD3	2.35	0.47
1:B:180:TRP:NE1	1:B:182:PRO:HG3	2.30	0.47
1:B:187:LEU:N	1:B:187:LEU:HD12	2.30	0.47
1:B:187:LEU:HD23	1:B:235:ALA:HB1	1.97	0.47
1:B:119:THR:HG22	1:B:120:PRO:N	2.28	0.47
1:A:170:ARG:HH21	1:A:184:HIS:CE1	2.32	0.47
1:B:227:PHE:O	1:B:231:PHE:HD1	1.98	0.47
1:B:27:TYR:CD1	1:B:28:PRO:CB	2.94	0.47
1:B:28:PRO:HD2	1:B:29:TYR:CD2	2.50	0.47
1:A:156:VAL:HG22	1:A:202:SER:HA	1.97	0.47
1:C:114:LYS:O	1:C:117:LYS:HB2	2.15	0.47
1:A:111:GLY:O	1:A:115:ILE:HG13	2.15	0.46
1:B:220:VAL:CG1	1:B:221:TYR:N	2.78	0.46
1:B:56:LYS:HG2	1:B:56:LYS:O	2.15	0.46
1:A:107:ALA:HB2	1:A:112:ILE:CG2	2.45	0.46
1:A:224:ILE:HG13	1:A:225:VAL:N	2.29	0.46
1:C:118:ILE:HG13	1:C:118:ILE:O	2.15	0.46
1:C:189:ARG:C	1:C:191:SER:N	2.68	0.46
1:A:18:GLY:CA	1:A:218:ASP:HB3	2.44	0.46
1:A:63:LEU:O	1:A:66:MET:HB2	2.15	0.46
1:B:32:VAL:HG13	1:B:96:LEU:HD21	1.98	0.46
1:B:151:SER:O	1:B:155:GLN:HG3	2.16	0.46
1:A:119:THR:N	1:A:120:PRO:HD2	2.31	0.46
1:A:214:THR:O	1:A:215:ALA:HB2	2.16	0.46
1:B:11:GLN:O	1:B:14:LEU:HB2	2.16	0.46
1:B:28:PRO:O	1:B:32:VAL:HG13	2.16	0.46
1:C:33:ALA:HA	1:C:125:LEU:HD22	1.97	0.46
1:C:80:LEU:HD13	1:C:143:HIS:CD2	2.50	0.46
1:B:147:LEU:CD1	1:B:147:LEU:H	2.29	0.46
1:C:168:ILE:HD11	2:C:301:PT5:H52	1.98	0.45
1:C:222:LEU:HD12	1:C:222:LEU:O	2.17	0.45
1:B:22:HIS:C	1:B:22:HIS:ND1	2.69	0.45
1:A:35:TYR:O	1:A:39:ILE:HG13	2.16	0.45
1:A:39:ILE:HG21	1:A:101:TRP:HA	1.99	0.45
1:C:108:PRO:C	1:C:110:ASP:H	2.20	0.45
1:B:180:TRP:CD1	1:B:182:PRO:HD3	2.52	0.45
1:C:46:LEU:HD13	1:C:53:PHE:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:PRO:O	1:B:193:ALA:HB3	2.16	0.44
1:C:209:SER:O	1:C:211:THR:N	2.51	0.44
1:B:27:TYR:HD1	1:B:28:PRO:CB	2.30	0.44
1:A:36:LEU:O	1:A:40:ILE:HG13	2.17	0.44
1:A:90:ARG:HE	1:A:90:ARG:HB2	1.42	0.44
1:C:220:VAL:O	1:C:223:VAL:CG2	2.56	0.44
1:C:144:ALA:HB3	1:C:155:GLN:HA	1.99	0.44
1:C:27:TYR:HA	1:C:28:PRO:HA	1.87	0.44
1:A:147:LEU:HD12	1:A:147:LEU:N	2.33	0.44
1:C:143:HIS:CE1	1:C:147:LEU:HD11	2.53	0.44
1:C:221:TYR:O	1:C:224:ILE:HG12	2.17	0.44
1:A:116:ALA:O	1:A:122:LYS:HB2	2.18	0.44
1:A:220:VAL:HG13	1:A:221:TYR:N	2.33	0.44
1:A:49:ALA:O	1:A:51:SER:N	2.51	0.44
1:B:181:LEU:CD1	1:B:183:THR:HG23	2.47	0.44
1:C:183:THR:C	1:C:185:ASN:N	2.71	0.44
1:B:229:VAL:O	1:B:233:LEU:HG	2.18	0.43
1:C:108:PRO:C	1:C:110:ASP:N	2.71	0.43
1:B:16:ASP:O	1:B:20:GLN:HG3	2.18	0.43
1:A:182:PRO:C	1:A:184:HIS:H	2.22	0.43
1:A:62:TRP:CZ2	1:A:66:MET:HG3	2.53	0.43
1:C:183:THR:C	1:C:185:ASN:H	2.19	0.43
1:A:180:TRP:O	1:A:181:LEU:HG	2.19	0.43
1:A:212:TYR:O	1:A:213:LEU:HG	2.19	0.43
1:C:52:ILE:HA	1:C:55:ARG:NH1	2.33	0.43
1:A:154:VAL:O	1:A:158:VAL:HG23	2.18	0.43
1:A:46:LEU:HB3	1:A:50:ALA:CB	2.48	0.43
1:A:112:ILE:HG23	1:A:113:TYR:N	2.34	0.42
1:B:29:TYR:HA	1:B:32:VAL:HG22	2.01	0.42
1:C:189:ARG:O	1:C:191:SER:N	2.52	0.42
1:A:190:PRO:HA	1:A:193:ALA:HB2	2.00	0.42
