Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 09:16 PM JST

PDB ID	:	6JXH
Title	:	K+-bound E2-MgF state of the gastric proton pump (Tyr799Trp)
Authors	:	Abe, K.; Irie, K.
Deposited on	:	2019-04-23
Resolution	:	2.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

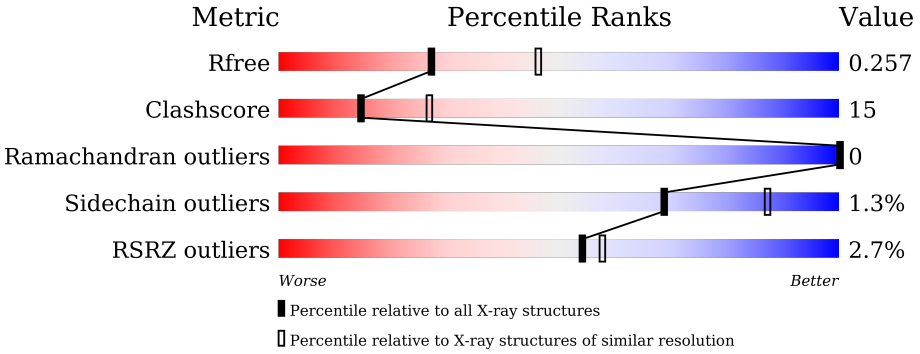
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	987	2% 75% 24% •
2	B	289	3% 68% 22% 9%

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
5	PCW	A	1103	-	-	-	X
5	PCW	A	1104	-	-	-	X
5	PCW	A	1105	-	-	-	X
8	CLR	B	302	-	-	-	X
9	NAG	B	306	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10512 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 Potassium-transporting ATPase alpha chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	987	7662	4893	1293	1422	54	0	0	0

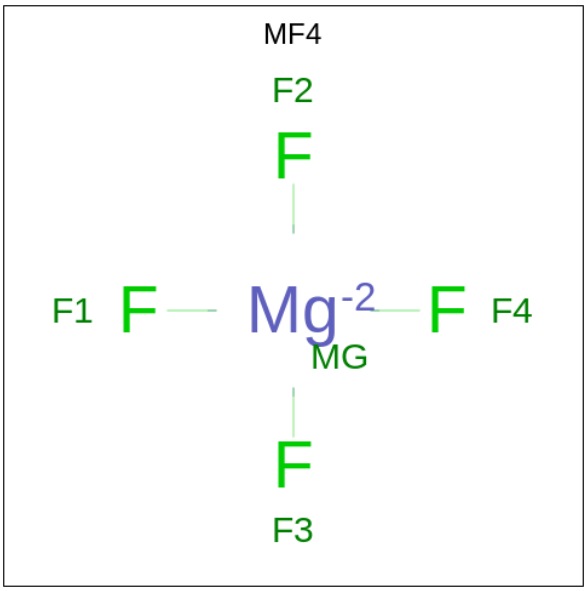
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	-	expression tag	UNP P19156
A	220	CYS	ARG	engineered mutation	UNP P19156
A	593	CYS	SER	engineered mutation	UNP P19156
A	799	TRP	TYR	engineered mutation	UNP P19156
A	1005	SER	GLY	engineered mutation	UNP P19156

- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	262	2100	1364	348	376	12	0	0	0

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F_4Mg).

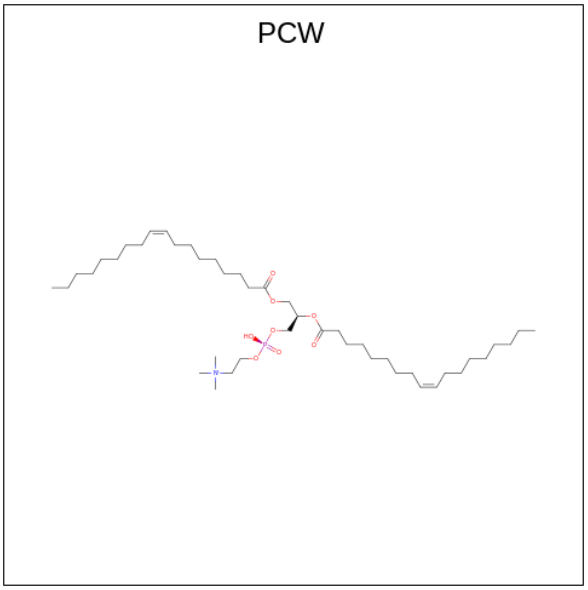


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total F Mg 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

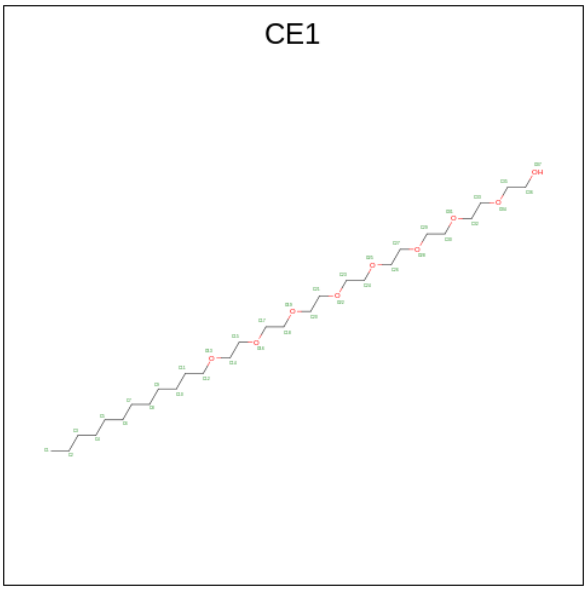
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	46	36	1	8	1	0	0
			Total	C	N	O	P		
5	A	1	47	37	1	8	1	0	0
			Total	C	N	O	P		
5	A	1	54	44	1	8	1	0	0
			Total	C	N	O	P		
5	B	1	54	44	1	8	1	0	0

- Molecule 6 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).

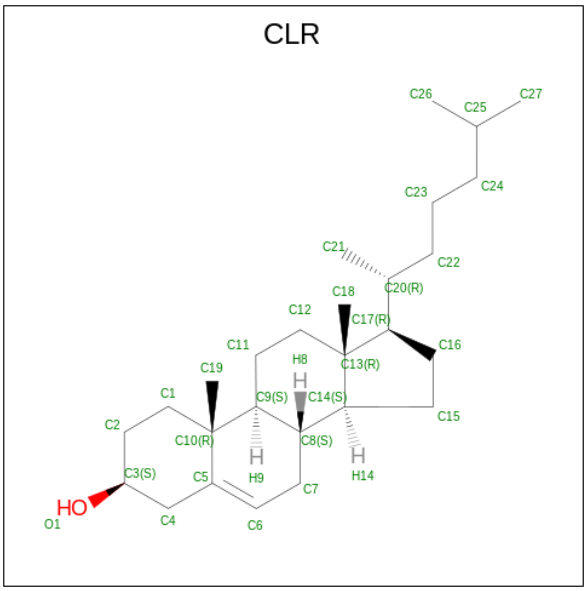


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	37	28	9	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

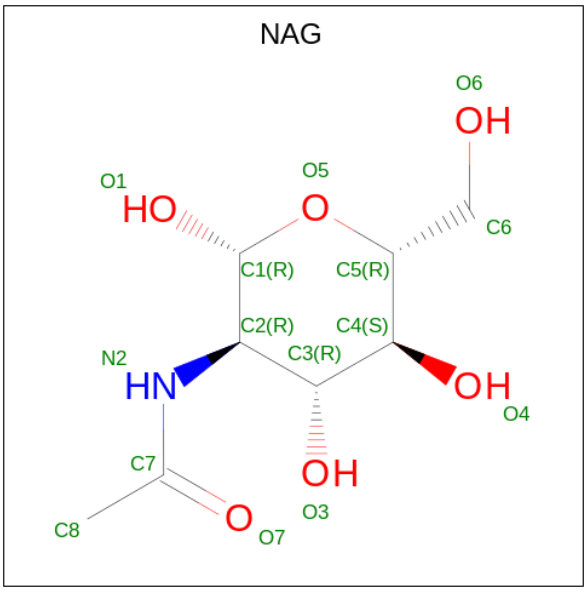
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	A	6	6	6	0	0

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	28	27	1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	B	1	14	8	1	5	0	0
			Total	C	N	O		
9	B	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	B	1	14	8	1	5	0	0
			Total	C	N	O		
9	B	1	14	8	1	5	0	0
			Total	C	N	O		
9	B	1	14	8	1	5	0	0
			Total	C	N	O		
9	B	1	14	8	1	5	0	0

- Molecule 10 is water.

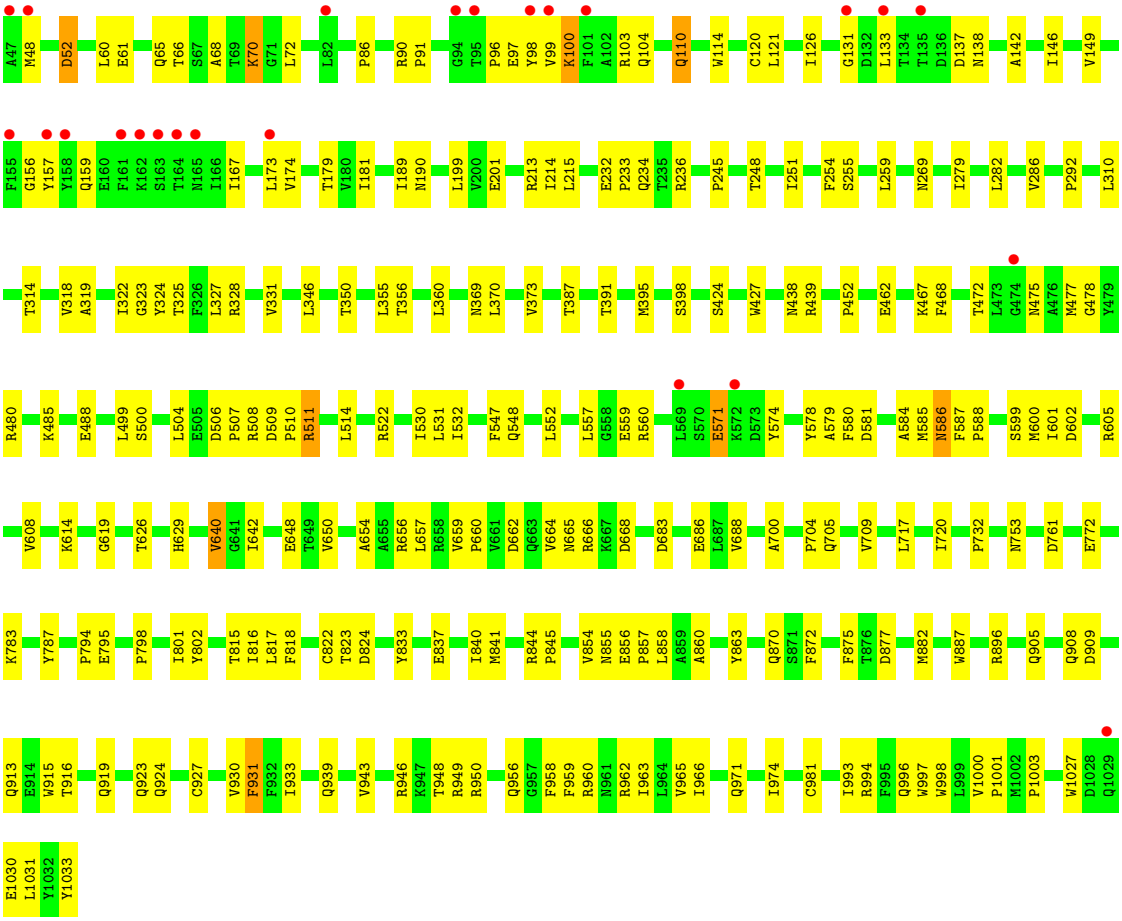
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	317	317	317	0	0
			Total	O		
10	B	71	71	71	0	0

