Full wwPDB EM Validation Report (i)

Nov 13, 2022 – 03:39 AM EST

PDB ID	:	6V35
EMDB ID	:	EMD-21028
Title	:	Cryo-EM structure of Ca2+-free hsSlo1-beta4 channel complex
Authors	:	Tao, X.; MacKinnon, R.
Deposited on	:	2019-11-25
Resolution	:	3.50 Å(reported)
Based on initial model	:	6V22

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

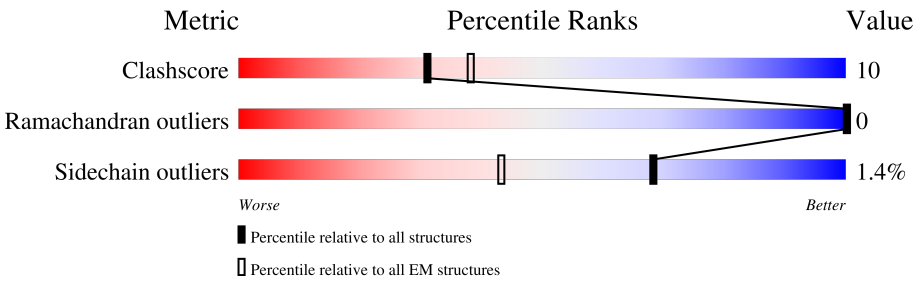
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1065	17% 67% 18% • 14%
1	B	1065	17% 67% 18% • 14%
1	C	1065	16% 67% 18% • 14%
1	D	1065	17% 67% 18% • 14%
2	E	219	37% 78% 13% 10%
2	F	219	36% 78% 12% 10%
2	G	219	37% 78% 13% 10%
2	H	219	34% 78% 13% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 36488 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	914	7287	4726	1193	1319	49	0	0
1	B	914	7287	4726	1193	1319	49	0	0
1	C	914	7287	4726	1193	1319	49	0	0
1	D	914	7287	4726	1193	1319	49	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1057	SER	-	expression tag	UNP Q12791
A	1058	ASN	-	expression tag	UNP Q12791
A	1059	SER	-	expression tag	UNP Q12791
A	1060	LEU	-	expression tag	UNP Q12791
A	1061	GLU	-	expression tag	UNP Q12791
A	1062	VAL	-	expression tag	UNP Q12791
A	1063	LEU	-	expression tag	UNP Q12791
A	1064	PHE	-	expression tag	UNP Q12791
A	1065	GLN	-	expression tag	UNP Q12791
B	1057	SER	-	expression tag	UNP Q12791
B	1058	ASN	-	expression tag	UNP Q12791
B	1059	SER	-	expression tag	UNP Q12791
B	1060	LEU	-	expression tag	UNP Q12791
B	1061	GLU	-	expression tag	UNP Q12791
B	1062	VAL	-	expression tag	UNP Q12791
B	1063	LEU	-	expression tag	UNP Q12791
B	1064	PHE	-	expression tag	UNP Q12791
B	1065	GLN	-	expression tag	UNP Q12791
C	1057	SER	-	expression tag	UNP Q12791
C	1058	ASN	-	expression tag	UNP Q12791
C	1059	SER	-	expression tag	UNP Q12791
C	1060	LEU	-	expression tag	UNP Q12791

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1061	GLU	-	expression tag	UNP Q12791
C	1062	VAL	-	expression tag	UNP Q12791
C	1063	LEU	-	expression tag	UNP Q12791
C	1064	PHE	-	expression tag	UNP Q12791
C	1065	GLN	-	expression tag	UNP Q12791
D	1057	SER	-	expression tag	UNP Q12791
D	1058	ASN	-	expression tag	UNP Q12791
D	1059	SER	-	expression tag	UNP Q12791
D	1060	LEU	-	expression tag	UNP Q12791
D	1061	GLU	-	expression tag	UNP Q12791
D	1062	VAL	-	expression tag	UNP Q12791
D	1063	LEU	-	expression tag	UNP Q12791
D	1064	PHE	-	expression tag	UNP Q12791
D	1065	GLN	-	expression tag	UNP Q12791

- Molecule 2 is a protein called Calcium-activated potassium channel subunit beta-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	198	1581	1012	262	294	13	0	0
2	F	198	1581	1012	262	294	13	0	0
2	G	198	1581	1012	262	294	13	0	0
2	H	198	1581	1012	262	294	13	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2211	SER	-	expression tag	UNP Q86W47
E	2212	ASN	-	expression tag	UNP Q86W47
E	2213	SER	-	expression tag	UNP Q86W47
E	2214	LEU	-	expression tag	UNP Q86W47
E	2215	GLU	-	expression tag	UNP Q86W47
E	2216	VAL	-	expression tag	UNP Q86W47
E	2217	LEU	-	expression tag	UNP Q86W47
E	2218	PHE	-	expression tag	UNP Q86W47
E	2219	GLN	-	expression tag	UNP Q86W47
F	2211	SER	-	expression tag	UNP Q86W47
F	2212	ASN	-	expression tag	UNP Q86W47
F	2213	SER	-	expression tag	UNP Q86W47

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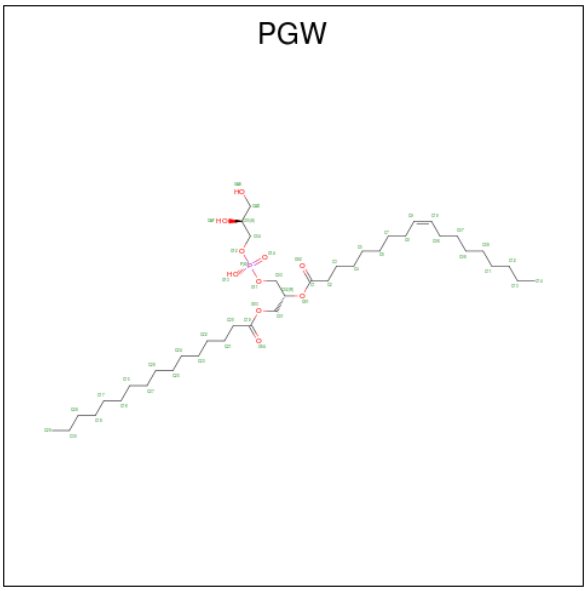
Chain	Residue	Modelled	Actual	Comment	Reference
F	2214	LEU	-	expression tag	UNP Q86W47
F	2215	GLU	-	expression tag	UNP Q86W47
F	2216	VAL	-	expression tag	UNP Q86W47
F	2217	LEU	-	expression tag	UNP Q86W47
F	2218	PHE	-	expression tag	UNP Q86W47
F	2219	GLN	-	expression tag	UNP Q86W47
G	2211	SER	-	expression tag	UNP Q86W47
G	2212	ASN	-	expression tag	UNP Q86W47
G	2213	SER	-	expression tag	UNP Q86W47
G	2214	LEU	-	expression tag	UNP Q86W47
G	2215	GLU	-	expression tag	UNP Q86W47
G	2216	VAL	-	expression tag	UNP Q86W47
G	2217	LEU	-	expression tag	UNP Q86W47
G	2218	PHE	-	expression tag	UNP Q86W47
G	2219	GLN	-	expression tag	UNP Q86W47
H	2211	SER	-	expression tag	UNP Q86W47
H	2212	ASN	-	expression tag	UNP Q86W47
H	2213	SER	-	expression tag	UNP Q86W47
H	2214	LEU	-	expression tag	UNP Q86W47
H	2215	GLU	-	expression tag	UNP Q86W47
H	2216	VAL	-	expression tag	UNP Q86W47
H	2217	LEU	-	expression tag	UNP Q86W47
H	2218	PHE	-	expression tag	UNP Q86W47
H	2219	GLN	-	expression tag	UNP Q86W47

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			160	129	28	3	
3	A	1	Total	C	O	P	0
			160	129	28	3	
3	A	1	Total	C	O	P	0
			160	129	28	3	
3	A	1	Total	C	O	P	0
			160	129	28	3	
3	A	1	Total	C	O	P	0
			160	129	28	3	
3	A	1	Total	C	O	P	0
			160	129	28	3	
3	A	1	Total	C	O	P	0
			160	129	28	3	
3	A	1	Total	C	O	P	0
			160	129	28	3	
3	E	1	Total	C			0
			13	13			
3	E	1	Total	C			0
			13	13			
3	B	1	Total	C	O	P	0
			184	144	36	4	
3	B	1	Total	C	O	P	0
			184	144	36	4	
3	B	1	Total	C	O	P	0
			184	144	36	4	
3	B	1	Total	C	O	P	0
			184	144	36	4	

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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	O	P	0
			184	144	36	4	
3	B	1	Total	C	O	P	0
			184	144	36	4	
3	B	1	Total	C	O	P	0
			184	144	36	4	
3	B	1	Total	C	O	P	0
			184	144	36	4	
3	B	1	Total	C	O	P	0
			184	144	36	4	
3	F	1	Total	C			0
			22	22			
3	F	1	Total	C			0
			22	22			
3	F	1	Total	C			0
			22	22			
3	C	1	Total	C	O	P	0
			121	99	20	2	
3	C	1	Total	C	O	P	0
			121	99	20	2	
3	C	1	Total	C	O	P	0
			121	99	20	2	
3	C	1	Total	C	O	P	0
			121	99	20	2	
3	C	1	Total	C	O	P	0
			121	99	20	2	
3	C	1	Total	C	O	P	0
			121	99	20	2	
3	G	1	Total	C			0
			13	13			
3	G	1	Total	C			0
			13	13			
3	D	1	Total	C	O	P	0
			145	114	28	3	
3	D	1	Total	C	O	P	0
			145	114	28	3	
3	D	1	Total	C	O	P	0
			145	114	28	3	
3	D	1	Total	C	O	P	0
			145	114	28	3	
3	D	1	Total	C	O	P	0
			145	114	28	3	

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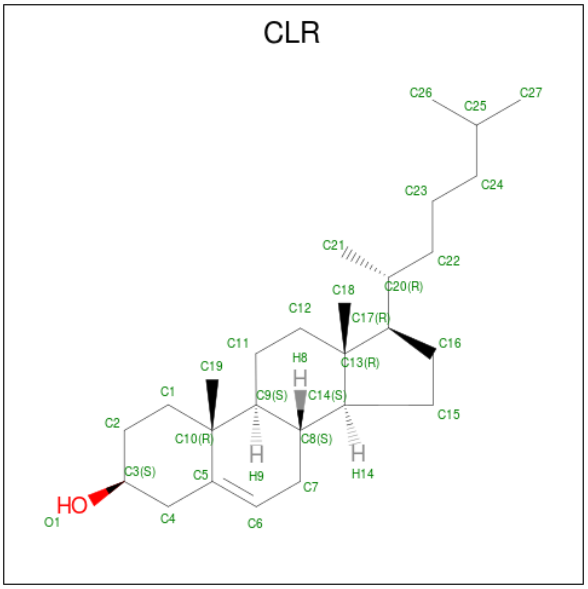
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
3	D	1	145	114	28	3	0
			Total	C	O	P	
3	D	1	145	114	28	3	0
			Total	C			
3	H	1	22	22			0
			Total	C			
3	H	1	22	22			0
			Total	C			
3	H	1	22	22			0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	A	1	28	27	1	0
			Total	C	O	
4	E	1	28	27	1	0
			Total	C	O	
4	B	1	28	27	1	0
			Total	C	O	
4	F	1	28	27	1	0
			Total	C	O	
4	C	1	28	27	1	0
			Total	C	O	
4	G	1	28	27	1	0

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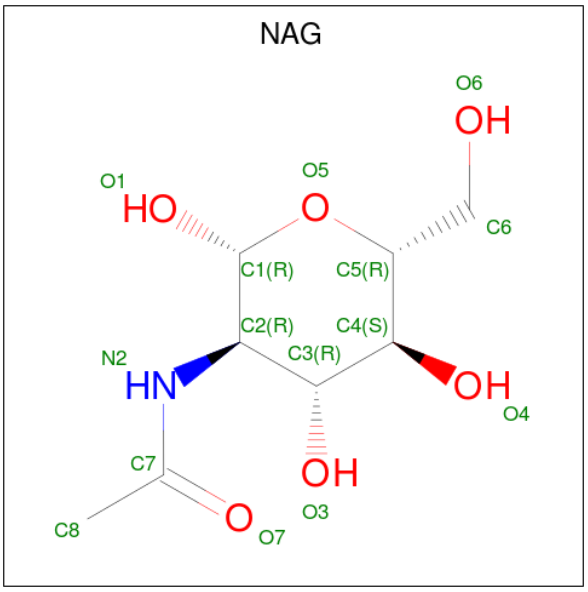
Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	O		0
			28	27	1		
4	H	1	Total	C	O		0
			28	27	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



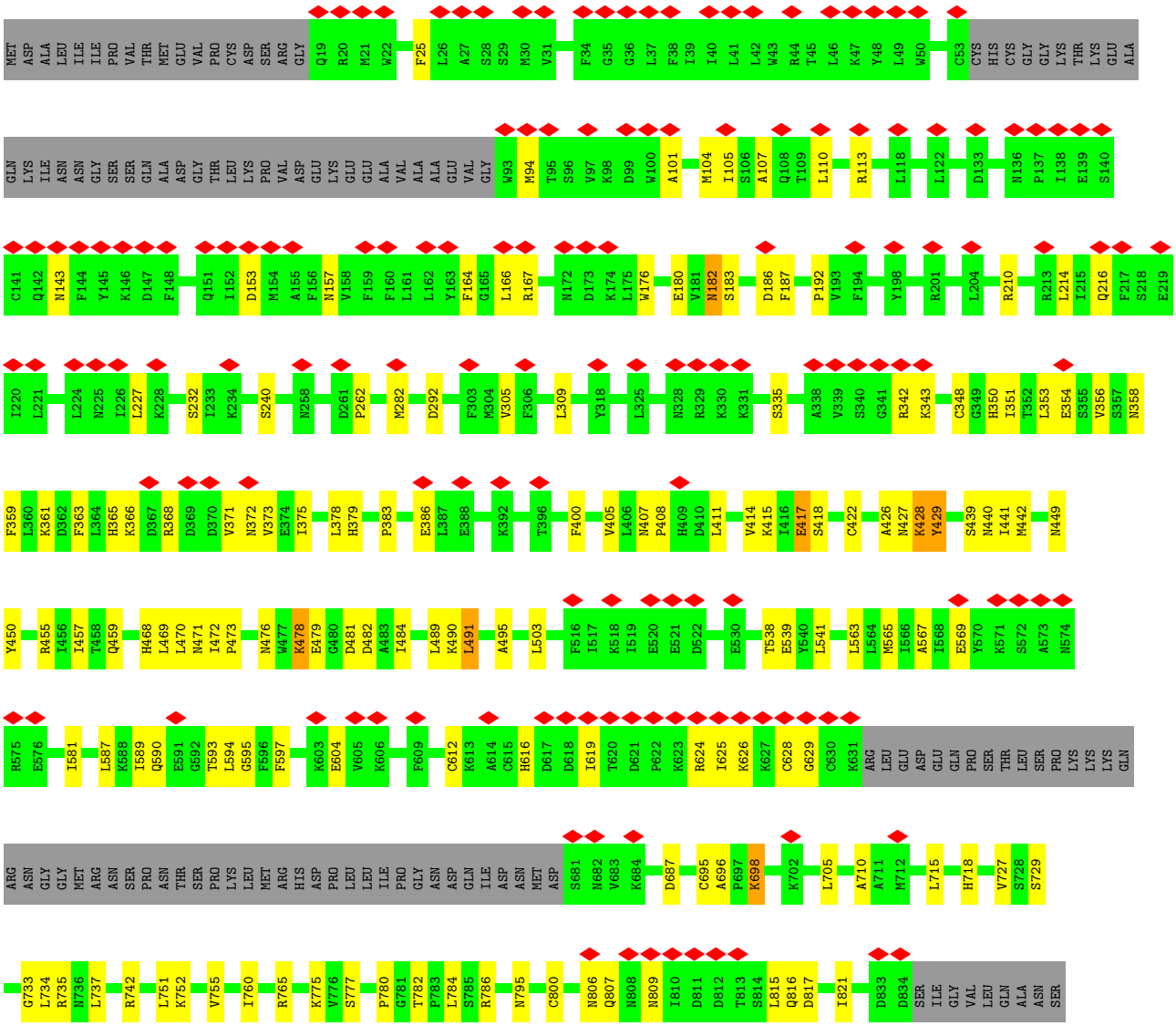
Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			28	16	2	10	
5	E	1	Total	C	N	O	0
			28	16	2	10	
5	F	1	Total	C	N	O	0
			28	16	2	10	
5	F	1	Total	C	N	O	0
			28	16	2	10	
5	G	1	Total	C	N	O	0
			28	16	2	10	
5	G	1	Total	C	N	O	0
			28	16	2	10	
5	H	1	Total	C	N	O	0
			28	16	2	10	
5	H	1	Total	C	N	O	0
			28	16	2	10	

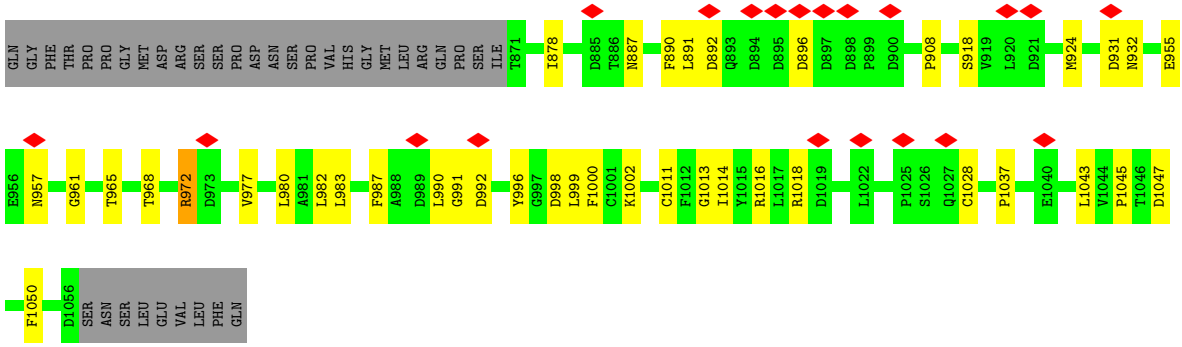
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Calcium-activated potassium channel subunit alpha-1

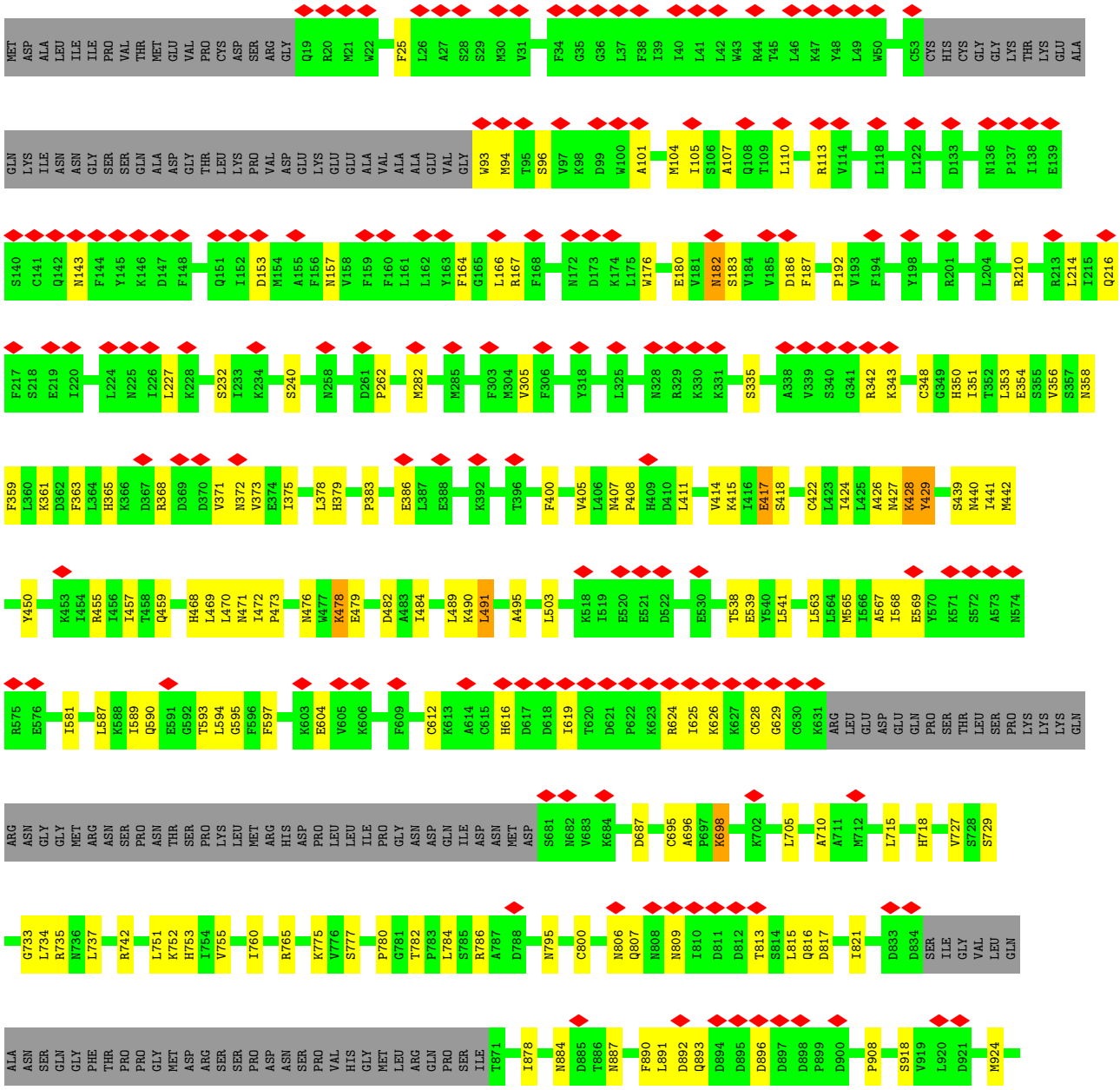
Chain A:

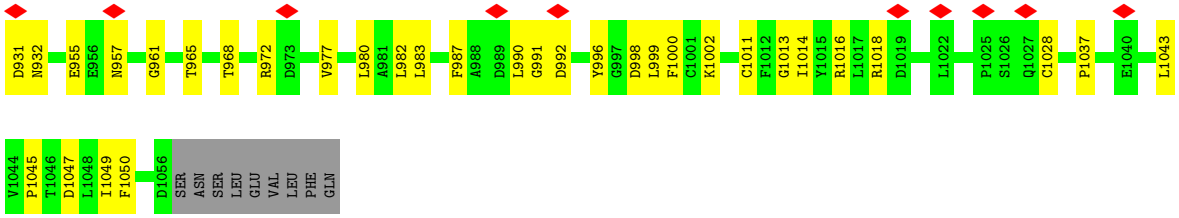




• Molecule 1: Calcium-activated potassium channel subunit alpha-1

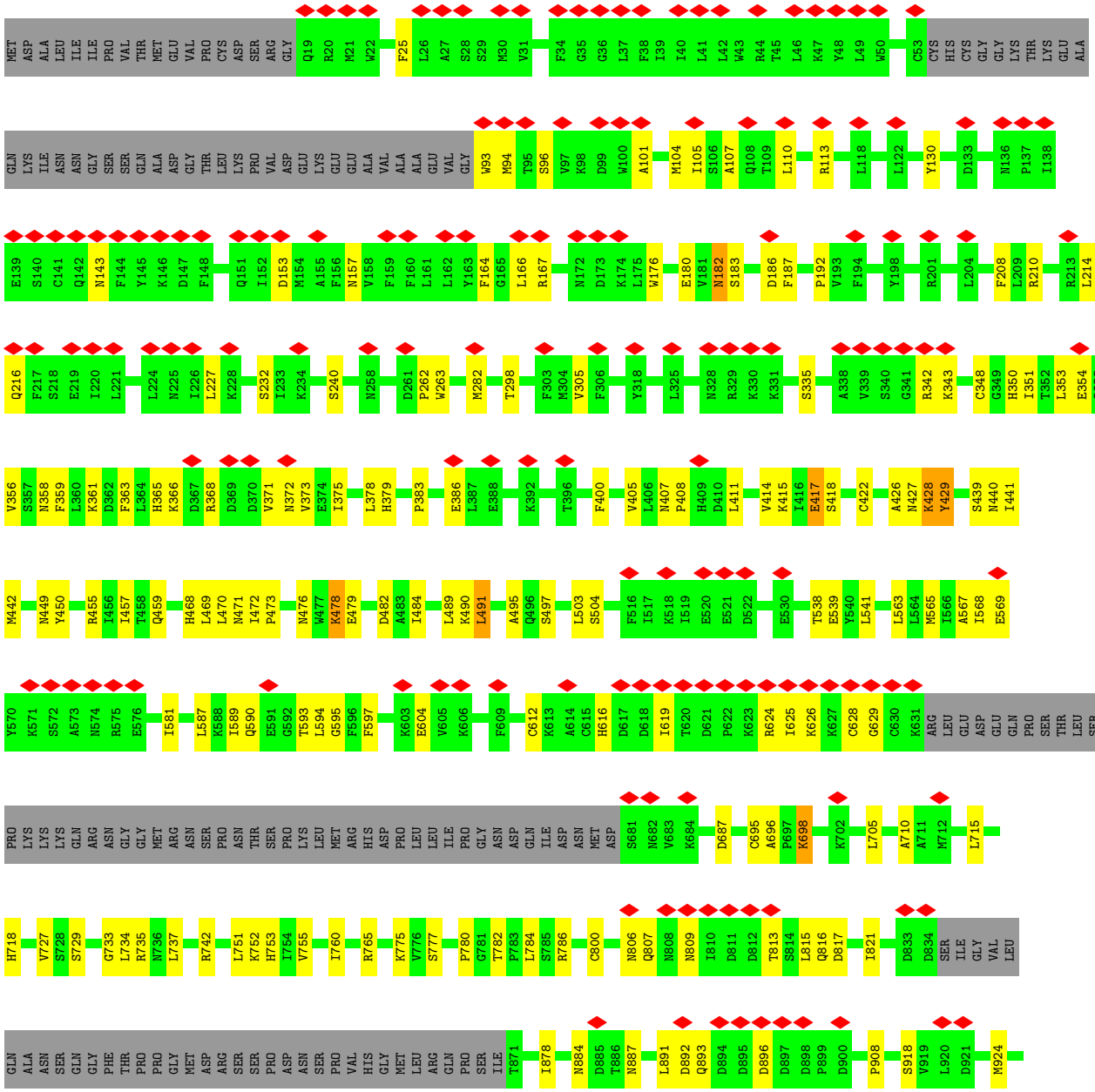
Chain B:

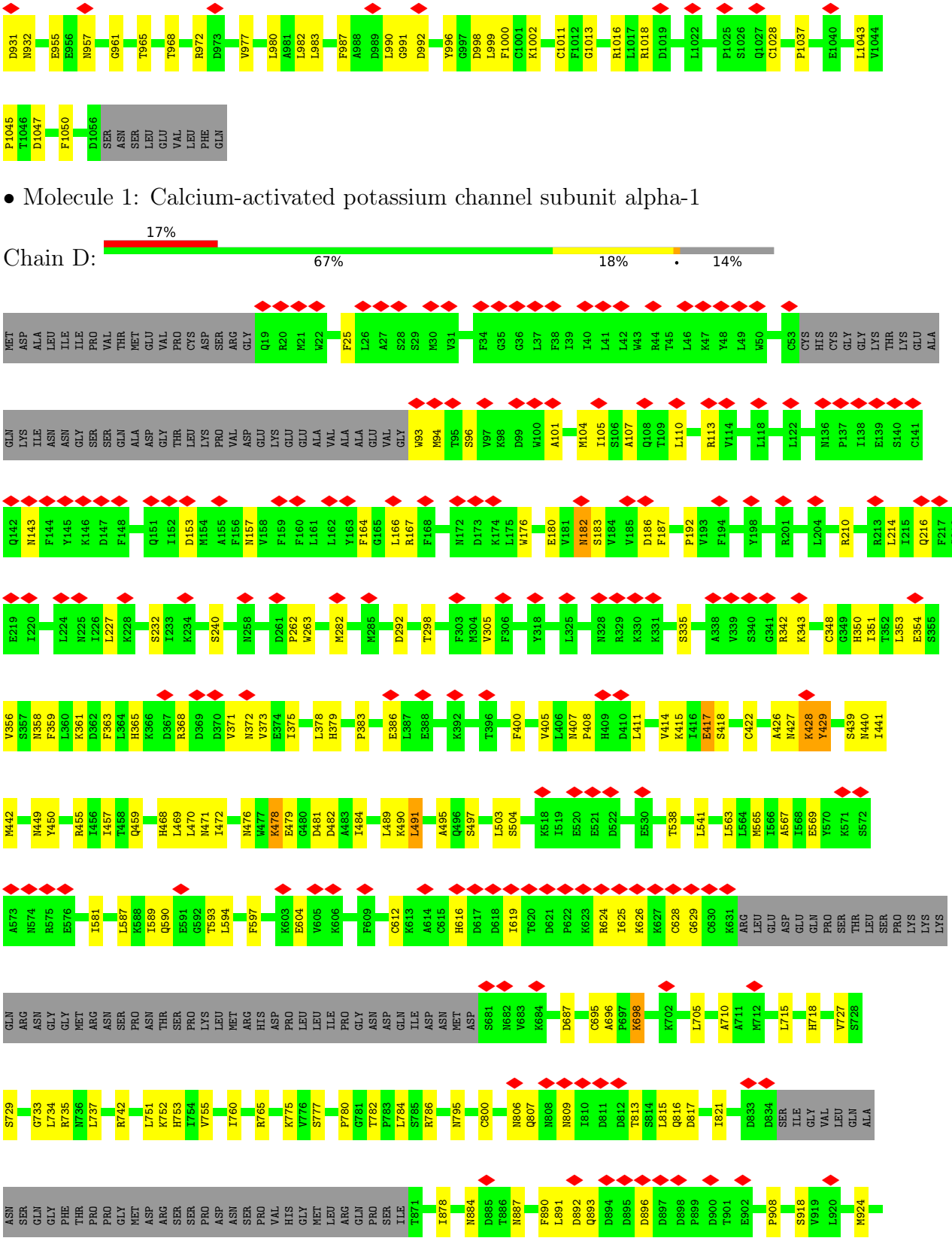


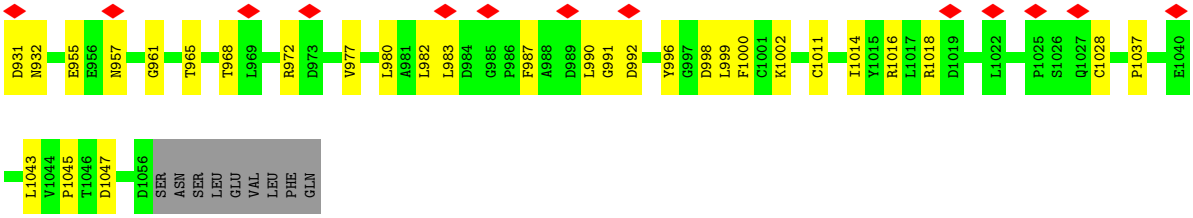


- Molecule 1: Calcium-activated potassium channel subunit alpha-1

Chain C:

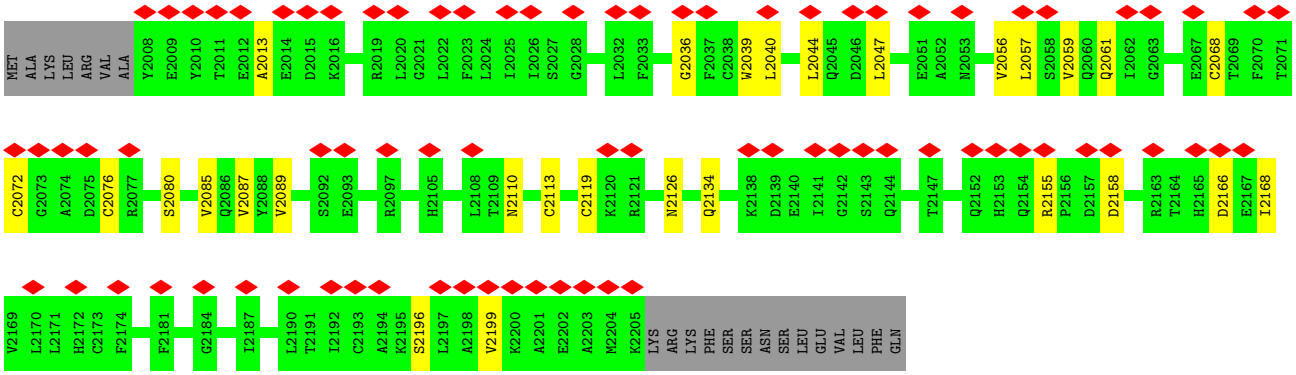



D931 N932 E955 E956 N957 G961 T965 T968 R972 D973 V977 L980 A981 L982 L983 F987 A988 D989 L990 G991 D992 Y996 G997 D998 L999 F1000 C1001 K1002 C1011 F1012 G1013 R1016 L1017 R1018 D1019 L1022 P1025 S1026 Q1027 C1028 P1037 E1040 L1043 V1044
P1045 T1046 D1047 F1050 D1056 SER ASN SER LEU GLU VAL LEU PHE GLN
• Molecule 1: Calcium-activated potassium channel subunit alpha-1
Chain D:
17%
67%
18%
14%
MET ASP ALA LEU ILE ILE PRO VAL THR MET GLU VAL PRO CYS ASP SER ARG GLY Q19 R20 M21 W22 F25 L26 A27 S28 S29 M30 V31 F34 G35 G36 L37 F38 I39 I40 L41 L42 W43 R44 T45 L46 K47 Y48 L49 W50 C53 CYS HIS CYS GLY GLY LYS THR LYS GLU ALA
GLN LYS ILE ASN ASN GLY SER SER GLN ALA ASP GLY THR LEU LYS PRO VAL ASP GLU LYS GLU GLU ALA VAL ALA ALA GLU VAL GLY W93 M94 T95 S96 V97 K98 D99 W100 A101 M104 I105 S106 A107 Q108 T109 L110 R113 V114 L118 L122 N136 P137 I138 E139 S140 C141
Q142 N143 F144 Y145 K146 D147 F148 Q151 I152 D153 M154 A155 F156 N157 V158 F159 F160 L161 L162 Y163 F164 G165 L166 R167 F168 N172 D173 K174 L175 W176 E180 V181 N182 S183 V184 V185 D186 F187 P192 V193 F194 Y198 R201 L204 R210 R213 L214 I215 Q216 F217 S218
E219 I220 L224 N225 I226 L227 K228 S232 I233 K234 S240 N258 D261 P262 W263 M282 M285 D292 T298 F303 M304 V305 F306 Y318 L325 N328 R329 K330 K331 S335 A338 V339 S340 G341 R342 K343 C348 G349 H350 I351 T352 L353 E354 S355
V356 S357 N358 F359 L360 K361 D362 F363 L364 H365 K366 D367 R368 D369 D370 V371 N372 V373 E374 I375 L378 H379 P383 E386 L387 E388 K392 T396 F400 V405 L406 N407 P408 H409 D410 L411 V414 K415 I416 E417 S418 C422 A426 N427 K428 Y429 S439 N440 I441
M442 N449 Y450 R455 I456 I457 T458 Q459 H468 L469 L470 N471 I472 N476 W477 K478 E479 G480 D481 D482 A483 I484 L489 K490 L491 A495 G496 S497 L503 S504 K518 I519 E520 E521 D522 E530 T538 L541 L563 L564 M565 I566 A567 I568 E569 Y570 K571 S572
A573 N574 R575 E576 I581 L587 K588 I589 Q590 E591 G592 T593 L594 F597 K603 E604 V605 K606 F609 C612 K613 A614 C615 H616 D617 D618 I619 T620 D621 P622 K623 R624 I625 K626 K627 C628 G629 C630 K631 ARG LEU GLU ASP GLU GLN PRO SER THR LEU SER PRO LYS LYS LYS
GLN ARG ASN GLY GLY MET ARG ASN SER PRO ASN THR SER PRO LYS LEU MET ARG HIS ASP PRO LEU LEU ILE PRO GLY ASN ASP GLN ILE ASP ASN MET ASP S681 N682 V683 K684 D687 C695 A696 P697 K698 K702 L705 A710 A711 M712 L715 H718 V727 S728
S729 G733 L734 R735 N736 L737 R742 L751 K752 H753 I754 V755 I760 R765 K775 V776 S777 P780 G781 T782 P783 L784 S785 R786 N795 C800 N806 Q807 N808 N809 I810 D811 D812 T813 S814 L815 Q816 D817 I821 D833 D834 SER ILE GLY VAL LEU GLN ALA
ASN SER GLN GLY PHE THR PRO PRO GLY MET ASP ARG SER SER PRO ASP ASN SER PRO VAL HIS GLY MET LEU ARG GLN PRO SER ILE T871 I878 N884 D885 T886 N887 F890 L891 D892 Q893 D894 D895 D896 D897 D898 P899 D900 T901 E902 P908 S918 Y919 L920 M924



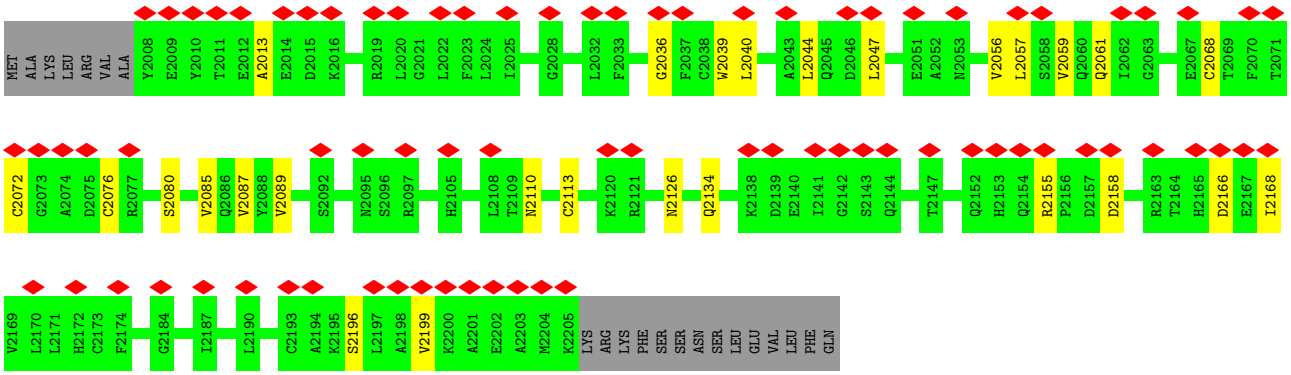
• Molecule 2: Calcium-activated potassium channel subunit beta-4

Chain E:



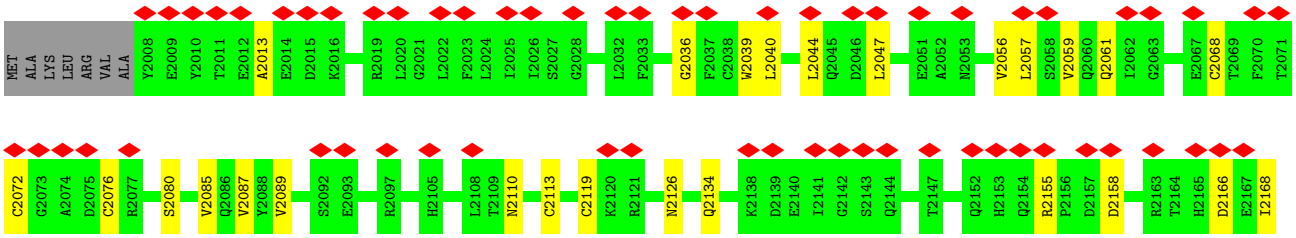
• Molecule 2: Calcium-activated potassium channel subunit beta-4

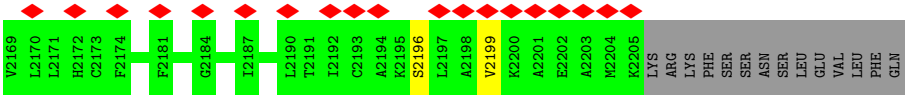
Chain F:



• Molecule 2: Calcium-activated potassium channel subunit beta-4

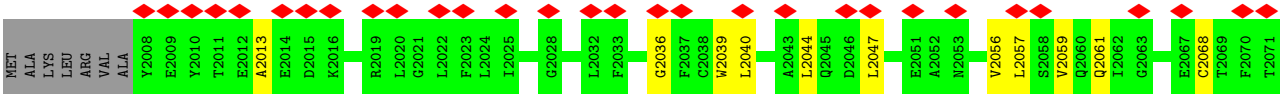
Chain G:

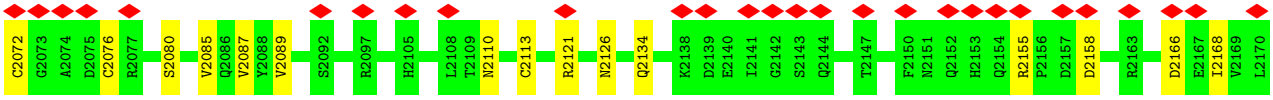


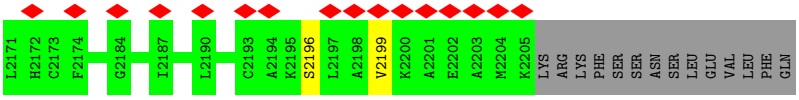


• Molecule 2: Calcium-activated potassium channel subunit beta-4

Chain H:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	42842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	21.471	Depositor
Minimum map value	-9.618	Depositor
Average map value	-0.342	Depositor
Map value standard deviation	1.078	Depositor
Recommended contour level	6.7	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

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: CLR, PGW, NAG

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	0.43	0/7456	0.55	0/10119
1	B	0.43	0/7456	0.55	0/10119
1	C	0.43	0/7456	0.55	0/10119
1	D	0.43	0/7456	0.55	0/10119
2	E	0.32	0/1619	0.48	0/2204
2	F	0.32	0/1619	0.49	0/2204
2	G	0.32	0/1619	0.48	0/2204
2	H	0.32	0/1619	0.48	0/2204
All	All	0.41	0/36300	0.54	0/49292

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	7287	0	7277	152	0
1	B	7287	0	7277	153	0
1	C	7287	0	7277	152	0
1	D	7287	0	7277	154	0
2	E	1581	0	1538	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1581	0	1538	16	0
2	G	1581	0	1538	20	0
2	H	1581	0	1538	19	0
3	A	160	0	215	1	0
3	B	184	0	236	2	0
3	C	121	0	168	1	0
3	D	145	0	189	3	0
3	E	13	0	18	0	0
3	F	22	0	32	0	0
3	G	13	0	18	0	0
3	H	22	0	32	0	0
4	A	28	0	44	6	0
4	B	28	0	44	6	0
4	C	28	0	44	5	0
4	D	28	0	44	6	0
4	E	28	0	45	5	0
4	F	28	0	45	8	0
4	G	28	0	45	8	0
4	H	28	0	45	7	0
5	E	28	0	26	0	0
5	F	28	0	26	0	0
5	G	28	0	26	0	0
5	H	28	0	26	0	0
All	All	36488	0	36628	707	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 10.