1:B:174:GLN:NE2	1:B:181:LEU:HB3	2.34	0.42
1:B:19:ALA:O	1:B:23:ARG:HG2	2.18	0.42
1:A:122:LYS:NZ	1:A:122:LYS:HB3	2.34	0.42
1:A:37:LEU:HD12	1:A:129:LYS:CD	2.37	0.42
1:C:199:VAL:C	1:C:201:ALA:N	2.72	0.42
1:B:138:SER:HA	1:B:204:LEU:HD13	2.02	0.42
1:C:103:LEU:C	1:C:112:ILE:HG21	2.40	0.42
1:C:192:PHE:HB3	1:C:231:PHE:CD2	2.54	0.42
1:C:34:HIS:O	1:C:38:MET:HG2	2.19	0.42
1:C:49:ALA:O	1:C:52:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASP:OD2	1:A:170:ARG:NH1	2.48	0.42
1:B:127:VAL:O	1:B:128:MET:C	2.57	0.42
1:A:62:TRP:CE2	1:A:66:MET:HG3	2.55	0.42
1:B:137:VAL:O	1:B:141:VAL:HG23	2.20	0.42
1:C:197:CYS:O	1:C:201:ALA:HB2	2.20	0.42
1:C:36:LEU:HA	1:C:100:ILE:CG2	2.50	0.42
1:C:130:GLU:CG	1:C:232:LYS:HG2	2.50	0.42
1:A:46:LEU:HB3	1:A:50:ALA:CA	2.50	0.41
1:B:45:ASP:C	1:B:47:GLY:N	2.74	0.41
1:B:162:LYS:HB3	1:B:162:LYS:HE3	1.88	0.41
1:B:186:GLU:HG3	2:B:301:PT5:O52	2.20	0.41
1:C:131:VAL:O	1:C:134:ALA:HB3	2.19	0.41
1:A:187:LEU:HD23	1:A:235:ALA:HB1	2.01	0.41
1:B:23:ARG:CG	1:B:23:ARG:HH11	2.28	0.41
1:C:139:HIS:H	1:C:139:HIS:HD1	1.66	0.41
2:B:301:PT5:H51	1:C:177:ARG:HG2	2.01	0.41
1:B:198:VAL:HG22	4:C:302:DMU:H16	2.01	0.41
1:A:26:MET:HA	1:A:30:PHE:CD2	2.56	0.41
1:A:46:LEU:CB	1:A:50:ALA:HB2	2.50	0.41
1:A:85:ILE:HG12	1:C:154:VAL:HG13	2.03	0.41
1:B:146:LYS:HB3	1:B:147:LEU:HD12	2.02	0.41
1:A:120:PRO:HG2	1:A:121:VAL:H	1.86	0.41
1:B:137:VAL:HG22	1:B:163:GLY:HA3	2.02	0.41
1:B:220:VAL:O	1:B:224:ILE:HG23	2.21	0.41
1:A:43:ARG:O	1:A:46:LEU:HB2	2.20	0.41
1:C:24:LEU:HD21	1:C:30:PHE:CE2	2.56	0.41
1:B:103:LEU:HD23	1:B:112:ILE:CD1	2.51	0.41
1:B:147:LEU:N	1:B:147:LEU:CD1	2.84	0.41
1:A:85:ILE:HA	1:A:85:ILE:HD12	1.93	0.41
1:C:180:TRP:CD1	1:C:182:PRO:HD3	2.56	0.41
1:C:130:GLU:HG2	1:C:232:LYS:HG2	2.03	0.41
1:C:46:LEU:HB2	1:C:50:ALA:CB	2.50	0.41
1:A:56:LYS:O	1:A:57:HIS:CD2	2.74	0.40
1:B:145:ALA:HA	1:B:155:GLN:HE21	1.86	0.40
1:B:232:LYS:O	1:B:236:VAL:HG23	2.20	0.40
1:C:174:GLN:HB3	1:C:179:VAL:O	2.20	0.40
1:A:145:ALA:O	1:A:149:PRO:HA	2.21	0.40
1:B:32:VAL:CG1	1:B:96:LEU:HD11	2.51	0.40
1:A:176:VAL:HA	1:C:171:THR:HG21	2.02	0.40
1:B:80:LEU:HD23	1:C:85:ILE:HG21	2.02	0.40
1:B:214:THR:O	1:B:215:ALA:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:HD13	1:B:94:ILE:HG21	2.02	0.40
1:C:30:PHE:CD1	1:C:128:MET:HB3	2.56	0.40
1:B:112:ILE:HG23	1:B:113:TYR:N	2.35	0.40
1:C:212:TYR:O	1:C:213:LEU:HB2	2.21	0.40
1:A:118:ILE:CD1	1:A:120:PRO:HG2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/257 (90%)	205 (89%)	19 (8%)	6 (3%)	5	27
1	B	231/257 (90%)	198 (86%)	28 (12%)	5 (2%)	6	30
1	C	230/257 (90%)	210 (91%)	18 (8%)	2 (1%)	17	48
All	All	691/771 (90%)	613 (89%)	65 (9%)	13 (2%)	8	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ALA
1	A	90	ARG
1	A	185	ASN
1	B	184	HIS
1	B	190	PRO
1	B	211	THR
1	C	210	GLY
1	C	138	SER
1	B	215	ALA
1	A	215	ALA
1	B	119	THR
1	A	120	PRO