3 Residue-property plots (i)

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

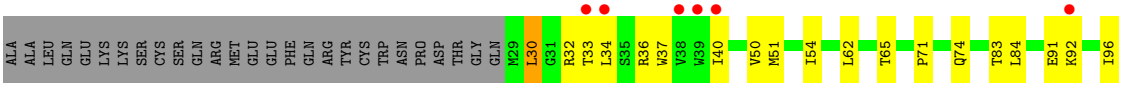
• Molecule 1: Potassium-transporting ATPase alpha chain 1

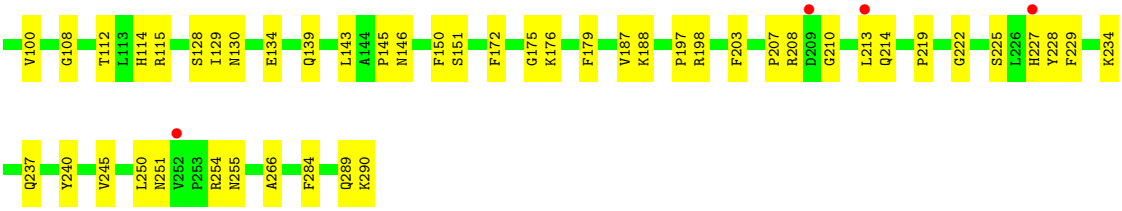
Chain A: 2% 75% 24%



• Molecule 2: Potassium-transporting ATPase subunit beta

Chain B: 3% 68% 22% 9%




V100
G108
T112
L113
H114
R115
S128
I129
N130
E134
Q139
L143
A144
P145
N146
F150
S151
F172
G175
K176
F179
V187
K188
P197
R198
F203
P207
R208
D209
G210
L213
Q214
P219
G222
S225
L226
H227
Y228
F229
K234
Q237
Y240
V245
L250
N251
V252
P253
R254
N255
A266
F284
Q289
K290

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.37Å 103.37Å 370.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.67 – 2.50 47.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.6 (47.67-2.50) 85.6 (47.67-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.201 , 0.257 0.201 , 0.257	Depositor DCC
R_{free} test set	3597 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10512	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

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: MG, CLR, NAG, MF4, CE1, K, PCW

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	0.45	0/7821	0.62	0/10625
2	B	0.44	0/2167	0.59	0/2947
All	All	0.45	0/9988	0.61	0/13572

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7662	0	7688	248	0
2	B	2100	0	2042	67	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	147	0	217	10	0
5	B	54	0	84	7	0
6	A	37	0	58	1	0
7	A	6	0	0	0	0
8	B	28	0	46	4	0
9	B	84	0	78	5	0
10	A	317	0	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	71	0	0	3	0
All	All	10512	0	10213	312	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 15.

