wwPDB EM Validation Summary Report

Oct 27, 2024 – 05:02 PM EDT

PDB ID	:	7RK6
EMDB ID	:	EMD-24493
Title	:	Aplysia Slo1 with Barium
Authors	:	Zhu, J.; Srivastava, S.; Cachau, R.; Holmgren, M.
Deposited on	:	2021-07-22
Resolution	:	2.91 Å(reported)
Based on initial model	:	5TJ6

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

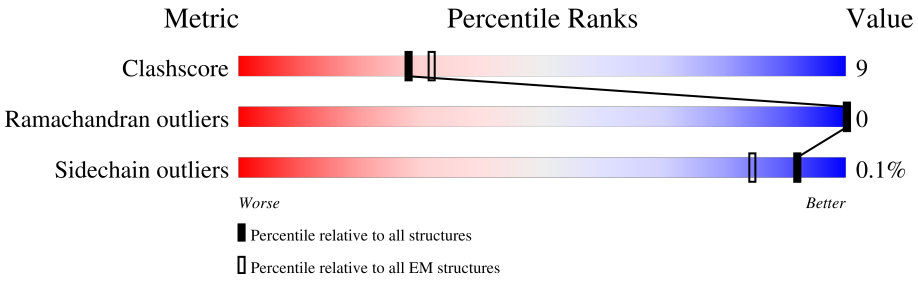
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.91 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1079	11% 62% 20% 17%
1	B	1079	11% 62% 20% 17%
1	C	1079	11% 62% 21% 17%
1	D	1079	11% 63% 20% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 28615 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 BK channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	891	Total	C	N	O	S	0	0
			7104	4598	1175	1289	42		
1	B	891	Total	C	N	O	S	0	0
			7104	4598	1175	1289	42		
1	C	891	Total	C	N	O	S	0	0
			7104	4598	1175	1289	42		
1	D	891	Total	C	N	O	S	0	0
			7104	4598	1175	1289	42		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	conflict	UNP Q5QJC5
A	1071	SER	-	expression tag	UNP Q5QJC5
A	1072	ASN	-	expression tag	UNP Q5QJC5
A	1073	PHE	-	expression tag	UNP Q5QJC5
A	1074	LEU	-	expression tag	UNP Q5QJC5
A	1075	GLU	-	expression tag	UNP Q5QJC5
A	1076	VAL	-	expression tag	UNP Q5QJC5
A	1077	LEU	-	expression tag	UNP Q5QJC5
A	1078	PHE	-	expression tag	UNP Q5QJC5
A	1079	GLN	-	expression tag	UNP Q5QJC5
B	2	ALA	THR	conflict	UNP Q5QJC5
B	1071	SER	-	expression tag	UNP Q5QJC5
B	1072	ASN	-	expression tag	UNP Q5QJC5
B	1073	PHE	-	expression tag	UNP Q5QJC5
B	1074	LEU	-	expression tag	UNP Q5QJC5
B	1075	GLU	-	expression tag	UNP Q5QJC5
B	1076	VAL	-	expression tag	UNP Q5QJC5
B	1077	LEU	-	expression tag	UNP Q5QJC5
B	1078	PHE	-	expression tag	UNP Q5QJC5
B	1079	GLN	-	expression tag	UNP Q5QJC5
C	2	ALA	THR	conflict	UNP Q5QJC5
C	1071	SER	-	expression tag	UNP Q5QJC5

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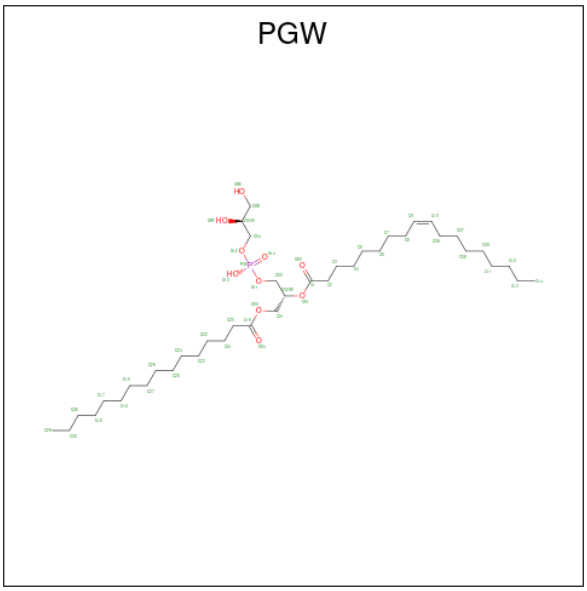
Chain	Residue	Modelled	Actual	Comment	Reference
C	1072	ASN	-	expression tag	UNP Q5QJC5
C	1073	PHE	-	expression tag	UNP Q5QJC5
C	1074	LEU	-	expression tag	UNP Q5QJC5
C	1075	GLU	-	expression tag	UNP Q5QJC5
C	1076	VAL	-	expression tag	UNP Q5QJC5
C	1077	LEU	-	expression tag	UNP Q5QJC5
C	1078	PHE	-	expression tag	UNP Q5QJC5
C	1079	GLN	-	expression tag	UNP Q5QJC5
D	2	ALA	THR	conflict	UNP Q5QJC5
D	1071	SER	-	expression tag	UNP Q5QJC5
D	1072	ASN	-	expression tag	UNP Q5QJC5
D	1073	PHE	-	expression tag	UNP Q5QJC5
D	1074	LEU	-	expression tag	UNP Q5QJC5
D	1075	GLU	-	expression tag	UNP Q5QJC5
D	1076	VAL	-	expression tag	UNP Q5QJC5
D	1077	LEU	-	expression tag	UNP Q5QJC5
D	1078	PHE	-	expression tag	UNP Q5QJC5
D	1079	GLN	-	expression tag	UNP Q5QJC5

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Ba 2 2	0
2	B	2	Total Ba 2 2	0
2	C	2	Total Ba 2 2	0
2	D	2	Total Ba 2 2	0

- 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 9 9	0
3	A	1	Total C 9 9	0
3	A	1	Total C 9 9	0
3	A	1	Total C O P 19 12 6 1	0
3	B	1	Total C 9 9	0
3	B	1	Total C 9 9	0
3	B	1	Total C 9 9	0
3	B	1	Total C O P 19 12 6 1	0
3	C	1	Total C 9 9	0
3	C	1	Total C 9 9	0
3	C	1	Total C 9 9	0
3	C	1	Total C O P 19 12 6 1	0
3	D	1	Total C 9 9	0
3	D	1	Total C 9 9	0

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Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total C 9 9	0
3	D	1	Total C O P 19 12 6 1	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
4	A	3	Total K 3 3	0

- Molecule 5 is water.