All (707) 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)
4:E:2305:CLR:C16	4:E:2305:CLR:C17	1.74	1.61
4:G:2305:CLR:C16	4:G:2305:CLR:C17	1.74	1.59
4:B:1110:CLR:C16	4:B:1110:CLR:C17	1.75	1.56
4:F:2306:CLR:C16	4:F:2306:CLR:C17	1.74	1.56
4:C:1107:CLR:C16	4:C:1107:CLR:C17	1.75	1.51
4:D:1108:CLR:C16	4:D:1108:CLR:C17	1.75	1.49
4:A:3006:CLR:C16	4:A:3006:CLR:C17	1.75	1.47
4:H:2306:CLR:C16	4:H:2306:CLR:C17	1.74	1.44
1:C:183:SER:O	1:C:187:PHE:HB2	1.68	0.93
1:A:183:SER:O	1:A:187:PHE:HB2	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:SER:O	1:B:187:PHE:HB2	1.68	0.93
1:C:491:LEU:HG	1:C:737:LEU:HB2	1.50	0.92
1:D:183:SER:O	1:D:187:PHE:HB2	1.68	0.92
1:A:491:LEU:HG	1:A:737:LEU:HB2	1.50	0.91
1:B:491:LEU:HG	1:B:737:LEU:HB2	1.50	0.90
1:D:491:LEU:HG	1:D:737:LEU:HB2	1.50	0.89
1:C:101:ALA:HB1	1:C:166:LEU:HD12	1.60	0.83
1:A:982:LEU:HD13	1:A:1043:LEU:HD21	1.61	0.83
1:A:101:ALA:HB1	1:A:166:LEU:HD12	1.60	0.83
1:B:982:LEU:HD13	1:B:1043:LEU:HD21	1.61	0.83
1:D:982:LEU:HD13	1:D:1043:LEU:HD21	1.61	0.82
1:B:101:ALA:HB1	1:B:166:LEU:HD12	1.61	0.82
1:C:982:LEU:HD13	1:C:1043:LEU:HD21	1.61	0.82
1:D:101:ALA:HB1	1:D:166:LEU:HD12	1.60	0.82
1:A:1002:LYS:CA	1:A:1002:LYS:HE2	2.11	0.81
1:B:1002:LYS:HE2	1:B:1002:LYS:CA	2.11	0.81
4:H:2306:CLR:C16	4:H:2306:CLR:C20	2.58	0.81
4:C:1107:CLR:C16	4:C:1107:CLR:C20	2.59	0.80
4:E:2305:CLR:C16	4:E:2305:CLR:C20	2.58	0.80
4:F:2306:CLR:C16	4:F:2306:CLR:C20	2.58	0.80
4:B:1110:CLR:C16	4:B:1110:CLR:C20	2.59	0.80
4:A:3006:CLR:C16	4:A:3006:CLR:C20	2.59	0.79
1:D:1002:LYS:CA	1:D:1002:LYS:HE2	2.11	0.79
1:C:1002:LYS:CA	1:C:1002:LYS:HE2	2.11	0.79
4:D:1108:CLR:C16	4:D:1108:CLR:C20	2.59	0.78
4:G:2305:CLR:C16	4:G:2305:CLR:C20	2.58	0.78
1:A:1002:LYS:HE2	1:A:1002:LYS:HA	1.67	0.76
1:B:1002:LYS:HE2	1:B:1002:LYS:HA	1.67	0.76
1:C:1002:LYS:HE2	1:C:1002:LYS:HA	1.67	0.76
1:D:1002:LYS:HE2	1:D:1002:LYS:HA	1.67	0.76
1:C:417:GLU:HG3	1:C:450:TYR:HE2	1.53	0.74
1:A:417:GLU:HG3	1:A:450:TYR:HE2	1.53	0.73
1:C:1002:LYS:HE2	1:C:1002:LYS:N	2.05	0.72
1:D:417:GLU:HG3	1:D:450:TYR:HE2	1.53	0.72
1:B:417:GLU:HG3	1:B:450:TYR:HE2	1.53	0.72
1:B:1002:LYS:HE2	1:B:1002:LYS:N	2.04	0.72
1:A:1002:LYS:HE2	1:A:1002:LYS:N	2.05	0.72
1:D:1002:LYS:HE2	1:D:1002:LYS:N	2.04	0.72
1:D:1000:PHE:HA	1:D:1011:CYS:SG	2.32	0.70
1:D:343:LYS:O	1:D:373:VAL:HA	1.91	0.70
1:A:1000:PHE:HA	1:A:1011:CYS:SG	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:O	1:B:373:VAL:HA	1.91	0.69
1:B:1000:PHE:HA	1:B:1011:CYS:SG	2.32	0.69
1:C:1000:PHE:HA	1:C:1011:CYS:SG	2.32	0.69
1:A:104:MET:HA	1:A:104:MET:CE	2.23	0.69
1:D:104:MET:HA	1:D:104:MET:CE	2.23	0.69
1:C:343:LYS:O	1:C:373:VAL:HA	1.91	0.69
1:A:343:LYS:O	1:A:373:VAL:HA	1.91	0.68
1:B:104:MET:HA	1:B:104:MET:CE	2.23	0.68
1:C:104:MET:CE	1:C:104:MET:HA	2.23	0.67
1:A:351:ILE:HG23	1:A:356:VAL:HG21	1.78	0.66
1:C:351:ILE:HG23	1:C:356:VAL:HG21	1.78	0.66
1:C:305:VAL:HG13	1:D:282:MET:HG2	1.77	0.66
1:B:351:ILE:HG23	1:B:356:VAL:HG21	1.78	0.66
1:D:351:ILE:HG23	1:D:356:VAL:HG21	1.78	0.66
2:F:2072:CYS:H	2:F:2076:CYS:HB2	1.61	0.65
2:E:2072:CYS:H	2:E:2076:CYS:HB2	1.61	0.65
1:D:470:LEU:C	1:D:470:LEU:HD23	2.18	0.64
1:B:470:LEU:HD23	1:B:470:LEU:C	2.18	0.64
1:C:358:ASN:HD22	1:C:918:SER:HB3	1.62	0.64
1:C:470:LEU:C	1:C:470:LEU:HD23	2.18	0.64
1:C:563:LEU:HD21	1:C:604:GLU:HB3	1.79	0.64
2:G:2072:CYS:H	2:G:2076:CYS:HB2	1.61	0.64
1:D:358:ASN:HD22	1:D:918:SER:HB3	1.62	0.64
2:H:2072:CYS:H	2:H:2076:CYS:HB2	1.61	0.64
1:A:353:LEU:HD22	1:A:386:GLU:OE1	1.98	0.64
1:A:358:ASN:HD22	1:A:918:SER:HB3	1.62	0.64
1:B:353:LEU:HD22	1:B:386:GLU:OE1	1.98	0.63
1:A:563:LEU:HD21	1:A:604:GLU:HB3	1.80	0.63
1:A:441:ILE:HD13	1:A:468:HIS:HB2	1.81	0.63
1:B:563:LEU:HD21	1:B:604:GLU:HB3	1.80	0.63
1:A:470:LEU:C	1:A:470:LEU:HD23	2.18	0.62
1:B:358:ASN:HD22	1:B:918:SER:HB3	1.62	0.62
1:C:353:LEU:HD22	1:C:386:GLU:OE1	1.98	0.62
1:D:353:LEU:HD22	1:D:386:GLU:OE1	1.98	0.62
1:D:563:LEU:HD21	1:D:604:GLU:HB3	1.80	0.62
1:C:439:SER:OG	1:D:815:LEU:HD21	1.99	0.62
1:B:441:ILE:HD13	1:B:468:HIS:HB2	1.81	0.62
2:F:2057:LEU:H	2:F:2089:VAL:HA	1.65	0.62
1:C:351:ILE:HG23	1:C:356:VAL:CG2	2.30	0.62
1:B:439:SER:OG	1:C:815:LEU:HD21	2.00	0.62
1:C:441:ILE:HD13	1:C:468:HIS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ILE:HG23	1:B:356:VAL:CG2	2.30	0.62
1:D:705:LEU:HD13	1:D:710:ALA:HB2	1.82	0.61
1:D:351:ILE:HG23	1:D:356:VAL:CG2	2.30	0.61
2:G:2057:LEU:H	2:G:2089:VAL:HA	1.65	0.61
1:D:441:ILE:HD13	1:D:468:HIS:HB2	1.81	0.61
1:A:351:ILE:HG23	1:A:356:VAL:CG2	2.30	0.61
1:A:705:LEU:HD13	1:A:710:ALA:HB2	1.82	0.61
1:C:612:CYS:H	1:C:616:HIS:HD2	1.49	0.61
2:H:2057:LEU:H	2:H:2089:VAL:HA	1.65	0.61
1:D:612:CYS:H	1:D:616:HIS:HD2	1.49	0.60
1:B:612:CYS:H	1:B:616:HIS:HD2	1.49	0.60
1:C:705:LEU:HD13	1:C:710:ALA:HB2	1.82	0.60
1:D:727:VAL:O	1:D:765:ARG:NH1	2.35	0.60
1:A:612:CYS:H	1:A:616:HIS:HD2	1.49	0.60
1:C:727:VAL:O	1:C:765:ARG:NH1	2.35	0.60
1:D:587:LEU:O	1:D:587:LEU:HD23	2.02	0.60
1:B:727:VAL:O	1:B:765:ARG:NH1	2.35	0.60
1:A:587:LEU:HD23	1:A:587:LEU:O	2.02	0.60
1:C:587:LEU:HD23	1:C:587:LEU:O	2.02	0.60
1:B:800:CYS:HB3	1:B:878:ILE:HG22	1.84	0.60
1:A:727:VAL:O	1:A:765:ARG:NH1	2.35	0.60
1:A:439:SER:OG	1:B:815:LEU:HD21	2.02	0.60
4:E:2305:CLR:C16	4:E:2305:CLR:H222	2.32	0.60
1:B:705:LEU:HD13	1:B:710:ALA:HB2	1.82	0.60
1:A:305:VAL:HG13	1:B:282:MET:HG2	1.82	0.60
1:A:479:GLU:OE1	1:A:479:GLU:HA	2.02	0.59
4:H:2306:CLR:C16	4:H:2306:CLR:H222	2.32	0.59
2:E:2057:LEU:H	2:E:2089:VAL:HA	1.65	0.59
1:B:742:ARG:NH2	1:B:775:LYS:O	2.36	0.59
1:B:619:ILE:HA	1:B:624:ARG:HG3	1.85	0.59
1:C:186:ASP:OD1	1:C:210:ARG:NH1	2.36	0.59
1:C:619:ILE:HA	1:C:624:ARG:HG3	1.85	0.59
4:G:2305:CLR:C16	4:G:2305:CLR:H222	2.32	0.59
1:D:186:ASP:OD1	1:D:210:ARG:NH1	2.36	0.59
1:D:479:GLU:HA	1:D:479:GLU:OE1	2.02	0.59
1:D:815:LEU:HG	1:D:815:LEU:O	2.03	0.59
4:F:2306:CLR:C16	4:F:2306:CLR:H222	2.32	0.59
1:C:742:ARG:NH2	1:C:775:LYS:O	2.36	0.59
1:C:800:CYS:HB3	1:C:878:ILE:HG22	1.84	0.59
1:C:815:LEU:O	1:C:815:LEU:HG	2.03	0.59
1:D:742:ARG:NH2	1:D:775:LYS:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1108:CLR:C16	4:D:1108:CLR:H222	2.33	0.59
1:B:815:LEU:HG	1:B:815:LEU:O	2.03	0.59
1:A:619:ILE:HA	1:A:624:ARG:HG3	1.85	0.59
1:A:742:ARG:NH2	1:A:775:LYS:O	2.36	0.59
1:D:619:ILE:HA	1:D:624:ARG:HG3	1.85	0.59
1:B:587:LEU:O	1:B:587:LEU:HD23	2.02	0.58
1:B:695:CYS:SG	1:B:696:ALA:N	2.76	0.58
4:A:3006:CLR:C16	4:A:3006:CLR:H222	2.33	0.58
1:B:479:GLU:HA	1:B:479:GLU:OE1	2.02	0.58
1:D:800:CYS:HB3	1:D:878:ILE:HG22	1.84	0.58
1:D:809:ASN:HD22	1:D:816:GLN:HG2	1.69	0.58
1:B:809:ASN:HD22	1:B:816:GLN:HG2	1.69	0.58
1:A:800:CYS:HB3	1:A:878:ILE:HG22	1.84	0.58
1:C:262:PRO:HB2	2:G:2039:TRP:HZ3	1.68	0.58
1:C:955:GLU:HG2	1:D:786:ARG:HD2	1.85	0.58
4:C:1107:CLR:C16	4:C:1107:CLR:H222	2.33	0.58
1:A:348:CYS:SG	1:A:422:CYS:SG	3.02	0.58
1:D:982:LEU:HD11	1:D:1047:ASP:HB2	1.86	0.58
1:A:262:PRO:HB2	2:E:2039:TRP:HZ3	1.68	0.58
1:B:348:CYS:SG	1:B:422:CYS:SG	3.02	0.58
1:C:479:GLU:OE1	1:C:479:GLU:HA	2.02	0.58
1:D:695:CYS:SG	1:D:696:ALA:N	2.76	0.58
1:A:695:CYS:SG	1:A:696:ALA:N	2.76	0.58
1:B:186:ASP:OD1	1:B:210:ARG:NH1	2.36	0.58
1:C:753:HIS:HD1	1:C:775:LYS:HB2	1.67	0.58
1:B:982:LEU:HD11	1:B:1047:ASP:HB2	1.86	0.58
1:C:695:CYS:SG	1:C:696:ALA:N	2.76	0.58
1:D:348:CYS:SG	1:D:422:CYS:SG	3.02	0.58
1:A:982:LEU:HD11	1:A:1047:ASP:HB2	1.86	0.58
4:B:1110:CLR:C16	4:B:1110:CLR:H222	2.33	0.58
1:B:262:PRO:HB2	2:F:2039:TRP:HZ3	1.68	0.58
1:C:809:ASN:HD22	1:C:816:GLN:HG2	1.69	0.58
1:A:809:ASN:HD22	1:A:816:GLN:HG2	1.69	0.57
1:C:982:LEU:HD11	1:C:1047:ASP:HB2	1.86	0.57
1:C:101:ALA:CB	1:C:166:LEU:HD12	2.33	0.57
1:C:348:CYS:SG	1:C:422:CYS:SG	3.02	0.57
1:A:227:LEU:HD22	1:A:232:SER:HB3	1.87	0.57
1:A:815:LEU:HD21	1:D:439:SER:OG	2.05	0.57
1:D:262:PRO:HB2	2:H:2039:TRP:HZ3	1.68	0.57
1:A:815:LEU:O	1:A:815:LEU:HG	2.03	0.57
1:D:227:LEU:HD22	1:D:232:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2036:GLY:HA2	2:F:2040:LEU:HD12	1.87	0.57
1:A:405:VAL:HA	1:A:411:LEU:HD11	1.87	0.56
2:E:2036:GLY:HA2	2:E:2040:LEU:HD12	1.87	0.56
1:B:227:LEU:HD22	1:B:232:SER:HB3	1.87	0.56
1:C:227:LEU:HD22	1:C:232:SER:HB3	1.87	0.56
1:A:101:ALA:CB	1:A:166:LEU:HD12	2.34	0.56
1:C:569:GLU:HG2	1:C:594:LEU:HB3	1.88	0.56
1:D:351:ILE:HD12	1:D:379:HIS:HB2	1.88	0.56
1:B:105:ILE:HD11	1:B:166:LEU:HG	1.87	0.56
1:B:101:ALA:CB	1:B:166:LEU:HD12	2.34	0.56
1:A:153:ASP:OD1	1:A:157:ASN:ND2	2.38	0.56
1:B:687:ASP:HA	1:B:961:GLY:HA2	1.88	0.56
1:C:405:VAL:HA	1:C:411:LEU:HD11	1.87	0.56
1:A:569:GLU:HG2	1:A:594:LEU:HB3	1.88	0.56
1:C:351:ILE:HD12	1:C:379:HIS:HB2	1.88	0.56
1:D:353:LEU:HD22	1:D:386:GLU:HB3	1.88	0.56
1:A:687:ASP:HA	1:A:961:GLY:HA2	1.88	0.56
1:B:1018:ARG:NH2	1:B:1028:CYS:SG	2.79	0.56
1:D:735:ARG:NH2	1:D:957:ASN:OD1	2.39	0.56
1:A:186:ASP:OD1	1:A:210:ARG:NH1	2.36	0.56
1:C:590:GLN:HB2	1:C:593:THR:HG23	1.88	0.56
1:A:459:GLN:NE2	1:A:924:MET:SD	2.80	0.55
1:B:353:LEU:HD22	1:B:386:GLU:HB3	1.88	0.55
1:D:105:ILE:HD11	1:D:166:LEU:HG	1.88	0.55
1:D:405:VAL:HA	1:D:411:LEU:HD11	1.87	0.55
1:A:282:MET:HG2	1:D:305:VAL:HG13	1.88	0.55
1:A:892:ASP:HB2	1:A:908:PRO:HG3	1.88	0.55
1:B:153:ASP:OD1	1:B:157:ASN:ND2	2.38	0.55
1:C:353:LEU:HD22	1:C:386:GLU:HB3	1.88	0.55
1:C:735:ARG:NH2	1:C:957:ASN:OD1	2.39	0.55
1:D:1018:ARG:NH2	1:D:1028:CYS:SG	2.79	0.55
2:H:2036:GLY:HA2	2:H:2040:LEU:HD12	1.87	0.55
4:A:3006:CLR:C16	4:A:3006:CLR:C22	2.85	0.55
1:B:590:GLN:HB2	1:B:593:THR:HG23	1.88	0.55
4:F:2306:CLR:C16	4:F:2306:CLR:C22	2.85	0.55
1:D:892:ASP:HB2	1:D:908:PRO:HG3	1.88	0.55
1:C:459:GLN:NE2	1:C:924:MET:SD	2.79	0.55
1:A:105:ILE:HD11	1:A:166:LEU:HG	1.88	0.55
1:A:1018:ARG:NH2	1:A:1028:CYS:SG	2.79	0.55
1:C:782:THR:HG22	1:C:784:LEU:H	1.72	0.55
1:A:735:ARG:NH2	1:A:957:ASN:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ILE:HD12	1:B:379:HIS:HB2	1.88	0.55
1:C:892:ASP:HB2	1:C:908:PRO:HG3	1.89	0.55
2:G:2036:GLY:HA2	2:G:2040:LEU:HD12	1.87	0.55
1:D:101:ALA:CB	1:D:166:LEU:HD12	2.34	0.55
1:D:569:GLU:HG2	1:D:594:LEU:HB3	1.88	0.55
1:A:782:THR:HG22	1:A:784:LEU:H	1.72	0.55
1:B:782:THR:HG22	1:B:784:LEU:H	1.72	0.55
1:C:1018:ARG:NH2	1:C:1028:CYS:SG	2.79	0.55
1:D:782:THR:HG22	1:D:784:LEU:H	1.72	0.55
1:B:735:ARG:NH2	1:B:957:ASN:OD1	2.39	0.55
1:A:351:ILE:HD12	1:A:379:HIS:HB2	1.88	0.55
1:B:405:VAL:HA	1:B:411:LEU:HD11	1.87	0.55
1:B:503:LEU:HD22	1:B:977:VAL:HG11	1.89	0.55
1:C:105:ILE:HD11	1:C:166:LEU:HG	1.88	0.55
1:C:628:CYS:SG	1:C:629:GLY:N	2.80	0.55
2:G:2056:VAL:HA	2:G:2089:VAL:HG12	1.89	0.55
1:D:982:LEU:CD1	1:D:1047:ASP:HB2	2.37	0.55
1:A:982:LEU:CD1	1:A:1047:ASP:HB2	2.37	0.55
1:B:982:LEU:CD1	1:B:1047:ASP:HB2	2.37	0.55
1:C:687:ASP:HA	1:C:961:GLY:HA2	1.88	0.55
1:C:715:LEU:O	1:C:718:HIS:ND1	2.40	0.55
1:D:459:GLN:NE2	1:D:924:MET:SD	2.80	0.55
1:D:590:GLN:HB2	1:D:593:THR:HG23	1.88	0.55
2:H:2056:VAL:HA	2:H:2089:VAL:HG12	1.89	0.55
1:A:590:GLN:HB2	1:A:593:THR:HG23	1.88	0.54
1:C:982:LEU:CD1	1:C:1047:ASP:HB2	2.37	0.54
1:D:350:HIS:CG	1:D:427:ASN:HB3	2.42	0.54
2:E:2056:VAL:HA	2:E:2089:VAL:HG12	1.89	0.54
2:F:2056:VAL:HA	2:F:2089:VAL:HG12	1.89	0.54
1:D:503:LEU:HD22	1:D:977:VAL:HG11	1.89	0.54
1:C:153:ASP:OD1	1:C:157:ASN:ND2	2.38	0.54
1:C:358:ASN:ND2	1:C:918:SER:HB3	2.22	0.54
4:C:1107:CLR:C16	4:C:1107:CLR:C22	2.85	0.54
1:D:358:ASN:ND2	1:D:918:SER:HB3	2.22	0.54
4:E:2305:CLR:C16	4:E:2305:CLR:C22	2.85	0.54
1:B:538:THR:HG21	1:B:932:ASN:HB2	1.90	0.54
4:G:2305:CLR:C16	4:G:2305:CLR:C22	2.85	0.54
1:D:153:ASP:OD1	1:D:157:ASN:ND2	2.38	0.54
1:B:459:GLN:NE2	1:B:924:MET:SD	2.80	0.54
1:B:892:ASP:HB2	1:B:908:PRO:HG3	1.88	0.54
1:A:538:THR:HG21	1:A:932:ASN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASN:ND2	1:B:918:SER:HB3	2.22	0.54
1:B:569:GLU:HG2	1:B:594:LEU:HB3	1.88	0.54
1:B:628:CYS:SG	1:B:629:GLY:N	2.80	0.54
1:C:538:THR:HG21	1:C:932:ASN:HB2	1.90	0.54
4:D:1108:CLR:C16	4:D:1108:CLR:C22	2.85	0.54
1:A:353:LEU:HD22	1:A:386:GLU:HB3	1.88	0.54
1:A:358:ASN:ND2	1:A:918:SER:HB3	2.22	0.54
1:A:817:ASP:OD1	1:A:887:ASN:ND2	2.41	0.54
1:D:687:ASP:HA	1:D:961:GLY:HA2	1.88	0.54
1:D:742:ARG:NH2	1:D:752:LYS:O	2.41	0.54
1:A:350:HIS:CG	1:A:427:ASN:HB3	2.42	0.54
1:D:817:ASP:OD1	1:D:887:ASN:ND2	2.41	0.54
1:A:503:LEU:HD22	1:A:977:VAL:HG11	1.89	0.54
1:B:350:HIS:CG	1:B:427:ASN:HB3	2.42	0.54
1:B:715:LEU:O	1:B:718:HIS:ND1	2.40	0.54
1:B:817:ASP:OD1	1:B:887:ASN:ND2	2.41	0.54
4:B:1110:CLR:C16	4:B:1110:CLR:C22	2.85	0.54
1:D:538:THR:HG21	1:D:932:ASN:HB2	1.90	0.54
4:H:2306:CLR:C16	4:H:2306:CLR:C22	2.85	0.54
1:C:182:ASN:OD1	1:C:216:GLN:NE2	2.41	0.53
1:C:350:HIS:CG	1:C:427:ASN:HB3	2.42	0.53
1:D:715:LEU:O	1:D:718:HIS:ND1	2.40	0.53
1:A:742:ARG:NH2	1:A:752:LYS:O	2.41	0.53
2:G:2061:GLN:NE2	2:G:2134:GLN:OE1	2.42	0.53
1:D:182:ASN:OD1	1:D:216:GLN:NE2	2.41	0.53
1:B:742:ARG:NH2	1:B:752:LYS:O	2.41	0.53
1:C:503:LEU:HD22	1:C:977:VAL:HG11	1.89	0.53
1:C:742:ARG:NH2	1:C:752:LYS:O	2.41	0.53
1:C:817:ASP:OD1	1:C:887:ASN:ND2	2.41	0.53
1:A:715:LEU:O	1:A:718:HIS:ND1	2.40	0.53
1:A:996:TYR:CG	1:A:1037:PRO:HG2	2.44	0.53
1:B:996:TYR:CG	1:B:1037:PRO:HG2	2.44	0.53
2:H:2061:GLN:NE2	2:H:2134:GLN:OE1	2.41	0.53
2:E:2061:GLN:NE2	2:E:2134:GLN:OE1	2.42	0.53
2:E:2110:ASN:ND2	2:E:2113:CYS:SG	2.82	0.53
1:B:182:ASN:OD1	1:B:216:GLN:NE2	2.41	0.53
2:F:2110:ASN:ND2	2:F:2113:CYS:SG	2.82	0.53
1:C:996:TYR:CG	1:C:1037:PRO:HG2	2.44	0.53
1:D:755:VAL:HG22	1:D:777:SER:HB2	1.91	0.53
1:A:182:ASN:OD1	1:A:216:GLN:NE2	2.41	0.53
1:B:305:VAL:HG13	1:C:282:MET:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2166:ASP:HB3	2:H:2168:ILE:HG22	1.91	0.53
1:D:353:LEU:CD2	1:D:386:GLU:OE1	2.57	0.53
1:D:628:CYS:SG	1:D:629:GLY:N	2.80	0.53
2:E:2166:ASP:HB3	2:E:2168:ILE:HG22	1.91	0.53
1:B:353:LEU:CD2	1:B:386:GLU:OE1	2.57	0.53
1:C:495:ALA:HB2	1:C:737:LEU:HD12	1.91	0.53
1:D:996:TYR:CG	1:D:1037:PRO:HG2	2.44	0.53
2:F:2166:ASP:HB3	2:F:2168:ILE:HG22	1.91	0.52
1:C:755:VAL:HG22	1:C:777:SER:HB2	1.91	0.52
2:H:2110:ASN:ND2	2:H:2113:CYS:SG	2.82	0.52
1:A:729:SER:O	1:A:765:ARG:NH2	2.35	0.52
2:F:2061:GLN:NE2	2:F:2134:GLN:OE1	2.41	0.52
2:G:2158:ASP:OD1	2:H:2121:ARG:NH2	2.42	0.52
1:D:495:ALA:HB2	1:D:737:LEU:HD12	1.91	0.52
2:G:2110:ASN:ND2	2:G:2113:CYS:SG	2.82	0.52
1:A:495:ALA:HB2	1:A:737:LEU:HD12	1.91	0.52
1:B:495:ALA:HB2	1:B:737:LEU:HD12	1.91	0.52
1:C:342:ARG:HD3	1:C:372:ASN:HB3	1.92	0.52
1:C:353:LEU:CD2	1:C:386:GLU:OE1	2.57	0.52
2:G:2166:ASP:HB3	2:G:2168:ILE:HG22	1.90	0.52
1:A:890:PHE:HD1	1:D:449:ASN:HD22	1.58	0.52
1:A:353:LEU:CD2	1:A:386:GLU:OE1	2.57	0.52
1:A:755:VAL:HG22	1:A:777:SER:HB2	1.91	0.52
1:B:729:SER:O	1:B:765:ARG:NH2	2.35	0.52
1:A:628:CYS:SG	1:A:629:GLY:N	2.80	0.52
1:A:815:LEU:CD1	1:D:442:MET:HG2	2.40	0.52
1:A:983:LEU:CD2	1:A:1045:PRO:HB2	2.41	0.51
1:C:1016:ARG:HH22	1:C:1043:LEU:HA	1.76	0.51
1:B:755:VAL:HG22	1:B:777:SER:HB2	1.91	0.51
1:C:983:LEU:CD2	1:C:1045:PRO:HB2	2.41	0.51
1:C:1000:PHE:HD1	1:C:1011:CYS:HB2	1.76	0.51
1:D:342:ARG:HD3	1:D:372:ASN:HB3	1.92	0.51
1:D:1016:ARG:HH22	1:D:1043:LEU:HA	1.76	0.51
1:A:955:GLU:HG2	1:B:786:ARG:HD2	1.93	0.51
1:B:476:ASN:OD1	1:B:478:LYS:HG3	2.11	0.51
1:B:983:LEU:CD2	1:B:1045:PRO:HB2	2.41	0.51
1:D:983:LEU:CD2	1:D:1045:PRO:HB2	2.41	0.51
1:A:342:ARG:HD3	1:A:372:ASN:HB3	1.92	0.51
1:A:476:ASN:OD1	1:A:478:LYS:HG3	2.11	0.50
1:A:1016:ARG:HH22	1:A:1043:LEU:HA	1.76	0.50
1:B:405:VAL:HA	1:B:411:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:VAL:HA	1:C:411:LEU:CD1	2.42	0.50
1:D:1000:PHE:HD1	1:D:1011:CYS:HB2	1.76	0.50
1:A:214:LEU:O	1:A:240:SER:OG	2.30	0.50
1:C:153:ASP:O	1:C:157:ASN:ND2	2.44	0.50
1:A:1000:PHE:HD1	1:A:1011:CYS:HB2	1.76	0.50
1:B:110:LEU:HD12	1:B:110:LEU:O	2.12	0.50
1:A:110:LEU:HD12	1:A:110:LEU:O	2.12	0.50
1:B:342:ARG:HD3	1:B:372:ASN:HB3	1.92	0.50
1:C:476:ASN:OD1	1:C:478:LYS:HG3	2.11	0.50
1:B:354:GLU:OE1	1:B:354:GLU:HA	2.12	0.50
1:B:1016:ARG:HH22	1:B:1043:LEU:HA	1.76	0.50
1:B:153:ASP:O	1:B:157:ASN:ND2	2.44	0.50
1:B:1000:PHE:HD1	1:B:1011:CYS:HB2	1.76	0.50
1:C:729:SER:O	1:C:765:ARG:NH2	2.35	0.50
1:D:153:ASP:O	1:D:157:ASN:ND2	2.45	0.50
1:D:405:VAL:HA	1:D:411:LEU:CD1	2.42	0.50
1:D:476:ASN:OD1	1:D:478:LYS:HG3	2.11	0.50
1:A:383:PRO:HD3	1:A:400:PHE:CE2	2.47	0.50
1:C:383:PRO:HD3	1:C:400:PHE:CE2	2.47	0.50
1:D:110:LEU:HD12	1:D:110:LEU:O	2.12	0.50
1:D:354:GLU:OE1	1:D:354:GLU:HA	2.12	0.50
1:D:214:LEU:O	1:D:240:SER:OG	2.30	0.50
1:D:383:PRO:HD3	1:D:400:PHE:CE2	2.47	0.50
1:A:354:GLU:HA	1:A:354:GLU:OE1	2.12	0.49
1:A:405:VAL:HA	1:A:411:LEU:CD1	2.42	0.49
1:B:214:LEU:O	1:B:240:SER:OG	2.30	0.49
1:B:383:PRO:HD3	1:B:400:PHE:CE2	2.47	0.49
1:B:955:GLU:HG2	1:C:786:ARG:HD2	1.94	0.49
1:C:354:GLU:HA	1:C:354:GLU:OE1	2.12	0.49
1:A:153:ASP:O	1:A:157:ASN:ND2	2.44	0.49
1:B:183:SER:O	1:B:187:PHE:CB	2.53	0.49
1:C:539:GLU:O	1:C:595:GLY:N	2.39	0.49
1:C:110:LEU:O	1:C:110:LEU:HD12	2.12	0.49
1:C:214:LEU:O	1:C:240:SER:OG	2.30	0.49
1:C:990:LEU:HD21	1:C:998:ASP:HB2	1.94	0.49
1:A:990:LEU:HD21	1:A:998:ASP:HB2	1.94	0.49
1:D:742:ARG:HG2	1:D:751:LEU:HD22	1.94	0.49
1:A:742:ARG:HG2	1:A:751:LEU:HD22	1.94	0.49
1:B:742:ARG:HG2	1:B:751:LEU:HD22	1.94	0.49
1:C:449:ASN:HD22	1:D:890:PHE:HD1	1.61	0.48
1:D:93:TRP:NE1	1:D:96:SER:OG	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:ARG:HG2	1:C:751:LEU:HD22	1.94	0.48
1:D:990:LEU:HD21	1:D:998:ASP:HB2	1.94	0.48
1:A:786:ARG:HD2	1:D:955:GLU:HG2	1.95	0.48
1:A:428:LYS:HD2	1:A:428:LYS:N	2.29	0.48
1:B:428:LYS:N	1:B:428:LYS:HD2	2.29	0.48
1:B:990:LEU:HD21	1:B:998:ASP:HB2	1.94	0.48
1:B:176:TRP:HB2	2:F:2013:ALA:HB2	1.96	0.48
1:C:428:LYS:HD2	1:C:428:LYS:N	2.29	0.48
1:C:455:ARG:NH1	1:C:931:ASP:OD1	2.47	0.48
1:D:176:TRP:HB2	2:H:2013:ALA:HB2	1.96	0.48
1:C:93:TRP:NE1	1:C:96:SER:OG	2.46	0.48
1:A:176:TRP:HB2	2:E:2013:ALA:HB2	1.96	0.48
1:B:455:ARG:NH1	1:B:931:ASP:OD1	2.47	0.48
1:B:1002:LYS:HA	1:B:1002:LYS:CE	2.40	0.47
1:C:491:LEU:HG	1:C:737:LEU:CB	2.35	0.47
1:D:417:GLU:CD	1:D:417:GLU:H	2.17	0.47
1:A:983:LEU:HD21	1:A:1045:PRO:HB2	1.96	0.47
1:D:417:GLU:OE1	1:D:418:SER:N	2.47	0.47
1:D:983:LEU:HD21	1:D:1045:PRO:HB2	1.96	0.47
1:B:991:GLY:O	1:B:1043:LEU:HD23	2.14	0.47
1:C:991:GLY:O	1:C:1043:LEU:HD23	2.14	0.47
1:C:983:LEU:HD21	1:C:1045:PRO:HB2	1.96	0.47
1:D:455:ARG:NH1	1:D:931:ASP:OD1	2.47	0.47
1:A:991:GLY:O	1:A:1043:LEU:HD23	2.14	0.47
1:C:176:TRP:HB2	2:G:2013:ALA:HB2	1.96	0.47
1:D:991:GLY:O	1:D:1043:LEU:HD23	2.14	0.47
1:A:455:ARG:NH1	1:A:931:ASP:OD1	2.47	0.47
4:E:2305:CLR:C16	4:E:2305:CLR:H181	2.45	0.47
1:B:616:HIS:CE1	1:B:626:LYS:H	2.33	0.47
1:C:616:HIS:CE1	1:C:626:LYS:H	2.33	0.47
1:D:428:LYS:N	1:D:428:LYS:HD2	2.29	0.47
1:A:1002:LYS:HA	1:A:1002:LYS:CE	2.40	0.47
1:D:616:HIS:CE1	1:D:626:LYS:H	2.33	0.47
1:A:476:ASN:HB3	1:A:479:GLU:HB2	1.97	0.47
1:D:497:SER:HG	1:D:504:SER:HG	1.57	0.47
1:D:587:LEU:HD23	1:D:587:LEU:C	2.36	0.47
4:H:2306:CLR:C16	4:H:2306:CLR:H181	2.45	0.46
1:A:417:GLU:CD	1:A:417:GLU:H	2.17	0.46
1:B:429:TYR:HD1	1:B:807:GLN:HB3	1.80	0.46
1:B:476:ASN:HB3	1:B:479:GLU:HB2	1.97	0.46
4:F:2306:CLR:C16	4:F:2306:CLR:H181	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:TYR:HD1	1:C:807:GLN:HB3	1.80	0.46
1:C:476:ASN:HB3	1:C:479:GLU:HB2	1.97	0.46
1:D:476:ASN:HB3	1:D:479:GLU:HB2	1.97	0.46
1:B:983:LEU:HD21	1:B:1045:PRO:HB2	1.96	0.46
1:C:965:THR:H	1:C:968:THR:HB	1.81	0.46
4:G:2305:CLR:C16	4:G:2305:CLR:H181	2.45	0.46
1:A:470:LEU:HD23	1:A:470:LEU:O	2.15	0.46
1:A:996:TYR:CD2	1:A:1037:PRO:HG2	2.51	0.46
1:B:470:LEU:HD23	1:B:470:LEU:O	2.15	0.46
1:C:491:LEU:CG	1:C:737:LEU:HB2	2.36	0.46
1:C:587:LEU:HD23	1:C:587:LEU:C	2.36	0.46
1:A:417:GLU:OE1	1:A:418:SER:N	2.47	0.46
1:A:616:HIS:CE1	1:A:626:LYS:H	2.33	0.46
1:C:25:PHE:HB3	1:C:192:PRO:HB3	1.98	0.46
1:D:965:THR:H	1:D:968:THR:HB	1.81	0.46
1:B:565:MET:HA	1:B:597:PHE:HB3	1.98	0.46
1:B:616:HIS:HE1	1:B:626:LYS:H	1.64	0.46
1:A:107:ALA:O	1:A:113:ARG:HG3	2.16	0.46
1:A:616:HIS:HE1	1:A:626:LYS:H	1.64	0.46
2:E:2059:VAL:HG22	2:E:2087:VAL:HG13	1.98	0.46
1:B:25:PHE:HB3	1:B:192:PRO:HB3	1.98	0.46
1:B:587:LEU:HD23	1:B:587:LEU:C	2.36	0.46
1:B:965:THR:H	1:B:968:THR:HB	1.81	0.46
1:C:616:HIS:HE1	1:C:626:LYS:H	1.64	0.46
1:D:616:HIS:HE1	1:D:626:LYS:H	1.64	0.46
2:H:2196:SER:HA	2:H:2199:VAL:HG12	1.98	0.46
1:C:999:LEU:HD12	1:C:999:LEU:O	2.16	0.46
2:G:2059:VAL:HG22	2:G:2087:VAL:HG13	1.98	0.46
1:D:25:PHE:HB3	1:D:192:PRO:HB3	1.98	0.46
1:A:587:LEU:HD23	1:A:587:LEU:C	2.36	0.46
2:E:2044:LEU:HD23	2:E:2047:LEU:HD12	1.98	0.46
1:D:729:SER:O	1:D:765:ARG:NH2	2.35	0.46
1:A:965:THR:H	1:A:968:THR:HB	1.81	0.45
2:G:2196:SER:HA	2:G:2199:VAL:HG12	1.98	0.45
1:D:565:MET:HA	1:D:597:PHE:HB3	1.98	0.45
1:B:996:TYR:CD2	1:B:1037:PRO:HG2	2.51	0.45
1:C:996:TYR:CD2	1:C:1037:PRO:HG2	2.51	0.45
1:D:429:TYR:HD1	1:D:807:GLN:HB3	1.80	0.45
1:B:110:LEU:HA	1:B:113:ARG:HE	1.82	0.45
1:B:999:LEU:O	1:B:999:LEU:HD12	2.16	0.45
1:C:110:LEU:HA	1:C:113:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2044:LEU:HD23	2:G:2047:LEU:HD12	1.98	0.45
1:D:996:TYR:CD2	1:D:1037:PRO:HG2	2.51	0.45
1:A:110:LEU:HA	1:A:113:ARG:HE	1.82	0.45
1:A:429:TYR:HD1	1:A:807:GLN:HB3	1.80	0.45
1:A:999:LEU:HD12	1:A:999:LEU:O	2.16	0.45
1:B:107:ALA:O	1:B:113:ARG:HG3	2.16	0.45
1:B:164:PHE:HA	1:B:167:ARG:HG2	1.99	0.45
1:B:417:GLU:OE1	1:B:418:SER:N	2.47	0.45
1:B:491:LEU:HG	1:B:737:LEU:CB	2.34	0.45
1:C:107:ALA:O	1:C:113:ARG:HG3	2.16	0.45
1:C:565:MET:HA	1:C:597:PHE:HB3	1.98	0.45
1:D:110:LEU:HA	1:D:113:ARG:HE	1.82	0.45
1:D:999:LEU:HD12	1:D:999:LEU:O	2.16	0.45
1:A:25:PHE:HB3	1:A:192:PRO:HB3	1.98	0.45
1:C:470:LEU:HD23	1:C:470:LEU:O	2.15	0.45
1:A:565:MET:HA	1:A:597:PHE:HB3	1.98	0.45
4:H:2306:CLR:H111	4:H:2306:CLR:H193	1.76	0.45
2:F:2059:VAL:HG22	2:F:2087:VAL:HG13	1.98	0.45
1:D:107:ALA:O	1:D:113:ARG:HG3	2.16	0.45
2:H:2044:LEU:HD23	2:H:2047:LEU:HD12	1.98	0.45
2:H:2059:VAL:HG22	2:H:2087:VAL:HG13	1.98	0.45
1:B:491:LEU:HD12	1:B:737:LEU:HD13	1.99	0.45
1:D:470:LEU:HD23	1:D:470:LEU:O	2.15	0.45
1:B:176:TRP:NE1	1:B:180:GLU:OE2	2.50	0.45
1:C:491:LEU:HD12	1:C:737:LEU:HD13	1.99	0.45
2:E:2196:SER:HA	2:E:2199:VAL:HG12	1.98	0.44
1:C:164:PHE:HA	1:C:167:ARG:HG2	1.99	0.44
1:C:896:ASP:N	1:C:896:ASP:OD1	2.51	0.44
1:D:335:SER:HB2	1:D:415:LYS:NZ	2.32	0.44
1:A:449:ASN:HD22	1:B:890:PHE:HD1	1.65	0.44
2:F:2044:LEU:HD23	2:F:2047:LEU:HD12	1.98	0.44
2:F:2196:SER:HA	2:F:2199:VAL:HG12	1.98	0.44
1:C:417:GLU:CD	1:C:417:GLU:H	2.17	0.44
1:C:473:PRO:HG2	1:D:893:GLN:NE2	2.32	0.44
1:B:335:SER:HB2	1:B:415:LYS:NZ	2.32	0.44
1:C:110:LEU:HD12	1:C:110:LEU:C	2.38	0.44
1:A:491:LEU:HD12	1:A:737:LEU:HD13	1.99	0.44
1:C:176:TRP:NE1	1:C:180:GLU:OE2	2.50	0.44
1:C:335:SER:HB2	1:C:415:LYS:NZ	2.32	0.44
1:C:442:MET:HG2	1:D:815:LEU:CD1	2.47	0.44
1:D:183:SER:O	1:D:187:PHE:CB	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PHE:HA	1:A:167:ARG:HG2	1.99	0.44
1:A:567:ALA:HB2	1:A:581:ILE:HD13	2.00	0.44
2:E:2080:SER:OG	2:E:2126:ASN:ND2	2.51	0.44
2:F:2080:SER:OG	2:F:2126:ASN:ND2	2.51	0.44
4:A:3006:CLR:H222	4:A:3006:CLR:H162	2.00	0.44
1:D:176:TRP:NE1	1:D:180:GLU:OE2	2.50	0.44
1:A:176:TRP:NE1	1:A:180:GLU:OE2	2.50	0.44
1:B:417:GLU:CD	1:B:417:GLU:H	2.17	0.44
1:D:110:LEU:HD12	1:D:110:LEU:C	2.38	0.44
1:D:164:PHE:HA	1:D:167:ARG:HG2	1.99	0.44
1:D:491:LEU:HG	1:D:737:LEU:CB	2.35	0.44
1:D:491:LEU:HD12	1:D:737:LEU:HD13	1.99	0.44
1:A:815:LEU:HD13	1:D:442:MET:HG2	2.00	0.44
1:A:982:LEU:HA	1:A:987:PHE:CE2	2.53	0.44
1:C:497:SER:HG	1:C:504:SER:HG	1.61	0.44
2:G:2080:SER:OG	2:G:2126:ASN:ND2	2.51	0.44
4:H:2306:CLR:H183	4:H:2306:CLR:H20	1.90	0.44
2:H:2080:SER:OG	2:H:2126:ASN:ND2	2.51	0.44
1:B:471:ASN:N	1:B:471:ASN:HD22	2.16	0.43
1:B:567:ALA:HB2	1:B:581:ILE:HD13	2.00	0.43
1:B:1013:GLY:O	1:B:1050:PHE:N	2.46	0.43
1:A:539:GLU:O	1:A:595:GLY:N	2.39	0.43
1:B:541:LEU:HD22	1:B:589:ILE:HG21	2.00	0.43
1:B:982:LEU:HA	1:B:987:PHE:CE2	2.53	0.43
1:C:417:GLU:OE1	1:C:418:SER:N	2.47	0.43
1:A:473:PRO:HG2	1:B:893:GLN:NE2	2.33	0.43
1:A:760:ILE:HB	1:A:780:PRO:HB3	2.00	0.43
4:F:2306:CLR:H111	4:F:2306:CLR:H193	1.76	0.43
1:D:982:LEU:HA	1:D:987:PHE:CE2	2.53	0.43
4:D:1108:CLR:H222	4:D:1108:CLR:H162	2.00	0.43
1:A:335:SER:HB2	1:A:415:LYS:NZ	2.32	0.43
1:B:491:LEU:HD23	1:B:733:GLY:O	2.19	0.43
1:C:426:ALA:HB2	1:C:440:ASN:ND2	2.34	0.43
1:C:982:LEU:HA	1:C:987:PHE:CE2	2.53	0.43
2:G:2158:ASP:OD2	2:H:2121:ARG:NH1	2.50	0.43
2:F:2061:GLN:HG2	2:F:2085:VAL:HG22	2.00	0.43
1:D:471:ASN:N	1:D:471:ASN:HD22	2.16	0.43
1:D:541:LEU:HD22	1:D:589:ILE:HG21	2.00	0.43
1:D:567:ALA:HB2	1:D:581:ILE:HD13	2.00	0.43
1:A:491:LEU:HD23	1:A:733:GLY:O	2.19	0.43
2:E:2068:CYS:HB2	2:E:2119:CYS:HB2	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:LEU:CG	1:B:737:LEU:HB2	2.36	0.43
1:C:471:ASN:N	1:C:471:ASN:HD22	2.16	0.43
1:D:795:ASN:OD1	1:D:795:ASN:N	2.50	0.43
1:A:795:ASN:OD1	1:A:795:ASN:N	2.50	0.43
1:A:1013:GLY:O	1:A:1050:PHE:N	2.46	0.43
1:B:896:ASP:OD1	1:B:896:ASP:N	2.51	0.43
1:A:471:ASN:N	1:A:471:ASN:HD22	2.16	0.43
1:B:365:HIS:O	1:B:368:ARG:HB2	2.18	0.43
1:B:407:ASN:OD1	1:B:408:PRO:HD2	2.19	0.43
1:C:183:SER:O	1:C:187:PHE:CB	2.53	0.43
1:C:365:HIS:O	1:C:368:ARG:HB2	2.19	0.43
1:C:491:LEU:HD23	1:C:733:GLY:O	2.19	0.43
1:C:983:LEU:HG	1:C:1045:PRO:O	2.19	0.43
1:A:426:ALA:HB2	1:A:440:ASN:ND2	2.34	0.43
1:B:426:ALA:HB2	1:B:440:ASN:ND2	2.34	0.43
4:F:2306:CLR:H183	4:F:2306:CLR:H20	1.90	0.43
1:C:407:ASN:OD1	1:C:408:PRO:HD2	2.19	0.43
2:G:2061:GLN:HG2	2:G:2085:VAL:HG22	2.00	0.43
1:D:491:LEU:CG	1:D:737:LEU:HB2	2.36	0.43
1:D:760:ILE:HB	1:D:780:PRO:HB3	2.00	0.43
1:D:983:LEU:HG	1:D:1045:PRO:O	2.19	0.43
1:B:110:LEU:HD12	1:B:110:LEU:C	2.38	0.43
4:C:1107:CLR:H222	4:C:1107:CLR:H162	2.00	0.43
1:A:442:MET:HG2	1:B:815:LEU:CD1	2.49	0.42
1:C:760:ILE:HB	1:C:780:PRO:HB3	2.00	0.42
1:D:426:ALA:HB2	1:D:440:ASN:ND2	2.34	0.42
1:B:760:ILE:HB	1:B:780:PRO:HB3	2.00	0.42
1:C:567:ALA:HB2	1:C:581:ILE:HD13	2.00	0.42
1:D:407:ASN:OD1	1:D:408:PRO:HD2	2.19	0.42
1:D:491:LEU:HD23	1:D:733:GLY:O	2.19	0.42
1:A:619:ILE:HD11	1:A:625:ILE:HD11	2.01	0.42
2:E:2061:GLN:HG2	2:E:2085:VAL:HG22	2.00	0.42
1:D:698:LYS:H	1:D:698:LYS:HD2	1.84	0.42
1:A:104:MET:HA	1:A:104:MET:HE1	1.98	0.42
1:A:371:VAL:O	1:A:371:VAL:HG23	2.20	0.42
1:A:541:LEU:HD22	1:A:589:ILE:HG21	2.00	0.42
1:B:619:ILE:HD11	1:B:625:ILE:HD11	2.01	0.42
1:B:983:LEU:HG	1:B:1045:PRO:O	2.19	0.42
3:B:1106:PGW:H26	3:B:1106:PGW:H23A	1.86	0.42
1:D:371:VAL:HG23	1:D:371:VAL:O	2.20	0.42
1:A:365:HIS:O	1:A:368:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:LYS:H	1:A:698:LYS:HD2	1.84	0.42
1:A:983:LEU:HG	1:A:1045:PRO:O	2.19	0.42
3:A:3002:PGW:H09	3:A:3002:PGW:H06	1.86	0.42
1:B:361:LYS:HE2	1:B:361:LYS:HB3	1.84	0.42
1:C:813:THR:O	1:C:884:ASN:ND2	2.46	0.42
1:D:365:HIS:O	1:D:368:ARG:HB2	2.19	0.42
1:D:1002:LYS:HA	1:D:1002:LYS:CE	2.40	0.42
1:B:821:ILE:HG22	1:B:891:LEU:HD21	2.02	0.42
4:D:1108:CLR:C22	4:D:1108:CLR:H162	2.50	0.42
2:E:2068:CYS:SG	2:E:2080:SER:OG	2.78	0.42
1:D:817:ASP:OD1	1:D:817:ASP:N	2.53	0.42
2:H:2061:GLN:HG2	2:H:2085:VAL:HG22	2.00	0.42
1:A:405:VAL:CA	1:A:411:LEU:HD11	2.50	0.42
1:A:407:ASN:OD1	1:A:408:PRO:HD2	2.19	0.42
1:B:371:VAL:HG23	1:B:371:VAL:O	2.20	0.42
1:B:405:VAL:CA	1:B:411:LEU:HD11	2.50	0.42
1:B:491:LEU:HD21	1:B:734:LEU:HD23	2.02	0.42
1:D:378:LEU:HD22	1:D:414:VAL:HG11	2.02	0.42
1:A:110:LEU:HD12	1:A:110:LEU:C	2.38	0.42
1:A:491:LEU:HD21	1:A:734:LEU:HD23	2.02	0.42
1:B:93:TRP:NE1	1:B:96:SER:OG	2.46	0.42
1:B:442:MET:HG2	1:C:815:LEU:CD1	2.50	0.42
1:B:469:LEU:HA	1:B:472:ILE:HD12	2.02	0.42
1:B:563:LEU:HD23	1:B:563:LEU:HA	1.88	0.42
2:F:2155:ARG:HB3	2:F:2158:ASP:HB2	2.02	0.42
1:C:1013:GLY:O	1:C:1050:PHE:N	2.46	0.42
4:G:2305:CLR:H183	4:G:2305:CLR:H20	1.90	0.42
1:D:405:VAL:CA	1:D:411:LEU:HD11	2.50	0.42
1:D:491:LEU:HD21	1:D:734:LEU:HD23	2.02	0.42
1:A:821:ILE:HG22	1:A:891:LEU:HD21	2.02	0.41
4:A:3006:CLR:C22	4:A:3006:CLR:H162	2.50	0.41
1:A:491:LEU:HG	1:A:737:LEU:CB	2.35	0.41
4:B:1110:CLR:H222	4:B:1110:CLR:H162	2.00	0.41
1:C:619:ILE:HD11	1:C:625:ILE:HD11	2.01	0.41
3:D:1105:PGW:H26	3:D:1105:PGW:H23A	1.86	0.41
1:A:183:SER:O	1:A:187:PHE:CB	2.53	0.41
1:A:996:TYR:CD1	1:A:1014:ILE:HD11	2.56	0.41
1:B:359:PHE:CE2	1:B:375:ILE:HD13	2.56	0.41
1:B:813:THR:O	1:B:884:ASN:ND2	2.46	0.41
1:D:896:ASP:OD1	1:D:896:ASP:N	2.51	0.41
1:A:366:LYS:H	1:A:366:LYS:HG3	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ILE:HG23	1:A:489:LEU:HD12	2.02	0.41
1:C:469:LEU:HA	1:C:472:ILE:HD12	2.02	0.41
1:C:491:LEU:HD21	1:C:734:LEU:HD23	2.02	0.41
2:H:2155:ARG:HB3	2:H:2158:ASP:HB2	2.02	0.41
1:B:378:LEU:HD22	1:B:414:VAL:HG11	2.02	0.41
1:B:457:ILE:HA	1:B:482:ASP:O	2.20	0.41
1:B:484:ILE:HG23	1:B:489:LEU:HD12	2.02	0.41
1:B:980:LEU:HB3	1:B:987:PHE:HZ	1.86	0.41
1:C:371:VAL:HG23	1:C:371:VAL:O	2.20	0.41
2:G:2068:CYS:HB2	2:G:2119:CYS:HB2	1.93	0.41
1:D:359:PHE:CE2	1:D:375:ILE:HD13	2.56	0.41
1:D:996:TYR:CD1	1:D:1014:ILE:HD11	2.55	0.41
1:A:896:ASP:N	1:A:896:ASP:OD1	2.50	0.41
1:C:104:MET:HA	1:C:104:MET:HE2	2.00	0.41
1:C:366:LYS:H	1:C:366:LYS:HG3	1.53	0.41
1:C:1002:LYS:CA	1:C:1002:LYS:CE	2.87	0.41
1:D:619:ILE:HD11	1:D:625:ILE:HD11	2.01	0.41
1:B:698:LYS:H	1:B:698:LYS:HD2	1.84	0.41
4:B:1110:CLR:C22	4:B:1110:CLR:H162	2.50	0.41
1:C:484:ILE:HG23	1:C:489:LEU:HD12	2.02	0.41
1:C:541:LEU:HD22	1:C:589:ILE:HG21	2.00	0.41
1:D:813:THR:O	1:D:884:ASN:ND2	2.46	0.41
3:D:1104:PGW:H4A	3:D:1104:PGW:H7	1.85	0.41
1:A:359:PHE:CE2	1:A:375:ILE:HD13	2.56	0.41
1:A:361:LYS:HB3	1:A:361:LYS:HE2	1.84	0.41
1:A:457:ILE:HA	1:A:482:ASP:O	2.20	0.41
1:A:980:LEU:HB3	1:A:987:PHE:CZ	2.56	0.41
3:B:1106:PGW:H09	3:B:1106:PGW:H06	1.86	0.41
1:C:359:PHE:CE2	1:C:375:ILE:HD13	2.56	0.41
1:C:378:LEU:HD22	1:C:414:VAL:HG11	2.02	0.41
1:C:457:ILE:HA	1:C:482:ASP:O	2.20	0.41
1:C:491:LEU:CD1	1:C:737:LEU:HD13	2.51	0.41
1:D:457:ILE:HA	1:D:482:ASP:O	2.20	0.41
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.90	0.41
1:A:469:LEU:HA	1:A:472:ILE:HD12	2.02	0.41
1:B:980:LEU:HB3	1:B:987:PHE:CZ	2.56	0.41
2:F:2068:CYS:SG	2:F:2080:SER:OG	2.78	0.41
1:C:821:ILE:HG22	1:C:891:LEU:HD21	2.02	0.41
1:C:980:LEU:HB3	1:C:987:PHE:HZ	1.86	0.41
2:G:2068:CYS:SG	2:G:2080:SER:OG	2.78	0.41
2:G:2155:ARG:HB3	2:G:2158:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:2305:CLR:H193	4:G:2305:CLR:H111	1.76	0.41
1:D:292:ASP:OD1	1:D:292:ASP:N	2.54	0.41
1:D:476:ASN:O	1:D:481:ASP:HB2	2.21	0.41
1:D:484:ILE:HG23	1:D:489:LEU:HD12	2.02	0.41
1:D:491:LEU:CD1	1:D:737:LEU:HD13	2.51	0.41
1:D:753:HIS:NE2	1:D:777:SER:OG	2.54	0.41
1:D:821:ILE:HG22	1:D:891:LEU:HD21	2.02	0.41
1:A:292:ASP:OD1	1:A:292:ASP:N	2.54	0.41
1:A:378:LEU:HD22	1:A:414:VAL:HG11	2.02	0.41
1:B:539:GLU:O	1:B:595:GLY:N	2.39	0.41
1:C:361:LYS:HB3	1:C:361:LYS:HE2	1.84	0.41
1:D:263:TRP:HZ2	1:D:298:THR:HB	1.86	0.41
1:A:491:LEU:CD1	1:A:737:LEU:HD13	2.51	0.40
1:D:361:LYS:HB3	1:D:361:LYS:HE2	1.84	0.40
1:A:476:ASN:O	1:A:481:ASP:HB2	2.21	0.40
1:B:473:PRO:HG2	1:C:893:GLN:NE2	2.36	0.40
1:B:568:ILE:HG13	1:B:593:THR:HB	2.03	0.40
1:B:753:HIS:NE2	1:B:777:SER:OG	2.54	0.40
1:C:698:LYS:H	1:C:698:LYS:HD2	1.84	0.40
1:D:469:LEU:HA	1:D:472:ILE:HD12	2.02	0.40
1:A:972:ARG:H	1:A:972:ARG:HG3	1.75	0.40
1:B:982:LEU:HD21	1:B:1049:ILE:HG22	2.03	0.40
4:F:2306:CLR:H222	4:F:2306:CLR:H161	2.04	0.40
1:C:130:TYR:CZ	1:C:208:PHE:HB3	2.57	0.40
1:C:263:TRP:HZ2	1:C:298:THR:HB	1.86	0.40
1:C:470:LEU:C	1:C:470:LEU:CD2	2.89	0.40
1:C:568:ILE:HG13	1:C:593:THR:HB	2.03	0.40
2:G:2155:ARG:HG3	2:H:2072:CYS:HB2	2.03	0.40
1:D:183:SER:HA	1:D:186:ASP:HB2	2.04	0.40
1:D:980:LEU:HB3	1:D:987:PHE:HZ	1.86	0.40
1:B:795:ASN:N	1:B:795:ASN:OD1	2.50	0.40
3:C:1103:PGW:H23A	3:C:1103:PGW:H26	1.86	0.40
4:G:2305:CLR:H222	4:G:2305:CLR:H161	2.04	0.40
1:D:980:LEU:HB3	1:D:987:PHE:CZ	2.56	0.40
1:A:183:SER:HA	1:A:186:ASP:HB2	2.04	0.40
2:E:2155:ARG:HB3	2:E:2158:ASP:HB2	2.02	0.40
1:B:348:CYS:SG	1:B:424:ILE:HG12	2.62	0.40
1:B:990:LEU:HD12	1:B:990:LEU:HA	1.95	0.40
1:B:996:TYR:CD1	1:B:1014:ILE:HD11	2.56	0.40
3:D:1105:PGW:H07A	3:D:1105:PGW:H11	1.93	0.40
2:H:2068:CYS:SG	2:H:2080:SER:OG	2.78	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 PDB entries followed by that with respect to all EM entries.