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Mol	Chain	Res	Type
1	A	81	GLY

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	195/219 (89%)	191 (98%)	4 (2%)	53	75
1	B	196/219 (90%)	189 (96%)	7 (4%)	35	63
1	C	195/219 (89%)	188 (96%)	7 (4%)	35	63
All	All	586/657 (89%)	568 (97%)	18 (3%)	40	67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	110	ASP
1	A	172	LEU
1	A	190	PRO
1	B	27	TYR
1	B	103	LEU
1	B	123	CYS
1	B	151	SER
1	B	173	GLU
1	B	212	TYR
1	B	224	ILE
1	C	28	PRO
1	C	103	LEU
1	C	123	CYS
1	C	148	TYR
1	C	172	LEU
1	C	173	GLU
1	C	183	THR

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

Mol	Chain	Res	Type
1	A	91	HIS
1	A	239	HIS
1	B	11	GLN
1	B	143	HIS
1	B	155	GLN
1	B	174	GLN
1	B	184	HIS
1	C	57	HIS
1	C	77	ASN
1	C	91	HIS
1	C	143	HIS
1	C	155	GLN
1	C	174	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
2	PT5	B	301	-	61,61,69	2.00	17 (27%)	75,79,87	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMU	C	302	-	34,34,34	1.50	6 (17%)	45,45,45	1.18	5 (11%)
2	PT5	A	301	-	61,61,69	1.96	16 (26%)	75,79,87	1.21	5 (6%)
2	PT5	C	301	-	61,61,69	2.03	17 (27%)	75,79,87	1.29	5 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PT5	B	301	-	-	30/58/82/90	0/1/1/1
4	DMU	C	302	-	-	14/19/59/59	0/2/2/2
2	PT5	A	301	-	-	30/58/82/90	0/1/1/1
2	PT5	C	301	-	-	27/58/82/90	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PT5	P5-O51	5.83	1.69	1.50
2	B	301	PT5	P5-O51	5.78	1.69	1.50
2	C	301	PT5	P5-O51	5.66	1.68	1.50
2	B	301	PT5	O18-C11	4.65	1.46	1.33
2	A	301	PT5	C16-C15	4.31	1.56	1.31
2	A	301	PT5	O18-C11	4.31	1.45	1.33
2	B	301	PT5	C16-C15	4.28	1.56	1.31
2	C	301	PT5	C16-C15	4.23	1.56	1.31
2	C	301	PT5	O18-C11	4.12	1.45	1.33
4	C	302	DMU	C2-C3	4.10	1.63	1.52
2	B	301	PT5	P4-O42	4.08	1.63	1.50
2	C	301	PT5	P1-O13	4.07	1.75	1.59
2	A	301	PT5	C22-C21	4.02	1.55	1.31
2	C	301	PT5	C22-C21	4.02	1.55	1.31
2	B	301	PT5	C22-C21	4.01	1.55	1.31
2	C	301	PT5	P4-O42	3.97	1.63	1.50
2	A	301	PT5	P4-O42	3.95	1.63	1.50
2	A	301	PT5	P1-O11	3.92	1.64	1.50
2	C	301	PT5	P1-O11	3.88	1.64	1.50
2	B	301	PT5	P1-O11	3.85	1.64	1.50
2	C	301	PT5	P4-O4	3.79	1.66	1.59
2	B	301	PT5	P1-O13	3.69	1.74	1.59
2	A	301	PT5	P1-O13	3.57	1.73	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	PT5	C24-C25	3.55	1.56	1.29
2	A	301	PT5	C24-C25	3.55	1.56	1.29
2	B	301	PT5	C24-C25	3.55	1.56	1.29
4	C	302	DMU	O3-C5	-3.53	1.34	1.43
2	B	301	PT5	P5-O5	3.46	1.65	1.59
2	A	301	PT5	P5-O53	3.33	1.67	1.54
2	B	301	PT5	P5-O53	3.32	1.67	1.54
2	C	301	PT5	P5-O53	3.20	1.67	1.54
2	C	301	PT5	P5-O5	3.16	1.65	1.59
2	C	301	PT5	C5-C4	3.15	1.58	1.52
4	C	302	DMU	C8-C9	3.03	1.59	1.53
4	C	302	DMU	O16-C6	2.94	1.45	1.40
4	C	302	DMU	O7-C10	2.82	1.49	1.41
2	A	301	PT5	P5-O5	2.82	1.64	1.59
2	A	301	PT5	P4-O4	2.70	1.64	1.59
2	B	301	PT5	O18-C9	2.69	1.51	1.45
2	A	301	PT5	O18-C9	2.68	1.51	1.45
2	B	301	PT5	P4-O4	2.52	1.64	1.59
2	A	301	PT5	C5-C4	2.51	1.57	1.52
2	C	301	PT5	O18-C9	2.45	1.50	1.45
2	B	301	PT5	C5-C4	2.35	1.57	1.52
2	C	301	PT5	C36-C35	-2.33	1.38	1.51
2	B	301	PT5	C36-C35	-2.29	1.38	1.51
2	C	301	PT5	C9-C8	2.25	1.57	1.50
2	B	301	PT5	C9-C8	2.23	1.57	1.50
2	A	301	PT5	C2-C1	2.21	1.58	1.52
4	C	302	DMU	O7-C3	2.19	1.49	1.43
2	B	301	PT5	O19-C11	2.17	1.29	1.22
2	A	301	PT5	C36-C35	-2.14	1.39	1.51
2	A	301	PT5	C9-C8	2.11	1.57	1.50
2	B	301	PT5	C6-C5	2.09	1.57	1.52
2	C	301	PT5	C7-C8	2.06	1.57	1.50
2	C	301	PT5	P4-O41	2.04	1.62	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	PT5	C5-C6-C1	5.04	119.41	108.96
2	C	301	PT5	C5-C6-C1	4.73	118.77	108.96
2	A	301	PT5	C5-C6-C1	3.61	116.45	108.96
4	C	302	DMU	O1-C9-C11	3.13	114.23	106.44
2	C	301	PT5	C39-C38-C37	3.09	130.11	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	302	DMU	C18-O16-C6	-2.99	108.88	113.84
4	C	302	DMU	C2-C3-C4	-2.98	104.08	110.93
2	A	301	PT5	C39-C38-C37	2.94	129.33	114.42
2	B	301	PT5	C39-C38-C37	2.84	128.84	114.42
2	A	301	PT5	O1-C1-C2	2.75	115.06	108.66
2	C	301	PT5	C6-C5-C4	2.62	117.65	111.66
2	A	301	PT5	O1-C1-C6	-2.62	102.57	108.66
4	C	302	DMU	O7-C10-O1	2.34	117.22	110.67
2	B	301	PT5	C6-C5-C4	2.34	117.00	111.66
4	C	302	DMU	C10-O7-C3	-2.31	112.24	117.96
2	B	301	PT5	C9-C8-C7	2.23	117.07	111.79
2	C	301	PT5	O12-P1-O1	2.21	115.49	106.78
2	A	301	PT5	O12-P1-O1	2.18	115.39	106.78
2	B	301	PT5	O12-P1-O1	2.18	115.37	106.78
2	C	301	PT5	C3-C4-C5	2.14	116.54	111.66

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	DMU	C1-C6-O16-C18
4	C	302	DMU	O5-C6-O16-C18
4	C	302	DMU	C19-C18-O16-C6
2	B	301	PT5	C7-O13-P1-O11
2	B	301	PT5	C15-C16-C17-C18
2	B	301	PT5	C21-C22-C23-C24
2	A	301	PT5	C7-O13-P1-O11
2	A	301	PT5	C2-C1-O1-P1
2	A	301	PT5	C12-C10-O16-C8
2	A	301	PT5	C19-C20-C21-C22
2	A	301	PT5	C23-C24-C25-C26
2	C	301	PT5	C7-O13-P1-O12
2	C	301	PT5	C7-O13-P1-O11
2	C	301	PT5	C7-O13-P1-O1
2	C	301	PT5	C12-C10-O16-C8
2	C	301	PT5	C23-C24-C25-C26
2	A	301	PT5	O19-C11-O18-C9
2	B	301	PT5	O17-C10-O16-C8
2	A	301	PT5	O17-C10-O16-C8
2	A	301	PT5	C31-C11-O18-C9
2	B	301	PT5	C12-C10-O16-C8
2	B	301	PT5	O19-C11-O18-C9