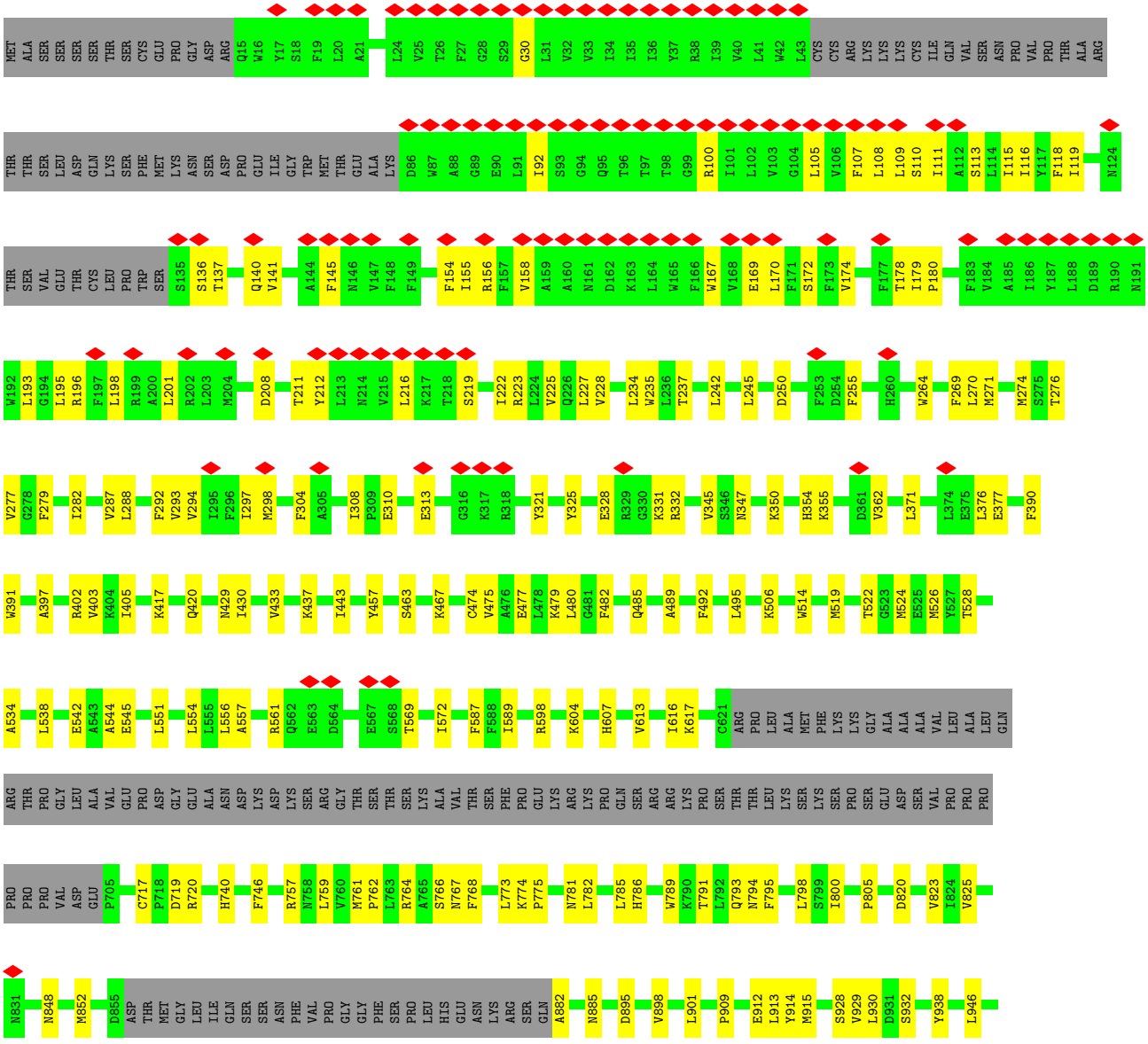
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total O 1 1	0
5	B	1	Total O 1 1	0
5	C	1	Total O 1 1	0
5	D	1	Total O 1 1	0

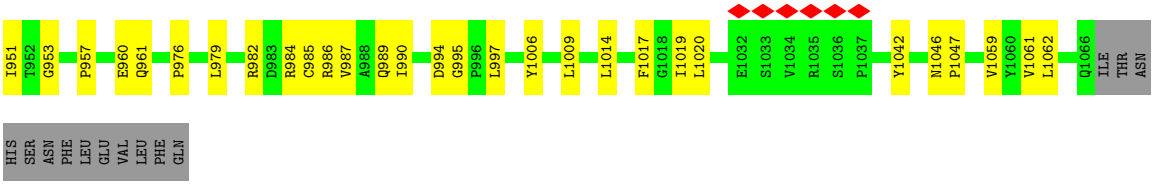
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: BK channel

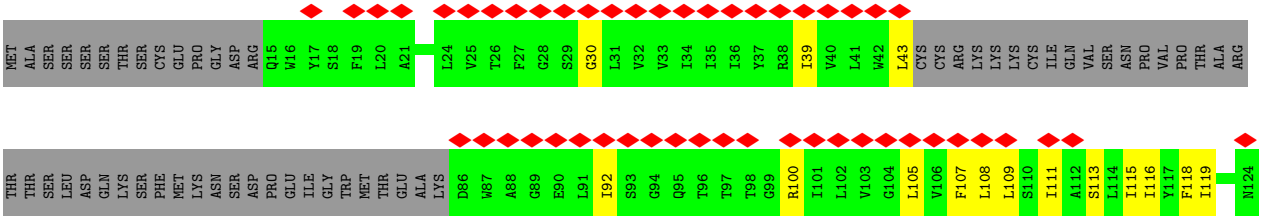
Chain A:

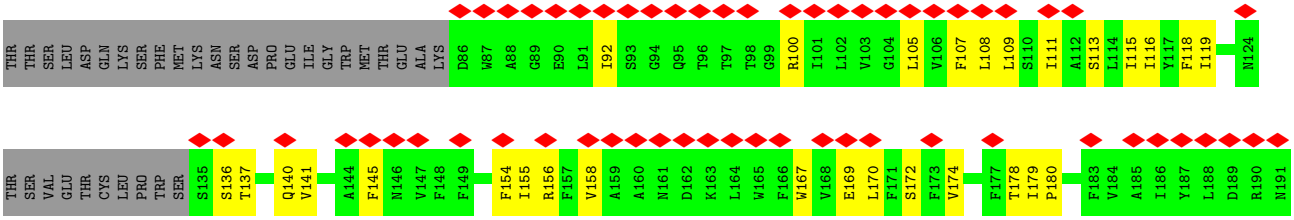


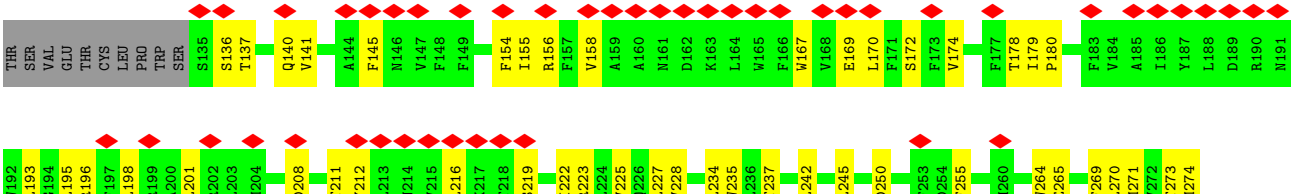


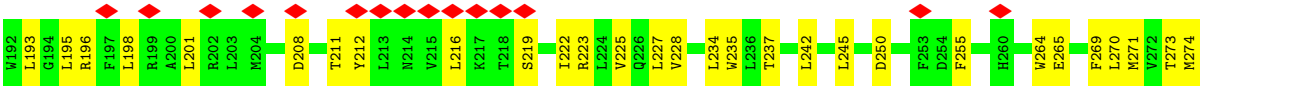
• Molecule 1: BK channel

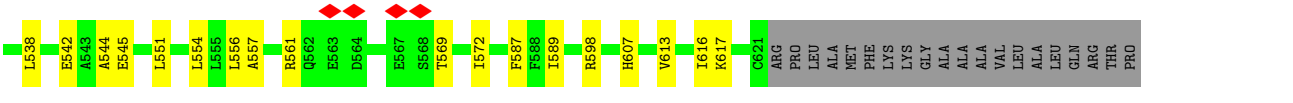
Chain B:

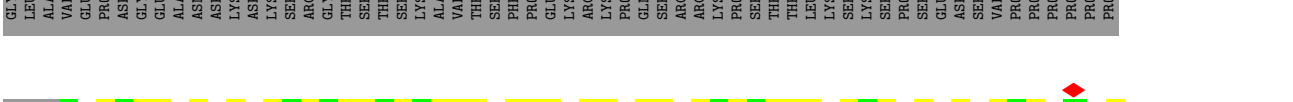


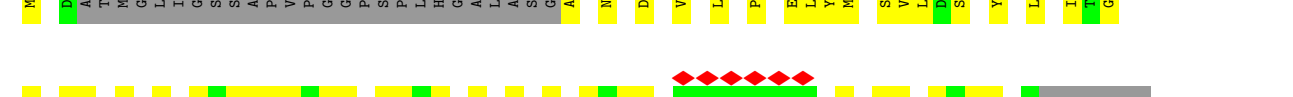


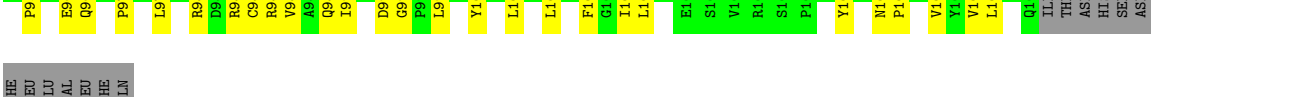






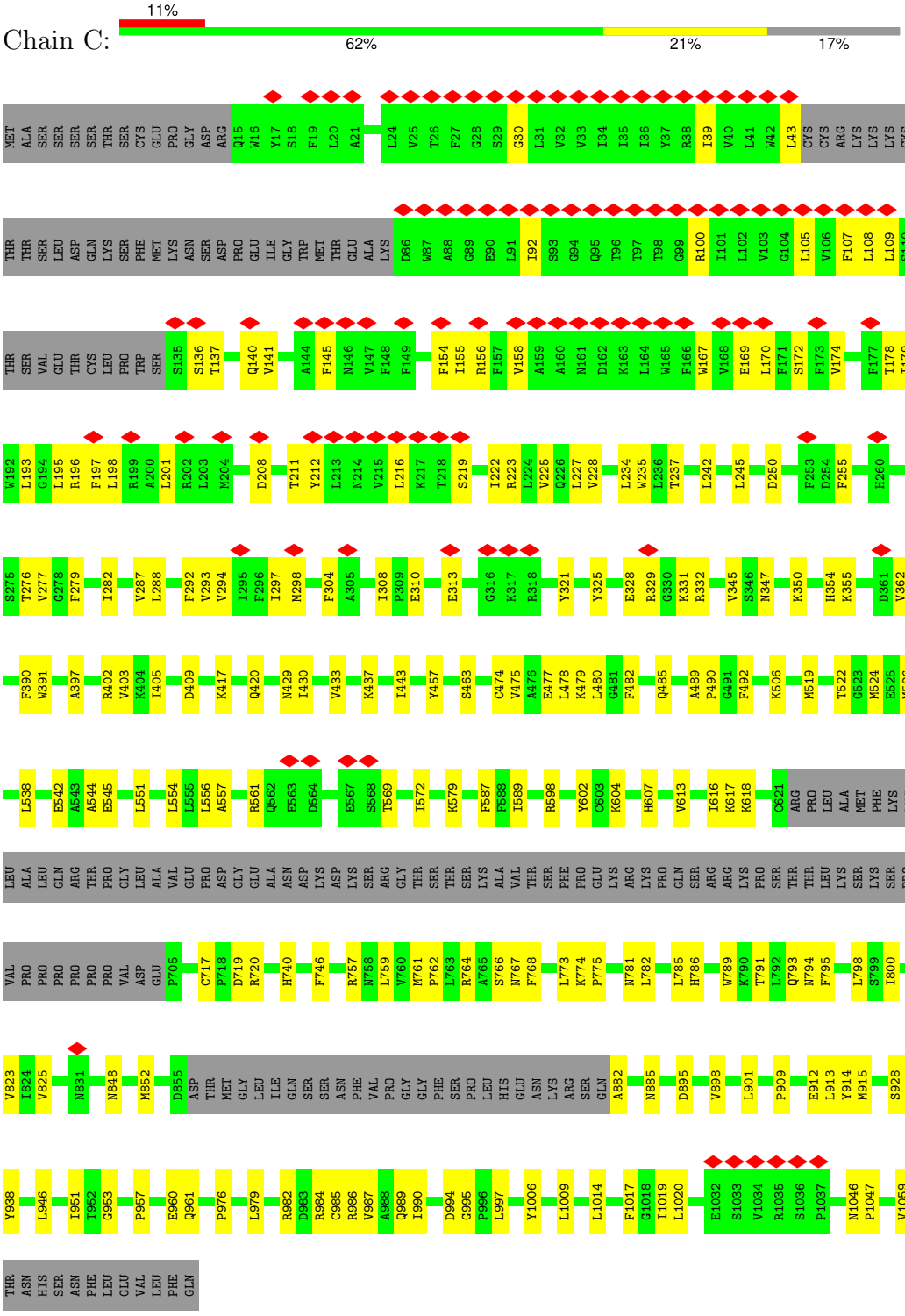






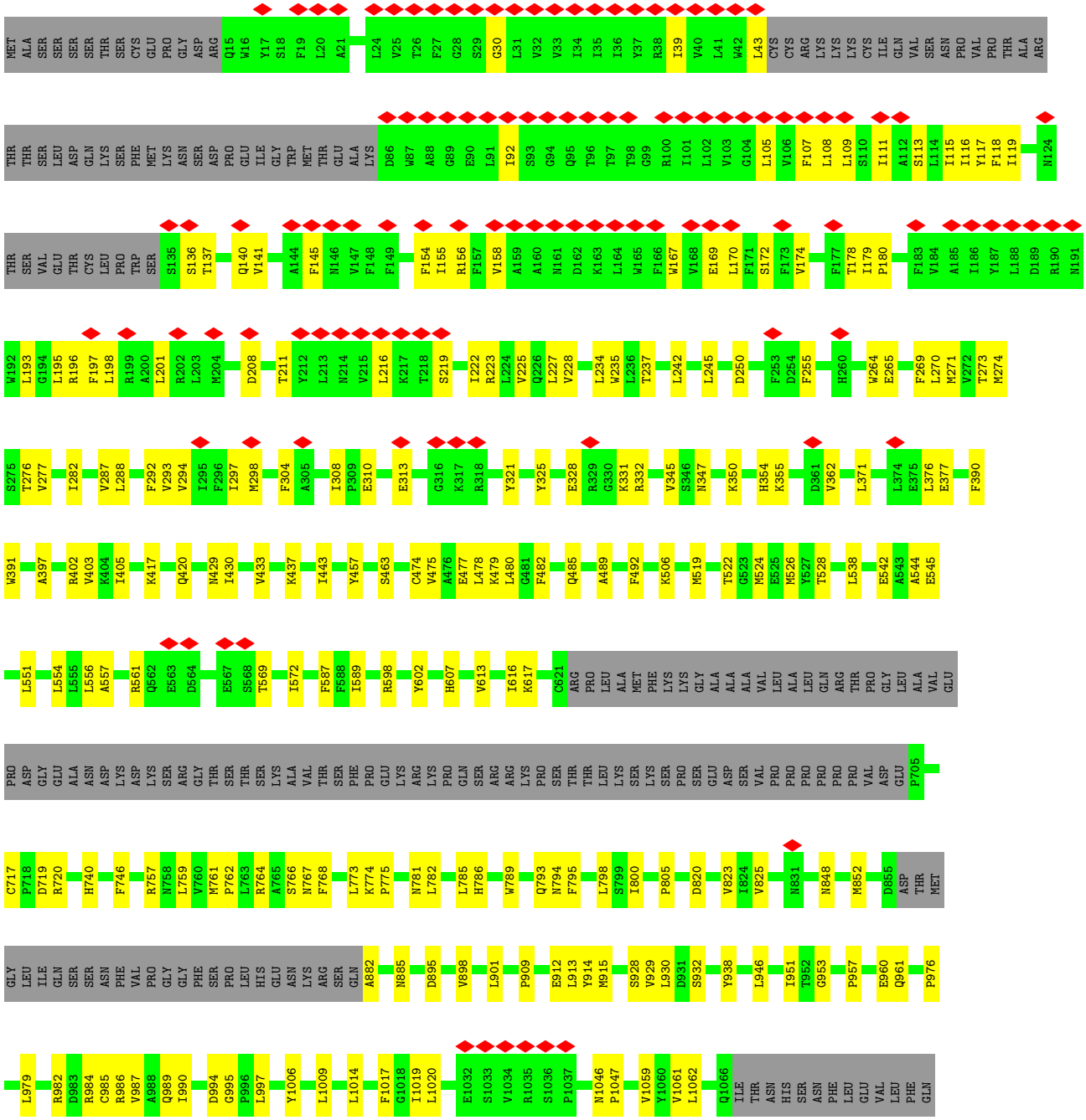
• Molecule 1: BK channel

Chain C:



• Molecule 1: BK channel

Chain D:


MET ALA SER SER SER SER THR SER CYS GLU PRO GLY ASP ARG Q15 W16 Y17 S18 F19 L20 A21 L24 V25 T26 F27 G28 S29 G30 L31 V32 V33 I34 I35 I36 Y37 R38 I39 V40 L41 W42 L43 CYS CYS ARG LYS LYS LYS CYS ILE GLN VAL SER ASN PRO VAL PRO THR ALA ARG
THR THR SER LEU ASP GLN LYS SER PHE MET LYS ASN SER ASP PRO GLU ILE GLY TRP MET THR GLU ALA LYS D86 W87 A88 G89 E90 L91 I92 S93 G94 Q95 T96 T97 T98 G99 R100 I101 L102 V103 G104 L105 V106 F107 L108 L109 S110 I111 A112 S113 K114 I115 I116 Y117 F118 I119 N124
THR SER VAL GLU THR CYS LEU PRO TRP SER S135 S136 T137 Q140 V141 A144 F145 N146 V147 F148 F149 F154 I155 R156 F157 V158 A159 A160 N161 D162 K163 L164 W165 F166 W167 V168 E169 L170 F171 S172 F173 V174 F177 T178 I179 P180 F183 V184 A185 I186 Y187 L188 D189 R190 N191
W192 L193 G194 L195 R196 F197 L198 R199 A200 L201 R202 L203 M204 D208 T211 Y212 L213 N214 V215 L216 K217 T218 S219 I222 R223 L224 V225 Q226 L227 V228 L234 W235 L236 T237 L242 L245 D250 F253 D254 F255 H260 W264 E265 F269 L270 M271 V272 T273 M274
S275 T276 V277 I282 V287 L288 F292 V293 V294 I295 F296 I297 M298 F304 A305 I308 P309 E310 E313 G316 K317 R318 Y321 Y325 E328 R329 G330 K331 R332 V345 S346 N347 K350 H354 K355 D361 V362 L371 L374 E375 L376 E377 F390
W391 A397 R402 V403 K404 I405 K417 Q420 N429 I430 V433 K437 I443 Y457 S463 C474 V475 A476 E477 L478 K479 L480 G481 F482 Q485 A489 F492 K506 M519 T522 G523 M524 E525 M526 Y527 T528 L538 E542 A543 A544 E545
L551 L554 L555 L556 A557 R561 Q562 E563 D564 E567 S568 T569 I572 F587 F588 I589 R598 Y602 H607 V613 I616 K617 C621 ARG PRO LEU ALA MET PHE LYS LYS GLY ALA ALA ALA VAL LEU ALA LEU GLN ARG THR PRO GLY LEU ALA VAL GLU
PRO ASP GLY GLU ALA ASN ASP LYS ASP LYS SER SER ARG GLY THR SER THR SER LYS ALA VAL THR SER PHE PRO GLU LYS ARG LYS PRO GLN SER ARG ARG ARG LYS PRO SER THR THR LEU LYS SER LYS SER PRO SER GLU ASP SER VAL PRO PRO PRO PRO PRO PRO VAL ASP GLU P705
C717 P718 D719 R720 H740 F746 R757 N758 L759 V760 M761 P762 L763 R764 A765 S766 N767 F768 L773 K774 P775 N781 L782 L785 H786 W789 Q793 N794 F795 L798 S799 I800 P805 D820 V823 I824 V825 N831 N848 M852 D855 ASP THR MET
GLY LEU ILE GLN SER SER ASN PHE VAL PRO GLY GLY PHE SER PRO LEU HIS GLU ASN LYS ARG SER GLN A882 N885 D895 V898 L901 P909 E912 L913 Y914 M915 S928 Y929 L930 D931 S932 Y938 L946 I951 T952 G953 P957 E960 Q961 P976
L979 R982 D983 R984 C985 R986 V987 A988 Q989 I990 D994 G995 P996 L997 Y1006 L1009 L1014 F1017 G1018 I1019 L1020 E1032 S1033 V1034 R1035 S1036 P1037 N1046 P1047 V1059 Y1060 V1061 L1062 Q1066 ILE THR ASN HIS SER ASN PHE LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	973760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	44.569	Depositor
Minimum map value	-20.460	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (Å)	340.48, 340.48, 340.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGW, BA, K

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	0.26	0/7272	0.47	0/9869
1	B	0.26	0/7272	0.47	0/9869
1	C	0.26	0/7272	0.47	0/9869
1	D	0.26	0/7272	0.47	0/9869
All	All	0.26	0/29088	0.47	0/39476

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

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	7104	0	7064	136	0
1	B	7104	0	7064	136	0
1	C	7104	0	7064	142	0
1	D	7104	0	7064	136	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	46	0	57	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	46	0	57	4	0
3	C	46	0	57	4	0
3	D	46	0	57	4	0
4	A	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	28615	0	28484	539	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 9.

The worst 5 of 539 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:SER:O	1:A:982:ARG:NH1	2.26	0.69
1:C:766:SER:O	1:C:982:ARG:NH1	2.26	0.69
1:C:480:LEU:HD22	1:C:759:LEU:HB2	1.76	0.68
1:B:480:LEU:HD22	1:B:759:LEU:HB2	1.76	0.68
1:D:766:SER:O	1:D:982:ARG:NH1	2.26	0.68

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	881/1079 (82%)	843 (96%)	38 (4%)	0	100	100
1	B	881/1079 (82%)	843 (96%)	38 (4%)	0	100	100
1	C	881/1079 (82%)	843 (96%)	38 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	881/1079 (82%)	843 (96%)	38 (4%)	0	100	100
All	All	3524/4316 (82%)	3372 (96%)	152 (4%)	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	777/945 (82%)	776 (100%)	1 (0%)	92	98
1	B	777/945 (82%)	776 (100%)	1 (0%)	92	98
1	C	777/945 (82%)	776 (100%)	1 (0%)	92	98
1	D	777/945 (82%)	776 (100%)	1 (0%)	92	98
All	All	3108/3780 (82%)	3104 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	LYS
1	B	355	LYS
1	C	355	LYS
1	D	355	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	460	ASN
1	D	406	GLN
1	D	460	ASN
1	D	454	ASN
1	B	383	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 11 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PGW	B	1106	-	18,18,50	2.33	3 (16%)	21,21,56	1.49	1 (4%)
3	PGW	C	1105	-	8,8,50	1.71	1 (12%)	7,7,56	0.90	0
3	PGW	A	1105	-	8,8,50	1.71	1 (12%)	7,7,56	0.91	0
3	PGW	B	1103	-	8,8,50	0.76	0	7,7,56	0.42	0
3	PGW	D	1105	-	8,8,50	1.71	1 (12%)	7,7,56	0.91	0
3	PGW	D	1106	-	18,18,50	2.33	3 (16%)	21,21,56	1.48	1 (4%)
3	PGW	A	1104	-	8,8,50	0.76	0	7,7,56	0.41	0
3	PGW	D	1104	-	8,8,50	0.76	0	7,7,56	0.41	0
3	PGW	C	1104	-	8,8,50	0.75	0	7,7,56	0.41	0
3	PGW	D	1103	-	8,8,50	0.76	0	7,7,56	0.42	0
3	PGW	A	1103	-	8,8,50	0.76	0	7,7,56	0.42	0
3	PGW	C	1106	-	18,18,50	2.33	3 (16%)	21,21,56	1.48	1 (4%)
3	PGW	B	1105	-	8,8,50	1.71	1 (12%)	7,7,56	0.91	0
3	PGW	B	1104	-	8,8,50	0.75	0	7,7,56	0.42	0
3	PGW	C	1103	-	8,8,50	0.76	0	7,7,56	0.42	0
3	PGW	A	1106	-	18,18,50	2.33	3 (16%)	21,21,56	1.48	1 (4%)