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	906/1065 (85%)	842 (93%)	64 (7%)	0	100	100
1	B	906/1065 (85%)	842 (93%)	64 (7%)	0	100	100
1	C	906/1065 (85%)	842 (93%)	64 (7%)	0	100	100
1	D	906/1065 (85%)	842 (93%)	64 (7%)	0	100	100
2	E	196/219 (90%)	183 (93%)	13 (7%)	0	100	100
2	F	196/219 (90%)	183 (93%)	13 (7%)	0	100	100
2	G	196/219 (90%)	183 (93%)	13 (7%)	0	100	100
2	H	196/219 (90%)	183 (93%)	13 (7%)	0	100	100
All	All	4408/5136 (86%)	4100 (93%)	308 (7%)	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 PDB entries followed by that with respect to all EM entries.

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	804/937 (86%)	790 (98%)	14 (2%)	60	82
1	B	804/937 (86%)	790 (98%)	14 (2%)	60	82
1	C	804/937 (86%)	790 (98%)	14 (2%)	60	82
1	D	804/937 (86%)	790 (98%)	14 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	180/199 (90%)	180 (100%)	0	100	100
2	F	180/199 (90%)	180 (100%)	0	100	100
2	G	180/199 (90%)	180 (100%)	0	100	100
2	H	180/199 (90%)	180 (100%)	0	100	100
All	All	3936/4544 (87%)	3880 (99%)	56 (1%)	68	85

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	MET
1	A	143	ASN
1	A	182	ASN
1	A	363	PHE
1	A	417	GLU
1	A	428	LYS
1	A	429	TYR
1	A	478	LYS
1	A	490	LYS
1	A	491	LEU
1	A	698	LYS
1	A	806	ASN
1	A	972	ARG
1	A	992	ASP
1	B	94	MET
1	B	143	ASN
1	B	182	ASN
1	B	363	PHE
1	B	417	GLU
1	B	428	LYS
1	B	429	TYR
1	B	478	LYS
1	B	490	LYS
1	B	491	LEU
1	B	698	LYS
1	B	806	ASN
1	B	972	ARG
1	B	992	ASP
1	C	94	MET
1	C	143	ASN
1	C	182	ASN
1	C	363	PHE

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Mol	Chain	Res	Type
1	C	417	GLU
1	C	428	LYS
1	C	429	TYR
1	C	478	LYS
1	C	490	LYS
1	C	491	LEU
1	C	698	LYS
1	C	806	ASN
1	C	972	ARG
1	C	992	ASP
1	D	94	MET
1	D	143	ASN
1	D	182	ASN
1	D	363	PHE
1	D	417	GLU
1	D	428	LYS
1	D	429	TYR
1	D	478	LYS
1	D	490	LYS
1	D	491	LEU
1	D	698	LYS
1	D	806	ASN
1	D	972	ARG
1	D	992	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	182	ASN
1	A	216	GLN
1	A	440	ASN
1	A	465	ASN
1	A	468	HIS
1	A	471	ASN
1	A	616	HIS
1	A	745	ASN
1	A	806	ASN
1	A	809	ASN
2	E	2106	GLN
1	B	143	ASN
1	B	182	ASN

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Mol	Chain	Res	Type
1	B	216	GLN
1	B	440	ASN
1	B	465	ASN
1	B	468	HIS
1	B	471	ASN
1	B	616	HIS
1	B	745	ASN
1	B	806	ASN
1	B	809	ASN
2	F	2106	GLN
1	C	143	ASN
1	C	182	ASN
1	C	216	GLN
1	C	440	ASN
1	C	465	ASN
1	C	468	HIS
1	C	471	ASN
1	C	616	HIS
1	C	745	ASN
1	C	806	ASN
1	C	809	ASN
2	G	2106	GLN
1	D	143	ASN
1	D	182	ASN
1	D	216	GLN
1	D	440	ASN
1	D	465	ASN
1	D	468	HIS
1	D	471	ASN
1	D	616	HIS
1	D	745	ASN
1	D	806	ASN
1	D	809	ASN
2	H	2106	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

56 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PGW	D	1104	-	28,28,50	1.18	2 (7%)	30,32,56	1.04	2 (6%)
3	PGW	C	1102	-	28,28,50	1.18	2 (7%)	30,32,56	1.04	2 (6%)
3	PGW	G	2301	-	6,6,50	0.31	0	5,5,56	0.65	0
3	PGW	D	1101	-	26,26,50	1.31	5 (19%)	30,31,56	1.44	4 (13%)
3	PGW	B	1105	-	26,26,50	1.32	5 (19%)	30,31,56	1.44	4 (13%)
3	PGW	B	1108	-	11,11,50	0.25	0	10,10,56	0.83	0
3	PGW	B	1107	-	8,8,50	0.28	0	7,7,56	0.80	0
3	PGW	D	1103	-	8,8,50	0.27	0	7,7,56	0.78	0
4	CLR	D	1108	-	31,31,31	4.23	14 (45%)	48,48,48	2.51	15 (31%)
3	PGW	F	2302	-	6,6,50	0.30	0	5,5,56	0.64	0
5	NAG	G	2303	2	14,14,15	0.53	0	17,19,21	2.11	3 (17%)
3	PGW	A	3009	-	11,11,50	0.28	0	10,10,56	0.74	0
5	NAG	H	2305	2	14,14,15	0.47	0	17,19,21	1.88	2 (11%)
3	PGW	A	3002	-	45,45,50	1.11	4 (8%)	48,51,56	1.11	3 (6%)
3	PGW	E	2301	-	6,6,50	0.30	0	5,5,56	0.64	0
5	NAG	F	2305	2	14,14,15	0.47	0	17,19,21	1.88	2 (11%)
5	NAG	F	2304	2	14,14,15	0.53	0	17,19,21	2.11	3 (17%)
4	CLR	H	2306	-	31,31,31	4.17	13 (41%)	48,48,48	2.72	19 (39%)
3	PGW	H	2301	-	8,8,50	0.27	0	7,7,56	0.78	0
3	PGW	B	1106	-	45,45,50	1.11	4 (8%)	48,51,56	1.11	3 (6%)
4	CLR	A	3006	-	31,31,31	4.23	13 (41%)	48,48,48	2.52	15 (31%)
3	PGW	C	1103	-	45,45,50	1.11	4 (8%)	48,51,56	1.11	3 (6%)
4	CLR	C	1107	-	31,31,31	4.23	13 (41%)	48,48,48	2.51	15 (31%)
4	CLR	F	2306	-	31,31,31	4.17	12 (38%)	48,48,48	2.71	19 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PGW	C	1104	-	8,8,50	0.28	0	7,7,56	0.80	0
3	PGW	D	1105	-	45,45,50	1.12	4 (8%)	48,51,56	1.11	3 (6%)
3	PGW	F	2301	-	8,8,50	0.27	0	7,7,56	0.78	0
3	PGW	H	2302	-	6,6,50	0.31	0	5,5,56	0.65	0
3	PGW	B	1103	-	8,8,50	0.27	0	7,7,56	0.78	0
3	PGW	D	1107	-	11,11,50	0.25	0	10,10,56	0.83	0
4	CLR	G	2305	-	31,31,31	4.17	12 (38%)	48,48,48	2.72	19 (39%)
3	PGW	C	1101	-	12,12,50	0.95	1 (8%)	12,12,56	1.17	0
3	PGW	F	2303	-	5,5,50	0.30	0	4,4,56	0.58	0
5	NAG	H	2304	2	14,14,15	0.53	0	17,19,21	2.10	3 (17%)
3	PGW	B	1109	-	11,11,50	0.29	0	10,10,56	0.75	0
3	PGW	B	1104	-	28,28,50	1.18	2 (7%)	30,32,56	1.04	2 (6%)
4	CLR	B	1110	-	31,31,31	4.23	14 (45%)	48,48,48	2.52	15 (31%)
3	PGW	G	2302	-	5,5,50	0.30	0	4,4,56	0.59	0
3	PGW	D	1106	-	8,8,50	0.28	0	7,7,56	0.79	0
3	PGW	A	3004	-	11,11,50	0.25	0	10,10,56	0.83	0
3	PGW	A	3005	-	11,11,50	0.29	0	10,10,56	0.74	0
3	PGW	A	3003	-	8,8,50	0.28	0	7,7,56	0.80	0
3	PGW	A	3008	-	12,12,50	0.94	1 (8%)	12,12,56	1.17	0
3	PGW	B	1101	-	26,26,50	1.31	5 (19%)	30,31,56	1.44	4 (13%)
3	PGW	B	1102	-	12,12,50	0.94	1 (8%)	12,12,56	1.17	0
3	PGW	C	1105	-	11,11,50	0.25	0	10,10,56	0.83	0
3	PGW	D	1102	-	12,12,50	0.94	1 (8%)	12,12,56	1.17	0
3	PGW	A	3001	-	28,28,50	1.18	2 (7%)	30,32,56	1.04	2 (6%)
5	NAG	G	2304	2	14,14,15	0.48	0	17,19,21	1.88	2 (11%)
3	PGW	E	2302	-	5,5,50	0.30	0	4,4,56	0.58	0
5	NAG	E	2304	2	14,14,15	0.48	0	17,19,21	1.88	2 (11%)
3	PGW	H	2303	-	5,5,50	0.30	0	4,4,56	0.59	0
4	CLR	E	2305	-	31,31,31	4.17	12 (38%)	48,48,48	2.72	19 (39%)
3	PGW	A	3007	-	26,26,50	1.32	5 (19%)	30,31,56	1.44	4 (13%)
3	PGW	C	1106	-	11,11,50	0.29	0	10,10,56	0.75	0
5	NAG	E	2303	2	14,14,15	0.53	0	17,19,21	2.11	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGW	D	1104	-	-	11/30/30/55	-
3	PGW	C	1102	-	-	12/30/30/55	-
3	PGW	G	2301	-	-	0/4/4/55	-
3	PGW	D	1101	-	-	11/28/28/55	-
3	PGW	B	1105	-	-	11/28/28/55	-
3	PGW	B	1108	-	-	5/9/9/55	-
3	PGW	B	1107	-	-	2/6/6/55	-
3	PGW	D	1103	-	-	3/6/6/55	-
4	CLR	D	1108	-	-	6/10/68/68	0/4/4/4
3	PGW	F	2302	-	-	0/4/4/55	-
5	NAG	G	2303	2	-	0/6/23/26	0/1/1/1
3	PGW	A	3009	-	-	4/9/9/55	-
5	NAG	H	2305	2	-	2/6/23/26	0/1/1/1
3	PGW	A	3002	-	-	16/50/50/55	-
3	PGW	E	2301	-	-	0/4/4/55	-
5	NAG	F	2305	2	-	2/6/23/26	0/1/1/1
5	NAG	F	2304	2	-	0/6/23/26	0/1/1/1
4	CLR	H	2306	-	-	9/10/68/68	0/4/4/4
3	PGW	H	2301	-	-	3/6/6/55	-
3	PGW	B	1106	-	-	16/50/50/55	-
4	CLR	A	3006	-	-	6/10/68/68	0/4/4/4
3	PGW	C	1103	-	-	16/50/50/55	-
4	CLR	C	1107	-	-	6/10/68/68	0/4/4/4
4	CLR	F	2306	-	-	9/10/68/68	0/4/4/4
3	PGW	C	1104	-	-	2/6/6/55	-
3	PGW	D	1105	-	-	16/50/50/55	-
3	PGW	F	2301	-	-	3/6/6/55	-
3	PGW	H	2302	-	-	0/4/4/55	-
3	PGW	B	1103	-	-	3/6/6/55	-
3	PGW	D	1107	-	-	5/9/9/55	-
4	CLR	G	2305	-	-	9/10/68/68	0/4/4/4
3	PGW	C	1101	-	-	5/10/10/55	-
3	PGW	F	2303	-	-	2/3/3/55	-
5	NAG	H	2304	2	-	0/6/23/26	0/1/1/1
3	PGW	B	1109	-	-	4/9/9/55	-
3	PGW	B	1104	-	-	11/30/30/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	B	1110	-	-	6/10/68/68	0/4/4/4
3	PGW	G	2302	-	-	2/3/3/55	-
3	PGW	D	1106	-	-	2/6/6/55	-
3	PGW	A	3004	-	-	5/9/9/55	-
3	PGW	A	3005	-	-	4/9/9/55	-
3	PGW	A	3003	-	-	2/6/6/55	-
3	PGW	A	3008	-	-	5/10/10/55	-
3	PGW	B	1101	-	-	11/28/28/55	-
3	PGW	B	1102	-	-	5/10/10/55	-
3	PGW	C	1105	-	-	5/9/9/55	-
3	PGW	D	1102	-	-	5/10/10/55	-
3	PGW	A	3001	-	-	12/30/30/55	-
5	NAG	G	2304	2	-	2/6/23/26	0/1/1/1
3	PGW	E	2302	-	-	2/3/3/55	-
5	NAG	E	2304	2	-	2/6/23/26	0/1/1/1
3	PGW	H	2303	-	-	2/3/3/55	-
4	CLR	E	2305	-	-	9/10/68/68	0/4/4/4
3	PGW	A	3007	-	-	11/28/28/55	-
3	PGW	C	1106	-	-	4/9/9/55	-
5	NAG	E	2303	2	-	0/6/23/26	0/1/1/1

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2306	CLR	C6-C5	11.32	1.57	1.33
4	E	2305	CLR	C6-C5	11.31	1.57	1.33
4	G	2305	CLR	C6-C5	11.31	1.57	1.33
4	F	2306	CLR	C6-C5	11.30	1.57	1.33
4	A	3006	CLR	C6-C5	10.94	1.57	1.33
4	C	1107	CLR	C6-C5	10.94	1.57	1.33
4	D	1108	CLR	C6-C5	10.92	1.57	1.33
4	B	1110	CLR	C6-C5	10.90	1.57	1.33
4	D	1108	CLR	C16-C17	10.01	1.75	1.54
4	A	3006	CLR	C16-C17	10.01	1.75	1.54
4	C	1107	CLR	C16-C17	10.01	1.75	1.54
4	B	1110	CLR	C16-C17	9.99	1.75	1.54
4	F	2306	CLR	C16-C17	9.69	1.74	1.54
4	E	2305	CLR	C16-C17	9.68	1.74	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2305	CLR	C16-C17	9.68	1.74	1.54
4	H	2306	CLR	C16-C17	9.68	1.74	1.54
4	H	2306	CLR	C20-C17	-9.63	1.37	1.54
4	E	2305	CLR	C20-C17	-9.62	1.37	1.54
4	G	2305	CLR	C20-C17	-9.62	1.37	1.54
4	F	2306	CLR	C20-C17	-9.60	1.37	1.54
4	B	1110	CLR	C20-C17	-9.57	1.37	1.54
4	A	3006	CLR	C20-C17	-9.56	1.37	1.54
4	C	1107	CLR	C20-C17	-9.56	1.37	1.54
4	D	1108	CLR	C20-C17	-9.56	1.37	1.54
4	C	1107	CLR	C8-C9	7.82	1.68	1.53
4	D	1108	CLR	C8-C9	7.79	1.68	1.53
4	B	1110	CLR	C8-C9	7.79	1.68	1.53
4	A	3006	CLR	C8-C9	7.78	1.68	1.53
4	F	2306	CLR	C8-C9	7.18	1.67	1.53
4	E	2305	CLR	C8-C9	7.17	1.67	1.53
4	G	2305	CLR	C8-C9	7.17	1.67	1.53
4	H	2306	CLR	C8-C9	7.13	1.67	1.53
4	E	2305	CLR	C12-C11	6.26	1.66	1.53
4	G	2305	CLR	C12-C11	6.26	1.66	1.53
4	H	2306	CLR	C12-C11	6.25	1.66	1.53
4	F	2306	CLR	C12-C11	6.24	1.66	1.53
4	A	3006	CLR	C12-C11	6.16	1.66	1.53
4	C	1107	CLR	C12-C11	6.16	1.66	1.53
4	D	1108	CLR	C12-C11	6.15	1.66	1.53
4	B	1110	CLR	C12-C11	6.14	1.66	1.53
4	B	1110	CLR	C13-C17	5.46	1.65	1.55
4	C	1107	CLR	C13-C17	5.46	1.65	1.55
4	D	1108	CLR	C13-C17	5.46	1.65	1.55
4	A	3006	CLR	C13-C17	5.45	1.65	1.55
4	D	1108	CLR	C7-C6	5.41	1.61	1.50
4	A	3006	CLR	C7-C6	5.41	1.61	1.50
4	C	1107	CLR	C7-C6	5.41	1.61	1.50
4	B	1110	CLR	C7-C6	5.40	1.61	1.50
4	E	2305	CLR	C7-C6	5.23	1.61	1.50
4	F	2306	CLR	C7-C6	5.23	1.61	1.50
4	G	2305	CLR	C7-C6	5.22	1.61	1.50
4	H	2306	CLR	C7-C6	5.21	1.61	1.50
4	F	2306	CLR	C13-C17	4.78	1.64	1.55
4	E	2305	CLR	C13-C17	4.76	1.64	1.55
4	H	2306	CLR	C13-C17	4.76	1.64	1.55
4	G	2305	CLR	C13-C17	4.75	1.64	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2305	CLR	C15-C14	3.96	1.62	1.54
4	G	2305	CLR	C15-C14	3.96	1.62	1.54
4	F	2306	CLR	C15-C14	3.94	1.62	1.54
4	H	2306	CLR	C15-C14	3.94	1.62	1.54
4	D	1108	CLR	C15-C14	3.90	1.62	1.54
4	A	3006	CLR	C15-C14	3.88	1.62	1.54
4	C	1107	CLR	C15-C14	3.88	1.62	1.54
4	B	1110	CLR	C15-C14	3.88	1.62	1.54
3	B	1106	PGW	C10-C9	3.62	1.52	1.31
3	D	1105	PGW	C10-C9	3.62	1.52	1.31
3	D	1104	PGW	C10-C9	3.61	1.52	1.31
3	A	3002	PGW	C10-C9	3.61	1.52	1.31
3	C	1103	PGW	C10-C9	3.61	1.52	1.31
3	B	1104	PGW	C10-C9	3.59	1.52	1.31
3	A	3001	PGW	C10-C9	3.59	1.52	1.31
3	C	1102	PGW	C10-C9	3.59	1.52	1.31
4	C	1107	CLR	C13-C14	3.52	1.61	1.55
4	D	1108	CLR	C13-C14	3.52	1.61	1.55
4	B	1110	CLR	C13-C14	3.51	1.61	1.55
4	A	3006	CLR	C13-C14	3.49	1.61	1.55
4	H	2306	CLR	C13-C14	3.35	1.61	1.55
4	E	2305	CLR	C13-C14	3.35	1.61	1.55
4	G	2305	CLR	C13-C14	3.35	1.61	1.55
4	F	2306	CLR	C13-C14	3.33	1.61	1.55
4	B	1110	CLR	C22-C20	3.05	1.62	1.54
4	A	3006	CLR	C22-C20	3.02	1.62	1.54
4	C	1107	CLR	C22-C20	3.02	1.62	1.54
4	D	1108	CLR	C22-C20	3.02	1.62	1.54
4	H	2306	CLR	C21-C20	2.97	1.60	1.53
4	H	2306	CLR	C22-C20	2.96	1.62	1.54
4	F	2306	CLR	C22-C20	2.95	1.62	1.54
4	E	2305	CLR	C21-C20	2.95	1.60	1.53
4	E	2305	CLR	C22-C20	2.95	1.62	1.54
4	G	2305	CLR	C21-C20	2.94	1.60	1.53
4	A	3006	CLR	C21-C20	2.94	1.60	1.53
4	B	1110	CLR	C21-C20	2.94	1.60	1.53
4	C	1107	CLR	C21-C20	2.94	1.60	1.53
4	F	2306	CLR	C21-C20	2.94	1.60	1.53
4	G	2305	CLR	C22-C20	2.93	1.61	1.54
4	D	1108	CLR	C21-C20	2.93	1.60	1.53
3	C	1101	PGW	O03-C19	2.82	1.40	1.30
3	B	1102	PGW	O03-C19	2.82	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1102	PGW	O03-C19	2.82	1.40	1.30
3	A	3008	PGW	O03-C19	2.81	1.40	1.30
4	H	2306	CLR	C8-C14	-2.70	1.48	1.53
3	B	1105	PGW	O01-C02	-2.68	1.39	1.46
3	A	3002	PGW	O03-C19	2.68	1.41	1.33
3	C	1103	PGW	O03-C19	2.68	1.41	1.33
4	E	2305	CLR	C8-C14	-2.68	1.48	1.53
4	G	2305	CLR	C8-C14	-2.68	1.48	1.53
3	B	1106	PGW	O03-C19	2.68	1.41	1.33
3	D	1105	PGW	O03-C19	2.67	1.41	1.33
3	B	1101	PGW	O01-C02	-2.67	1.39	1.46
3	A	3007	PGW	O01-C02	-2.66	1.39	1.46
3	A	3007	PGW	P-O12	2.65	1.65	1.54
3	B	1105	PGW	P-O12	2.65	1.65	1.54
4	F	2306	CLR	C8-C14	-2.65	1.48	1.53
3	B	1101	PGW	P-O12	2.64	1.65	1.54
3	D	1101	PGW	P-O12	2.64	1.65	1.54
3	D	1101	PGW	O01-C02	-2.64	1.40	1.46
4	A	3006	CLR	C8-C14	-2.63	1.48	1.53
4	C	1107	CLR	C8-C14	-2.63	1.48	1.53
4	D	1108	CLR	C8-C14	-2.63	1.48	1.53
4	B	1110	CLR	C8-C14	-2.60	1.48	1.53
3	B	1105	PGW	O03-C19	2.45	1.40	1.33
3	C	1103	PGW	O01-C02	-2.44	1.40	1.46
3	D	1105	PGW	O01-C02	-2.44	1.40	1.46
3	A	3002	PGW	O01-C02	-2.44	1.40	1.46
3	B	1101	PGW	O03-C19	2.42	1.40	1.33
3	D	1101	PGW	O03-C19	2.42	1.40	1.33
3	B	1106	PGW	O01-C02	-2.42	1.40	1.46
3	B	1104	PGW	O01-C1	2.42	1.40	1.33
3	A	3007	PGW	O03-C19	2.42	1.40	1.33
3	D	1104	PGW	O01-C1	2.40	1.40	1.33
3	C	1102	PGW	O01-C1	2.40	1.40	1.33
3	A	3001	PGW	O01-C1	2.39	1.40	1.33
4	D	1108	CLR	C7-C8	2.30	1.57	1.53
4	A	3006	CLR	C7-C8	2.28	1.57	1.53
4	B	1110	CLR	C7-C8	2.27	1.57	1.53
4	C	1107	CLR	C7-C8	2.25	1.56	1.53
3	A	3002	PGW	O01-C1	2.24	1.40	1.34
3	C	1103	PGW	O01-C1	2.24	1.40	1.34
3	D	1105	PGW	O01-C1	2.23	1.40	1.34
3	B	1106	PGW	O01-C1	2.23	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3007	PGW	P-O13	-2.21	1.46	1.54
3	B	1101	PGW	P-O13	-2.20	1.46	1.54
3	D	1101	PGW	P-O13	-2.20	1.46	1.54
3	B	1105	PGW	P-O13	-2.19	1.46	1.54
3	A	3007	PGW	O03-C01	-2.17	1.40	1.45
3	B	1105	PGW	O03-C01	-2.16	1.40	1.45
3	B	1101	PGW	O03-C01	-2.13	1.40	1.45
3	D	1101	PGW	O03-C01	-2.13	1.40	1.45
4	B	1110	CLR	C4-C5	2.02	1.56	1.51
4	D	1108	CLR	C4-C5	2.00	1.56	1.51
4	H	2306	CLR	C4-C5	2.00	1.56	1.51

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1110	CLR	C4-C5-C6	-8.56	108.27	120.61
4	A	3006	CLR	C4-C5-C6	-8.56	108.27	120.61
4	C	1107	CLR	C4-C5-C6	-8.56	108.27	120.61
4	D	1108	CLR	C4-C5-C6	-8.53	108.32	120.61
4	H	2306	CLR	C4-C5-C6	-8.03	109.04	120.61
4	E	2305	CLR	C4-C5-C6	-8.00	109.08	120.61
4	G	2305	CLR	C4-C5-C6	-8.00	109.08	120.61
4	F	2306	CLR	C4-C5-C6	-7.97	109.12	120.61
5	E	2304	NAG	C1-O5-C5	6.73	121.30	112.19
5	G	2304	NAG	C1-O5-C5	6.73	121.30	112.19
5	F	2305	NAG	C1-O5-C5	6.70	121.28	112.19
5	H	2305	NAG	C1-O5-C5	6.70	121.27	112.19
5	F	2304	NAG	C1-O5-C5	6.59	121.12	112.19
5	G	2303	NAG	C1-O5-C5	6.58	121.11	112.19
5	E	2303	NAG	C1-O5-C5	6.56	121.08	112.19
5	H	2304	NAG	C1-O5-C5	6.54	121.05	112.19
4	C	1107	CLR	C10-C5-C6	-6.49	112.97	122.90
4	A	3006	CLR	C10-C5-C6	-6.48	112.98	122.90
4	B	1110	CLR	C10-C5-C6	-6.47	113.00	122.90
4	D	1108	CLR	C10-C5-C6	-6.47	113.01	122.90
4	A	3006	CLR	C7-C6-C5	-6.11	113.79	125.06
4	C	1107	CLR	C7-C6-C5	-6.11	113.79	125.06
4	D	1108	CLR	C7-C6-C5	-6.10	113.81	125.06
4	B	1110	CLR	C7-C6-C5	-6.10	113.81	125.06
4	G	2305	CLR	C12-C13-C17	5.10	124.21	116.57
4	F	2306	CLR	C12-C13-C17	5.08	124.18	116.57
4	H	2306	CLR	C12-C13-C17	5.08	124.17	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2305	CLR	C12-C13-C17	5.08	124.17	116.57
4	H	2306	CLR	C7-C8-C9	-4.94	103.72	109.71
4	E	2305	CLR	C7-C8-C9	-4.93	103.74	109.71
4	G	2305	CLR	C7-C8-C9	-4.93	103.74	109.71
4	F	2306	CLR	C7-C8-C9	-4.90	103.77	109.71
4	B	1110	CLR	C14-C8-C9	4.66	115.33	109.09
4	A	3006	CLR	C14-C8-C9	4.65	115.32	109.09
4	D	1108	CLR	C14-C8-C9	4.64	115.30	109.09
4	H	2306	CLR	C1-C2-C3	4.64	116.42	110.47
4	E	2305	CLR	C1-C2-C3	4.63	116.41	110.47
4	G	2305	CLR	C7-C6-C5	-4.62	116.53	125.06
4	C	1107	CLR	C14-C8-C9	4.61	115.27	109.09
4	G	2305	CLR	C1-C2-C3	4.61	116.38	110.47
4	F	2306	CLR	C1-C2-C3	4.60	116.37	110.47
4	E	2305	CLR	C7-C6-C5	-4.60	116.58	125.06
4	F	2306	CLR	C7-C6-C5	-4.60	116.58	125.06
4	H	2306	CLR	C7-C6-C5	-4.59	116.59	125.06
4	E	2305	CLR	C18-C13-C17	-4.50	103.31	111.71
4	G	2305	CLR	C18-C13-C17	-4.50	103.32	111.71
4	H	2306	CLR	C18-C13-C17	-4.50	103.33	111.71
4	F	2306	CLR	C18-C13-C17	-4.49	103.33	111.71
4	H	2306	CLR	C14-C8-C9	4.35	114.92	109.09
4	E	2305	CLR	C14-C8-C9	4.34	114.90	109.09
4	G	2305	CLR	C14-C8-C9	4.34	114.90	109.09
3	A	3007	PGW	O01-C1-C2	4.33	120.83	111.50
3	D	1101	PGW	O01-C1-C2	4.33	120.83	111.50
3	B	1101	PGW	O01-C1-C2	4.33	120.83	111.50
3	B	1105	PGW	O01-C1-C2	4.32	120.82	111.50
4	B	1110	CLR	C12-C13-C17	4.32	123.03	116.57
4	C	1107	CLR	C12-C13-C17	4.30	123.01	116.57
4	F	2306	CLR	C14-C8-C9	4.30	114.85	109.09
4	D	1108	CLR	C12-C13-C17	4.30	123.00	116.57
4	A	3006	CLR	C12-C13-C17	4.29	122.99	116.57
4	G	2305	CLR	C18-C13-C14	-4.10	104.07	111.71
4	E	2305	CLR	C18-C13-C14	-4.09	104.09	111.71
4	H	2306	CLR	C18-C13-C14	-4.09	104.09	111.71
4	F	2306	CLR	C18-C13-C14	-4.08	104.10	111.71
4	H	2306	CLR	C21-C20-C22	-3.99	104.11	110.36
4	D	1108	CLR	C7-C8-C9	-3.98	104.90	109.71
4	C	1107	CLR	C7-C8-C9	-3.97	104.90	109.71
4	A	3006	CLR	C7-C8-C9	-3.97	104.90	109.71
4	E	2305	CLR	C21-C20-C22	-3.96	104.15	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1110	CLR	C7-C8-C9	-3.96	104.91	109.71
4	G	2305	CLR	C21-C20-C22	-3.96	104.16	110.36
4	F	2306	CLR	C21-C20-C22	-3.94	104.18	110.36
4	G	2305	CLR	C9-C10-C5	3.92	115.79	109.65
4	G	2305	CLR	C17-C13-C14	3.92	104.71	100.07
4	H	2306	CLR	C17-C13-C14	3.90	104.70	100.07
4	H	2306	CLR	C9-C10-C5	3.90	115.77	109.65
4	F	2306	CLR	C17-C13-C14	3.90	104.69	100.07
4	E	2305	CLR	C17-C13-C14	3.90	104.69	100.07
4	F	2306	CLR	C9-C10-C5	3.89	115.75	109.65
4	E	2305	CLR	C9-C10-C5	3.89	115.74	109.65
4	B	1110	CLR	C18-C13-C14	-3.72	104.77	111.71
4	H	2306	CLR	C10-C5-C6	-3.72	117.21	122.90
4	D	1108	CLR	C18-C13-C14	-3.71	104.80	111.71
4	C	1107	CLR	C18-C13-C14	-3.70	104.81	111.71
4	A	3006	CLR	C18-C13-C14	-3.70	104.81	111.71
4	E	2305	CLR	C10-C5-C6	-3.70	117.25	122.90
4	G	2305	CLR	C10-C5-C6	-3.70	117.25	122.90
4	F	2306	CLR	C10-C5-C6	-3.69	117.25	122.90
3	D	1105	PGW	O01-C1-C2	3.64	119.35	111.50
3	A	3002	PGW	O01-C1-C2	3.63	119.33	111.50
3	C	1103	PGW	O01-C1-C2	3.63	119.33	111.50
3	B	1106	PGW	O01-C1-C2	3.62	119.30	111.50
4	B	1110	CLR	C21-C20-C22	-3.57	104.76	110.36
4	A	3006	CLR	C21-C20-C22	-3.55	104.79	110.36
4	C	1107	CLR	C21-C20-C22	-3.55	104.79	110.36
4	D	1108	CLR	C21-C20-C22	-3.55	104.80	110.36
5	E	2303	NAG	O5-C1-C2	3.44	116.73	111.29
5	F	2304	NAG	O5-C1-C2	3.44	116.72	111.29
5	H	2304	NAG	O5-C1-C2	3.43	116.71	111.29
5	G	2303	NAG	O5-C1-C2	3.42	116.69	111.29
5	G	2303	NAG	C4-C3-C2	3.37	115.95	111.02
5	E	2303	NAG	C4-C3-C2	3.34	115.92	111.02
5	F	2304	NAG	C4-C3-C2	3.33	115.89	111.02
5	H	2304	NAG	C4-C3-C2	3.32	115.89	111.02
4	F	2306	CLR	C1-C10-C5	3.08	114.39	108.75
4	E	2305	CLR	C1-C10-C5	3.07	114.37	108.75
4	F	2306	CLR	C16-C17-C13	-3.06	100.15	103.84
4	H	2306	CLR	C1-C10-C5	3.06	114.36	108.75
4	G	2305	CLR	C16-C17-C13	-3.06	100.16	103.84
4	H	2306	CLR	C16-C17-C13	-3.06	100.16	103.84
4	E	2305	CLR	C16-C17-C13	-3.05	100.16	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2305	CLR	C1-C10-C5	3.05	114.34	108.75
4	A	3006	CLR	C18-C13-C12	-2.92	105.97	110.59
4	C	1107	CLR	C18-C13-C12	-2.92	105.97	110.59
4	B	1110	CLR	C18-C13-C12	-2.91	105.99	110.59
4	D	1108	CLR	C18-C13-C12	-2.90	106.00	110.59
4	E	2305	CLR	C19-C10-C9	-2.86	108.27	111.68
4	F	2306	CLR	C19-C10-C9	-2.86	108.27	111.68
4	H	2306	CLR	C19-C10-C9	-2.86	108.28	111.68
4	G	2305	CLR	C19-C10-C9	-2.85	108.28	111.68
4	F	2306	CLR	C4-C5-C10	-2.67	112.87	116.42
4	H	2306	CLR	C4-C5-C10	-2.66	112.88	116.42
4	E	2305	CLR	C4-C5-C10	-2.66	112.89	116.42
4	G	2305	CLR	C4-C5-C10	-2.66	112.89	116.42
3	D	1101	PGW	O03-C19-C20	2.60	120.05	111.91
3	A	3007	PGW	O03-C19-C20	2.59	120.04	111.91
3	B	1101	PGW	O03-C19-C20	2.58	120.02	111.91
3	B	1105	PGW	O03-C19-C20	2.58	120.02	111.91
4	A	3006	CLR	C17-C13-C14	2.56	103.11	100.07
4	C	1107	CLR	C17-C13-C14	2.56	103.10	100.07
4	D	1108	CLR	C17-C13-C14	2.55	103.10	100.07
3	C	1102	PGW	O01-C1-C2	2.55	119.91	111.91
3	A	3001	PGW	O01-C1-C2	2.54	119.89	111.91
3	D	1104	PGW	O01-C1-C2	2.54	119.87	111.91
3	B	1104	PGW	O01-C1-C2	2.54	119.86	111.91
4	B	1110	CLR	C17-C13-C14	2.52	103.06	100.07
4	B	1110	CLR	C12-C13-C14	2.48	111.13	107.27
3	D	1101	PGW	O13-P-O14	-2.48	100.97	110.68
3	B	1105	PGW	O13-P-O14	-2.47	101.01	110.68
4	D	1108	CLR	C12-C13-C14	2.47	111.10	107.27
4	A	3006	CLR	C12-C13-C14	2.47	111.10	107.27
3	B	1101	PGW	O13-P-O14	-2.47	101.02	110.68
3	A	3007	PGW	O13-P-O14	-2.46	101.03	110.68
4	C	1107	CLR	C12-C13-C14	2.45	111.07	107.27
4	C	1107	CLR	C9-C10-C5	2.39	113.41	109.65
4	A	3006	CLR	C9-C10-C5	2.37	113.37	109.65
4	B	1110	CLR	C9-C10-C5	2.37	113.36	109.65
4	D	1108	CLR	C9-C10-C5	2.36	113.34	109.65
3	B	1104	PGW	O13-P-O14	-2.33	100.73	112.24
3	D	1104	PGW	O13-P-O14	-2.33	100.73	112.24
4	H	2306	CLR	C2-C3-C4	2.32	113.49	110.31
3	A	3001	PGW	O13-P-O14	-2.32	100.75	112.24
3	C	1102	PGW	O13-P-O14	-2.32	100.75	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2305	CLR	C2-C3-C4	2.32	113.49	110.31
4	F	2306	CLR	C2-C3-C4	2.31	113.47	110.31
4	E	2305	CLR	C2-C3-C4	2.30	113.45	110.31
3	B	1106	PGW	O03-C19-C20	2.29	119.10	111.91
3	D	1105	PGW	O03-C19-C20	2.28	119.08	111.91
3	A	3002	PGW	O03-C19-C20	2.28	119.06	111.91
3	C	1103	PGW	O03-C19-C20	2.28	119.05	111.91
3	B	1106	PGW	O13-P-O14	-2.27	100.99	112.24
4	A	3006	CLR	C1-C10-C5	2.27	112.92	108.75
4	D	1108	CLR	C1-C10-C5	2.27	112.91	108.75
3	A	3002	PGW	O13-P-O14	-2.27	101.03	112.24
4	B	1110	CLR	C1-C10-C5	2.27	112.90	108.75
3	D	1105	PGW	O13-P-O14	-2.26	101.04	112.24
4	D	1108	CLR	C18-C13-C17	-2.26	107.49	111.71
3	C	1103	PGW	O13-P-O14	-2.26	101.07	112.24
4	C	1107	CLR	C1-C10-C5	2.26	112.89	108.75
4	B	1110	CLR	C18-C13-C17	-2.25	107.52	111.71
4	A	3006	CLR	C18-C13-C17	-2.25	107.53	111.71
4	C	1107	CLR	C18-C13-C17	-2.24	107.53	111.71
3	A	3007	PGW	C02-O01-C1	-2.23	112.30	117.79
3	B	1101	PGW	C02-O01-C1	-2.22	112.32	117.79
3	D	1101	PGW	C02-O01-C1	-2.22	112.32	117.79
3	B	1105	PGW	C02-O01-C1	-2.22	112.32	117.79
4	D	1108	CLR	C1-C2-C3	2.21	113.30	110.47
4	B	1110	CLR	C1-C2-C3	2.21	113.30	110.47
4	C	1107	CLR	C1-C2-C3	2.21	113.30	110.47
4	A	3006	CLR	C1-C2-C3	2.21	113.30	110.47
4	G	2305	CLR	C19-C10-C5	-2.19	104.79	108.34
4	H	2306	CLR	C19-C10-C5	-2.18	104.81	108.34
4	E	2305	CLR	C19-C10-C5	-2.18	104.81	108.34
4	F	2306	CLR	C19-C10-C5	-2.17	104.84	108.34
4	F	2306	CLR	C1-C10-C9	-2.16	105.71	108.73
4	G	2305	CLR	C1-C10-C9	-2.13	105.75	108.73
4	E	2305	CLR	C1-C10-C9	-2.13	105.75	108.73
4	H	2306	CLR	C1-C10-C9	-2.12	105.77	108.73
5	H	2305	NAG	O5-C1-C2	2.08	114.58	111.29
5	F	2305	NAG	O5-C1-C2	2.07	114.56	111.29
5	E	2304	NAG	O5-C1-C2	2.07	114.56	111.29
5	G	2304	NAG	O5-C1-C2	2.07	114.56	111.29