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Mol	Chain	Res	Type	Atoms
2	B	301	PT5	C31-C11-O18-C9
4	C	302	DMU	O5-C4-C57-O61
2	C	301	PT5	C14-C15-C16-C17
2	C	301	PT5	O17-C10-O16-C8
4	C	302	DMU	C3-C4-C57-O61
2	C	301	PT5	C31-C11-O18-C9
2	B	301	PT5	C11-C31-C32-C33
2	C	301	PT5	C10-C12-C13-C14
2	C	301	PT5	O19-C11-O18-C9
4	C	302	DMU	O16-C18-C19-C22
4	C	302	DMU	C25-C28-C31-C34
2	C	301	PT5	C34-C35-C36-C37
2	C	301	PT5	C39-C40-C41-C42
2	A	301	PT5	C31-C32-C33-C34
2	A	301	PT5	C6-C1-O1-P1
2	C	301	PT5	C31-C32-C33-C34
2	B	301	PT5	C37-C38-C39-C40
2	B	301	PT5	C35-C36-C37-C38
2	A	301	PT5	C37-C38-C39-C40
2	C	301	PT5	C37-C38-C39-C40
4	C	302	DMU	C19-C22-C25-C28
2	B	301	PT5	C38-C39-C40-C41
2	A	301	PT5	C33-C34-C35-C36
4	C	302	DMU	C31-C34-C37-C40
2	A	301	PT5	C20-C21-C22-C23
2	B	301	PT5	C20-C21-C22-C23
2	A	301	PT5	C12-C13-C14-C15
2	C	301	PT5	C38-C39-C40-C41
2	A	301	PT5	O16-C8-C9-O18
2	B	301	PT5	C31-C32-C33-C34
4	C	302	DMU	C22-C25-C28-C31
2	C	301	PT5	C12-C13-C14-C15
4	C	302	DMU	C34-C37-C40-C43
2	B	301	PT5	C2-C1-O1-P1
2	B	301	PT5	C40-C41-C42-C43
2	C	301	PT5	C17-C18-C19-C20
2	C	301	PT5	C32-C33-C34-C35
2	B	301	PT5	O13-C7-C8-C9
4	C	302	DMU	C4-C3-O7-C10
2	A	301	PT5	C40-C41-C42-C43
2	A	301	PT5	C7-C8-C9-O18
2	C	301	PT5	C1-O1-P1-O12

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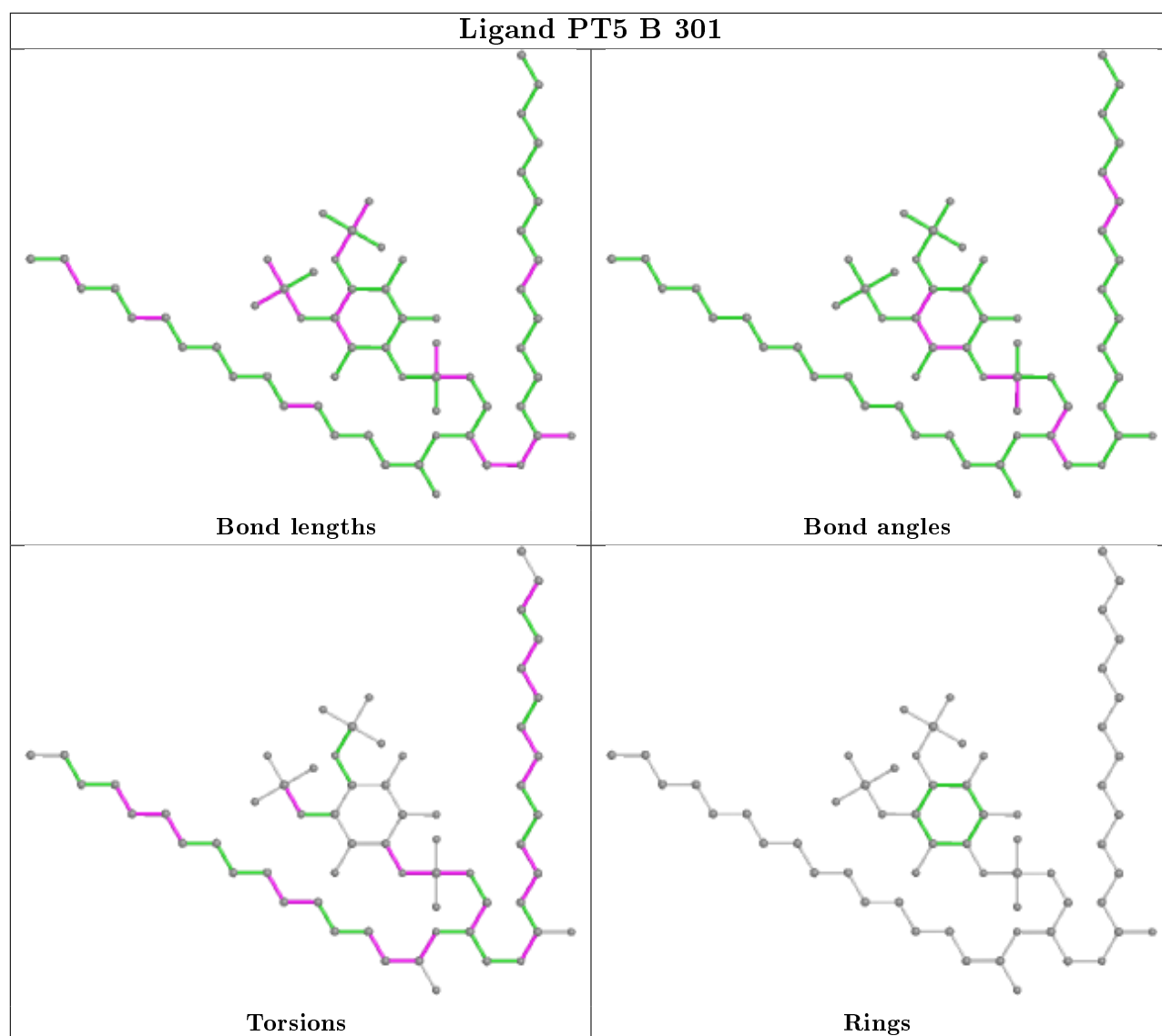
Mol	Chain	Res	Type	Atoms
2	C	301	PT5	C1-O1-P1-O11
2	B	301	PT5	C19-C20-C21-C22
2	A	301	PT5	C15-C16-C17-C18
2	A	301	PT5	C18-C19-C20-C21
2	C	301	PT5	C15-C16-C17-C18
2	C	301	PT5	C18-C19-C20-C21
2	C	301	PT5	C19-C20-C21-C22
2	C	301	PT5	C21-C22-C23-C24
2	B	301	PT5	O13-C7-C8-O16
2	B	301	PT5	C14-C15-C16-C17
2	B	301	PT5	C1-O1-P1-O13
2	C	301	PT5	C40-C41-C42-C43
2	B	301	PT5	C5-O5-P5-O51
2	C	301	PT5	C5-O5-P5-O51
2	B	301	PT5	C6-C1-O1-P1
2	B	301	PT5	C10-C12-C13-C14
2	B	301	PT5	C7-O13-P1-O12
2	A	301	PT5	C7-O13-P1-O12
2	A	301	PT5	C10-C12-C13-C14
2	B	301	PT5	C34-C35-C36-C37
4	C	302	DMU	C28-C31-C34-C37
4	C	302	DMU	C2-C3-O7-C10
2	A	301	PT5	C7-O13-P1-O1
2	A	301	PT5	C8-C9-O18-C11
2	B	301	PT5	C1-O1-P1-O12
2	B	301	PT5	C1-O1-P1-O11
2	A	301	PT5	O13-C7-C8-O16
2	C	301	PT5	C1-O1-P1-O13
2	A	301	PT5	C4-O4-P4-O42
2	B	301	PT5	O16-C10-C12-C13
2	A	301	PT5	C13-C14-C15-C16
2	A	301	PT5	O13-C7-C8-C9
2	B	301	PT5	C5-O5-P5-O53
2	A	301	PT5	C4-O4-P4-O41
2	A	301	PT5	C8-C7-O13-P1
2	B	301	PT5	O17-C10-C12-C13
2	A	301	PT5	O18-C11-C31-C32