All (312) 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:97:GLU:OE1	1:A:100:LYS:NZ	1.56	1.37
1:A:97:GLU:OE2	1:A:100:LYS:CE	1.79	1.30
1:A:97:GLU:CD	1:A:100:LYS:HZ2	1.40	1.23
1:A:840:ILE:HD12	1:A:841:MET:N	1.58	1.16
1:A:97:GLU:CD	1:A:100:LYS:CE	2.15	1.15
1:A:48:MET:CE	1:A:269:ASN:HD21	1.67	1.08
1:A:322:ILE:HD11	1:A:324:TYR:CD1	1.93	1.04
1:A:322:ILE:CD1	1:A:324:TYR:CD1	2.41	1.02
1:A:97:GLU:CD	1:A:100:LYS:HE3	1.75	1.02
1:A:97:GLU:CD	1:A:100:LYS:NZ	2.02	1.02
1:A:571:GLU:HA	1:A:574:TYR:O	1.60	1.01
1:A:97:GLU:OE2	1:A:100:LYS:HE3	1.51	1.01
1:A:933:ILE:HD12	1:A:993:ILE:HD11	1.38	1.01
1:A:97:GLU:OE2	1:A:100:LYS:HE2	1.61	1.00
1:A:97:GLU:HA	1:A:100:LYS:HE3	1.43	1.00
1:A:531:LEU:C	1:A:532:ILE:HD12	1.88	0.94
1:A:322:ILE:HD11	1:A:324:TYR:HD1	1.33	0.93
1:A:322:ILE:CD1	1:A:324:TYR:HD1	1.81	0.89
2:B:225:SER:HB3	2:B:227:HIS:CE1	2.08	0.89
1:A:509:ASP:OD1	1:A:511:ARG:HG3	1.73	0.87
2:B:227:HIS:NE2	2:B:228:TYR:CE2	2.47	0.82
1:A:173:LEU:O	1:A:255:SER:HB2	1.79	0.82
1:A:322:ILE:CD1	1:A:324:TYR:CE1	2.62	0.82
1:A:48:MET:CE	1:A:269:ASN:ND2	2.42	0.82
1:A:840:ILE:HD12	1:A:841:MET:H	1.47	0.80
1:A:398:SER:HB2	1:A:601:ILE:HG22	1.64	0.80
1:A:531:LEU:O	1:A:532:ILE:HD12	1.81	0.80
1:A:133:LEU:HD13	2:B:92:LYS:CE	2.10	0.80
1:A:840:ILE:CD1	1:A:841:MET:HG2	2.10	0.80
1:A:560:ARG:HH21	1:A:600:MET:HE2	1.46	0.80
2:B:234:LYS:NZ	10:B:402:HOH:O	2.15	0.79
2:B:130:ASN:HD21	9:B:304:NAG:H5	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PRO:HD2	1:A:90:ARG:HH22	1.49	0.78
1:A:318:VAL:O	1:A:322:ILE:HG13	1.85	0.77
1:A:48:MET:HE3	1:A:269:ASN:HD21	1.50	0.76
1:A:560:ARG:HH21	1:A:600:MET:CE	1.99	0.76
1:A:1003:PRO:HB3	5:A:1103:PCW:H221	1.67	0.75
2:B:172:PHE:O	10:B:401:HOH:O	2.03	0.75
1:A:131:GLY:O	2:B:92:LYS:NZ	2.14	0.74
1:A:322:ILE:O	5:A:1105:PCW:H31	1.89	0.73
1:A:133:LEU:HD13	2:B:92:LYS:HE2	1.71	0.72
1:A:96:PRO:HD2	1:A:99:VAL:HG11	1.72	0.72
2:B:84:LEU:O	2:B:84:LEU:HD12	1.90	0.72
1:A:860:ALA:HB1	8:B:302:CLR:H6	1.71	0.72
1:A:650:VAL:HG21	1:A:666:ARG:HD3	1.72	0.71
1:A:629:HIS:ND1	10:A:1206:HOH:O	2.22	0.71
1:A:48:MET:HE3	1:A:48:MET:O	1.90	0.71
1:A:322:ILE:HD11	1:A:324:TYR:CE1	2.22	0.71
2:B:227:HIS:NE2	2:B:228:TYR:CZ	2.57	0.70
1:A:98:TYR:HD2	10:A:1426:HOH:O	1.73	0.70
1:A:322:ILE:HD13	1:A:324:TYR:CE1	2.27	0.70
1:A:994:ARG:HA	6:A:1106:CE1:H232	1.72	0.70
2:B:225:SER:CB	2:B:227:HIS:CE1	2.74	0.70
1:A:732:PRO:O	10:A:1201:HOH:O	2.09	0.70
2:B:37:TRP:HZ3	8:B:302:CLR:H193	1.56	0.70
1:A:854:VAL:HG13	1:A:858:LEU:HD22	1.73	0.69
2:B:84:LEU:HD12	2:B:84:LEU:C	2.14	0.68
1:A:97:GLU:HG3	1:A:157:TYR:OH	1.93	0.68
1:A:840:ILE:HD11	1:A:841:MET:HG2	1.74	0.68
1:A:507:PRO:HG2	1:A:508:ARG:CD	2.25	0.67
1:A:508:ARG:N	1:A:508:ARG:HD2	2.10	0.67
1:A:98:TYR:CD2	10:A:1426:HOH:O	2.48	0.66
1:A:662:ASP:OD2	1:A:662:ASP:N	2.26	0.66
1:A:530:ILE:HG12	1:A:532:ILE:CD1	2.24	0.66
1:A:579:ALA:O	1:A:586:ASN:ND2	2.29	0.66
2:B:197:PRO:HB3	2:B:266:ALA:HB2	1.78	0.66
2:B:187:VAL:HG12	2:B:188:LYS:HG2	1.77	0.65
1:A:310:LEU:O	1:A:314:THR:HG23	1.97	0.65
1:A:468:PHE:O	1:A:472:THR:HG23	1.97	0.64
1:A:507:PRO:HG2	1:A:508:ARG:HD2	1.80	0.64
2:B:91:GLU:OE2	2:B:91:GLU:HA	1.96	0.64
1:A:580:PHE:HA	1:A:586:ASN:HD21	1.63	0.63
2:B:71:PRO:HG2	2:B:74:GLN:HE21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ILE:HG12	1:A:532:ILE:HD11	1.80	0.63
1:A:602:ASP:HB3	10:A:1246:HOH:O	1.99	0.62
1:A:863:TYR:OH	10:A:1202:HOH:O	2.14	0.62
1:A:950:ARG:NH2	10:A:1213:HOH:O	2.31	0.62
1:A:52:ASP:HB3	1:A:60:LEU:HD21	1.81	0.62
1:A:86:PRO:HD2	1:A:90:ARG:NH2	2.15	0.62
1:A:181:ILE:HB	1:A:199:LEU:HD23	1.81	0.62
1:A:395:MET:HG2	10:A:1432:HOH:O	1.99	0.61
2:B:50:VAL:O	2:B:54:ILE:HG13	2.00	0.61
1:A:199:LEU:HA	10:A:1216:HOH:O	2.00	0.60
2:B:129:ILE:HD12	2:B:130:ASN:O	2.02	0.60
1:A:586:ASN:OD1	1:A:586:ASN:N	2.34	0.60
1:A:601:ILE:HG12	1:A:602:ASP:N	2.18	0.59
1:A:1027:TRP:CZ3	1:A:1031:LEU:HD12	2.37	0.59
1:A:840:ILE:HD12	1:A:840:ILE:C	2.21	0.59
1:A:245:PRO:HA	1:A:248:THR:HG22	1.84	0.59
2:B:33:THR:HG23	2:B:36:ARG:H	1.68	0.58
2:B:96:ILE:HD13	2:B:179:PHE:HE2	1.68	0.58
5:A:1103:PCW:H51	10:A:1242:HOH:O	2.03	0.58
1:A:97:GLU:O	1:A:100:LYS:HG3	2.04	0.58
1:A:91:PRO:HA	1:A:167:ILE:HD13	1.85	0.58
1:A:571:GLU:CD	1:A:571:GLU:H	2.07	0.58
2:B:255:ASN:OD1	2:B:289:GLN:HA	2.04	0.58
1:A:933:ILE:HD12	1:A:993:ILE:CD1	2.25	0.57
2:B:289:GLN:HB3	9:B:303:NAG:H82	1.87	0.57
1:A:530:ILE:HG23	1:A:532:ILE:HD13	1.85	0.57
1:A:660:PRO:HB2	1:A:662:ASP:OD2	2.04	0.57
1:A:96:PRO:HD2	1:A:99:VAL:CG1	2.34	0.57
1:A:571:GLU:N	1:A:571:GLU:OE1	2.38	0.57
1:A:114:TRP:CZ2	1:A:149:VAL:HG11	2.40	0.57
1:A:587:PHE:HB2	1:A:588:PRO:HD2	1.87	0.56
2:B:62:LEU:O	2:B:65:THR:HG22	2.04	0.56
1:A:840:ILE:CD1	1:A:841:MET:N	2.51	0.56
1:A:48:MET:HE1	1:A:269:ASN:OD1	2.06	0.56
1:A:650:VAL:HG21	1:A:666:ARG:CD	2.35	0.56
2:B:130:ASN:HD21	9:B:304:NAG:C5	2.18	0.55
2:B:146:ASN:HD21	9:B:308:NAG:C7	2.19	0.55
1:A:199:LEU:HD12	10:A:1216:HOH:O	2.06	0.55
2:B:139:GLN:NE2	2:B:150:PHE:O	2.36	0.55
2:B:176:LYS:HG2	2:B:250:LEU:HA	1.90	0.54
2:B:207:PRO:HG2	2:B:210:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:THR:HG21	10:A:1452:HOH:O	2.08	0.54
1:A:585:MET:HE3	10:A:1440:HOH:O	2.07	0.53
1:A:103:ARG:HG3	1:A:103:ARG:O	2.08	0.53
1:A:840:ILE:HD12	1:A:841:MET:HG2	1.89	0.53
1:A:1030:GLU:CD	2:B:40:ILE:HD11	2.28	0.53
1:A:232:GLU:O	1:A:234:GLN:NE2	2.39	0.53
1:A:823:THR:O	1:A:971:GLN:HG3	2.08	0.53
1:A:286:VAL:HG21	10:A:1201:HOH:O	2.09	0.53
1:A:504:LEU:HG	1:A:511:ARG:O	2.08	0.53
1:A:532:ILE:HD12	1:A:532:ILE:N	2.23	0.53
1:A:855:ASN:ND2	1:A:857:PRO:HD2	2.23	0.53
1:A:650:VAL:HG13	1:A:664:VAL:HB	1.91	0.52
1:A:657:LEU:O	1:A:659:VAL:HG23	2.08	0.52
2:B:143:LEU:HB2	2:B:150:PHE:CE2	2.44	0.52
1:A:370:LEU:O	1:A:373:VAL:HG12	2.09	0.52
1:A:48:MET:HE1	1:A:269:ASN:ND2	2.25	0.52
1:A:174:VAL:HG13	1:A:254:PHE:CZ	2.45	0.52
1:A:322:ILE:HD12	1:A:324:TYR:HD1	1.72	0.52
1:A:522:ARG:HH11	1:A:522:ARG:HB3	1.75	0.52
1:A:96:PRO:HB2	1:A:99:VAL:HG12	1.92	0.52
2:B:37:TRP:CZ3	8:B:302:CLR:H193	2.42	0.52
1:A:65:GLN:NE2	10:A:1222:HOH:O	2.43	0.51
1:A:323:GLY:HA3	5:A:1105:PCW:H31	1.92	0.51
1:A:963:ILE:HA	1:A:966:ILE:HD12	1.91	0.51
2:B:175:GLY:HA3	2:B:254:ARG:HH21	1.76	0.51
1:A:475:ASN:ND2	10:A:1223:HOH:O	2.43	0.51
1:A:772:GLU:HG3	1:A:840:ILE:HD11	1.93	0.51
1:A:48:MET:HE2	1:A:269:ASN:ND2	2.26	0.51
2:B:128:SER:HB3	2:B:151:SER:OG	2.10	0.51
1:A:783:LYS:HD3	1:A:946:ARG:O	2.11	0.50
1:A:509:ASP:OD1	1:A:511:ARG:CG	2.52	0.50
1:A:665:ASN:HB3	1:A:668:ASP:OD2	2.11	0.50
1:A:506:ASP:OD1	1:A:508:ARG:HB2	2.12	0.50
1:A:605:ARG:HB2	1:A:608:VAL:HG23	1.94	0.50
1:A:179:THR:OG1	1:A:201:GLU:HB3	2.12	0.50
1:A:882:MET:CE	1:A:923:GLN:HG3	2.41	0.49
2:B:129:ILE:CD1	2:B:130:ASN:O	2.60	0.49
1:A:499:LEU:HD21	1:A:514:LEU:HG	1.94	0.49
2:B:112:THR:HG22	2:B:115:ARG:NH1	2.27	0.49
1:A:322:ILE:HD12	1:A:324:TYR:CD1	2.41	0.49
2:B:225:SER:HG	2:B:227:HIS:CE1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD11	1:A:213:ARG:HG2	1.93	0.49
1:A:214:ILE:HD13	1:A:236:ARG:HB3	1.93	0.49
1:A:654:ALA:HB2	1:A:664:VAL:HG21	1.95	0.49
1:A:114:TRP:CE2	1:A:149:VAL:HG11	2.48	0.49
1:A:580:PHE:HA	1:A:586:ASN:ND2	2.28	0.49
1:A:356:THR:HG22	1:A:373:VAL:HG22	1.95	0.49
1:A:72:LEU:N	10:A:1210:HOH:O	2.46	0.48
1:A:156:GLY:O	1:A:159:GLN:HG2	2.13	0.48
1:A:578:TYR:OH	1:A:586:ASN:HB2	2.13	0.48
1:A:142:ALA:O	1:A:146:ILE:HG13	2.14	0.48
1:A:581:ASP:HB3	1:A:584:ALA:HB3	1.96	0.48
1:A:61:GLU:HG2	1:A:66:THR:O	2.13	0.48
1:A:159:GLN:O	1:A:369:ASN:HA	2.13	0.48
5:A:1105:PCW:H331	10:A:1354:HOH:O	2.14	0.48
2:B:84:LEU:CD2	2:B:284:PHE:CD1	2.95	0.48
1:A:783:LYS:HE2	1:A:949:ARG:HG3	1.95	0.48
1:A:322:ILE:HD13	1:A:324:TYR:HE1	1.77	0.48
1:A:325:THR:HG23	1:A:328:ARG:H	1.79	0.48
1:A:477:MET:HG2	1:A:480:ARG:HH21	1.79	0.48
1:A:511:ARG:HG3	1:A:511:ARG:H	1.51	0.48
2:B:134:GLU:OE2	2:B:225:SER:OG	2.31	0.48
1:A:137:ASP:OD2	10:A:1203:HOH:O	2.20	0.48
1:A:530:ILE:CG1	1:A:532:ILE:HD11	2.43	0.48
1:A:452:PRO:O	1:A:467:LYS:NZ	2.46	0.48
1:A:508:ARG:CD	1:A:508:ARG:N	2.76	0.48
1:A:798:PRO:HG3	1:A:931:PHE:CZ	2.48	0.48
1:A:801:ILE:HG13	5:B:301:PCW:H412	1.96	0.48
1:A:104:GLN:NE2	1:A:156:GLY:O	2.47	0.47
2:B:129:ILE:HD12	2:B:129:ILE:C	2.35	0.47
1:A:1030:GLU:OE1	2:B:32:ARG:NH1	2.46	0.47
1:A:52:ASP:OD1	1:A:52:ASP:N	2.48	0.47
1:A:924:GLN:O	1:A:927:CYS:HB2	2.14	0.47
1:A:233:PRO:HB3	1:A:259:LEU:HD12	1.96	0.47
1:A:557:LEU:HB2	1:A:559:GLU:HG3	1.96	0.47
1:A:956:GLN:O	1:A:960:ARG:HD3	2.15	0.47
2:B:108:GLY:O	2:B:112:THR:HG23	2.15	0.47
1:A:548:GLN:O	1:A:552:LEU:HG	2.14	0.47
1:A:508:ARG:HD2	1:A:508:ARG:H	1.79	0.46
1:A:908:GLN:HA	1:A:913:GLN:O	2.15	0.46
1:A:916:THR:HG23	1:A:919:GLN:OE1	2.16	0.46
1:A:802:TYR:CE1	1:A:896:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:PHE:CD2	2:B:213:LEU:HB2	2.50	0.46
1:A:688:VAL:HG23	1:A:717:LEU:HD11	1.98	0.46
1:A:823:THR:HG22	1:A:974:ILE:HG23	1.98	0.46
1:A:875:PHE:CD2	5:B:301:PCW:H431	2.51	0.46
1:A:994:ARG:HG3	1:A:997:TRP:CZ3	2.51	0.46
2:B:214:GLN:HG2	2:B:251:ASN:HD22	1.79	0.46
1:A:475:ASN:OD1	1:A:478:GLY:N	2.45	0.45
5:A:1104:PCW:H252	5:B:301:PCW:H283	1.99	0.45
1:A:930:VAL:HG23	1:A:997:TRP:HB3	1.98	0.45
2:B:96:ILE:HD13	2:B:179:PHE:CE2	2.50	0.45
1:A:279:ILE:HD11	1:A:704:PRO:HG2	1.97	0.45
1:A:97:GLU:CA	1:A:100:LYS:HE3	2.30	0.45
1:A:887:TRP:HZ2	1:A:915:TRP:CD2	2.35	0.45
1:A:499:LEU:HD23	1:A:500:SER:N	2.32	0.45
2:B:30:LEU:HG	2:B:37:TRP:NE1	2.32	0.45
2:B:34:LEU:HA	2:B:37:TRP:HB2	1.98	0.45
2:B:219:PRO:HD2	2:B:245:VAL:HG22	1.99	0.45
1:A:508:ARG:CD	1:A:508:ARG:H	2.30	0.44
1:A:648:GLU:OE1	1:A:656:ARG:NH1	2.50	0.44
1:A:840:ILE:HD12	1:A:841:MET:CA	2.42	0.44
1:A:840:ILE:CD1	1:A:840:ILE:C	2.85	0.44
1:A:877:ASP:CG	1:A:930:VAL:HG22	2.37	0.44
1:A:438:ASN:OD1	1:A:462:GLU:HB3	2.18	0.44
1:A:856:GLU:OE2	10:A:1204:HOH:O	2.21	0.44
1:A:858:LEU:HA	1:A:1033:TYR:HB2	2.00	0.44
5:B:301:PCW:H272	8:B:302:CLR:H262	1.99	0.44
1:A:126:ILE:HD13	1:A:327:LEU:HD11	1.98	0.44
2:B:227:HIS:C	2:B:229:PHE:H	2.20	0.44
2:B:214:GLN:HB2	2:B:251:ASN:HB2	1.99	0.44
1:A:110:GLN:HG2	10:A:1397:HOH:O	2.17	0.44
1:A:787:TYR:CE2	1:A:943:VAL:HB	2.52	0.44
1:A:126:ILE:HD13	1:A:327:LEU:CD1	2.48	0.44
1:A:346:LEU:O	1:A:350:THR:HG23	2.17	0.44
1:A:439:ARG:HD2	1:A:488:GLU:OE2	2.18	0.43
1:A:214:ILE:CD1	1:A:236:ARG:HB3	2.49	0.43
1:A:958:PHE:HB2	1:A:959:PHE:CE2	2.53	0.43
5:A:1104:PCW:H382	5:B:301:PCW:H382	2.00	0.43
1:A:360:LEU:HD11	10:A:1341:HOH:O	2.19	0.43
1:A:626:THR:HG23	1:A:700:ALA:HA	1.99	0.43
1:A:600:MET:HE3	1:A:600:MET:HB2	1.82	0.43
2:B:227:HIS:CE1	2:B:228:TYR:CE2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ARG:NH2	1:A:600:MET:CE	2.77	0.43
1:A:360:LEU:HD12	1:A:373:VAL:HG23	2.01	0.43
1:A:818:PHE:O	1:A:822:CYS:HB3	2.19	0.43
1:A:97:GLU:HA	1:A:100:LYS:CE	2.29	0.43
1:A:282:LEU:O	1:A:286:VAL:HG23	2.19	0.43
1:A:640:VAL:CG1	1:A:642:ILE:HG13	2.48	0.43
1:A:840:ILE:HG13	10:A:1442:HOH:O	2.17	0.43
2:B:145:PRO:HB2	9:B:308:NAG:H61	1.99	0.43
1:A:485:LYS:HD3	1:A:488:GLU:HB2	2.01	0.43
1:A:1030:GLU:OE2	2:B:40:ILE:HD11	2.19	0.43
1:A:48:MET:CE	1:A:269:ASN:OD1	2.66	0.42
1:A:322:ILE:HG21	5:A:1105:PCW:H412	2.01	0.42
2:B:129:ILE:HD12	2:B:130:ASN:C	2.39	0.42
1:A:753:ASN:HD22	1:A:753:ASN:HA	1.61	0.42
2:B:198:ARG:HA	2:B:222:GLY:O	2.19	0.42
1:A:824:ASP:OD2	1:A:939:GLN:HG3	2.20	0.42
1:A:956:GLN:NE2	10:A:1237:HOH:O	2.52	0.42
1:A:70:LYS:HE3	1:A:70:LYS:HB3	1.69	0.42
1:A:97:GLU:CG	1:A:100:LYS:HE3	2.45	0.42
5:B:301:PCW:H82	5:B:301:PCW:H42	1.81	0.42
2:B:143:LEU:HB2	2:B:150:PHE:HE2	1.85	0.42
1:A:530:ILE:CD1	1:A:532:ILE:HD11	2.49	0.42
1:A:1031:LEU:HD23	1:A:1031:LEU:HA	1.86	0.42
2:B:203:PHE:CE2	2:B:213:LEU:HB2	2.54	0.42
1:A:133:LEU:HD13	2:B:92:LYS:HE3	1.95	0.42
1:A:962:ARG:O	1:A:965:VAL:HG22	2.19	0.42
1:A:994:ARG:HB3	1:A:996:GLN:HE22	1.85	0.42
1:A:996:GLN:O	1:A:1000:VAL:HG23	2.19	0.42
2:B:40:ILE:HD13	2:B:40:ILE:HA	1.81	0.42
2:B:100:VAL:HG22	2:B:290:LYS:HA	2.01	0.42
1:A:292:PRO:HG3	1:A:720:ILE:HD13	2.02	0.42
1:A:905:GLN:HB2	2:B:83:THR:HG22	2.01	0.42
2:B:214:GLN:H	2:B:251:ASN:HB2	1.85	0.42
1:A:504:LEU:HD12	1:A:509:ASP:OD2	2.20	0.42
1:A:872:PHE:CE2	2:B:51:MET:HB3	2.55	0.42
1:A:560:ARG:O	1:A:599:SER:HA	2.20	0.41
1:A:619:GLY:HA3	1:A:845:PRO:HD3	2.01	0.41
1:A:683:ASP:HB2	1:A:686:GLU:HG3	2.03	0.41
2:B:237:GLN:HB3	2:B:240:TYR:HB2	2.01	0.41
1:A:601:ILE:CG1	1:A:602:ASP:N	2.82	0.41
1:A:794:PRO:HG3	1:A:870:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:PRO:HG3	5:A:1103:PCW:H162	2.03	0.41
1:A:68:ALA:HB1	1:A:215:LEU:HD13	2.01	0.41
1:A:761:ASP:O	10:A:1205:HOH:O	2.22	0.41
1:A:909:ASP:OD2	1:A:913:GLN:HB2	2.21	0.41
1:A:547:PHE:CD1	1:A:547:PHE:C	2.93	0.41
1:A:998:TRP:O	1:A:1001:PRO:HD2	2.21	0.41
1:A:322:ILE:O	5:A:1105:PCW:C3	2.66	0.41
1:A:795:GLU:HB3	1:A:816:ILE:HD13	2.03	0.41
1:A:958:PHE:HB2	1:A:959:PHE:CD2	2.56	0.41
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.68	0.41
1:A:355:LEU:HD13	1:A:833:TYR:OH	2.20	0.41
1:A:930:VAL:CG2	1:A:997:TRP:HB3	2.50	0.41
1:A:213:ARG:HA	1:A:251:ILE:HD13	2.02	0.41
1:A:817:LEU:HD23	1:A:817:LEU:HA	1.79	0.41
1:A:844:ARG:HA	1:A:844:ARG:HD3	1.89	0.41
2:B:175:GLY:O	2:B:254:ARG:NH2	2.54	0.41
2:B:255:ASN:OD1	2:B:290:LYS:N	2.54	0.41
1:A:189:ILE:HG23	1:A:190:ASN:O	2.21	0.40
1:A:424:SER:HB3	1:A:427:TRP:HB3	2.02	0.40
1:A:993:ILE:H	1:A:993:ILE:HG12	1.62	0.40
1:A:48:MET:CE	1:A:269:ASN:CG	2.89	0.40
1:A:120:CYS:HB3	1:A:138:ASN:O	2.22	0.40
1:A:327:LEU:O	1:A:331:VAL:HG23	2.22	0.40
1:A:877:ASP:OD2	1:A:930:VAL:HG22	2.21	0.40
1:A:994:ARG:HB3	1:A:996:GLN:NE2	2.35	0.40
2:B:114:HIS:HB2	10:B:456:HOH:O	2.21	0.40
1:A:387:THR:HA	1:A:391:THR:OG1	2.21	0.40
1:A:509:ASP:HA	1:A:510:PRO:HD3	1.90	0.40
1:A:705:GLN:O	1:A:709:VAL:HG23	2.21	0.40
1:A:798:PRO:HB2	10:A:1265:HOH:O	2.20	0.40
1:A:872:PHE:CE1	5:B:301:PCW:H442	2.57	0.40
1:A:319:ALA:O	1:A:322:ILE:CD1	2.70	0.40
1:A:477:MET:HG2	1:A:480:ARG:NH2	2.37	0.40
1:A:837:GLU:OE2	1:A:948:THR:HA	2.22	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	985/987 (100%)	968 (98%)	17 (2%)	0	100	100
2	B	260/289 (90%)	256 (98%)	4 (2%)	0	100	100
All	All	1245/1276 (98%)	1224 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	834/834 (100%)	822 (99%)	12 (1%)	67	86
2	B	229/253 (90%)	227 (99%)	2 (1%)	78	92
All	All	1063/1087 (98%)	1049 (99%)	14 (1%)	69	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	70	LYS
1	A	100	LYS
1	A	110	GLN
1	A	511	ARG
1	A	571	GLU
1	A	586	ASN
1	A	614	LYS