There are no chirality outliers.

All (306) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3001	PGW	C04-C05-CAD-OAE
3	A	3001	PGW	C03-O11-P-O13
3	A	3001	PGW	C03-O11-P-O14
3	A	3001	PGW	O01-C02-C03-O11
3	A	3002	PGW	OAF-C05-CAD-OAE
3	A	3002	PGW	C04-C05-CAD-OAE
3	A	3007	PGW	C03-O11-P-O12
3	A	3007	PGW	C03-O11-P-O13
3	A	3007	PGW	C03-O11-P-O14
3	A	3007	PGW	C2-C1-O01-C02
3	B	1101	PGW	C03-O11-P-O12
3	B	1101	PGW	C03-O11-P-O13
3	B	1101	PGW	C03-O11-P-O14
3	B	1101	PGW	C2-C1-O01-C02
3	B	1104	PGW	C04-C05-CAD-OAE
3	B	1104	PGW	C03-O11-P-O13
3	B	1104	PGW	C03-O11-P-O14
3	B	1104	PGW	O01-C02-C03-O11
3	B	1105	PGW	C03-O11-P-O12
3	B	1105	PGW	C03-O11-P-O13
3	B	1105	PGW	C03-O11-P-O14
3	B	1105	PGW	C2-C1-O01-C02
3	B	1106	PGW	OAF-C05-CAD-OAE
3	B	1106	PGW	C04-C05-CAD-OAE
3	C	1102	PGW	C04-C05-CAD-OAE
3	C	1102	PGW	C03-O11-P-O13
3	C	1102	PGW	C03-O11-P-O14
3	C	1102	PGW	O01-C02-C03-O11
3	C	1103	PGW	OAF-C05-CAD-OAE
3	C	1103	PGW	C04-C05-CAD-OAE
3	D	1101	PGW	C03-O11-P-O12
3	D	1101	PGW	C03-O11-P-O13
3	D	1101	PGW	C03-O11-P-O14
3	D	1101	PGW	C2-C1-O01-C02
3	D	1104	PGW	C04-C05-CAD-OAE
3	D	1104	PGW	C03-O11-P-O13
3	D	1104	PGW	C03-O11-P-O14
3	D	1104	PGW	O01-C02-C03-O11
3	D	1105	PGW	OAF-C05-CAD-OAE
3	D	1105	PGW	C04-C05-CAD-OAE
3	A	3007	PGW	O02-C1-O01-C02
3	B	1101	PGW	O02-C1-O01-C02
3	B	1105	PGW	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
3	D	1101	PGW	O02-C1-O01-C02
3	A	3002	PGW	C20-C19-O03-C01
3	B	1106	PGW	C20-C19-O03-C01
3	C	1103	PGW	C20-C19-O03-C01
3	D	1105	PGW	C20-C19-O03-C01
3	A	3002	PGW	O04-C19-O03-C01
3	B	1106	PGW	O04-C19-O03-C01
3	C	1103	PGW	O04-C19-O03-C01
3	D	1105	PGW	O04-C19-O03-C01
4	A	3006	CLR	C17-C20-C22-C23
4	B	1110	CLR	C17-C20-C22-C23
4	C	1107	CLR	C17-C20-C22-C23
4	D	1108	CLR	C17-C20-C22-C23
4	A	3006	CLR	C21-C20-C22-C23
4	B	1110	CLR	C21-C20-C22-C23
4	C	1107	CLR	C21-C20-C22-C23
4	D	1108	CLR	C21-C20-C22-C23
4	E	2305	CLR	C17-C20-C22-C23
4	F	2306	CLR	C17-C20-C22-C23
4	G	2305	CLR	C17-C20-C22-C23
4	H	2306	CLR	C17-C20-C22-C23
4	E	2305	CLR	C21-C20-C22-C23
4	F	2306	CLR	C21-C20-C22-C23
4	G	2305	CLR	C21-C20-C22-C23
4	H	2306	CLR	C21-C20-C22-C23
5	E	2304	NAG	C4-C5-C6-O6
5	F	2305	NAG	C4-C5-C6-O6
5	G	2304	NAG	C4-C5-C6-O6
5	H	2305	NAG	C4-C5-C6-O6
5	E	2304	NAG	O5-C5-C6-O6
5	F	2305	NAG	O5-C5-C6-O6
5	G	2304	NAG	O5-C5-C6-O6
5	H	2305	NAG	O5-C5-C6-O6
3	A	3007	PGW	C1-C2-C3-C4
3	B	1101	PGW	C1-C2-C3-C4
3	B	1105	PGW	C1-C2-C3-C4
3	D	1101	PGW	C1-C2-C3-C4
4	E	2305	CLR	C20-C22-C23-C24
4	F	2306	CLR	C20-C22-C23-C24
4	G	2305	CLR	C20-C22-C23-C24
4	H	2306	CLR	C20-C22-C23-C24
4	C	1107	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	A	3006	CLR	C22-C23-C24-C25
4	B	1110	CLR	C22-C23-C24-C25
4	D	1108	CLR	C22-C23-C24-C25
4	E	2305	CLR	C22-C23-C24-C25
4	F	2306	CLR	C22-C23-C24-C25
4	G	2305	CLR	C22-C23-C24-C25
4	H	2306	CLR	C22-C23-C24-C25
3	A	3001	PGW	C03-O11-P-O12
3	B	1104	PGW	C03-O11-P-O12
3	C	1102	PGW	C03-O11-P-O12
3	D	1104	PGW	C03-O11-P-O12
3	A	3001	PGW	C10-C06-C07-C08
3	B	1104	PGW	C10-C06-C07-C08
3	C	1102	PGW	C10-C06-C07-C08
3	D	1104	PGW	C10-C06-C07-C08
3	A	3004	PGW	C22-C23-C24-C25
3	B	1108	PGW	C22-C23-C24-C25
3	C	1105	PGW	C22-C23-C24-C25
3	D	1107	PGW	C22-C23-C24-C25
3	A	3002	PGW	C5-C6-C7-C8
3	A	3007	PGW	C2-C3-C4-C5
3	B	1101	PGW	C2-C3-C4-C5
3	B	1105	PGW	C2-C3-C4-C5
3	B	1106	PGW	C5-C6-C7-C8
3	C	1103	PGW	C5-C6-C7-C8
3	D	1101	PGW	C2-C3-C4-C5
3	D	1105	PGW	C5-C6-C7-C8
3	A	3004	PGW	C21-C22-C23-C24
3	A	3005	PGW	C16-C15-C27-C26
3	A	3009	PGW	C16-C15-C27-C26
3	B	1108	PGW	C21-C22-C23-C24
3	B	1109	PGW	C16-C15-C27-C26
3	C	1105	PGW	C21-C22-C23-C24
3	C	1106	PGW	C16-C15-C27-C26
3	D	1107	PGW	C21-C22-C23-C24
3	A	3008	PGW	C23-C24-C25-C26
3	B	1102	PGW	C23-C24-C25-C26
3	C	1101	PGW	C23-C24-C25-C26
3	D	1102	PGW	C23-C24-C25-C26
3	H	2301	PGW	C3-C4-C5-C6
3	B	1103	PGW	C3-C4-C5-C6
3	F	2301	PGW	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	D	1103	PGW	C3-C4-C5-C6
3	F	2303	PGW	C2-C3-C4-C5
3	G	2302	PGW	C2-C3-C4-C5
3	E	2302	PGW	C2-C3-C4-C5
3	H	2303	PGW	C2-C3-C4-C5
3	A	3005	PGW	C25-C26-C27-C15
3	A	3009	PGW	C25-C26-C27-C15
3	B	1109	PGW	C25-C26-C27-C15
3	C	1106	PGW	C25-C26-C27-C15
3	A	3008	PGW	C21-C22-C23-C24
3	B	1102	PGW	C21-C22-C23-C24
3	C	1101	PGW	C21-C22-C23-C24
3	D	1102	PGW	C21-C22-C23-C24
3	A	3004	PGW	C23-C24-C25-C26
3	B	1108	PGW	C23-C24-C25-C26
3	C	1105	PGW	C23-C24-C25-C26
3	D	1107	PGW	C23-C24-C25-C26
3	B	1104	PGW	C06-C07-C08-C09
3	D	1104	PGW	C06-C07-C08-C09
3	A	3001	PGW	C06-C07-C08-C09
3	C	1102	PGW	C06-C07-C08-C09
3	B	1107	PGW	C5-C6-C7-C8
3	A	3003	PGW	C5-C6-C7-C8
3	C	1104	PGW	C5-C6-C7-C8
3	D	1106	PGW	C5-C6-C7-C8
3	A	3004	PGW	C25-C26-C27-C15
3	B	1108	PGW	C25-C26-C27-C15
3	C	1105	PGW	C25-C26-C27-C15
3	D	1107	PGW	C25-C26-C27-C15
3	A	3008	PGW	C25-C26-C27-C15
3	B	1102	PGW	C25-C26-C27-C15
3	C	1101	PGW	C25-C26-C27-C15
3	D	1102	PGW	C25-C26-C27-C15
3	A	3005	PGW	C23-C24-C25-C26
3	A	3009	PGW	C23-C24-C25-C26
3	B	1109	PGW	C23-C24-C25-C26
3	C	1106	PGW	C23-C24-C25-C26
3	A	3002	PGW	C07-C06-C10-C9
3	B	1106	PGW	C07-C06-C10-C9
3	C	1103	PGW	C07-C06-C10-C9
3	D	1105	PGW	C07-C06-C10-C9
3	A	3001	PGW	OAF-C05-CAD-OAE

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Mol	Chain	Res	Type	Atoms
3	B	1104	PGW	OAF-C05-CAD-OAE
3	C	1102	PGW	OAF-C05-CAD-OAE
3	D	1104	PGW	OAF-C05-CAD-OAE
3	A	3005	PGW	C21-C22-C23-C24
3	A	3009	PGW	C21-C22-C23-C24
3	C	1106	PGW	C21-C22-C23-C24
3	B	1109	PGW	C21-C22-C23-C24
3	A	3001	PGW	C06-C10-C9-C8
3	B	1104	PGW	C06-C10-C9-C8
3	C	1102	PGW	C06-C10-C9-C8
3	D	1104	PGW	C06-C10-C9-C8
4	E	2305	CLR	C13-C17-C20-C21
4	F	2306	CLR	C13-C17-C20-C21
4	G	2305	CLR	C13-C17-C20-C21
4	H	2306	CLR	C13-C17-C20-C21
3	B	1101	PGW	C3-C4-C5-C6
3	B	1105	PGW	C3-C4-C5-C6
3	D	1101	PGW	C3-C4-C5-C6
3	A	3007	PGW	C3-C4-C5-C6
3	A	3002	PGW	C04-O12-P-O11
3	B	1106	PGW	C04-O12-P-O11
3	C	1103	PGW	C04-O12-P-O11
3	D	1105	PGW	C04-O12-P-O11
3	A	3007	PGW	O03-C01-C02-O01
3	B	1101	PGW	O03-C01-C02-O01
3	B	1105	PGW	O03-C01-C02-O01
3	D	1101	PGW	O03-C01-C02-O01
4	E	2305	CLR	C23-C24-C25-C26
4	F	2306	CLR	C23-C24-C25-C26
4	G	2305	CLR	C23-C24-C25-C26
4	H	2306	CLR	C23-C24-C25-C26
3	E	2302	PGW	C3-C4-C5-C6
3	G	2302	PGW	C3-C4-C5-C6
3	H	2303	PGW	C3-C4-C5-C6
3	F	2303	PGW	C3-C4-C5-C6
3	A	3007	PGW	O03-C01-C02-C03
3	B	1101	PGW	O03-C01-C02-C03
3	B	1105	PGW	O03-C01-C02-C03
3	D	1101	PGW	O03-C01-C02-C03
4	A	3006	CLR	C13-C17-C20-C21
4	B	1110	CLR	C13-C17-C20-C21
4	C	1107	CLR	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
4	D	1108	CLR	C13-C17-C20-C21
3	A	3007	PGW	C20-C21-C22-C23
3	B	1101	PGW	C20-C21-C22-C23
3	B	1105	PGW	C20-C21-C22-C23
3	D	1101	PGW	C20-C21-C22-C23
3	A	3002	PGW	C09-C11-C12-C13
3	B	1106	PGW	C09-C11-C12-C13
3	C	1103	PGW	C09-C11-C12-C13
3	D	1105	PGW	C09-C11-C12-C13
3	B	1103	PGW	C4-C5-C6-C7
3	D	1103	PGW	C4-C5-C6-C7
3	H	2301	PGW	C4-C5-C6-C7
4	A	3006	CLR	C23-C24-C25-C27
4	B	1110	CLR	C23-C24-C25-C27
4	C	1107	CLR	C23-C24-C25-C27
4	D	1108	CLR	C23-C24-C25-C27
3	F	2301	PGW	C4-C5-C6-C7
3	A	3001	PGW	C04-O12-P-O11
3	B	1104	PGW	C04-O12-P-O11
3	C	1102	PGW	C04-O12-P-O11
3	D	1104	PGW	C04-O12-P-O11
3	A	3002	PGW	C05-C04-O12-P
3	B	1106	PGW	C05-C04-O12-P
3	C	1103	PGW	C05-C04-O12-P
3	D	1105	PGW	C05-C04-O12-P
3	B	1106	PGW	C08-C09-C11-C12
3	C	1103	PGW	C08-C09-C11-C12
3	D	1105	PGW	C08-C09-C11-C12
3	A	3002	PGW	C08-C09-C11-C12
3	A	3004	PGW	C20-C21-C22-C23
3	B	1108	PGW	C20-C21-C22-C23
3	C	1105	PGW	C20-C21-C22-C23
3	D	1107	PGW	C20-C21-C22-C23
3	A	3002	PGW	C03-O11-P-O12
3	B	1106	PGW	C03-O11-P-O12
3	C	1103	PGW	C03-O11-P-O12
3	D	1105	PGW	C03-O11-P-O12
3	A	3002	PGW	C7-C8-C9-C10
3	B	1106	PGW	C7-C8-C9-C10
3	C	1103	PGW	C7-C8-C9-C10
3	D	1105	PGW	C7-C8-C9-C10
4	C	1107	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	A	3006	CLR	C20-C22-C23-C24
4	B	1110	CLR	C20-C22-C23-C24
4	E	2305	CLR	C13-C17-C20-C22
4	F	2306	CLR	C13-C17-C20-C22
4	H	2306	CLR	C13-C17-C20-C22
4	D	1108	CLR	C20-C22-C23-C24
4	G	2305	CLR	C13-C17-C20-C22
4	E	2305	CLR	C23-C24-C25-C27
4	F	2306	CLR	C23-C24-C25-C27
4	G	2305	CLR	C23-C24-C25-C27
4	H	2306	CLR	C23-C24-C25-C27
3	F	2301	PGW	C6-C7-C8-C9
3	B	1103	PGW	C6-C7-C8-C9
3	D	1103	PGW	C6-C7-C8-C9
3	H	2301	PGW	C6-C7-C8-C9
3	A	3008	PGW	O03-C19-C20-C21
3	B	1102	PGW	O03-C19-C20-C21
3	C	1101	PGW	O03-C19-C20-C21
3	D	1102	PGW	O03-C19-C20-C21
3	B	1102	PGW	O04-C19-C20-C21
3	D	1102	PGW	O04-C19-C20-C21
3	A	3002	PGW	O03-C19-C20-C21
3	B	1106	PGW	O03-C19-C20-C21
3	C	1103	PGW	O03-C19-C20-C21
3	D	1105	PGW	O03-C19-C20-C21
3	A	3008	PGW	O04-C19-C20-C21
3	C	1101	PGW	O04-C19-C20-C21
3	A	3002	PGW	O01-C02-C03-O11
3	B	1106	PGW	O01-C02-C03-O11
3	C	1103	PGW	O01-C02-C03-O11
3	D	1105	PGW	O01-C02-C03-O11
3	A	3002	PGW	O04-C19-C20-C21
3	C	1103	PGW	O04-C19-C20-C21
3	D	1105	PGW	O04-C19-C20-C21
3	B	1106	PGW	O04-C19-C20-C21
3	C	1103	PGW	C2-C3-C4-C5
3	A	3001	PGW	C04-O12-P-O14
3	B	1104	PGW	C04-O12-P-O14
3	C	1102	PGW	C04-O12-P-O14
3	D	1104	PGW	C04-O12-P-O14
3	A	3002	PGW	C2-C3-C4-C5
3	B	1106	PGW	C2-C3-C4-C5

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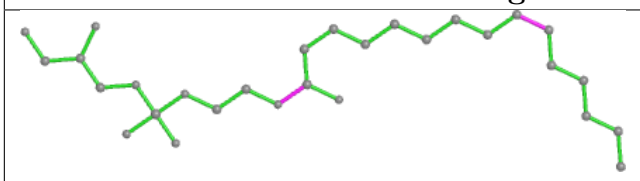
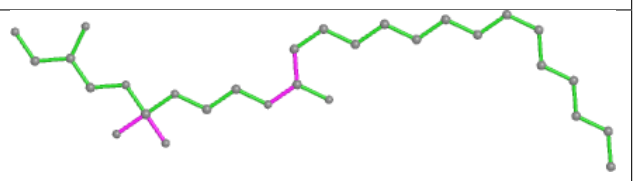
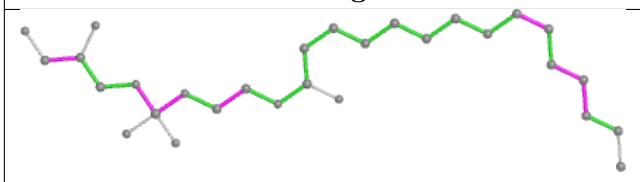
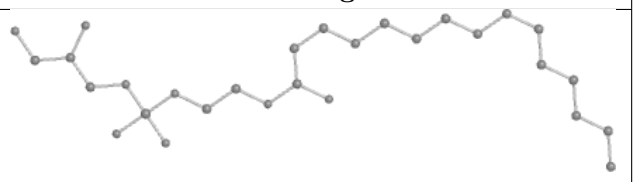
Mol	Chain	Res	Type	Atoms
3	D	1105	PGW	C2-C3-C4-C5
3	A	3003	PGW	C6-C7-C8-C9
3	B	1107	PGW	C6-C7-C8-C9
3	C	1104	PGW	C6-C7-C8-C9
4	E	2305	CLR	C16-C17-C20-C21
4	F	2306	CLR	C16-C17-C20-C21
4	G	2305	CLR	C16-C17-C20-C21
4	H	2306	CLR	C16-C17-C20-C21
3	D	1106	PGW	C6-C7-C8-C9
3	A	3001	PGW	C07-C06-C10-C9
3	C	1102	PGW	C07-C06-C10-C9

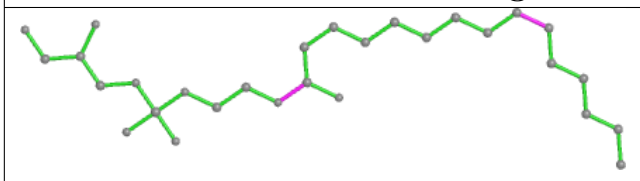
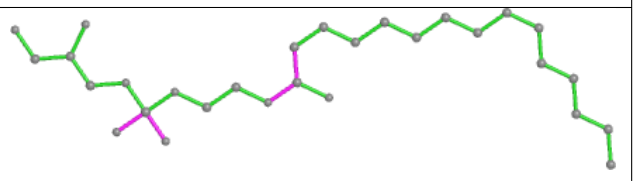
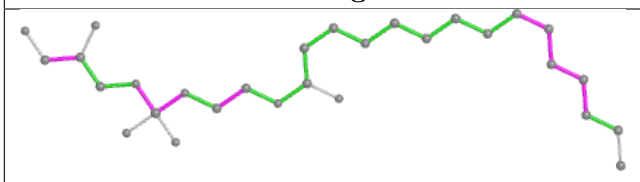
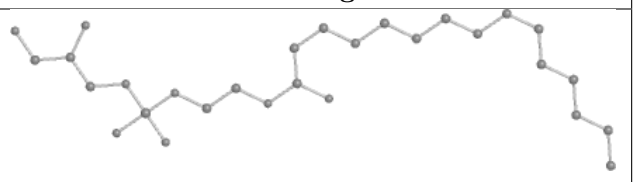
There are no ring outliers.

13 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1104	PGW	1	0
4	D	1108	CLR	6	0
3	A	3002	PGW	1	0
4	H	2306	CLR	7	0
3	B	1106	PGW	2	0
4	A	3006	CLR	6	0
3	C	1103	PGW	1	0
4	C	1107	CLR	5	0
4	F	2306	CLR	8	0
3	D	1105	PGW	2	0
4	G	2305	CLR	8	0
4	B	1110	CLR	6	0
4	E	2305	CLR	5	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 PGW D 1104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGW C 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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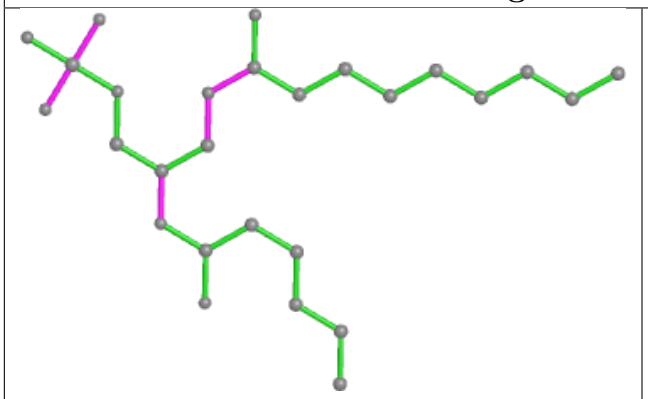
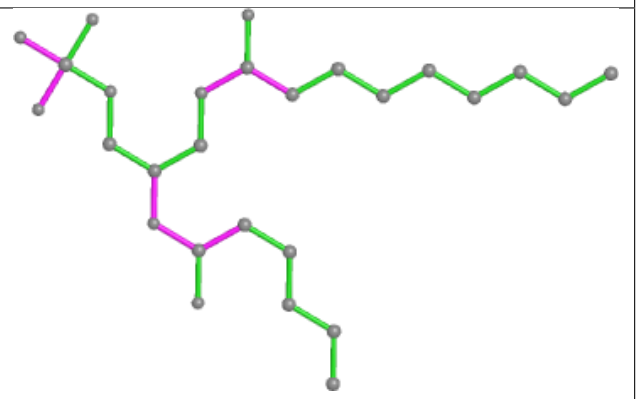
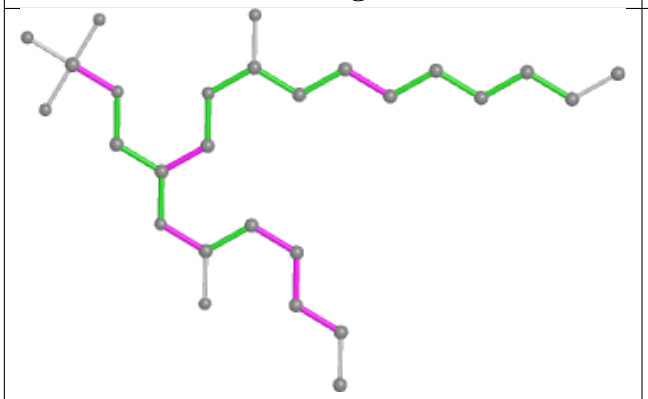


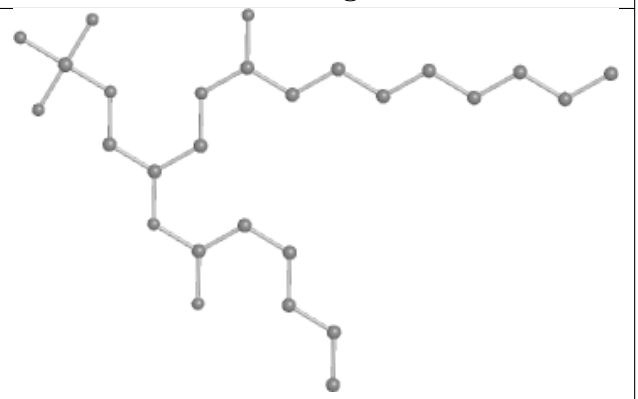
Bond lengths



Bond angles



Torsions



Rings

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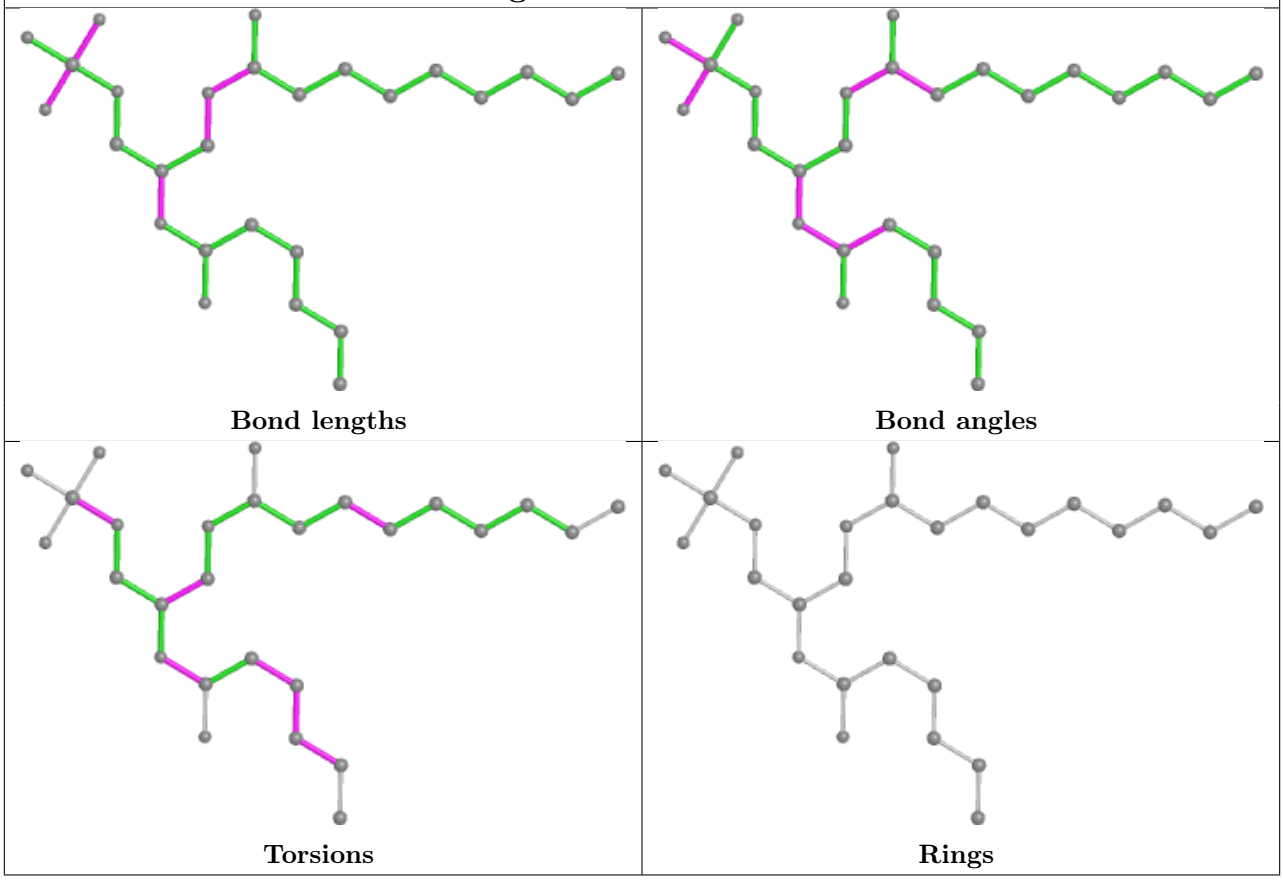

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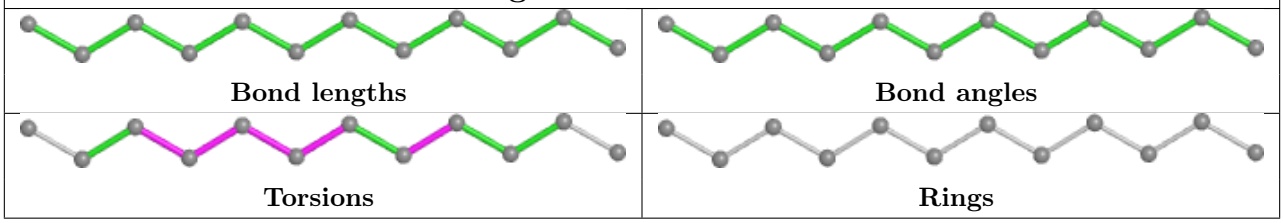