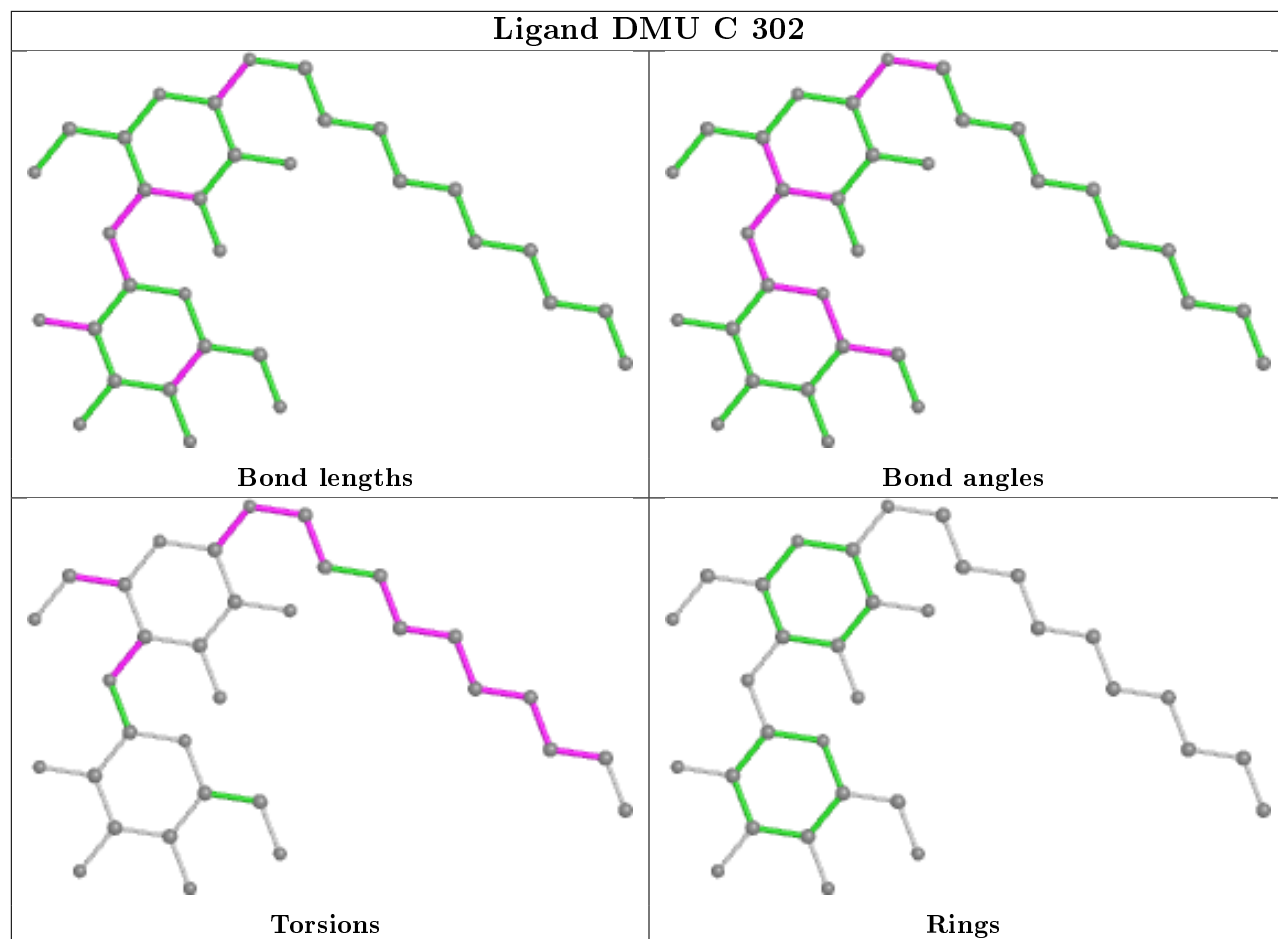
There are no ring outliers.