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Mol	Chain	Res	Type
1	A	640	VAL
1	A	815	THR
1	A	931	PHE
1	A	981	CYS
2	B	30	LEU
2	B	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	269	ASN
1	A	663	GLN
1	A	753	ASN
2	B	74	GLN
2	B	130	ASN
2	B	251	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
9	NAG	B	307	2	14,14,15	0.89	1 (7%)	17,19,21	0.84	1 (5%)
5	PCW	B	301	-	53,53,53	0.93	2 (3%)	59,61,61	1.01	3 (5%)
5	PCW	A	1104	-	46,46,53	1.08	2 (4%)	52,54,61	0.91	2 (3%)
9	NAG	B	305	2	14,14,15	0.26	0	17,19,21	0.80	1 (5%)
5	PCW	A	1103	-	45,45,53	1.09	2 (4%)	51,53,61	0.94	2 (3%)
5	PCW	A	1105	-	53,53,53	0.95	2 (3%)	59,61,61	1.06	3 (5%)
6	CE1	A	1106	-	36,36,36	0.53	0	35,35,35	0.45	0
9	NAG	B	303	2	14,14,15	0.61	0	17,19,21	0.54	0
8	CLR	B	302	-	31,31,31	0.60	0	48,48,48	1.11	3 (6%)
9	NAG	B	304	-	14,14,15	1.68	2 (14%)	17,19,21	1.53	4 (23%)
9	NAG	B	306	-	14,14,15	0.38	0	17,19,21	0.46	0
3	MF4	A	1101	1	0,4,4	-	-	-		
9	NAG	B	308	2	14,14,15	0.69	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	307	2	-	2/6/23/26	0/1/1/1
5	PCW	B	301	-	-	9/57/57/57	-
5	PCW	A	1104	-	-	21/50/50/57	-
9	NAG	B	305	2	-	0/6/23/26	0/1/1/1
5	PCW	A	1103	-	-	25/49/49/57	-
5	PCW	A	1105	-	-	29/57/57/57	-
6	CE1	A	1106	-	-	11/34/34/34	-
8	CLR	B	302	-	-	5/10/68/68	0/4/4/4
9	NAG	B	304	-	-	2/6/23/26	0/1/1/1
9	NAG	B	306	-	-	0/6/23/26	0/1/1/1
9	NAG	B	303	2	-	2/6/23/26	0/1/1/1
9	NAG	B	308	2	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	304	NAG	C1-C2	5.76	1.60	1.52
5	A	1103	PCW	O2-C31	4.67	1.47	1.34
5	A	1104	PCW	O2-C31	4.57	1.47	1.34
5	A	1104	PCW	O3-C11	4.54	1.46	1.33
5	A	1103	PCW	O3-C11	4.37	1.46	1.33
5	A	1105	PCW	O3-C11	4.30	1.45	1.33
5	A	1105	PCW	O2-C31	4.28	1.46	1.34
5	B	301	PCW	O3-C11	4.12	1.45	1.33
5	B	301	PCW	O2-C31	4.10	1.45	1.34
9	B	307	NAG	C1-C2	2.68	1.56	1.52
9	B	304	NAG	C3-C2	2.13	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1105	PCW	O2-C31-C32	4.82	121.88	111.50
5	B	301	PCW	O2-C31-C32	4.14	120.43	111.50
5	A	1103	PCW	O2-C31-C32	3.86	119.83	111.50
9	B	304	NAG	C2-N2-C7	3.66	128.11	122.90
5	A	1104	PCW	O2-C31-C32	3.65	119.36	111.50
8	B	302	CLR	C8-C7-C6	-3.35	107.92	112.73
9	B	304	NAG	C4-C3-C2	3.31	115.86	111.02
5	B	301	PCW	O3-C11-C12	2.85	120.86	111.91
5	A	1105	PCW	O2-C31-O31	-2.78	116.98	123.70
9	B	307	NAG	C1-O5-C5	2.66	115.79	112.19
5	A	1105	PCW	O3-C11-C12	2.63	120.17	111.91
9	B	304	NAG	C1-C2-N2	2.60	114.94	110.49
5	A	1103	PCW	O3-C11-C12	2.59	120.02	111.91
8	B	302	CLR	C9-C10-C5	2.48	113.54	109.65
9	B	304	NAG	O5-C5-C4	-2.43	104.91	110.83
9	B	305	NAG	C1-O5-C5	2.29	115.29	112.19
8	B	302	CLR	C1-C10-C9	2.09	111.65	108.73
5	A	1104	PCW	C3-C2-C1	-2.06	106.92	111.79
5	B	301	PCW	O3-C11-O11	-2.03	118.47	123.59