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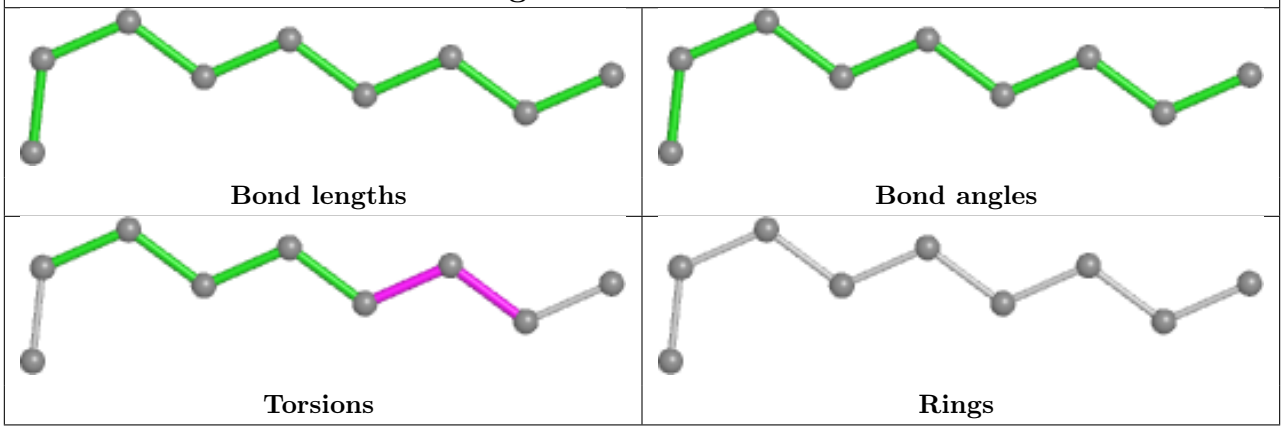
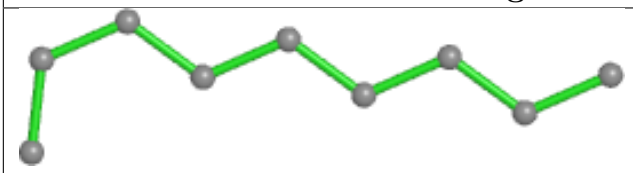
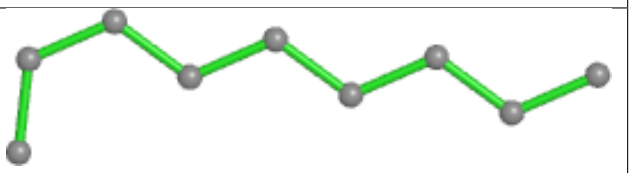


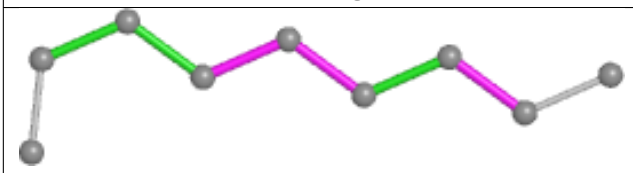
Ligand PGW D 1103



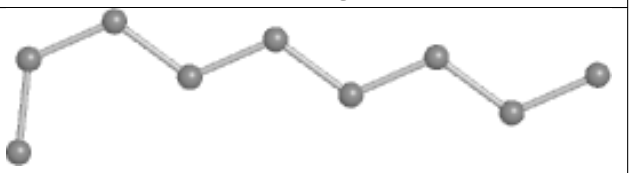
Bond lengths



Bond angles

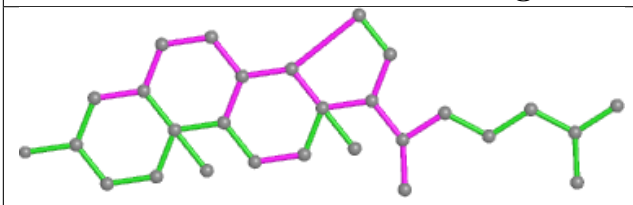


Torsions



Rings

Ligand CLR D 1108



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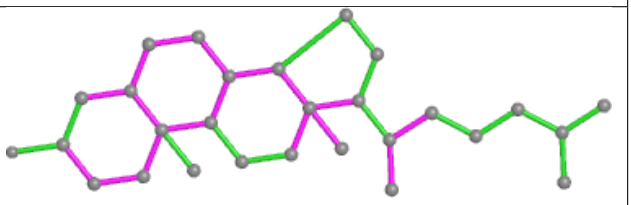
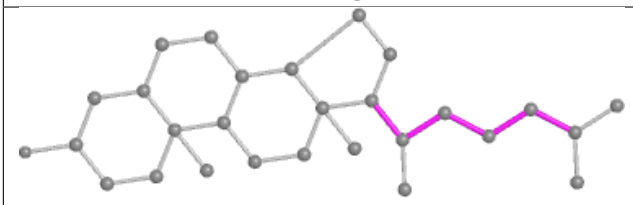


Bond angles



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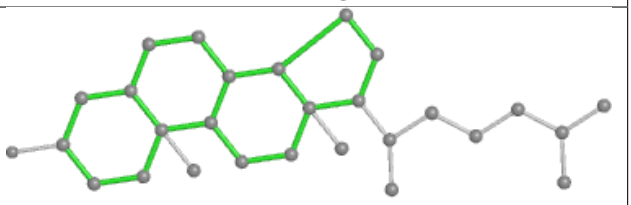
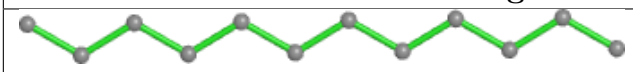
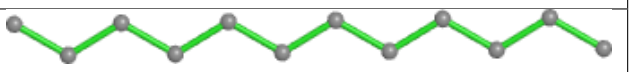


Rings

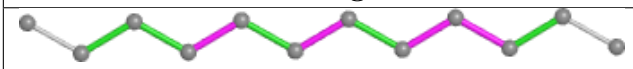
Ligand PGW A 3009



Bond lengths



Bond angles



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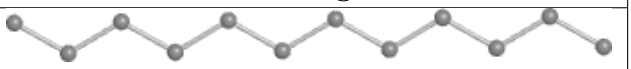
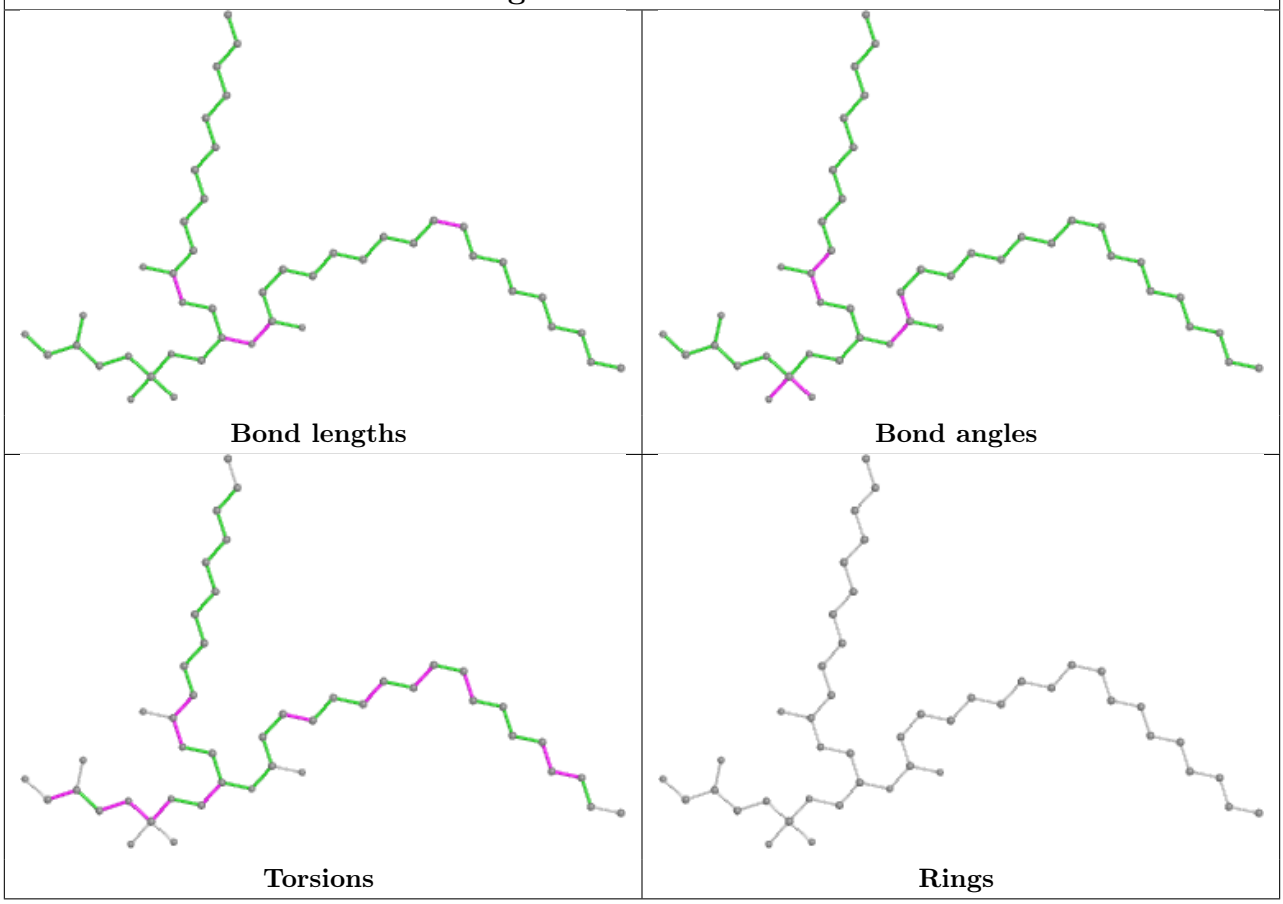
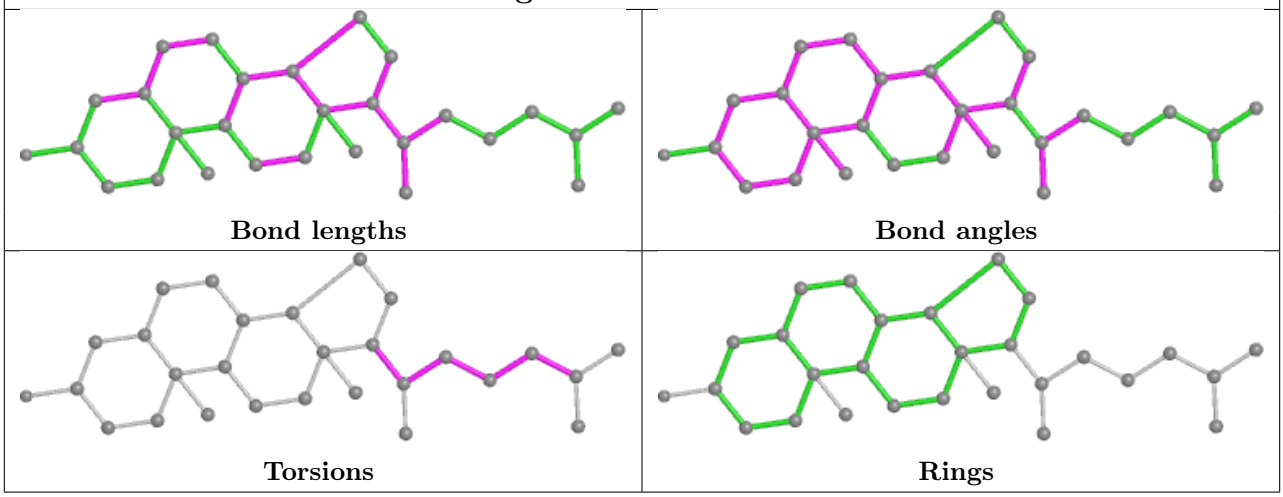


Rings

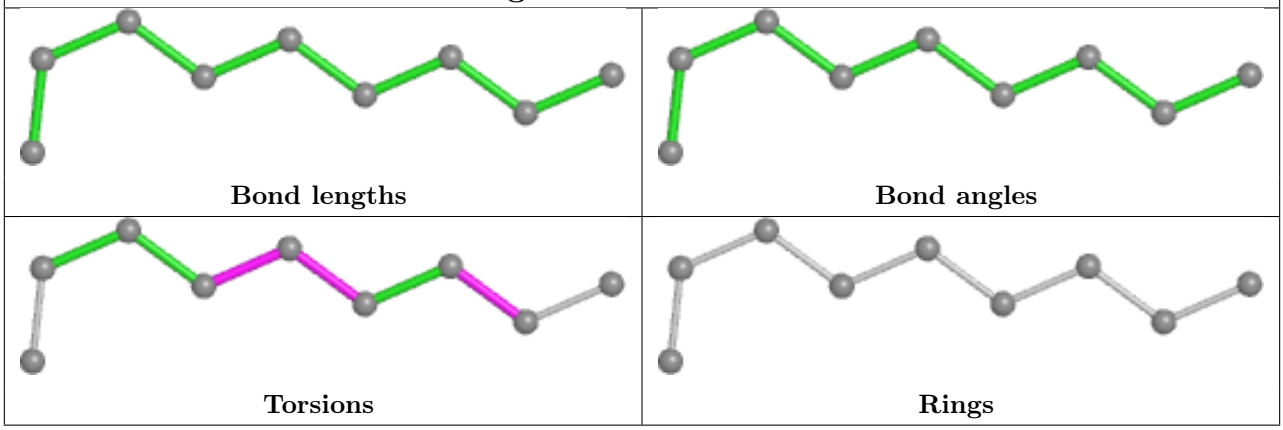
Ligand PGW A 3002



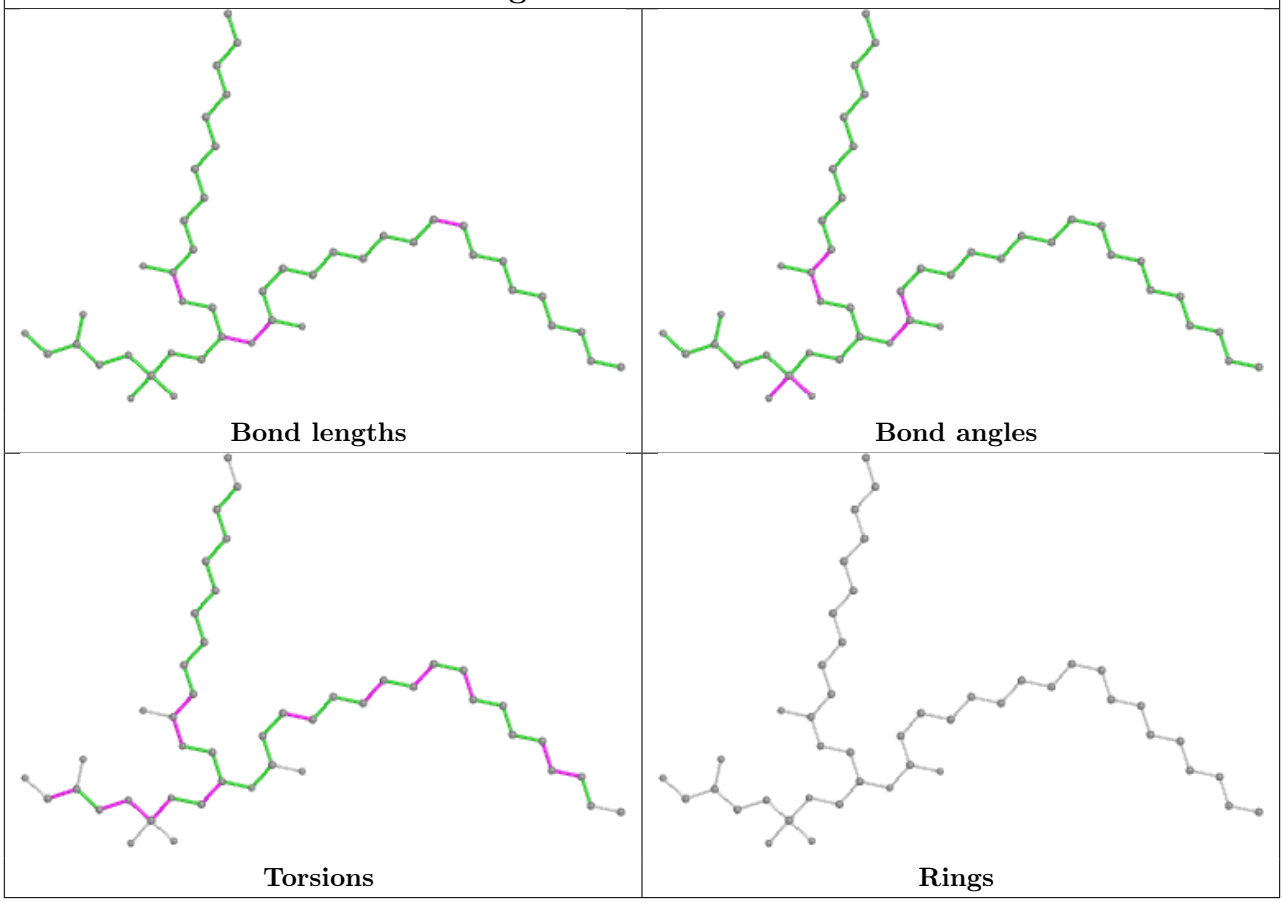
Ligand CLR H 2306



Ligand PGW H 2301



Ligand PGW B 1106



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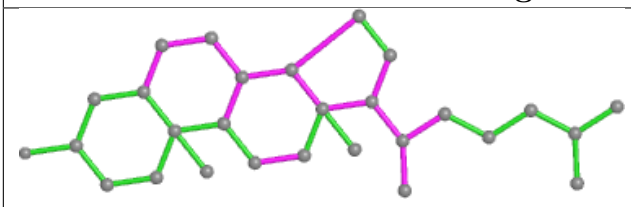
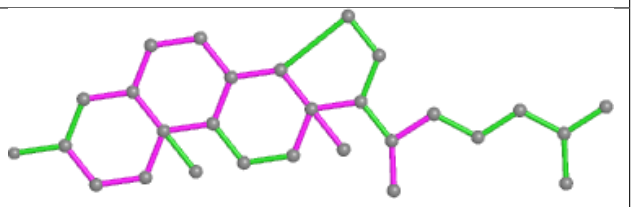
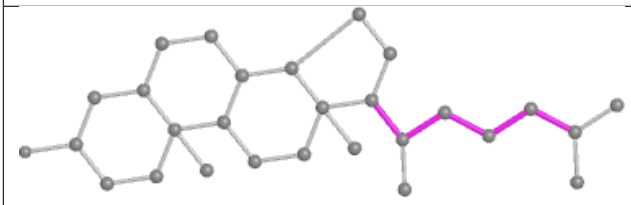


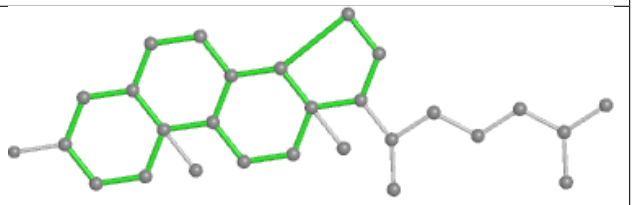
Bond lengths



Bond angles

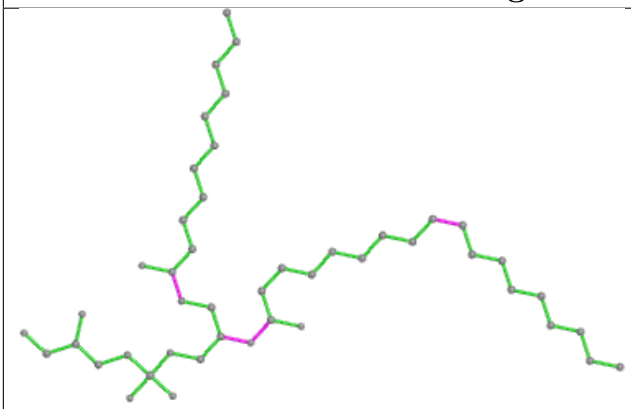


Torsions



Rings

Ligand PGW C 1103



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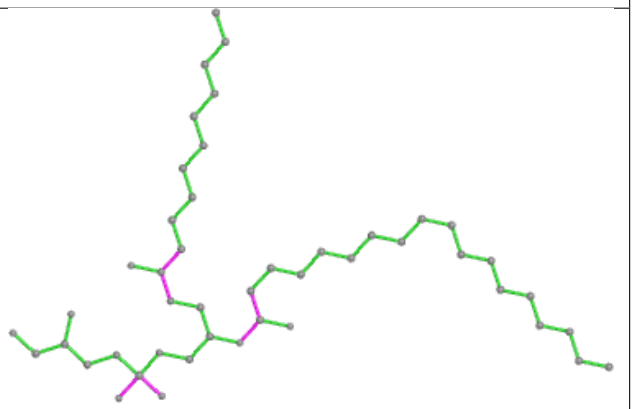
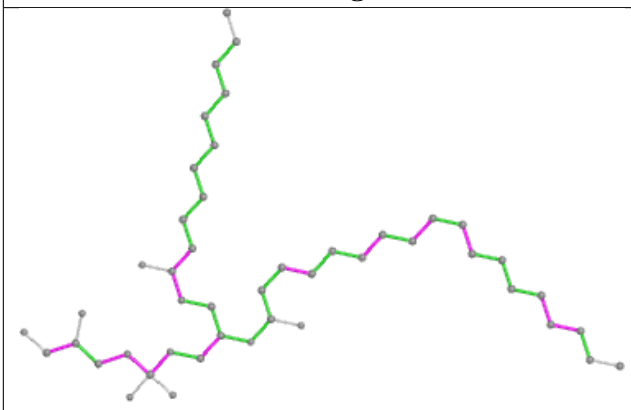
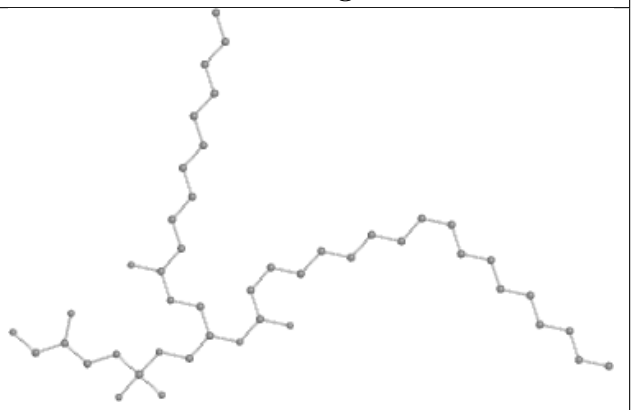