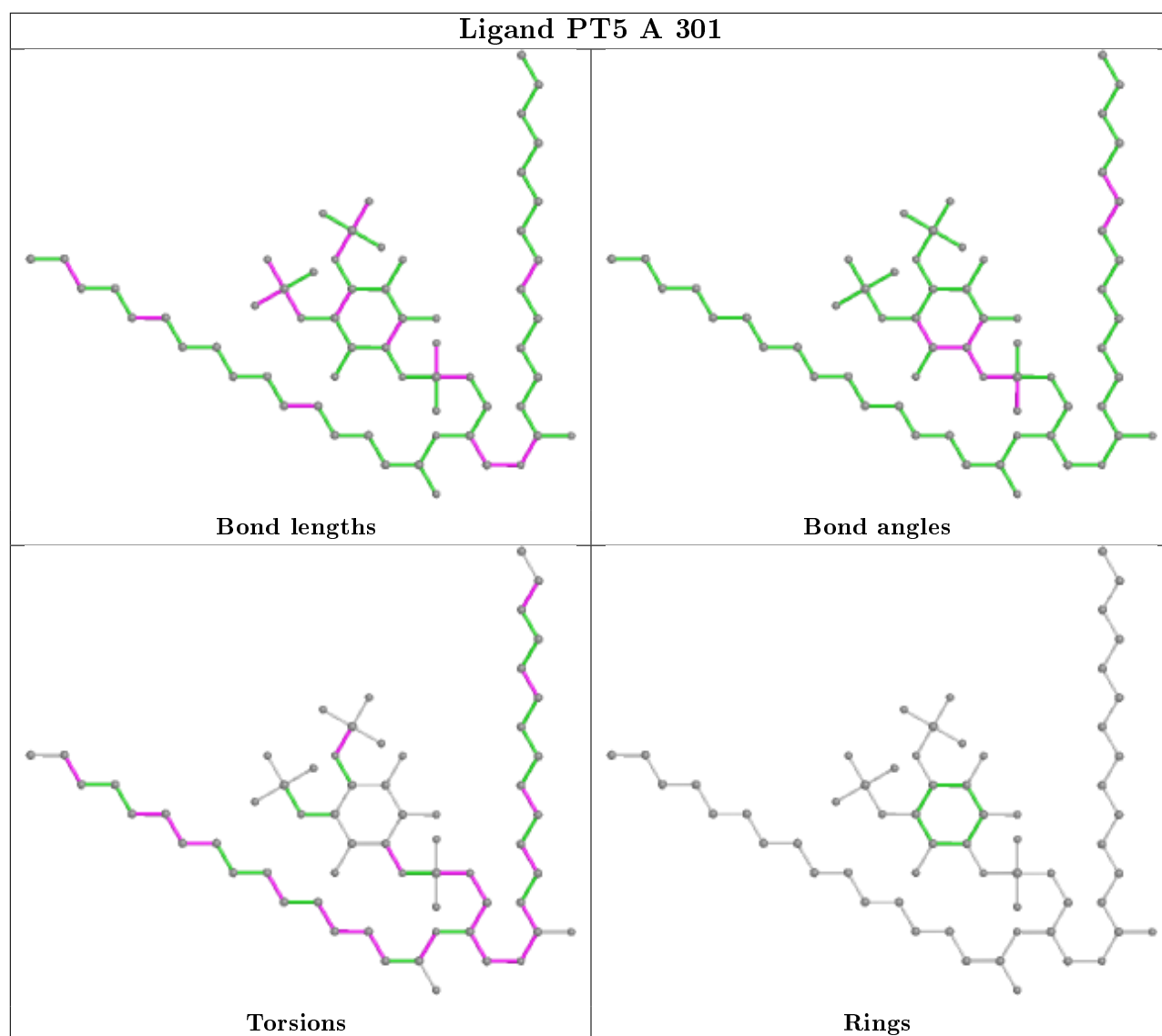
4 monomers are involved in 14 short contacts:

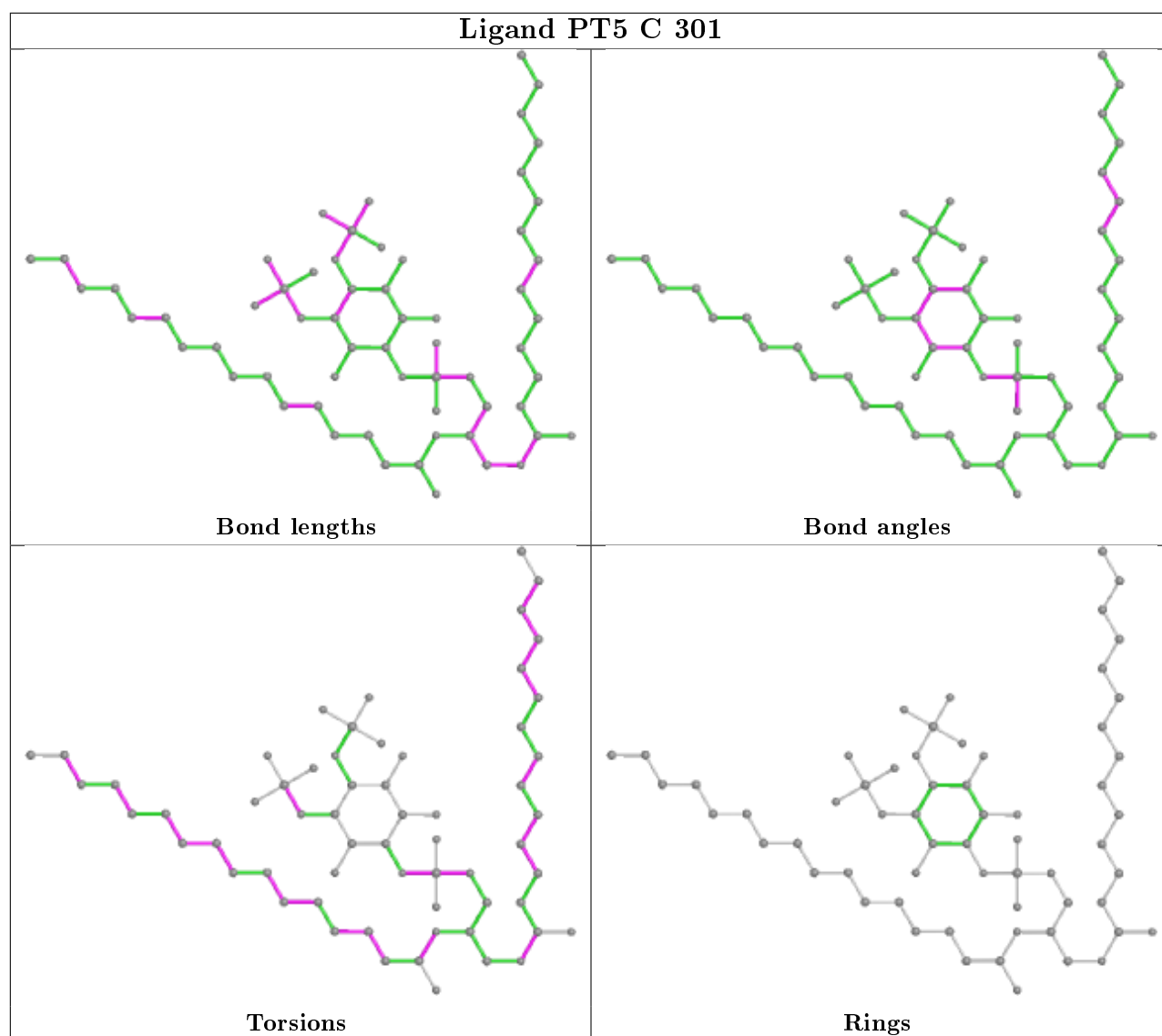
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	PT5	5	0
4	C	302	DMU	3	0
2	A	301	PT5	2	0
2	C	301	PT5	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/257 (90%)	0.15	17 (7%) 15 15	76, 115, 198, 220	0
1	B	233/257 (90%)	-0.01	10 (4%) 35 34	67, 98, 170, 203	0
1	C	232/257 (90%)	0.08	14 (6%) 21 21	69, 105, 191, 221	0
All	All	697/771 (90%)	0.07	41 (5%) 22 22	67, 105, 190, 221	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ILE	9.7
1	A	238	LEU	9.0
1	A	184	HIS	8.1
1	C	14	LEU	8.0
1	B	242	ASP	7.2
1	C	13	ILE	7.1
1	A	12	GLU	5.9
1	C	188	LEU	5.7
1	B	241	THR	5.4
1	B	191	SER	5.2
1	C	17	ALA	5.1
1	A	236	VAL	4.9
1	B	240	VAL	4.7
1	A	213	LEU	4.6
1	A	211	THR	4.5
1	C	12	GLU	4.4
1	A	13	ILE	4.1
1	A	239	HIS	4.1
1	A	234	SER	4.0
1	A	14	LEU	3.8
1	A	235	ALA	3.8
1	B	239	HIS	3.2
1	C	237	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	55	ARG	3.2
1	A	188	LEU	2.7
1	C	189	ARG	2.7
1	B	189	ARG	2.7
1	A	212	TYR	2.7
1	C	191	SER	2.5
1	C	109	PHE	2.5
1	C	16	ASP	2.4
1	A	187	LEU	2.3
1	B	214	THR	2.2
1	B	192	PHE	2.2
1	B	146	LYS	2.2
1	A	214	THR	2.2
1	C	27	TYR	2.1
1	B	190	PRO	2.1
1	A	185	ASN	2.1
1	C	25	LYS	2.0
1	C	239	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

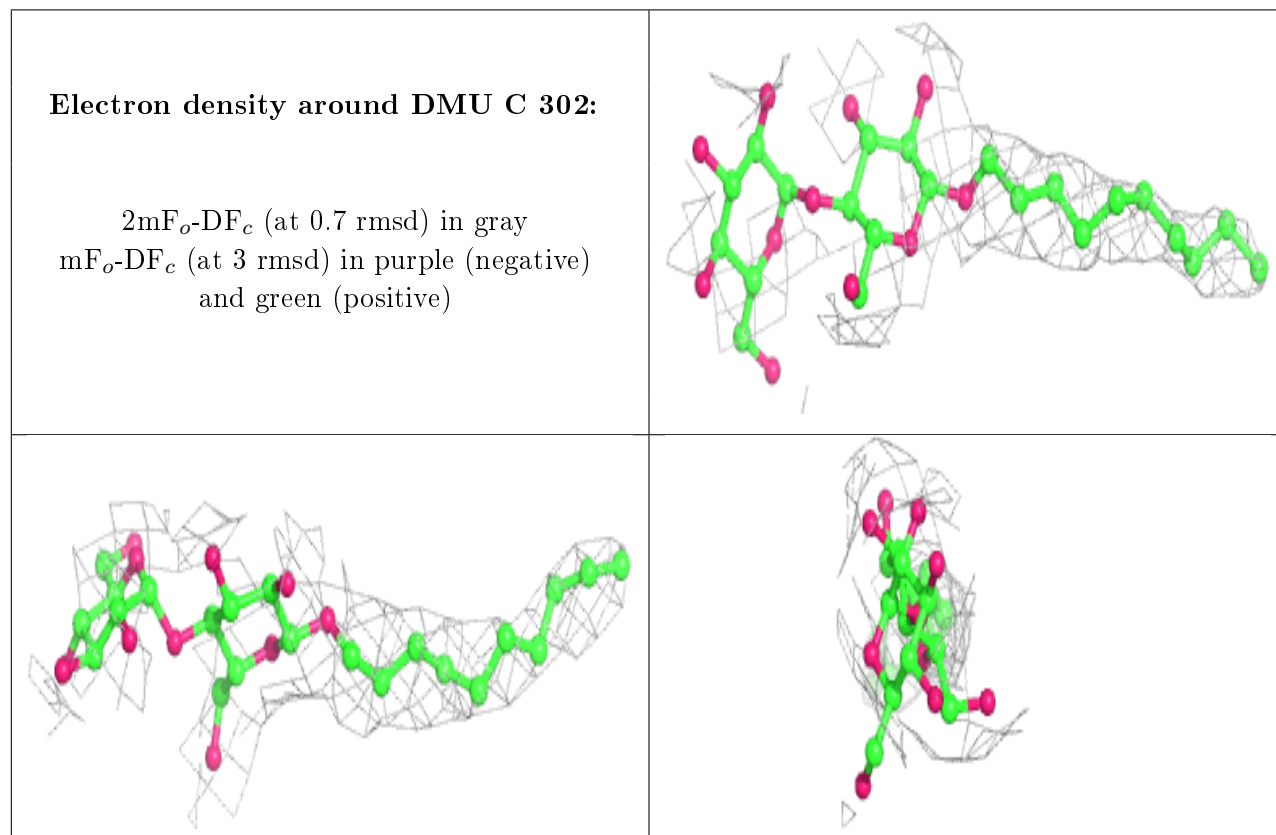
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