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1103	PCW	C4-O4P-P-O2P
5	A	1104	PCW	O2-C2-C3-O3
5	A	1104	PCW	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
5	A	1104	PCW	C1-O3P-P-O2P
5	A	1104	PCW	C4-O4P-P-O3P
5	A	1105	PCW	O4P-C4-C5-N
5	A	1105	PCW	C32-C31-O2-C2
5	A	1105	PCW	C4-O4P-P-O2P
5	B	301	PCW	O4P-C4-C5-N
9	B	304	NAG	C1-C2-N2-C7
5	A	1105	PCW	O31-C31-O2-C2
9	B	303	NAG	O5-C5-C6-O6
9	B	303	NAG	C4-C5-C6-O6
9	B	307	NAG	O5-C5-C6-O6
6	A	1106	CE1	O22-C23-C24-O25
9	B	307	NAG	C4-C5-C6-O6
9	B	308	NAG	O5-C5-C6-O6
6	A	1106	CE1	O16-C17-C18-O19
5	A	1104	PCW	C31-C32-C33-C34
8	B	302	CLR	C17-C20-C22-C23
6	A	1106	CE1	O19-C20-C21-O22
8	B	302	CLR	C21-C20-C22-C23
5	A	1105	PCW	C31-C32-C33-C34
5	A	1103	PCW	C23-C24-C25-C26
5	A	1103	PCW	C34-C35-C36-C37
5	A	1105	PCW	C21-C22-C23-C24
5	A	1105	PCW	C34-C35-C36-C37
5	A	1103	PCW	C32-C33-C34-C35
5	A	1104	PCW	C23-C24-C25-C26
5	B	301	PCW	C33-C34-C35-C36
5	A	1105	PCW	C16-C17-C18-C19
5	A	1105	PCW	C23-C24-C25-C26
5	A	1103	PCW	C22-C23-C24-C25
5	B	301	PCW	C34-C35-C36-C37
8	B	302	CLR	C23-C24-C25-C27
5	A	1103	PCW	C21-C22-C23-C24
5	A	1105	PCW	C14-C15-C16-C17
5	A	1105	PCW	C40-C41-C42-C43
5	A	1105	PCW	C36-C37-C38-C39
5	A	1104	PCW	C12-C11-O3-C3
5	A	1103	PCW	C32-C31-O2-C2
5	A	1105	PCW	C13-C14-C15-C16
8	B	302	CLR	C23-C24-C25-C26
5	A	1103	PCW	O31-C31-O2-C2
9	B	308	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1105	PCW	C4-O4P-P-O3P
5	A	1104	PCW	O3P-C1-C2-C3
5	A	1103	PCW	C12-C13-C14-C15
5	A	1104	PCW	O11-C11-O3-C3
9	B	304	NAG	O5-C5-C6-O6
5	A	1103	PCW	C1-C2-C3-O3
5	A	1104	PCW	C1-C2-C3-O3
5	A	1104	PCW	C20-C21-C22-C23
5	A	1104	PCW	C36-C37-C38-C39
6	A	1106	CE1	C1-C2-C3-C4
5	A	1103	PCW	C25-C26-C27-C28
5	A	1105	PCW	C35-C36-C37-C38
5	A	1105	PCW	O2-C31-C32-C33
5	B	301	PCW	C12-C11-O3-C3
5	A	1105	PCW	C12-C11-O3-C3
5	A	1104	PCW	O3P-C1-C2-O2
5	A	1103	PCW	C33-C34-C35-C36
5	A	1103	PCW	C13-C14-C15-C16
5	A	1104	PCW	C2-C1-O3P-P
6	A	1106	CE1	C2-C3-C4-C5
5	A	1105	PCW	C41-C42-C43-C44
6	A	1106	CE1	C32-C33-O34-C35
5	B	301	PCW	O11-C11-O3-C3
6	A	1106	CE1	C27-C26-O25-C24
5	A	1105	PCW	C1-C2-C3-O3
6	A	1106	CE1	C20-C21-O22-C23
5	A	1105	PCW	O11-C11-O3-C3
5	A	1103	PCW	O2-C2-C3-O3
8	B	302	CLR	C20-C22-C23-C24
5	A	1105	PCW	C42-C43-C44-C45
5	A	1104	PCW	C25-C26-C27-C28
6	A	1106	CE1	C24-C23-O22-C21
5	A	1103	PCW	C4-O4P-P-O3P
5	A	1104	PCW	C1-O3P-P-O4P
5	A	1104	PCW	C1-O3P-P-O1P
5	A	1104	PCW	C4-O4P-P-O1P
6	A	1106	CE1	C11-C10-C9-C8
5	A	1103	PCW	O4P-C4-C5-N
5	A	1105	PCW	O2-C2-C3-O3
5	A	1105	PCW	C32-C33-C34-C35
5	A	1105	PCW	C33-C34-C35-C36
5	A	1103	PCW	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
5	A	1103	PCW	C1-O3P-P-O4P
5	B	301	PCW	C1-O3P-P-O4P
5	B	301	PCW	C4-O4P-P-O3P
5	A	1105	PCW	C2-C1-O3P-P
5	A	1103	PCW	C17-C18-C19-C20
5	A	1104	PCW	C32-C33-C34-C35
5	A	1103	PCW	C3-C2-O2-C31
5	A	1103	PCW	C14-C15-C16-C17
5	A	1104	PCW	O2-C31-C32-C33
5	A	1105	PCW	C17-C18-C19-C20
5	A	1103	PCW	O2-C31-C32-C33
5	A	1105	PCW	O31-C31-C32-C33
5	A	1105	PCW	C12-C13-C14-C15
5	B	301	PCW	C19-C20-C21-C22
5	A	1103	PCW	C37-C38-C39-C40
5	A	1103	PCW	O31-C31-C32-C33
6	A	1106	CE1	O13-C14-C15-O16
5	B	301	PCW	C4-O4P-P-O2P
5	A	1104	PCW	C5-C4-O4P-P
5	A	1105	PCW	C1-C2-O2-C31
5	A	1103	PCW	C4-C5-N-C8

There are no ring outliers.