Bond angles

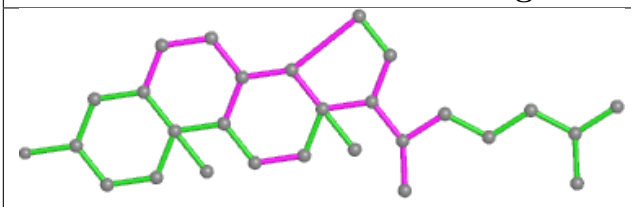


Torsions

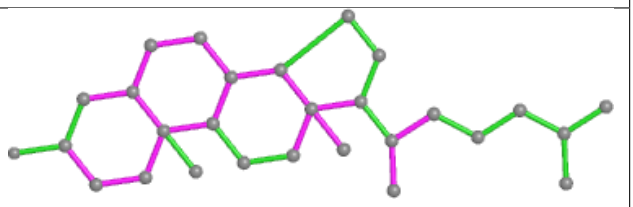


Rings

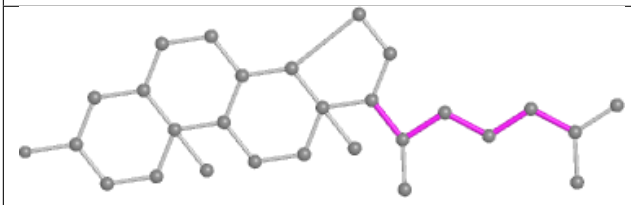
Ligand CLR C 1107



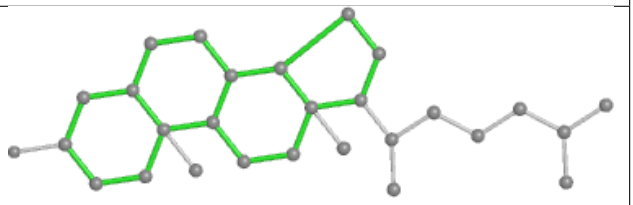
Bond lengths



Bond angles

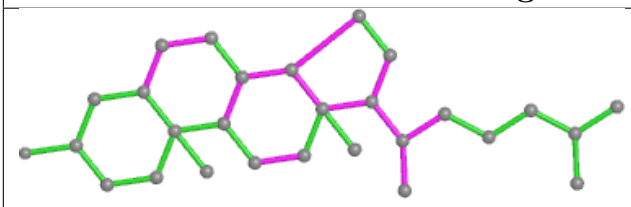


Torsions

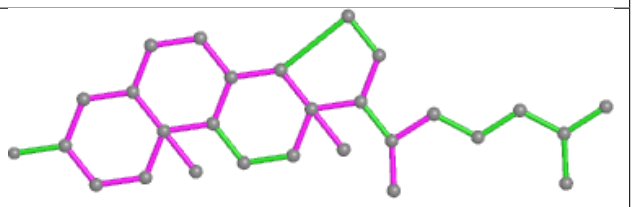


Rings

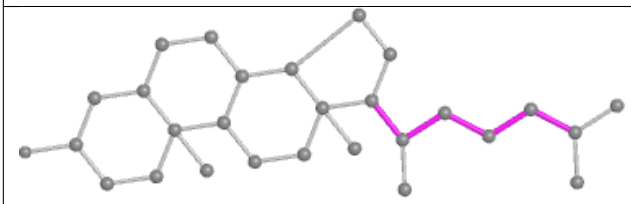
Ligand CLR F 2306



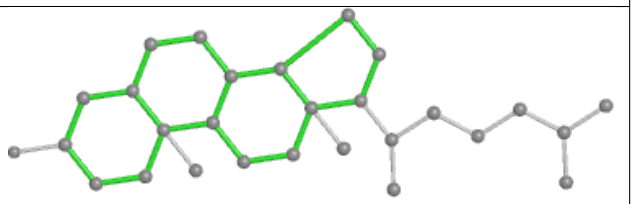
Bond lengths



Bond angles

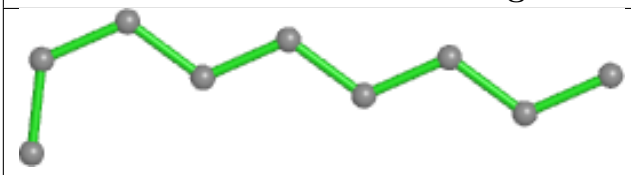


Torsions

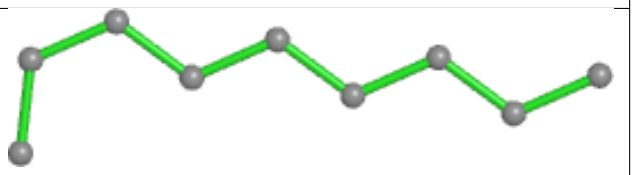


Rings

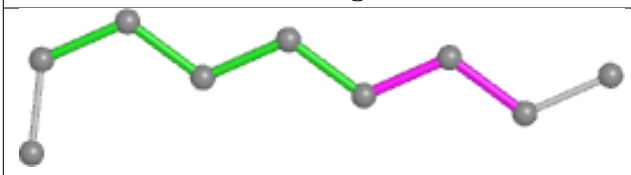
Ligand PGW C 1104



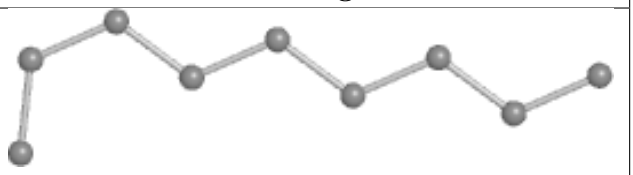
Bond lengths



Bond angles

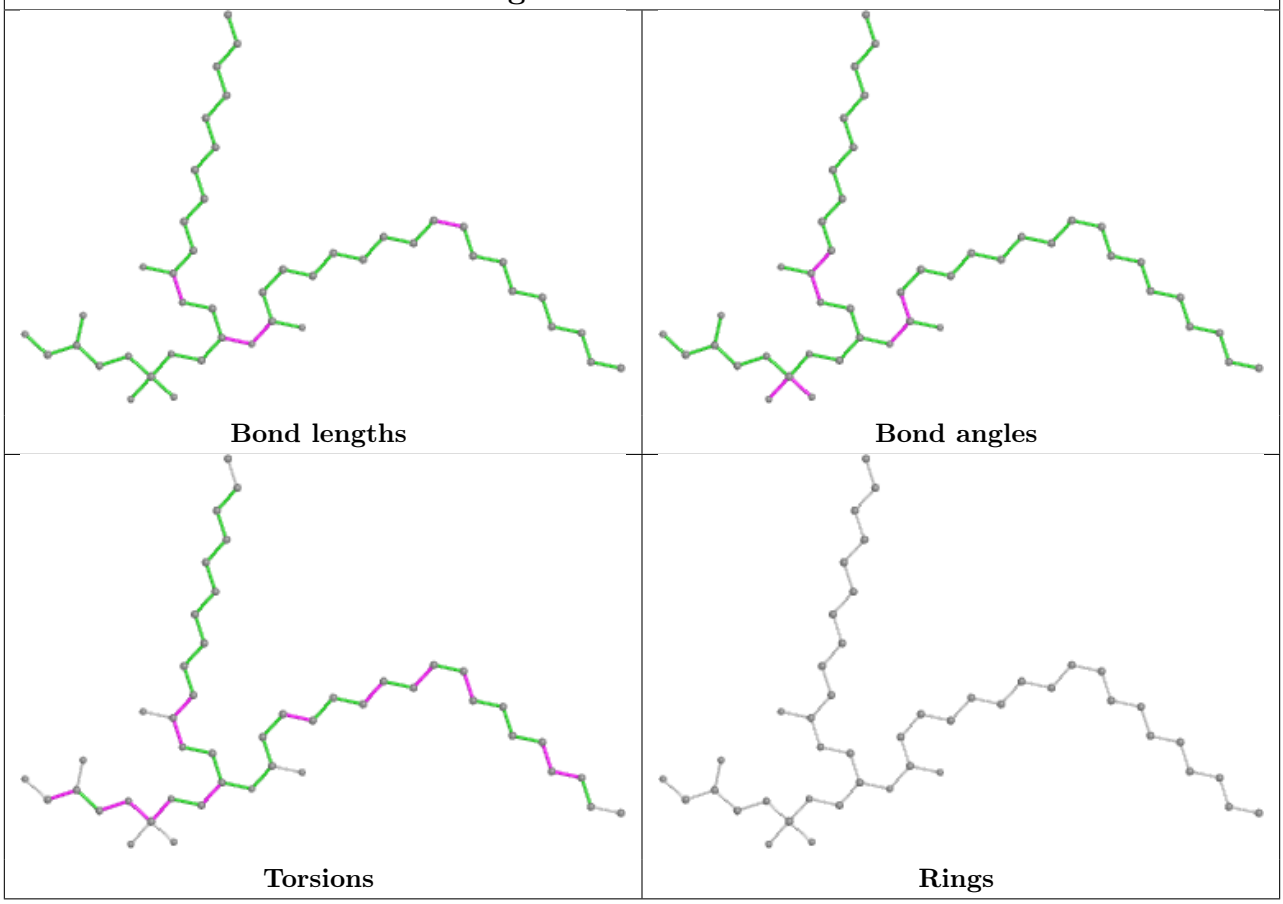


Torsions

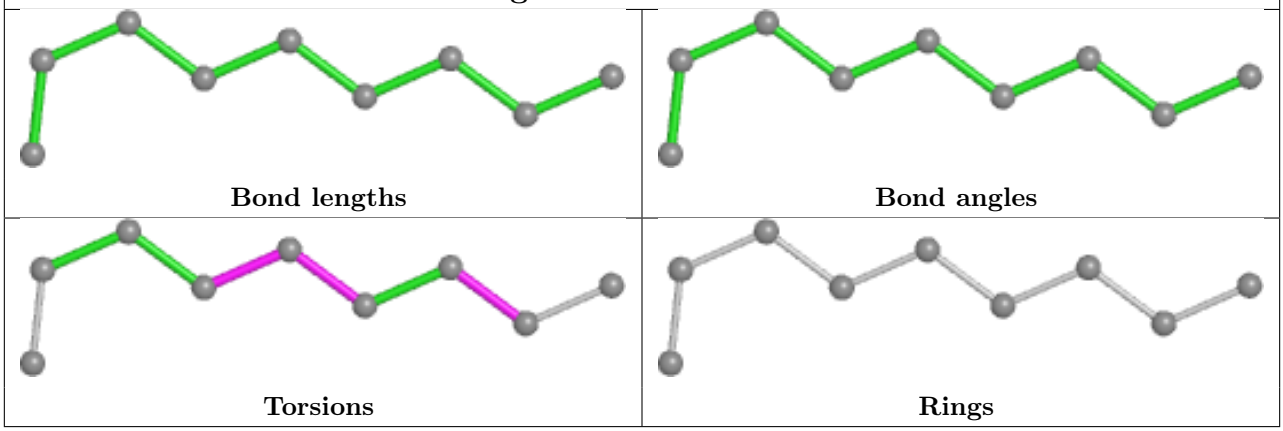


Rings

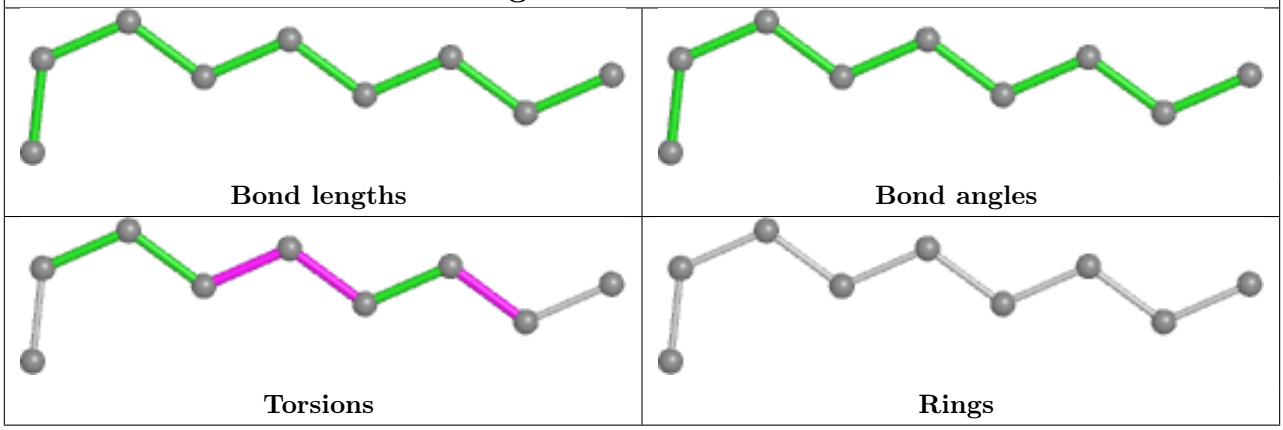
Ligand PGW D 1105



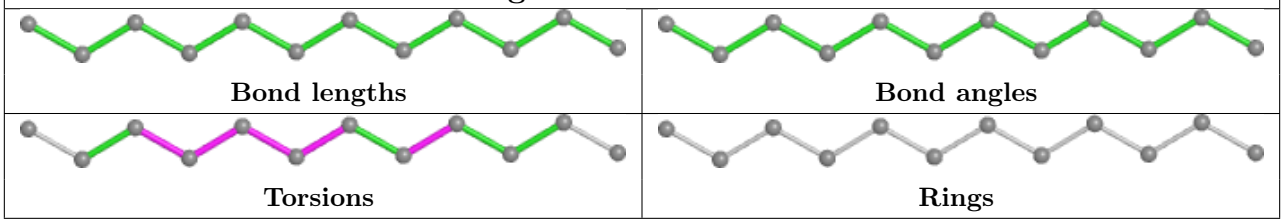
Ligand PGW F 2301



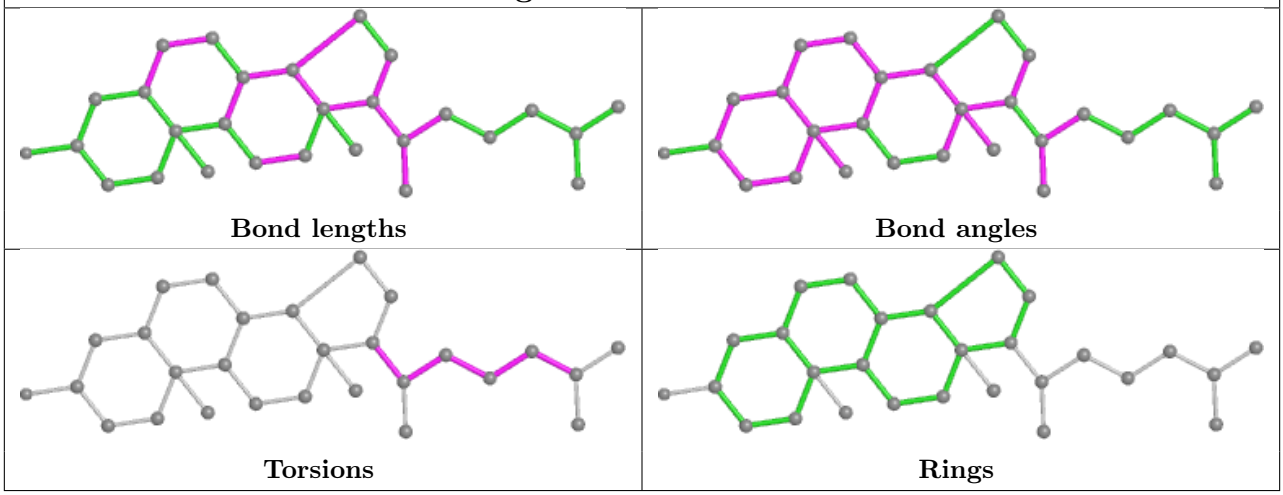
Ligand PGW B 1103



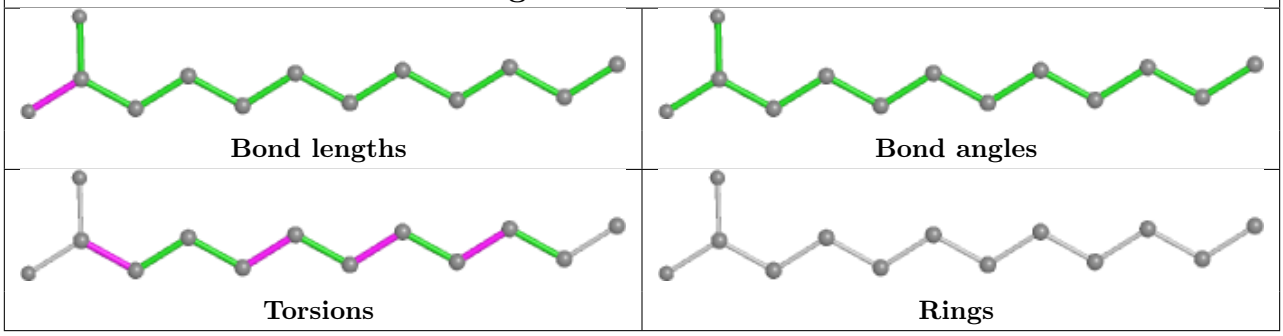
Ligand PGW D 1107



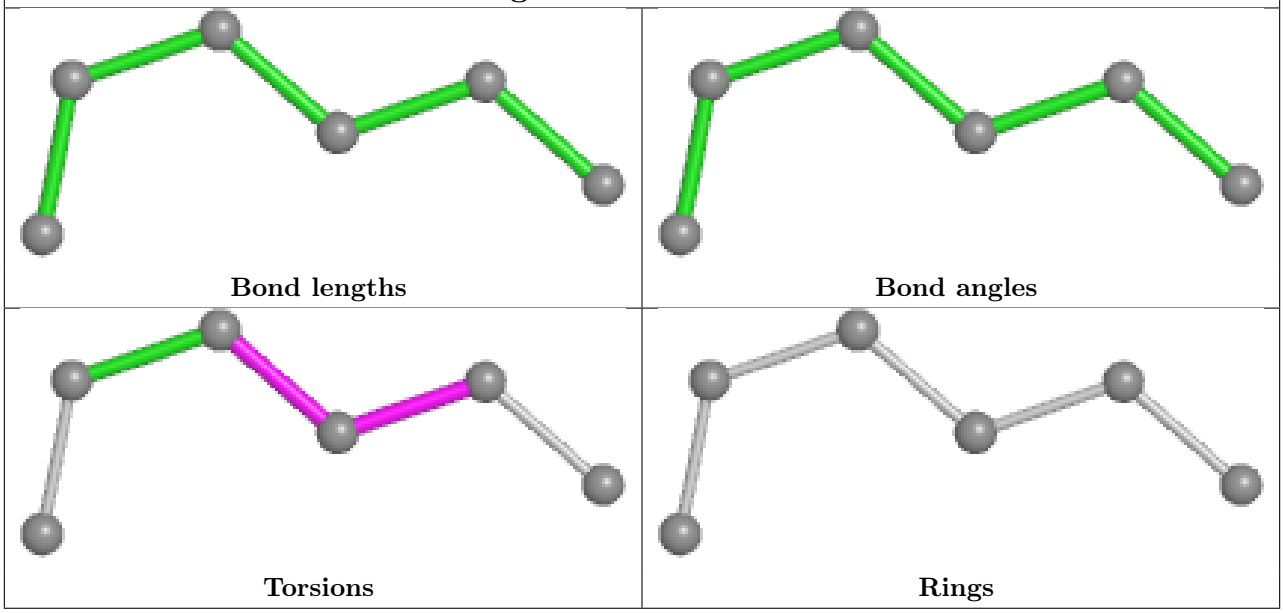
Ligand CLR G 2305



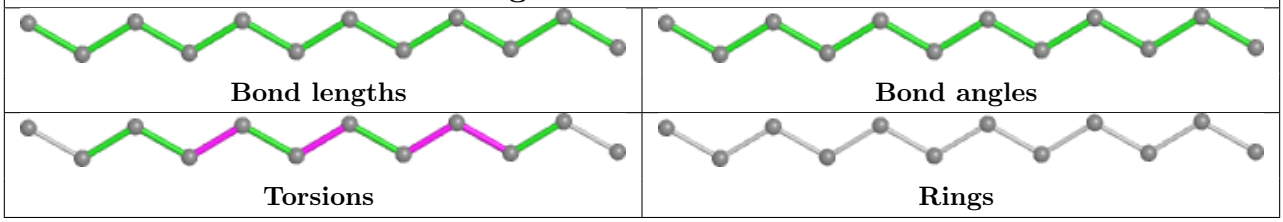
Ligand PGW C 1101



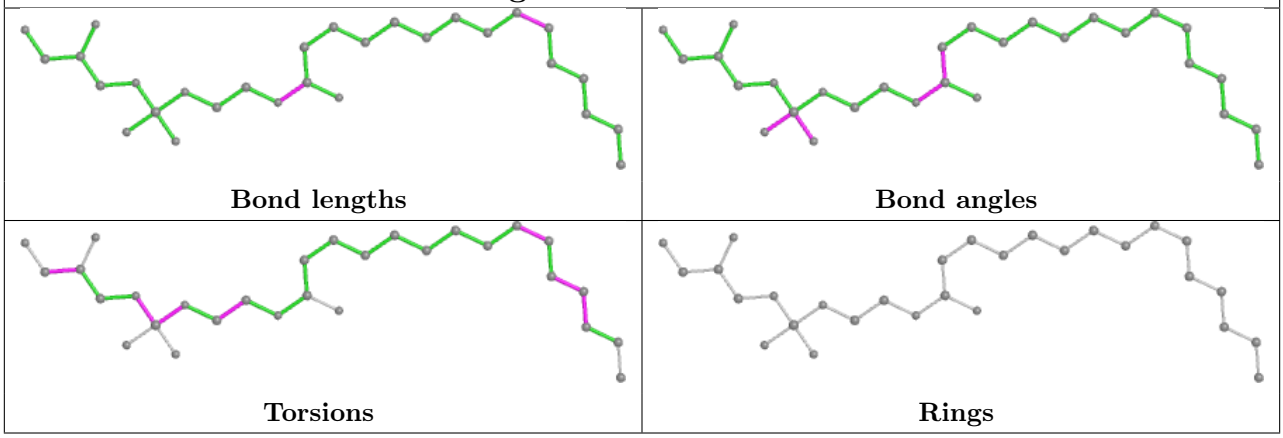
Ligand PGW F 2303



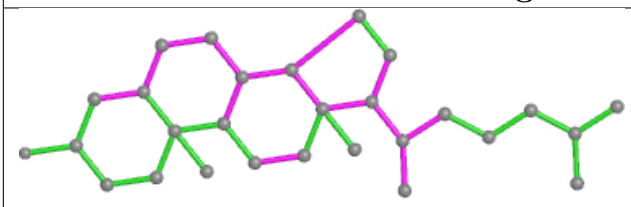
Ligand PGW B 1109



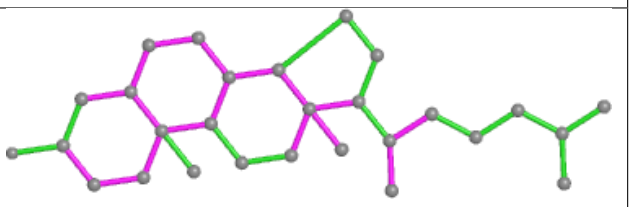
Ligand PGW B 1104



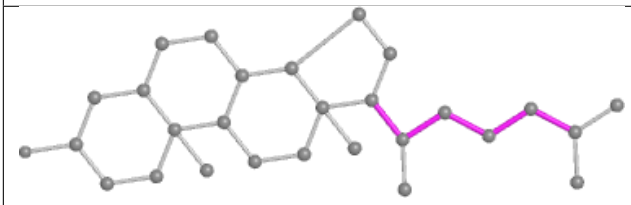
Ligand CLR B 1110



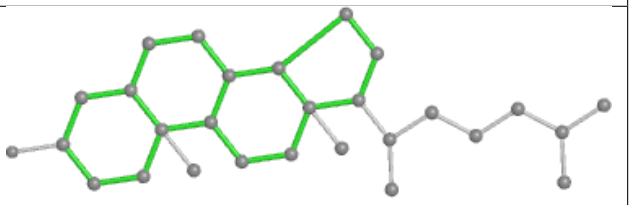
Bond lengths



Bond angles

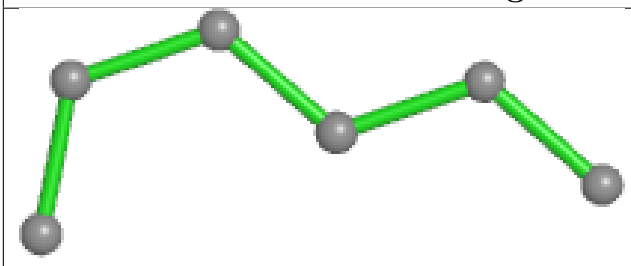


Torsions

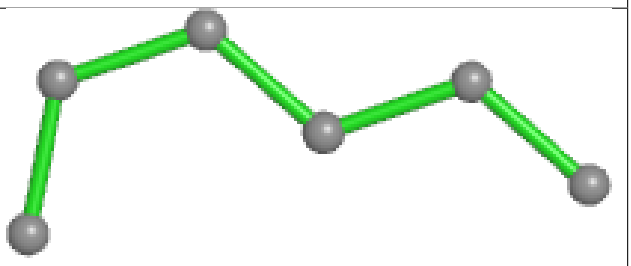


Rings

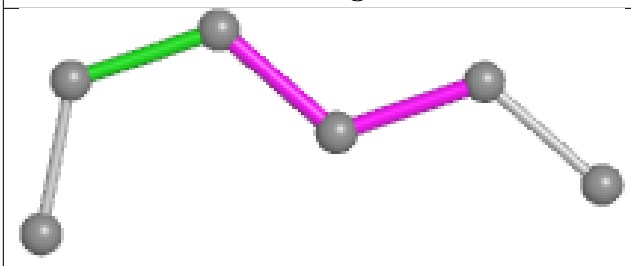
Ligand PGW G 2302



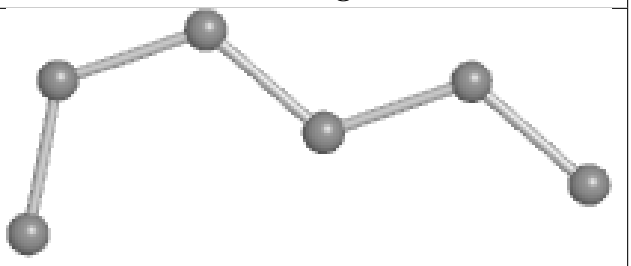
Bond lengths



Bond angles

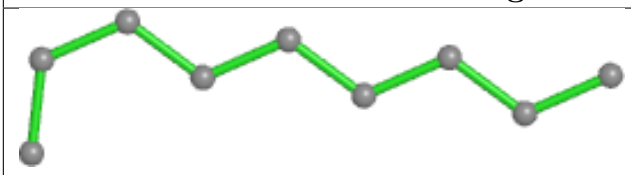


Torsions



Rings

Ligand PGW D 1106



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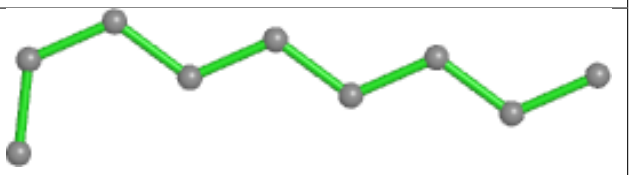
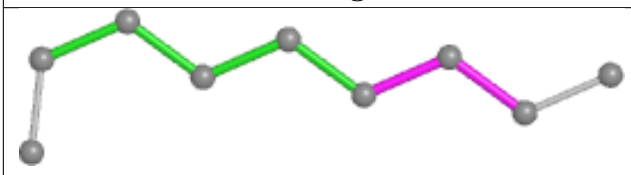
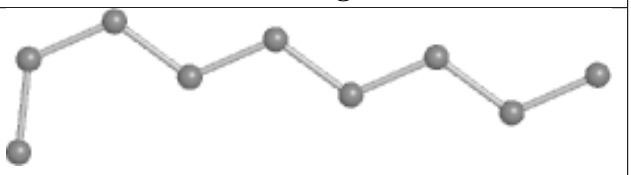