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	B	1106	-	-	10/17/17/55	-
3	PGW	C	1105	-	-	2/6/6/55	-
3	PGW	A	1105	-	-	2/6/6/55	-
3	PGW	B	1103	-	-	6/6/6/55	-
3	PGW	D	1105	-	-	2/6/6/55	-
3	PGW	D	1106	-	-	10/17/17/55	-
3	PGW	A	1104	-	-	6/6/6/55	-
3	PGW	D	1104	-	-	6/6/6/55	-
3	PGW	C	1104	-	-	6/6/6/55	-
3	PGW	D	1103	-	-	6/6/6/55	-
3	PGW	A	1103	-	-	6/6/6/55	-
3	PGW	C	1106	-	-	10/17/17/55	-
3	PGW	B	1105	-	-	2/6/6/55	-
3	PGW	B	1104	-	-	6/6/6/55	-
3	PGW	C	1103	-	-	6/6/6/55	-
3	PGW	A	1106	-	-	10/17/17/55	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1106	PGW	P-O14	7.40	1.73	1.50
3	A	1106	PGW	P-O14	7.39	1.73	1.50
3	C	1106	PGW	P-O14	7.39	1.73	1.50
3	D	1106	PGW	P-O14	7.39	1.73	1.50
3	A	1106	PGW	P-O11	4.52	1.74	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1106	PGW	O13-P-O12	5.12	127.01	107.80
3	A	1106	PGW	O13-P-O12	5.11	126.96	107.80
3	C	1106	PGW	O13-P-O12	5.11	126.96	107.80
3	D	1106	PGW	O13-P-O12	5.11	126.96	107.80

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

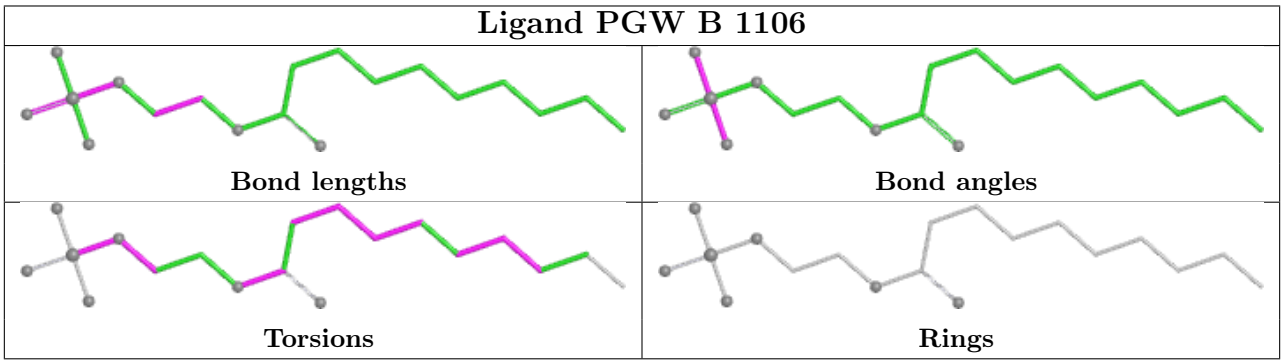
Mol	Chain	Res	Type	Atoms
3	A	1106	PGW	C03-O11-P-O13
3	A	1106	PGW	C02-C03-O11-P
3	B	1106	PGW	C03-O11-P-O13
3	B	1106	PGW	C02-C03-O11-P
3	C	1106	PGW	C03-O11-P-O13

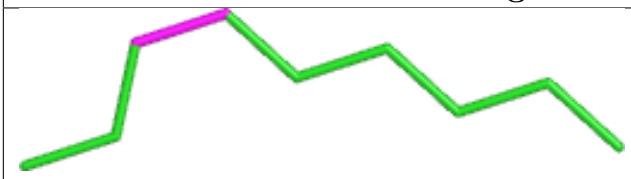
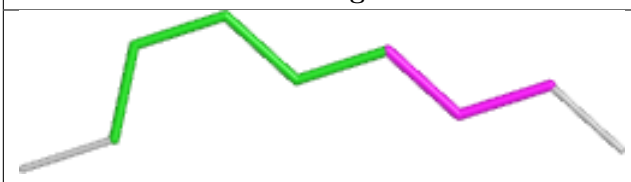
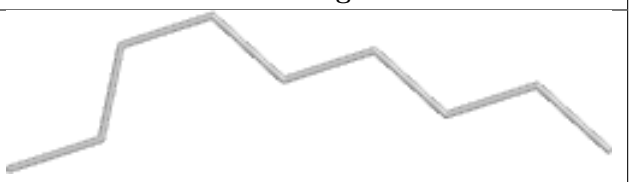
There are no ring outliers.

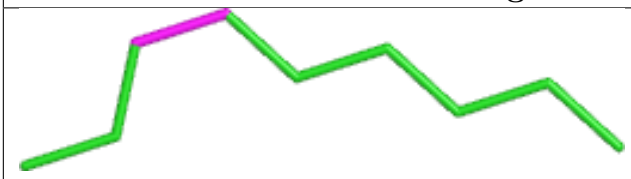
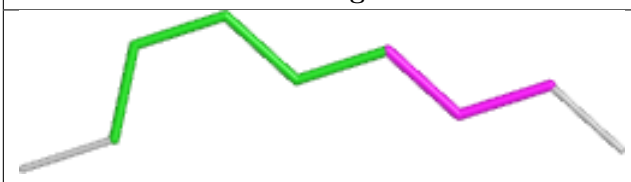
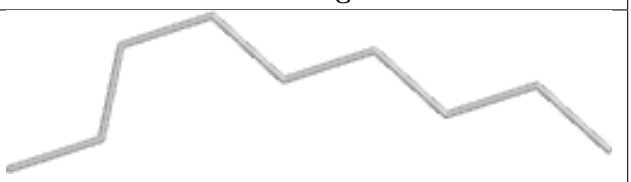
8 monomers are involved in 15 short contacts:

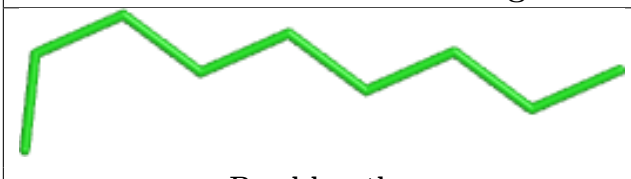
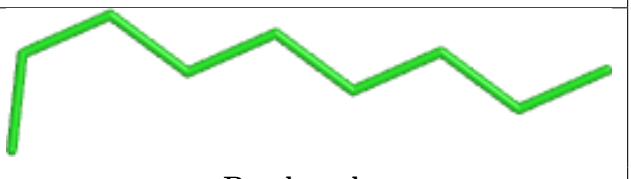
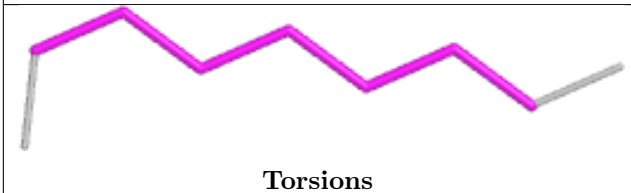
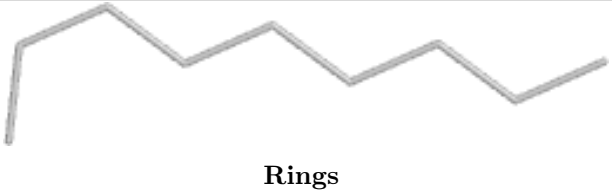
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1106	PGW	3	0
3	B	1103	PGW	1	0
3	D	1106	PGW	3	0
3	D	1103	PGW	1	0
3	A	1103	PGW	1	0
3	C	1106	PGW	3	0
3	C	1103	PGW	1	0
3	A	1106	PGW	2	0

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

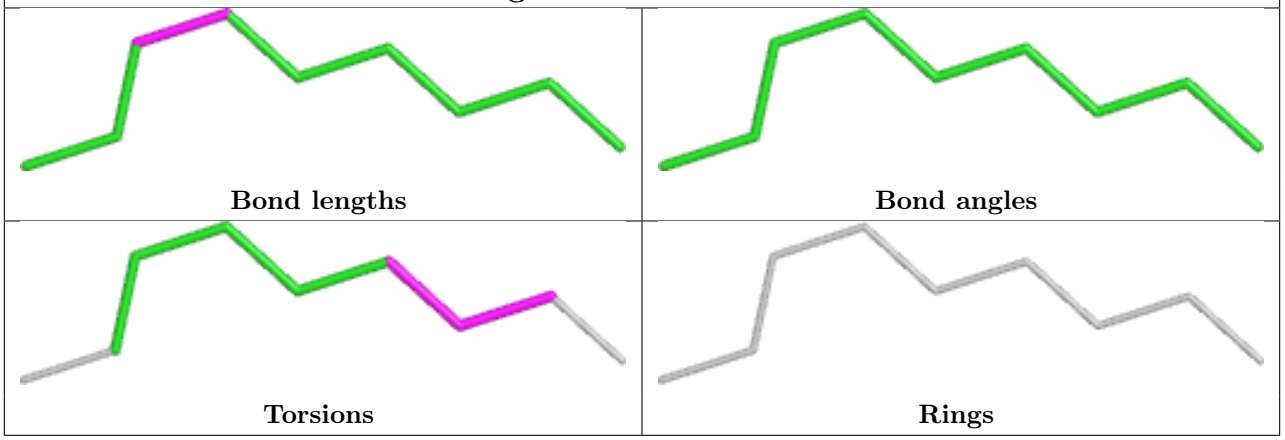


Ligand PGW C 1105	
 Bond lengths	Bond angles
 Torsions	 Rings

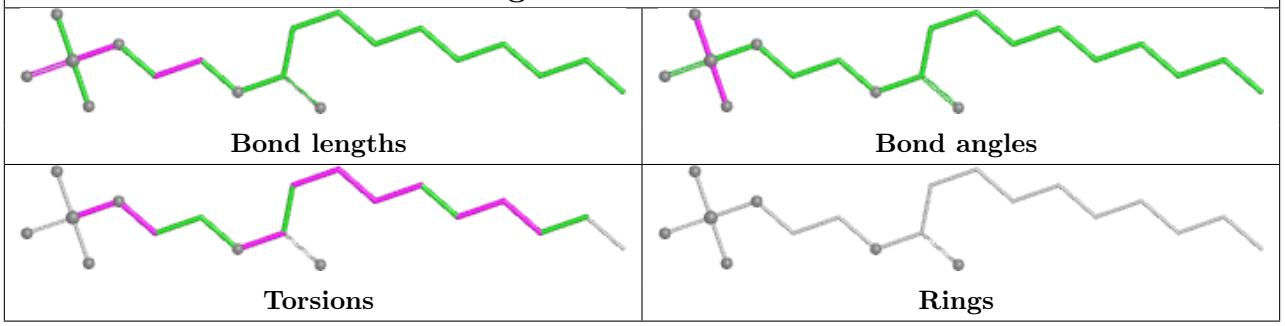
Ligand PGW A 1105	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand PGW B 1103	
 Bond lengths	 Bond angles
 Torsions	 Rings