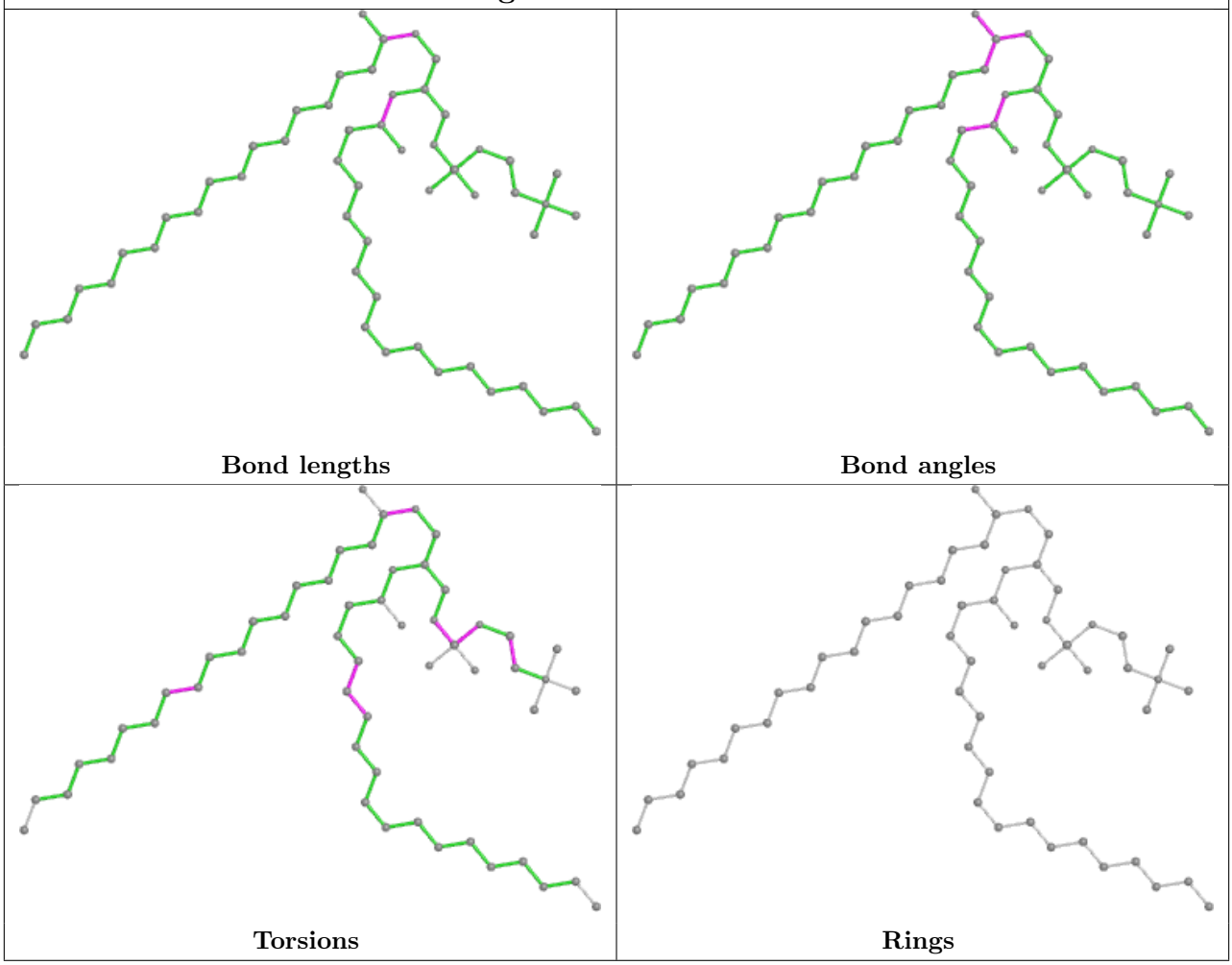
9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	PCW	7	0
5	A	1104	PCW	2	0
5	A	1103	PCW	3	0
5	A	1105	PCW	5	0
6	A	1106	CE1	1	0
9	B	303	NAG	1	0
8	B	302	CLR	4	0
9	B	304	NAG	2	0
9	B	308	NAG	2	0

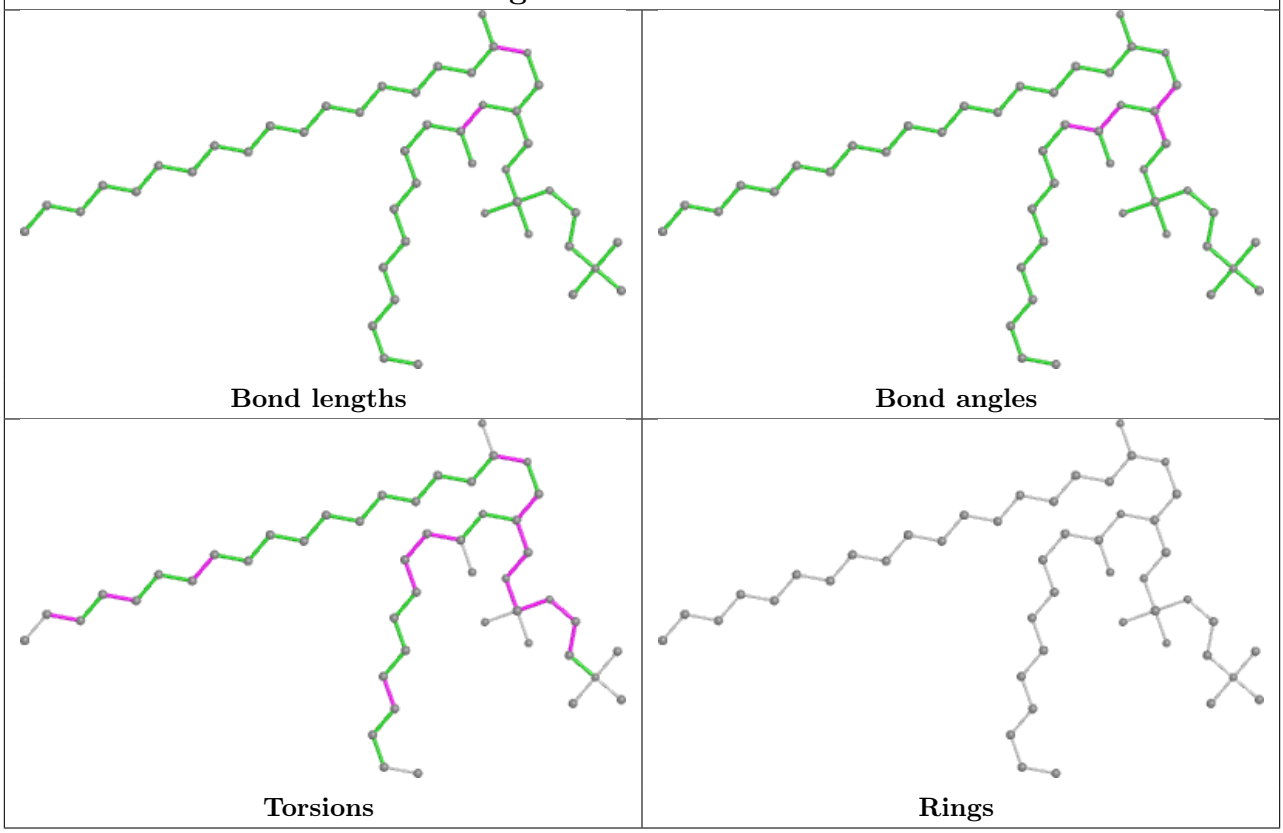
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