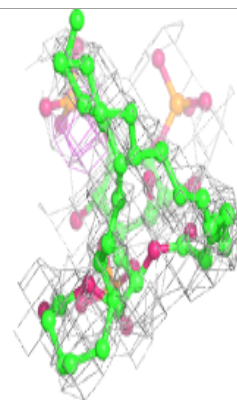
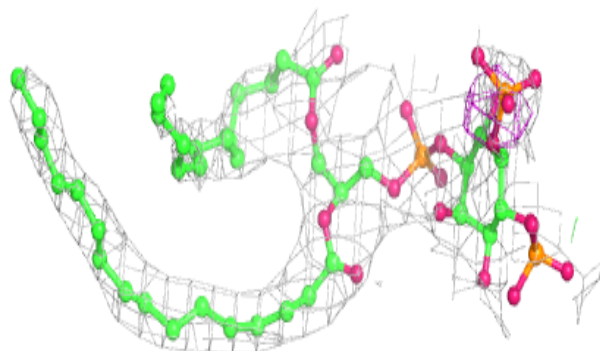
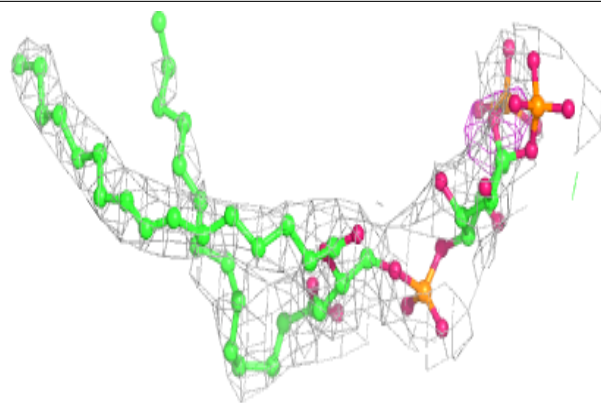
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DMU	C	302	33/33	0.77	0.24	83,136,156,157	0
2	PT5	B	301	61/69	0.86	0.38	58,123,151,154	0
2	PT5	C	301	61/69	0.88	0.38	72,138,157,160	0
2	PT5	A	301	61/69	0.89	0.39	52,136,149,152	0
3	CA	B	302	1/1	0.97	0.26	114,114,114,114	1

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.

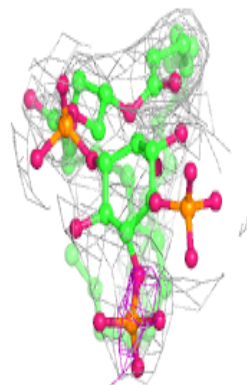
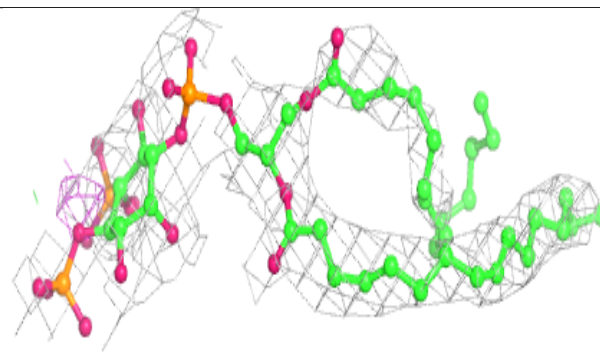
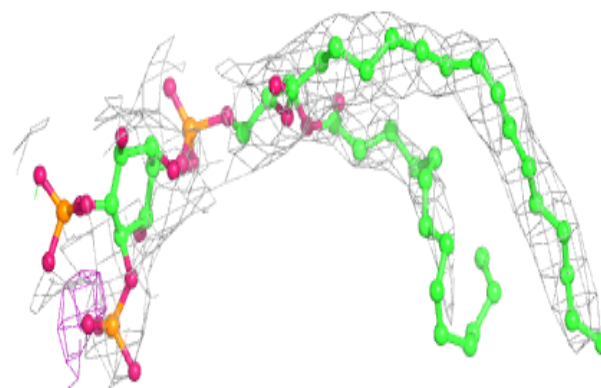


Electron density around PT5 B 301:

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

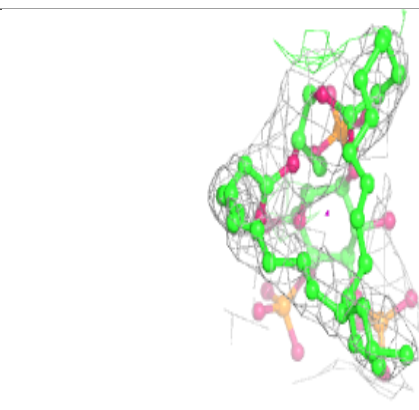
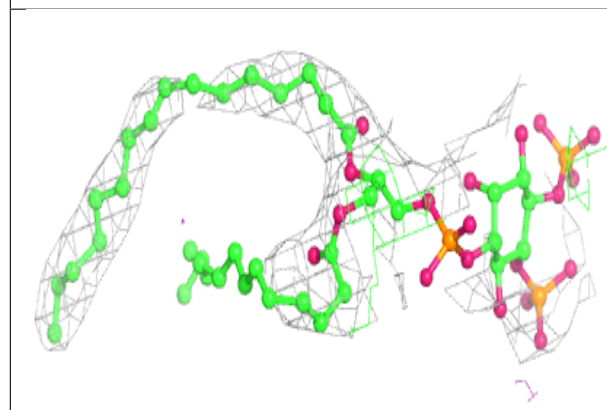
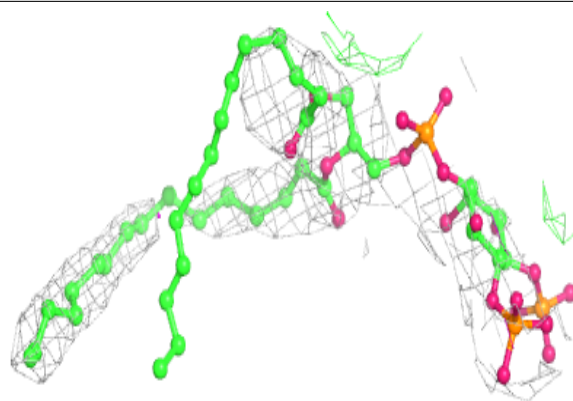
**Electron density around PT5 C 301:**

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



Electron density around PT5 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.