Bond angles

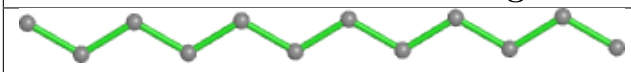


Torsions

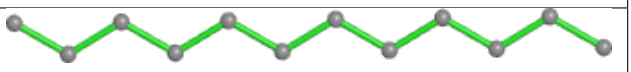


Rings

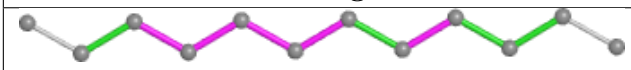
Ligand PGW A 3004



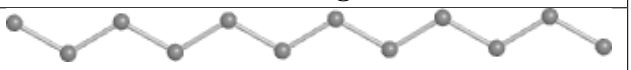
Bond lengths



Bond angles

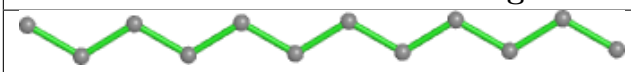


Torsions



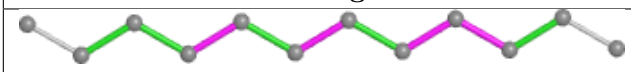
Rings

Ligand PGW A 3005

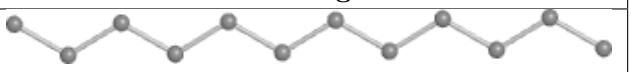


Bond lengths

Bond angles

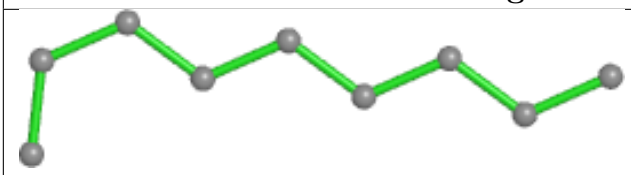


Torsions

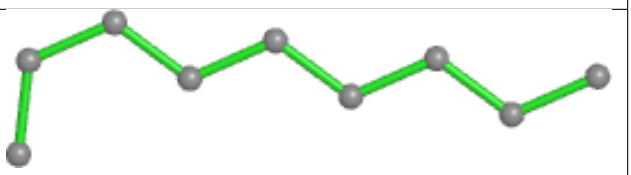


Rings

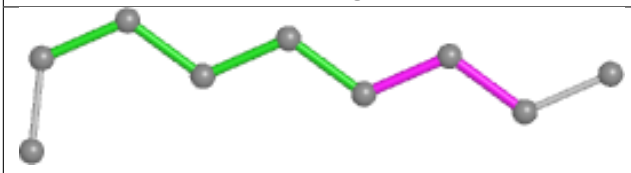
Ligand PGW A 3003



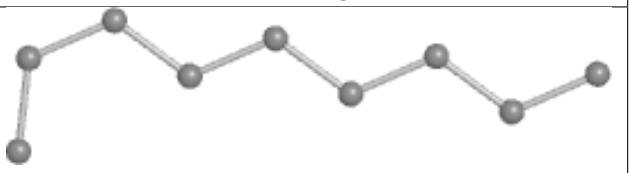
Bond lengths



Bond angles

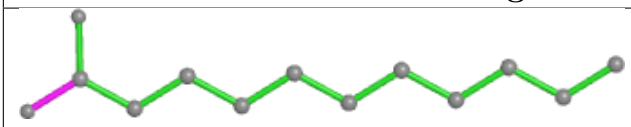


Torsions

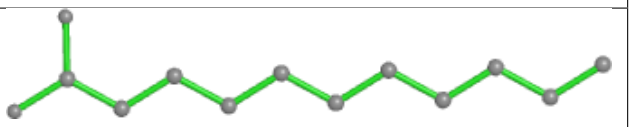


Rings

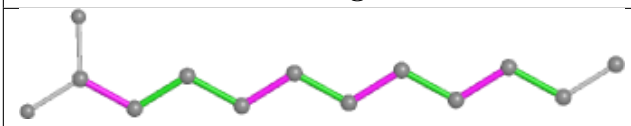
Ligand PGW A 3008



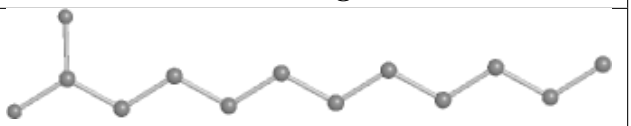
Bond lengths



Bond angles

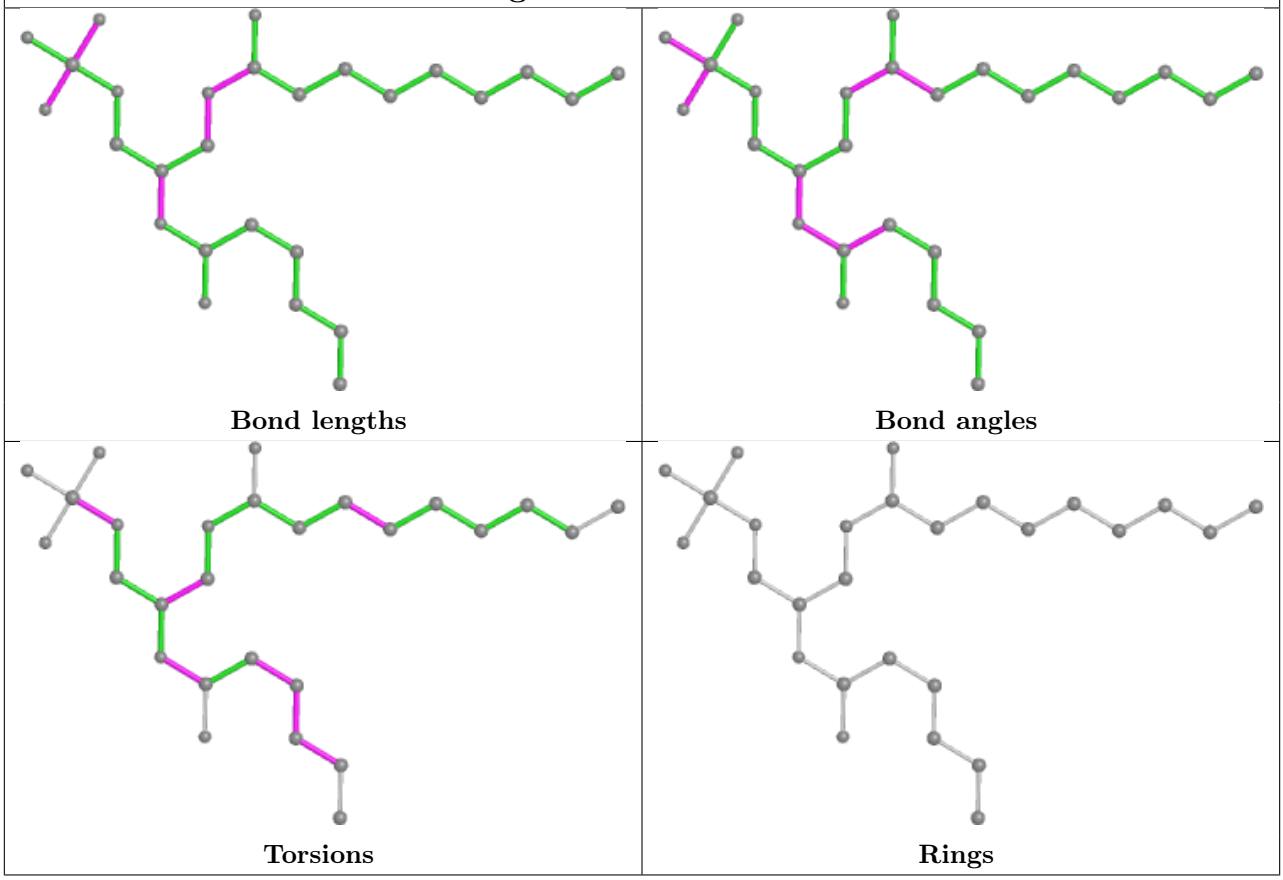


Torsions

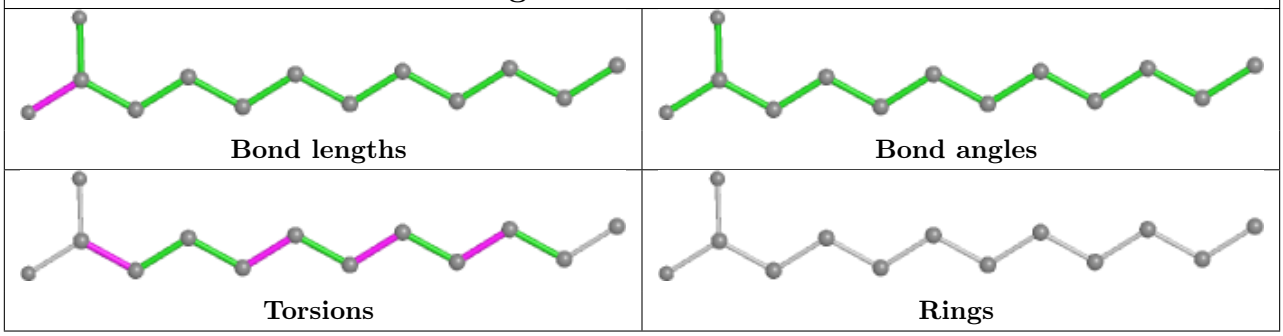


Rings

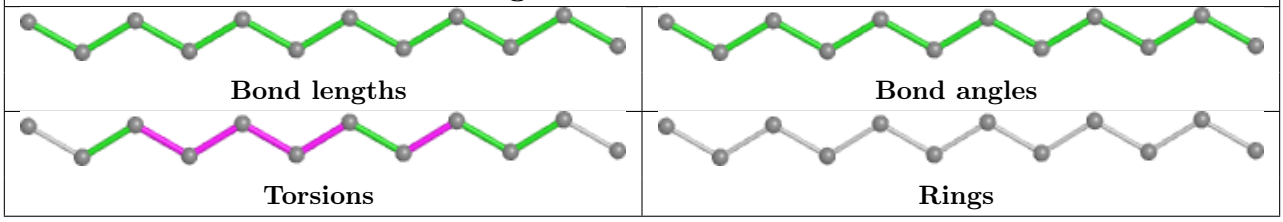
Ligand PGW B 1101



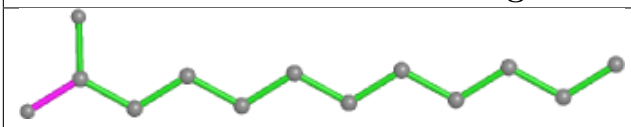
Ligand PGW B 1102



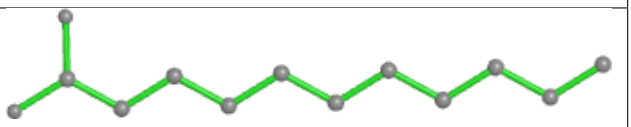
Ligand PGW C 1105



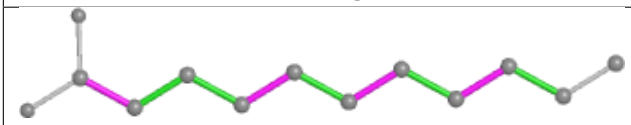
Ligand PGW D 1102



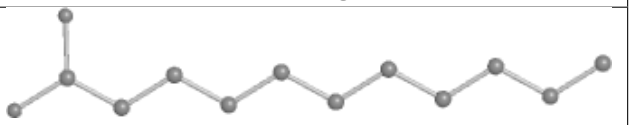
Bond lengths



Bond angles

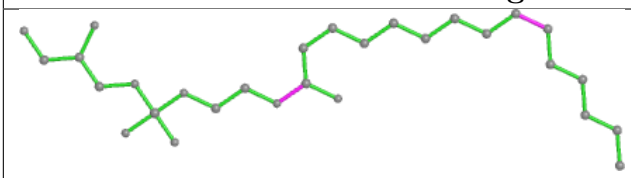


Torsions

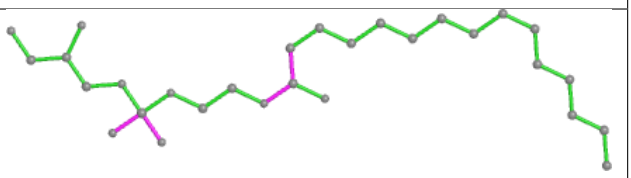


Rings

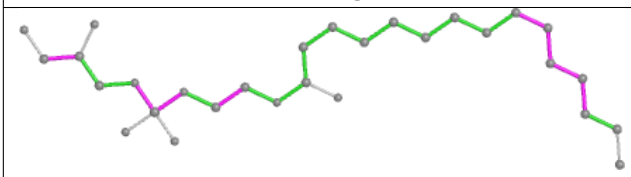
Ligand PGW A 3001



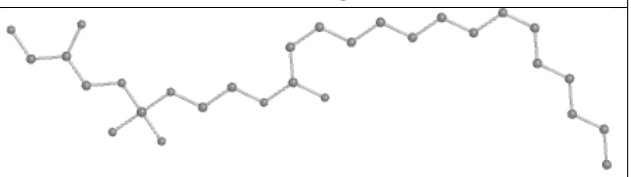
Bond lengths



Bond angles

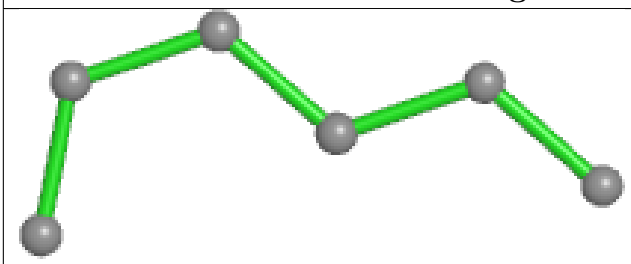


Torsions

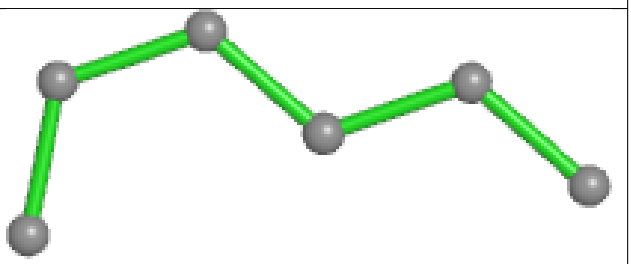


Rings

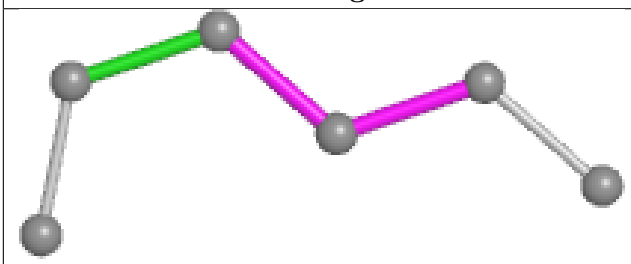
Ligand PGW E 2302



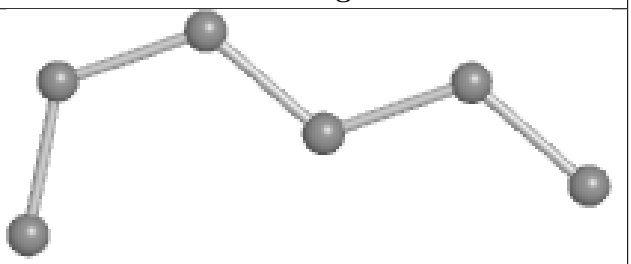
Bond lengths



Bond angles

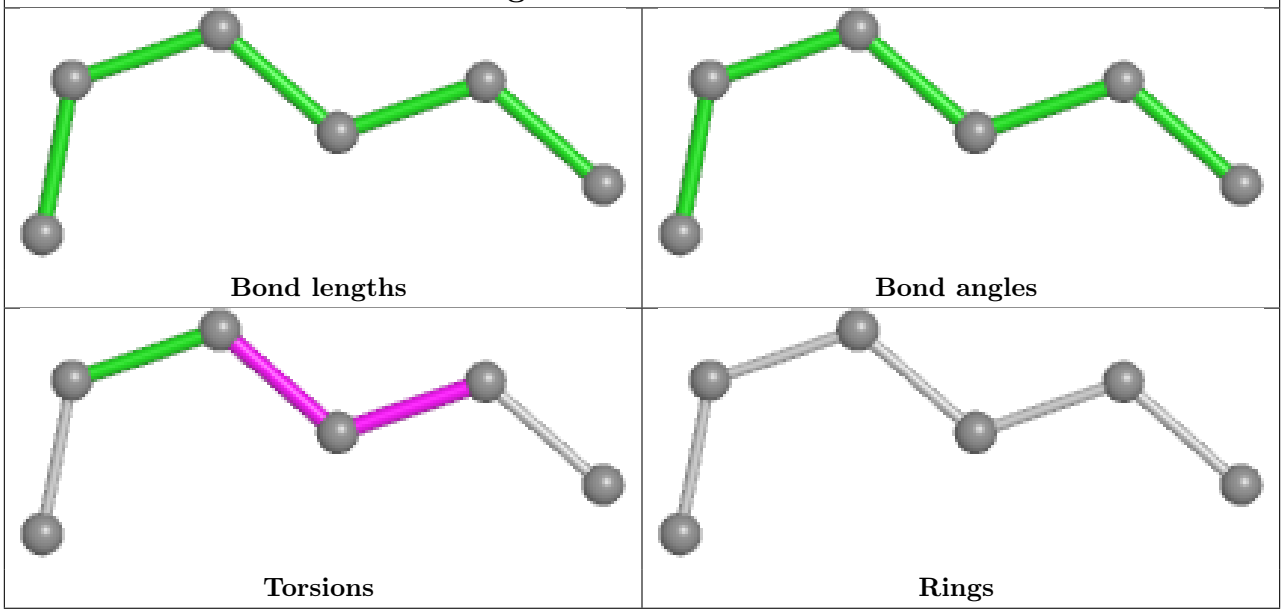


Torsions

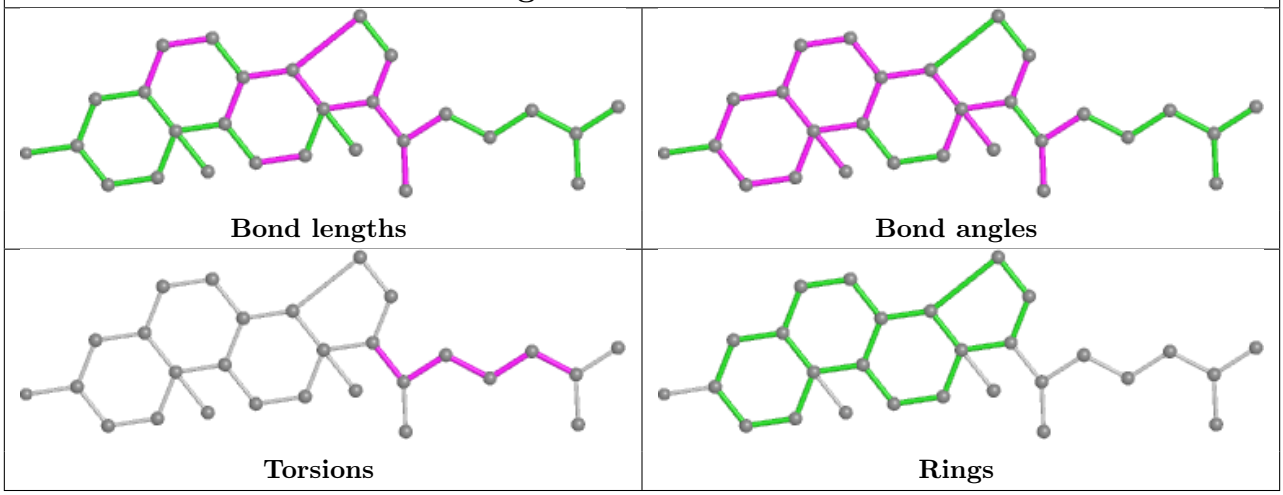


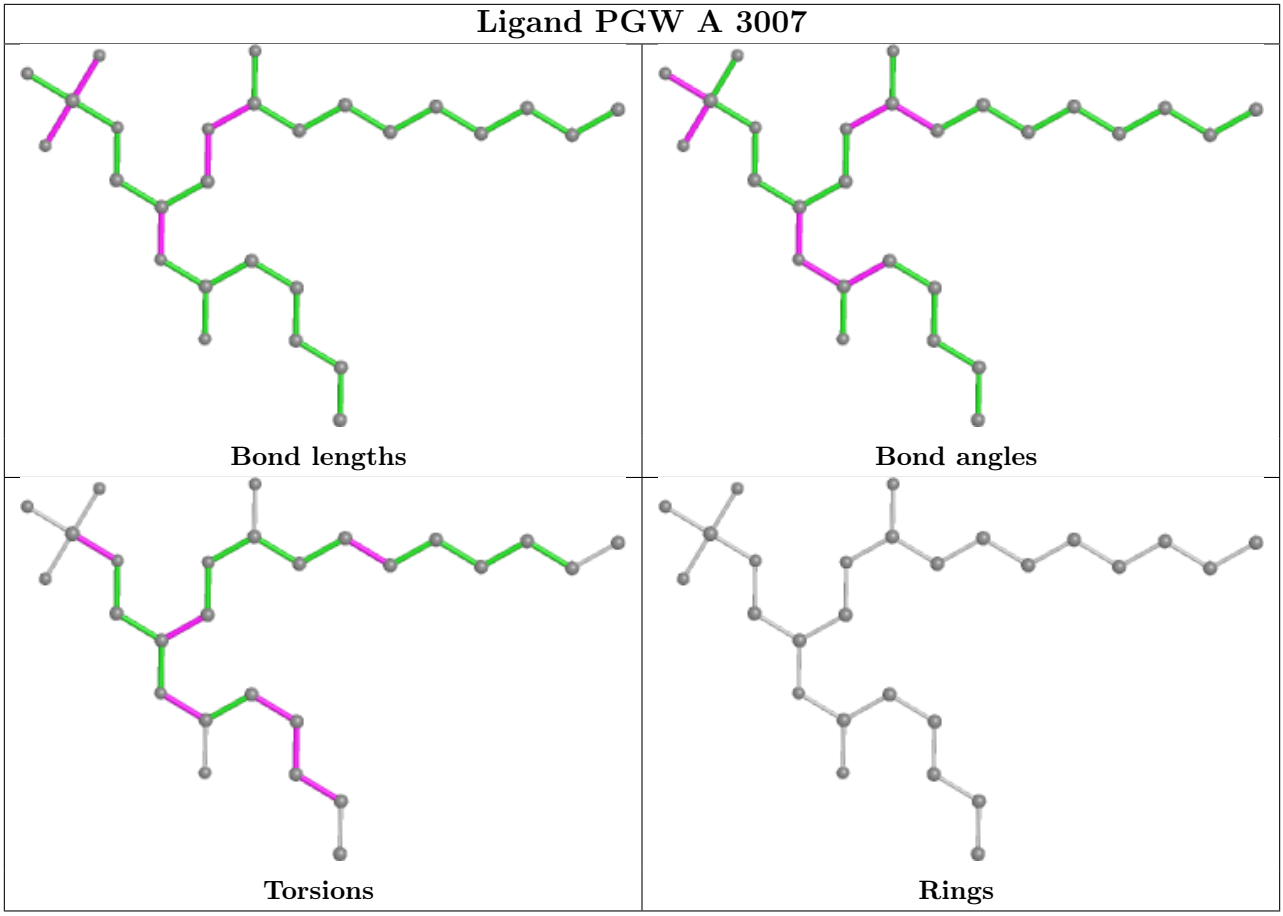
Rings

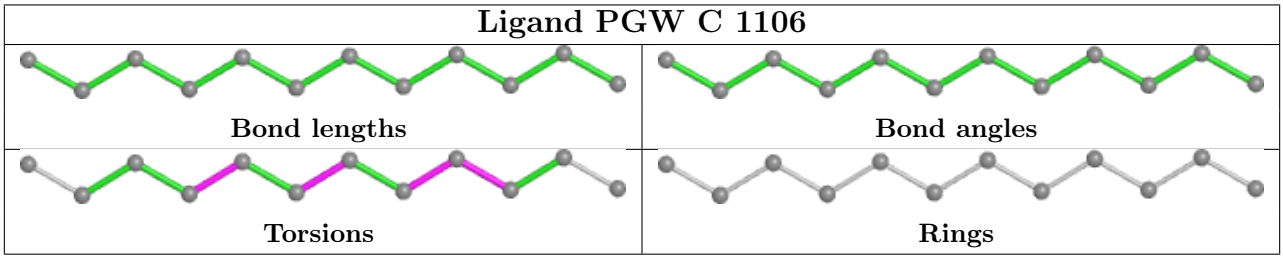
Ligand PGW H 2303



Ligand CLR E 2305







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.

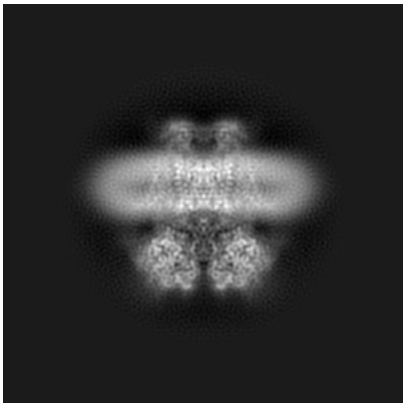
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21028. These allow visual inspection of the internal detail of the map and identification of artifacts.

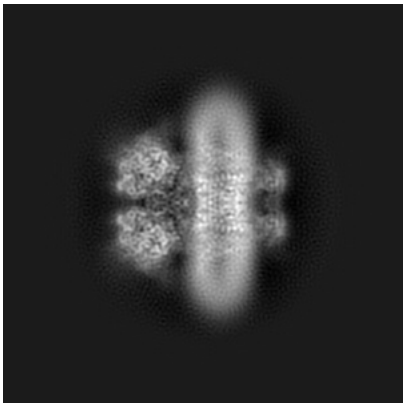
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

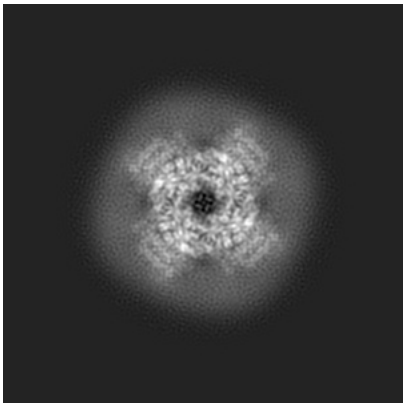
6.1.1 Primary map



X



Y

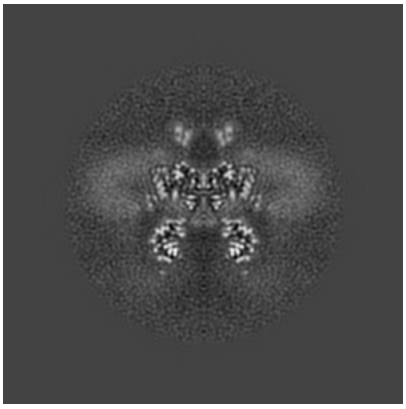


Z

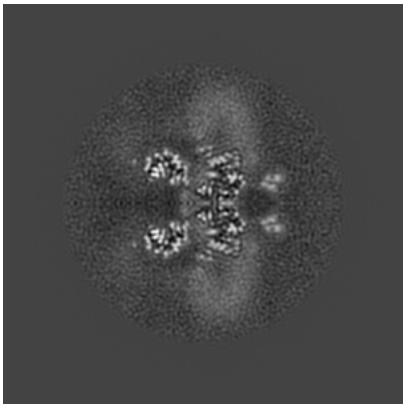
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

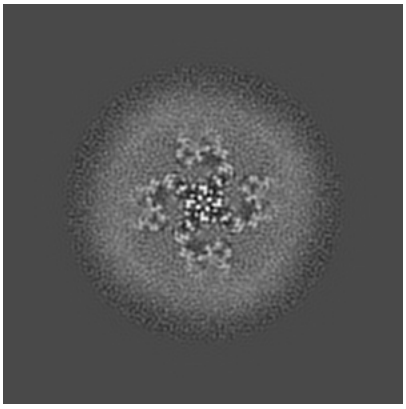
6.2.1 Primary map



X Index: 128



Y Index: 128

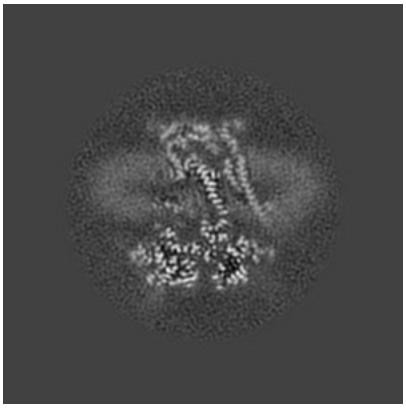


Z Index: 128

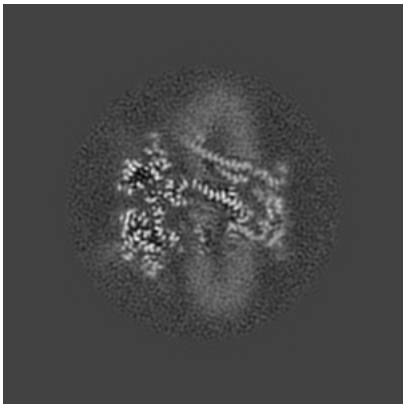
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

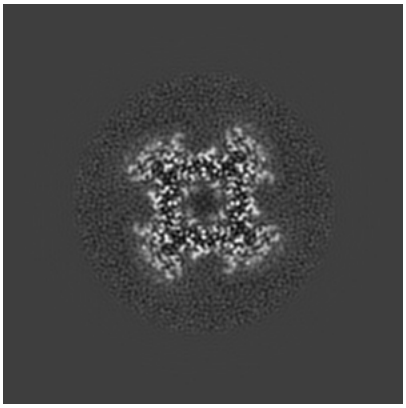
6.3.1 Primary map



X Index: 112



Y Index: 144

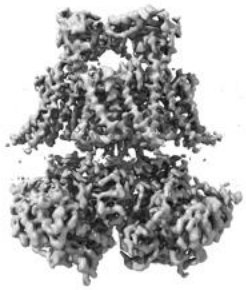


Z Index: 97

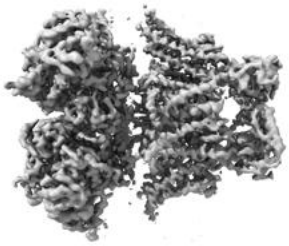
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

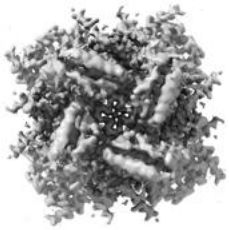
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

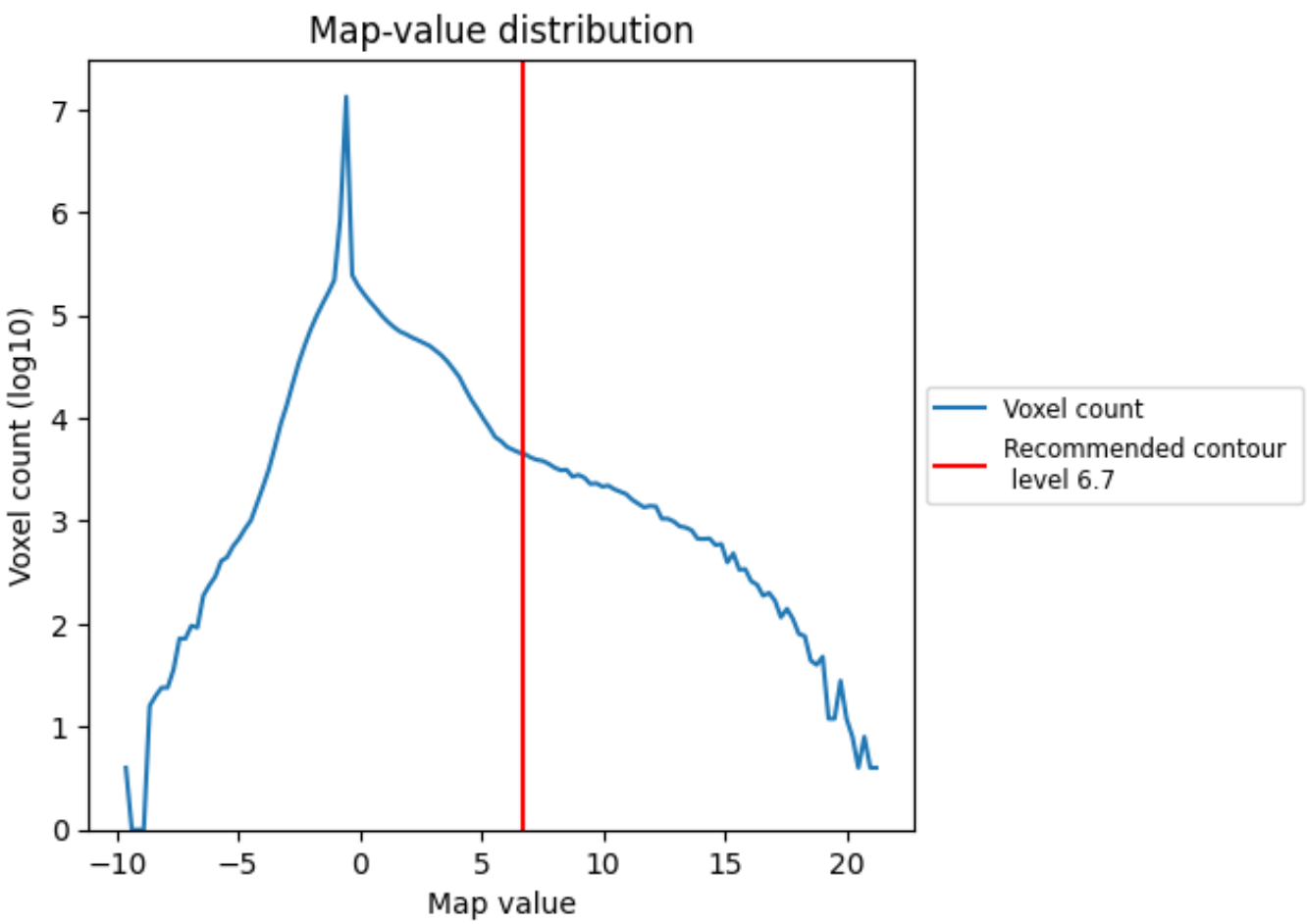
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

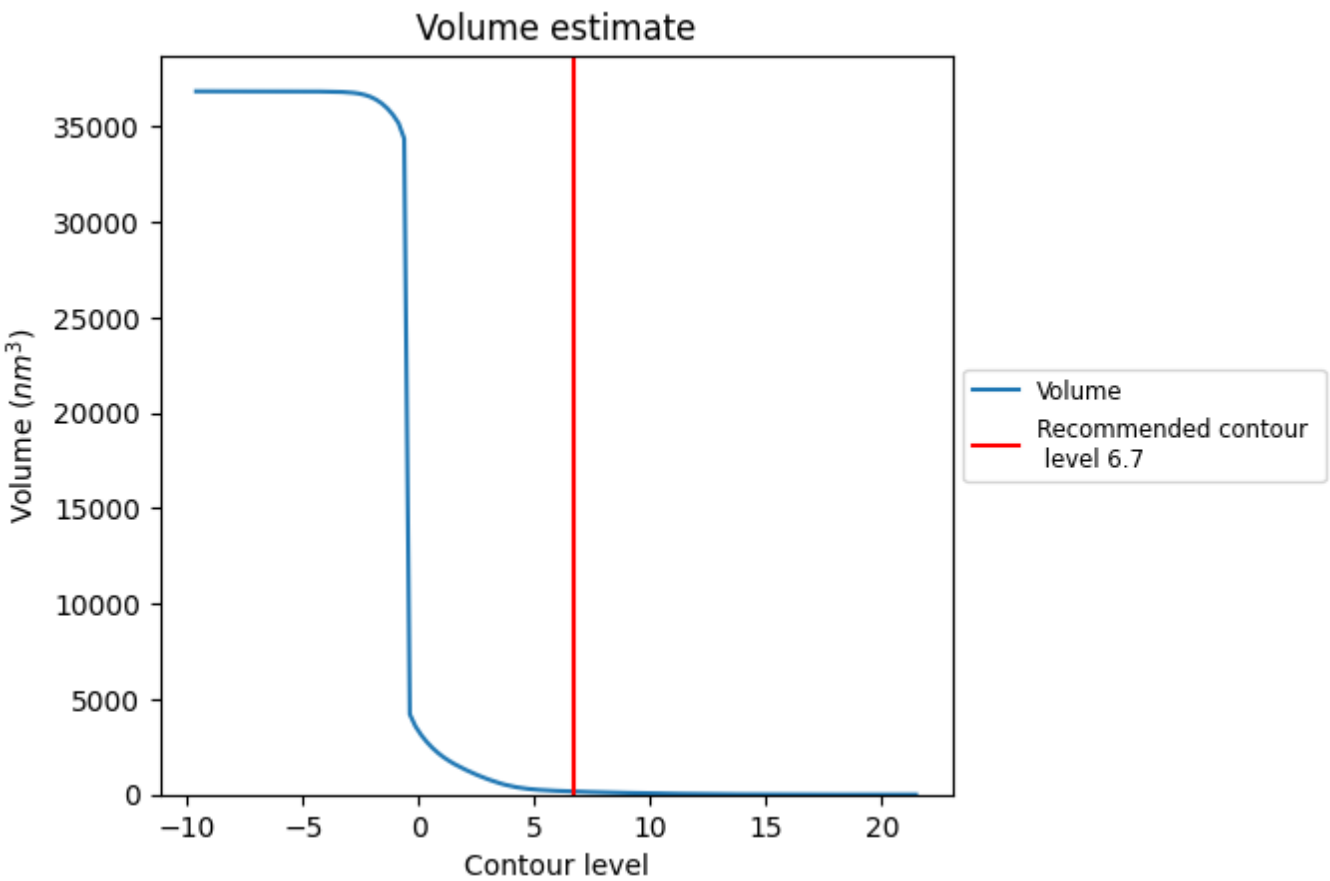
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

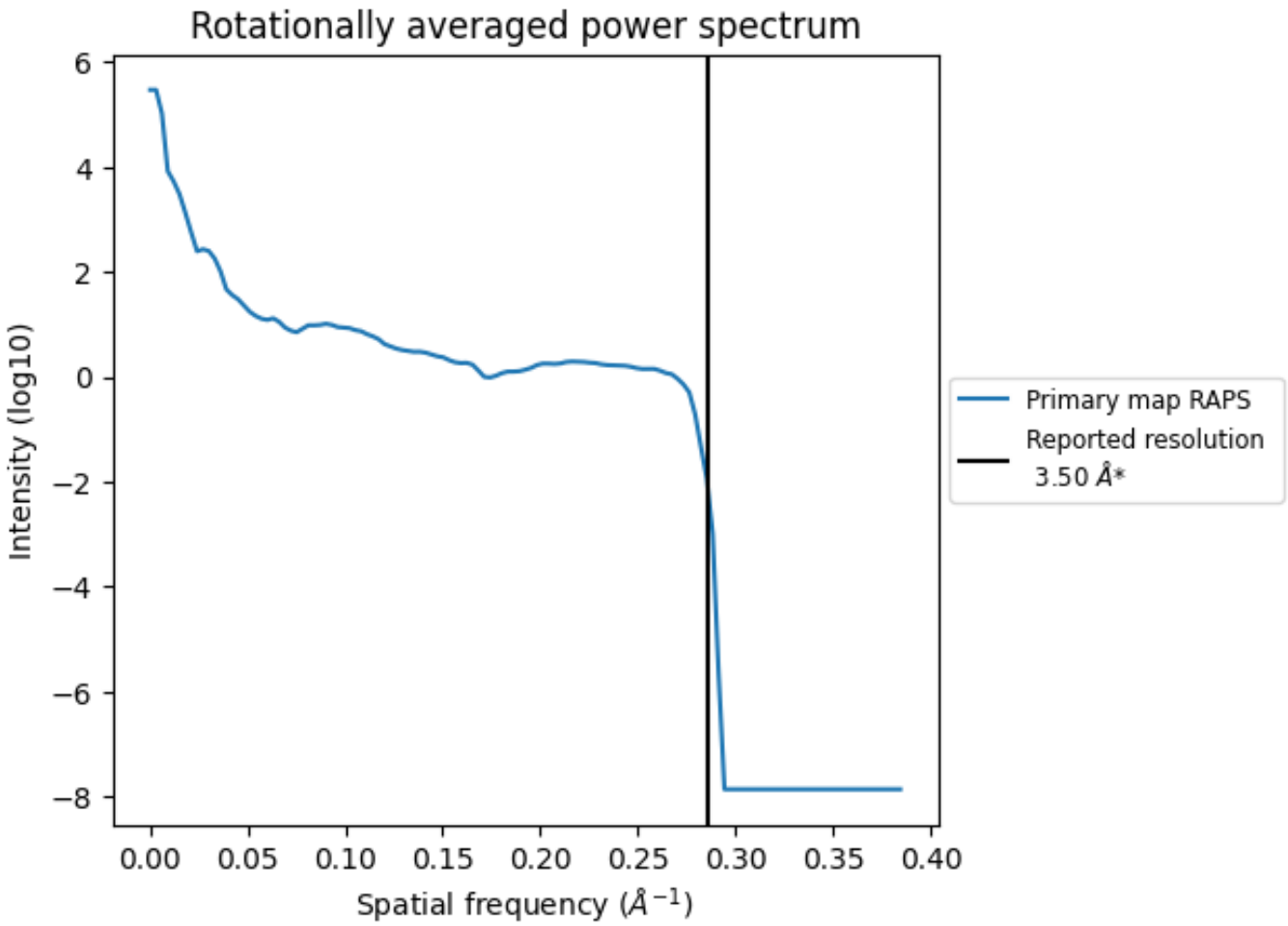
7.2 Volume estimate (i)



The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 146 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

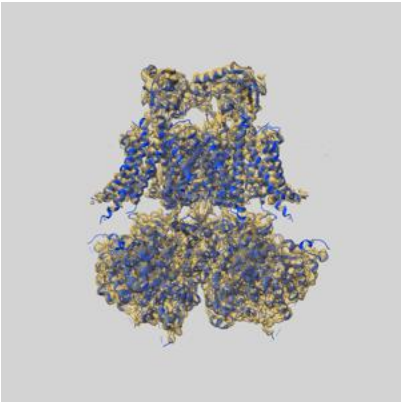
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

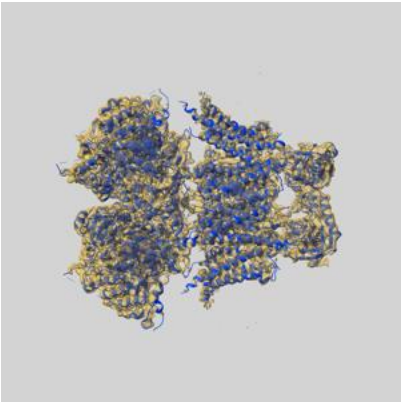
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21028 and PDB model 6V35. Per-residue inclusion information can be found in section 3 on page 10.

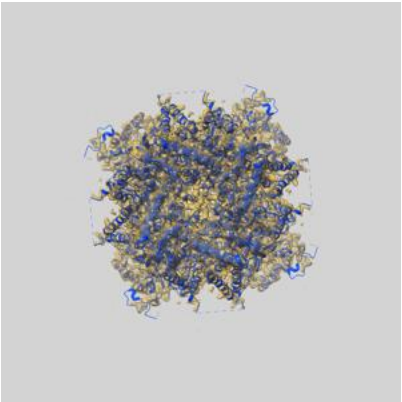
9.1 Map-model overlay (i)



X



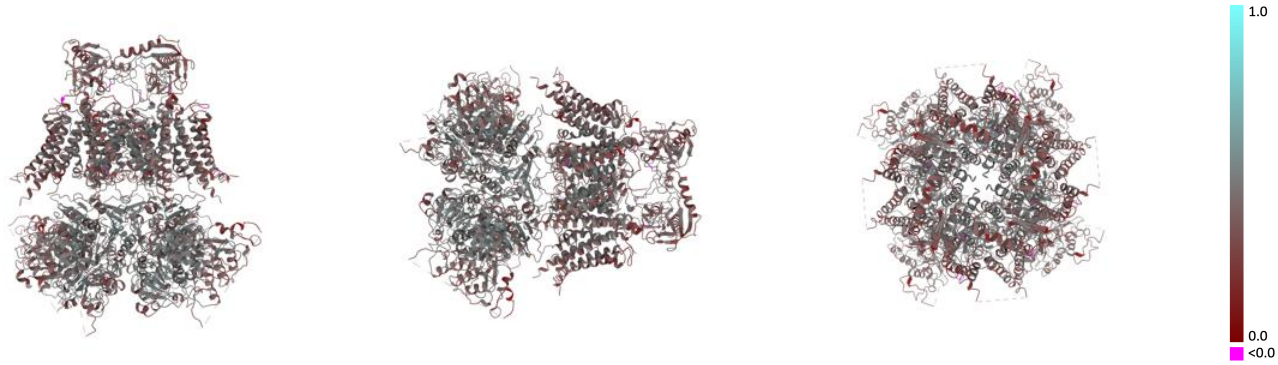
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

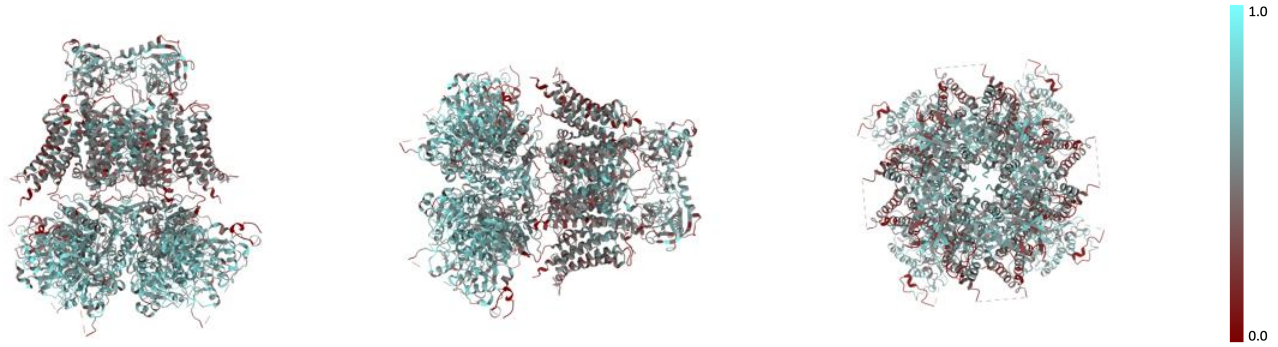
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

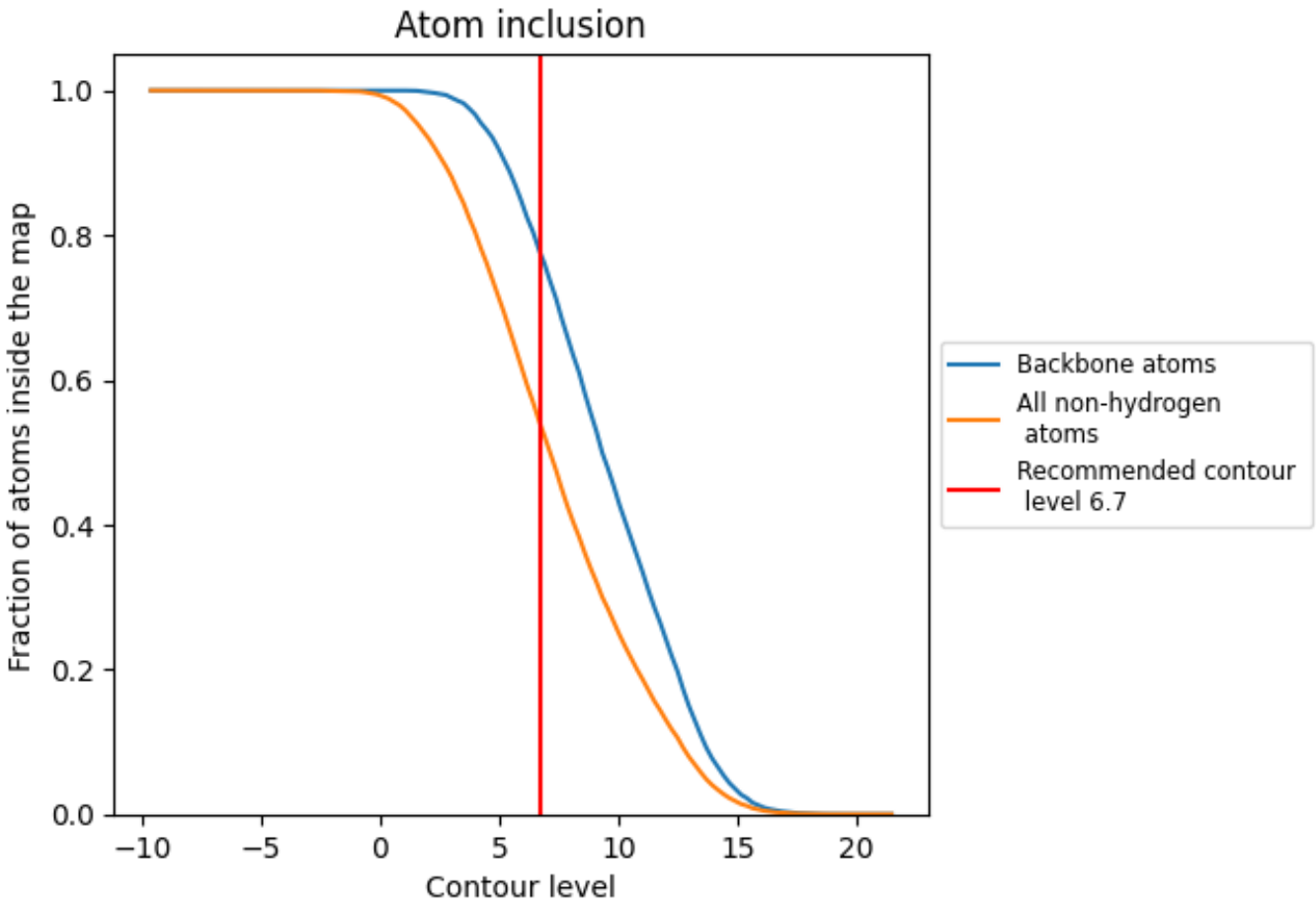
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.7).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (6.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5409	0.4120
A	0.5644	0.4240
B	0.5648	0.4240
C	0.5657	0.4220
D	0.5658	0.4230
E	0.4315	0.3620
F	0.4303	0.3650
G	0.4315	0.3610
H	0.4328	0.3620