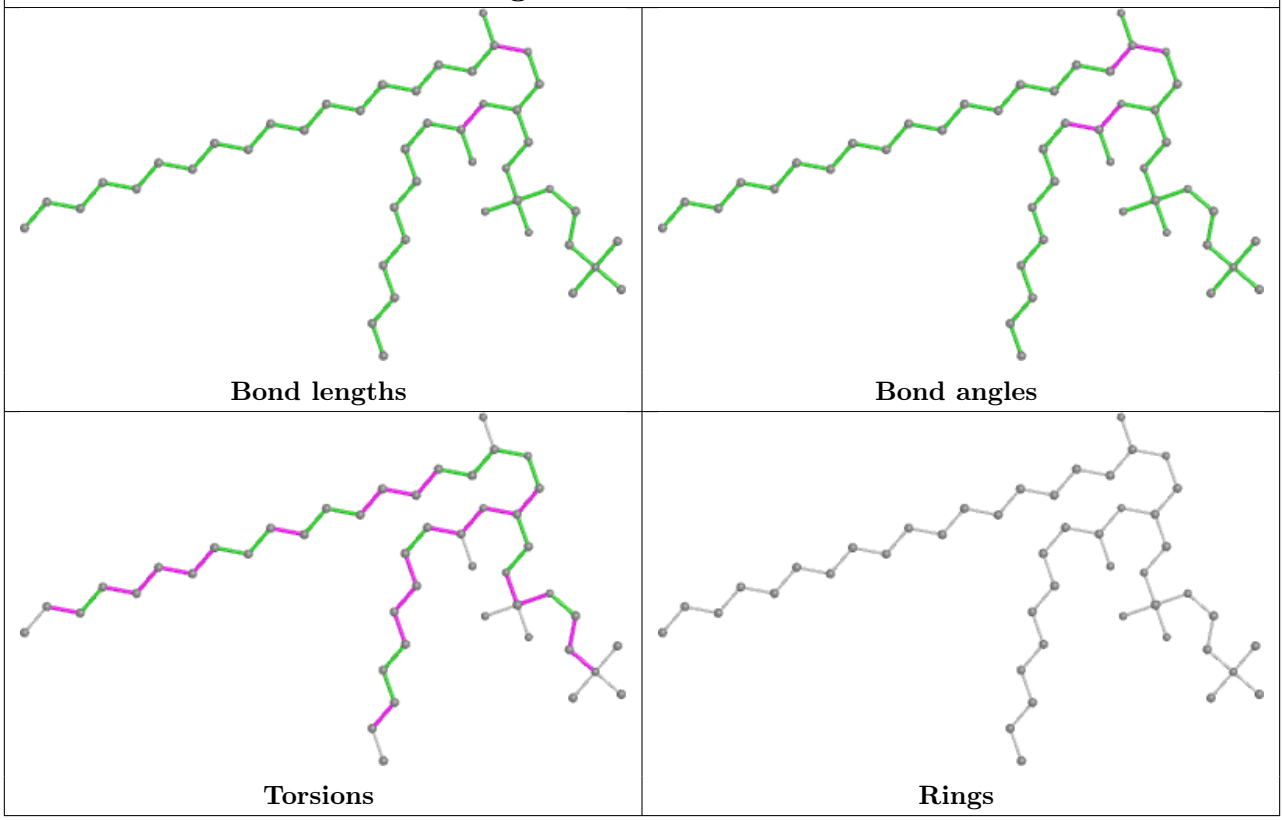
Ligand PCW B 301



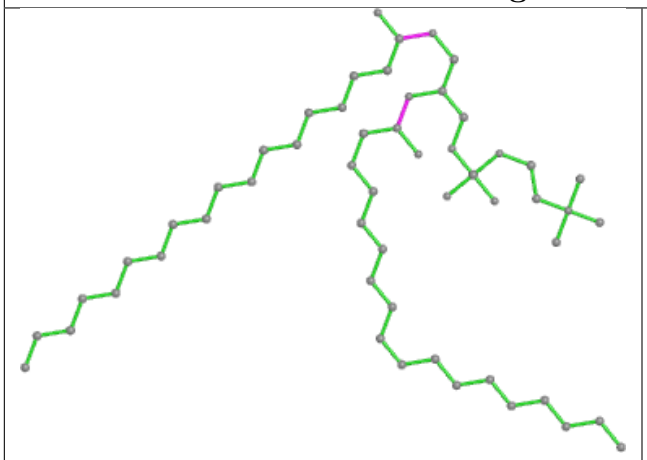
Ligand PCW A 1104



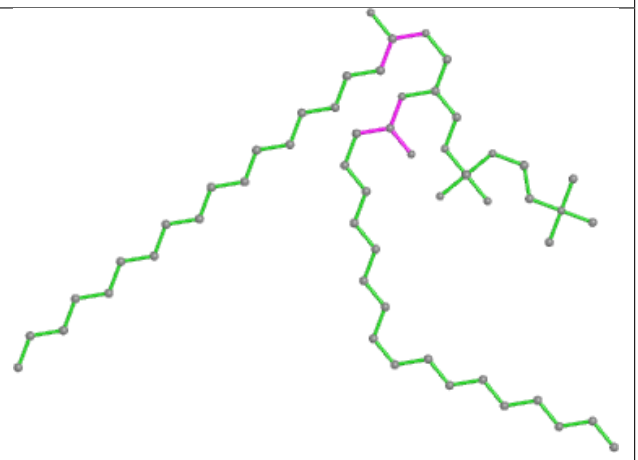
Ligand PCW A 1103



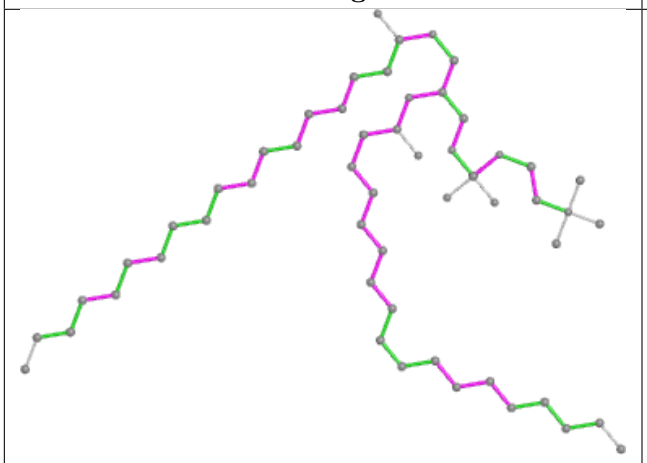
Ligand PCW A 1105



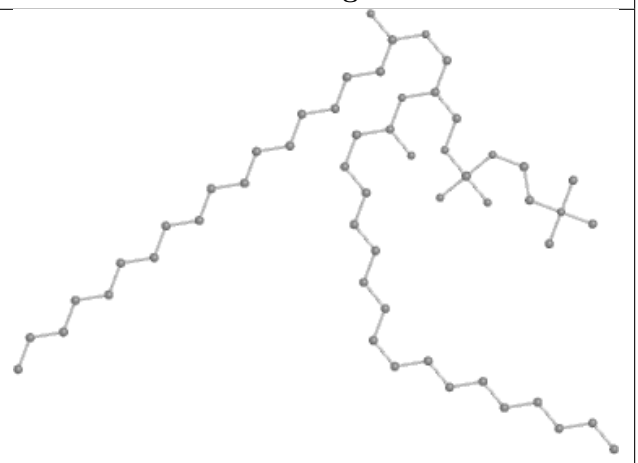
Bond lengths



Bond angles



Torsions

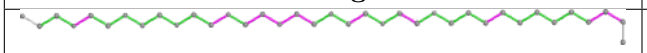


Rings

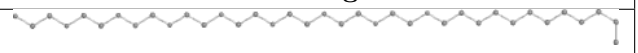
Ligand CE1 A 1106

Bond lengths

Bond angles

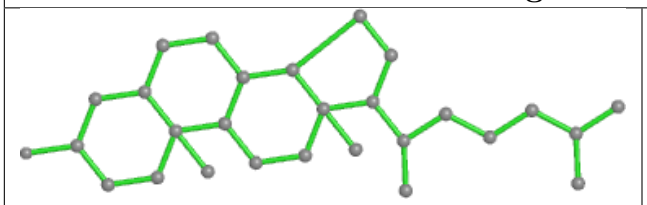


Torsions

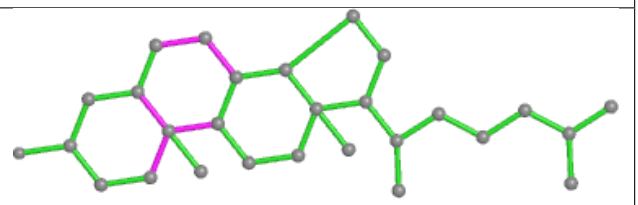


Rings

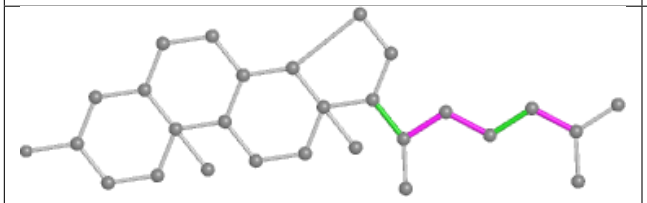
Ligand CLR B 302



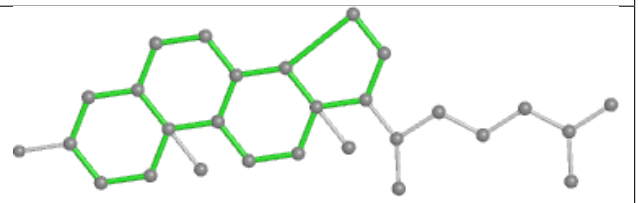
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	987/987 (100%)	-0.17	24 (2%)	59	62	36, 64, 115, 192	0
2	B	262/289 (90%)	-0.16	10 (3%)	40	43	49, 74, 121, 211	0
All	All	1249/1276 (97%)	-0.17	34 (2%)	54	58	36, 67, 118, 211	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	TYR	5.6
1	A	165	ASN	4.6
1	A	98	TYR	4.5
1	A	474	GLY	4.2
1	A	131	GLY	3.9
1	A	47	ALA	3.8
1	A	572	LYS	3.7
1	A	135	THR	3.6
1	A	162	LYS	3.6
2	B	39	TRP	3.4
2	B	209	ASP	3.2
1	A	133	LEU	3.2
2	B	92	LYS	3.2
1	A	48	MET	3.1
2	B	227	HIS	3.1
1	A	161	PHE	3.0
2	B	34	LEU	3.0
2	B	40	ILE	3.0
1	A	164	THR	2.9
1	A	101	PHE	2.7
1	A	94	GLY	2.7
1	A	157	TYR	2.6
1	A	99	VAL	2.5
1	A	95	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1029	GLN	2.4
1	A	155	PHE	2.3
1	A	82	LEU	2.3
1	A	569	LEU	2.3
2	B	38	VAL	2.2
2	B	213	LEU	2.2
1	A	173	LEU	2.2
1	A	163	SER	2.2
2	B	252	VAL	2.2
2	B	33	THR	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PCW	A	1105	54/54	0.67	0.55	70,111,191,204	0
8	CLR	B	302	28/28	0.71	0.57	134,146,153,157	0
9	NAG	B	306	14/15	0.75	0.53	156,166,184,190	0
5	PCW	A	1104	47/54	0.76	0.45	67,97,180,196	0
5	PCW	A	1103	46/54	0.76	0.41	93,123,151,156	0
6	CE1	A	1106	37/37	0.78	0.30	61,113,142,143	0
7	K	A	1107	1/1	0.82	0.28	126,126,126,126	0
9	NAG	B	308	14/15	0.85	0.43	175,178,182,183	0
9	NAG	B	307	14/15	0.86	0.34	131,145,152,162	0
9	NAG	B	304	14/15	0.86	0.20	132,148,154,159	0
7	K	A	1111	1/1	0.88	0.44	127,127,127,127	0
9	NAG	B	305	14/15	0.89	0.18	92,103,113,121	0
5	PCW	B	301	54/54	0.90	0.36	54,93,140,154	0

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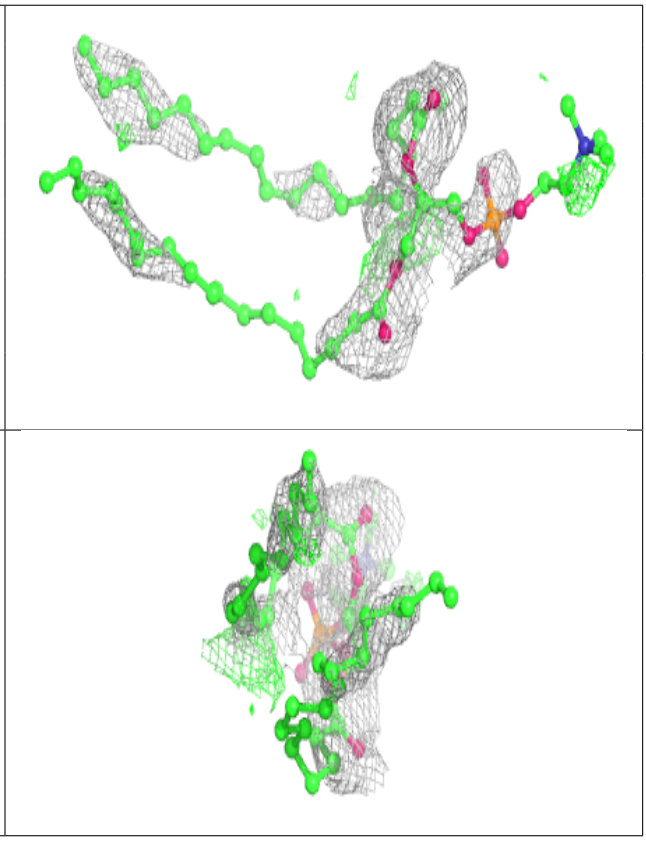
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	B	303	14/15	0.94	0.15	90,103,124,126	0
4	MG	A	1102	1/1	0.94	0.18	49,49,49,49	0
7	K	A	1110	1/1	0.94	0.11	103,103,103,103	0
3	MF4	A	1101	5/5	0.95	0.20	41,45,50,54	0
7	K	A	1108	1/1	0.96	0.09	91,91,91,91	0
7	K	A	1112	1/1	1.00	0.17	56,56,56,56	0
7	K	A	1109	1/1	1.00	0.13	63,63,63,63	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.

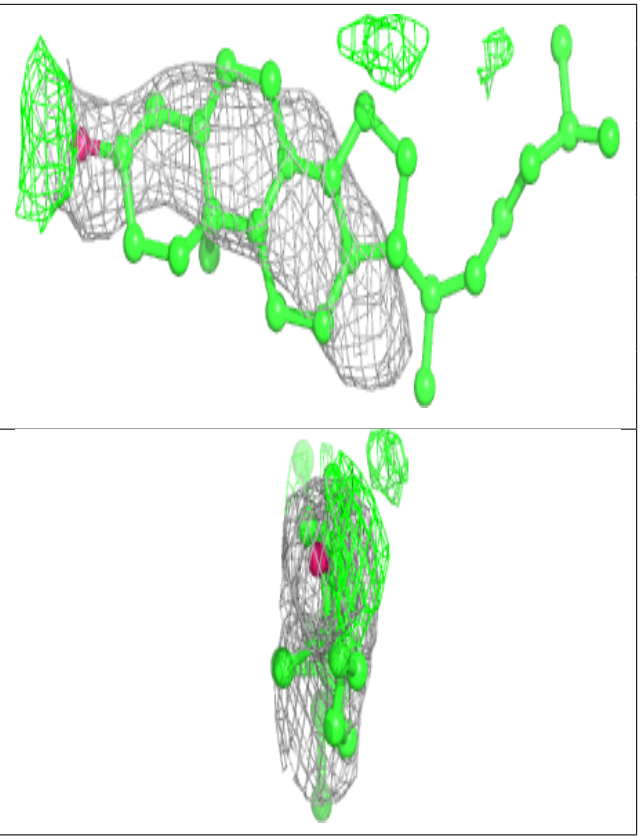
Electron density around PCW A 1105:

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



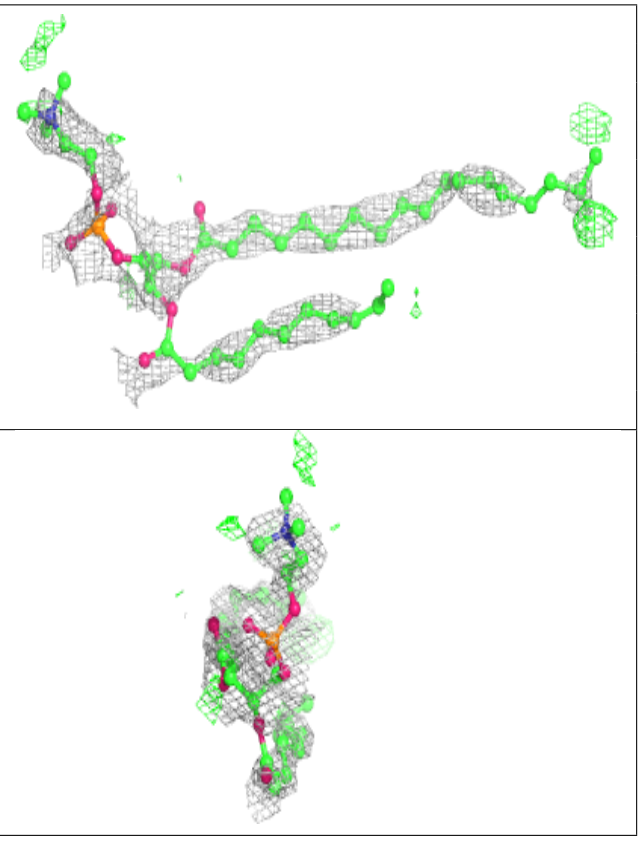
Electron density around CLR B 302:

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



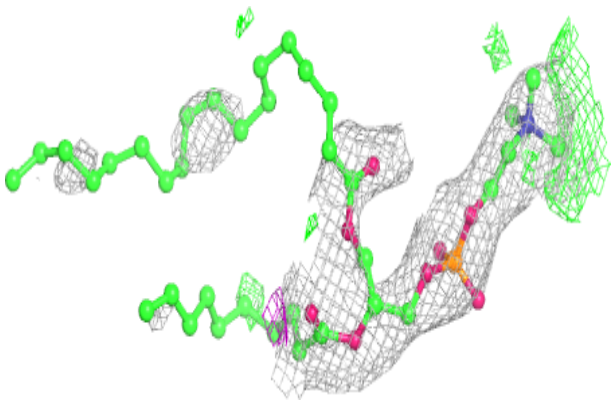
Electron density around PCW A 1104:

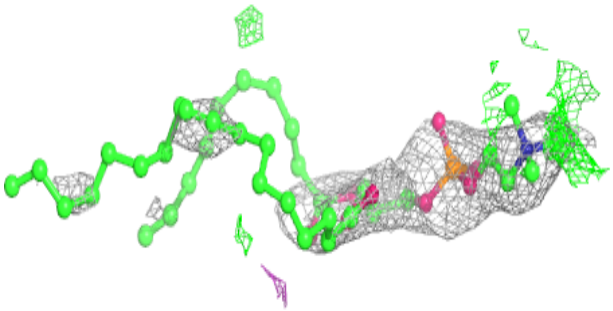
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

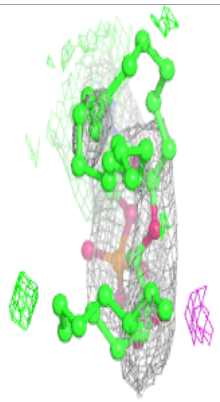


Electron density around PCW A 1103:

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

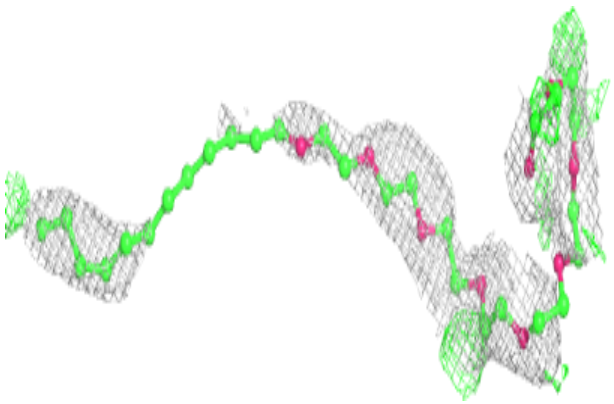


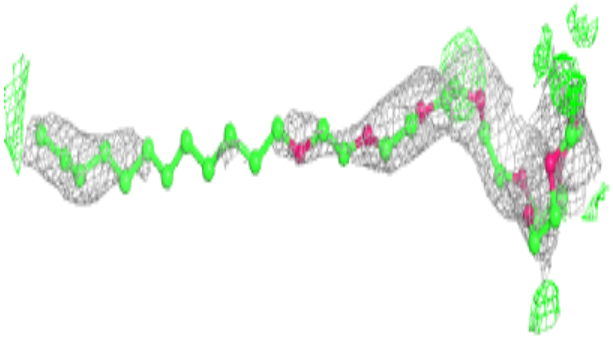




Electron density around CE1 A 1106:

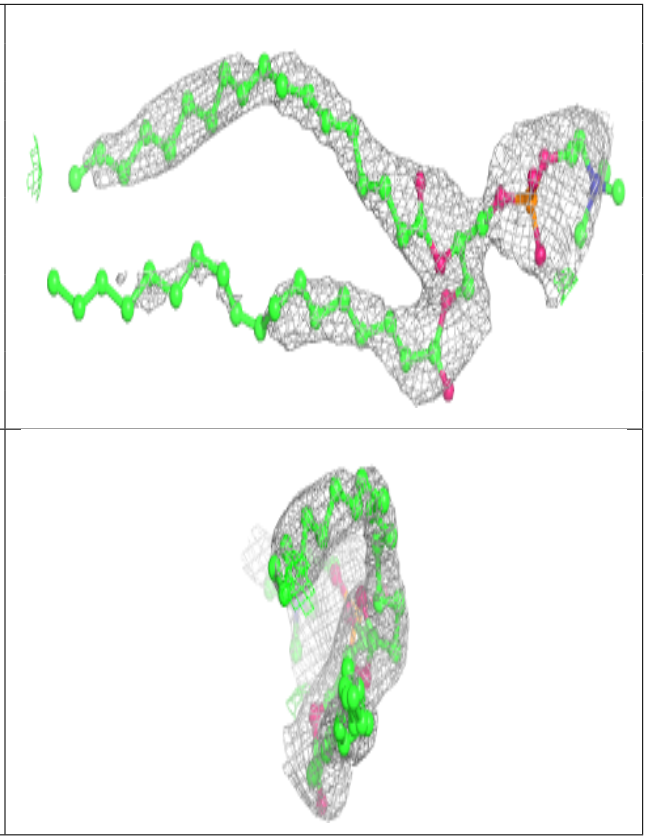
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around PCW 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)



6.5 Other polymers (i)

There are no such residues in this entry.