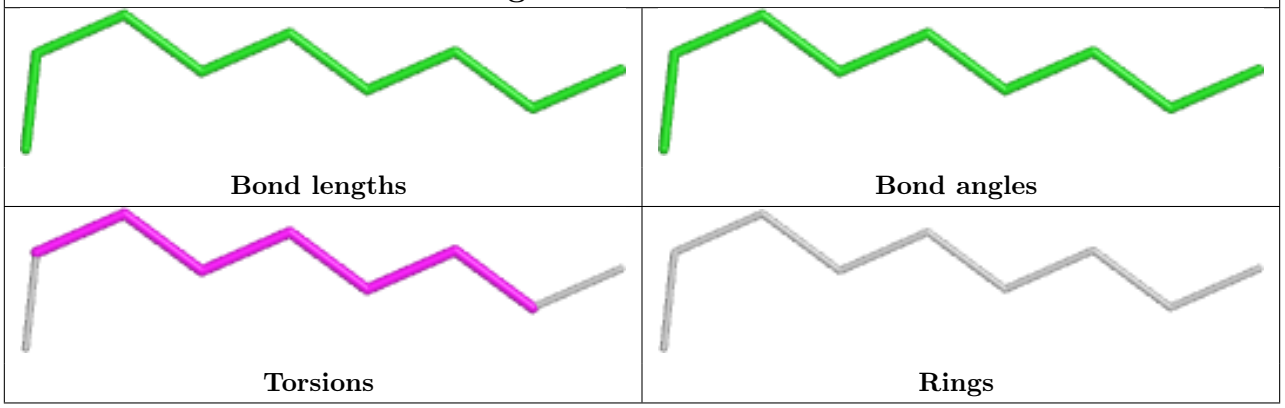
Ligand PGW D 1105



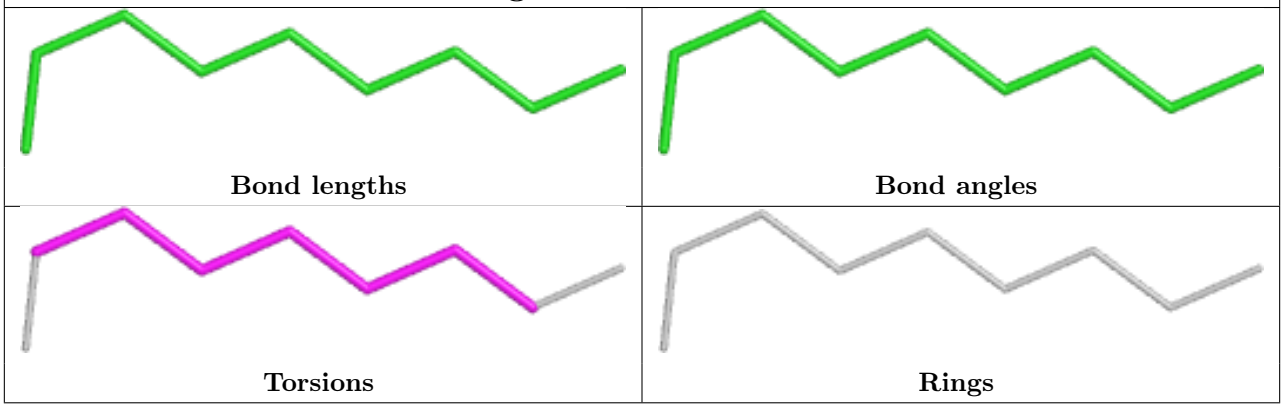
Ligand PGW D 1106



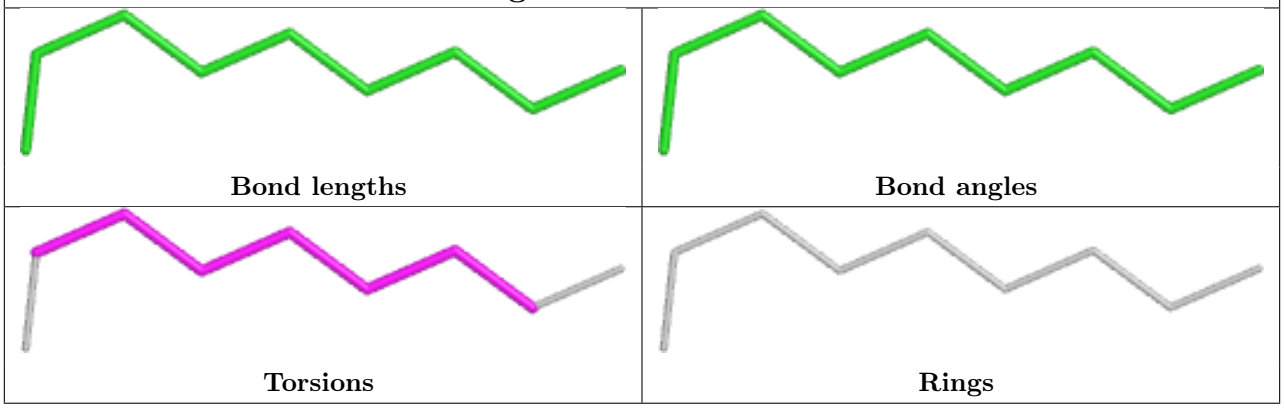
Ligand PGW A 1104



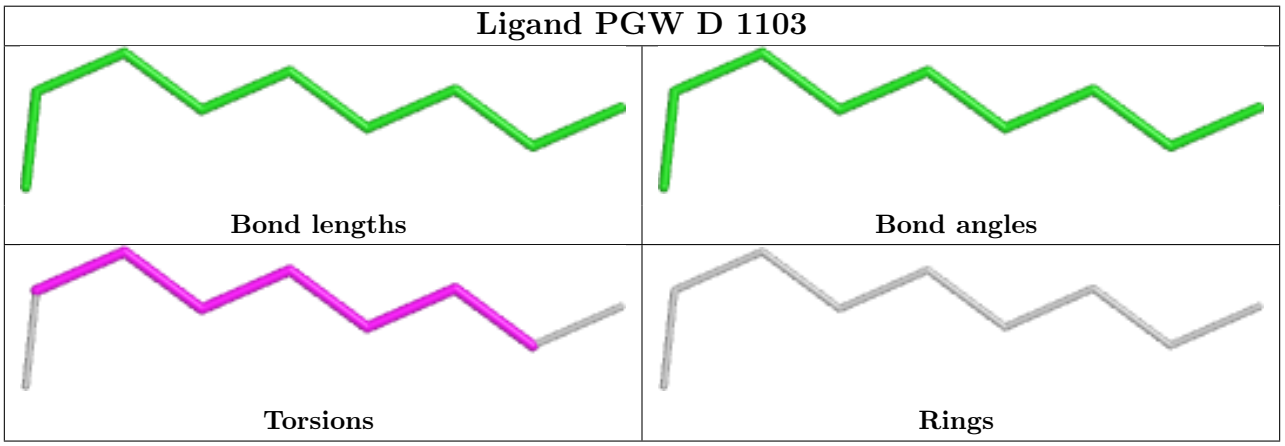
Ligand PGW D 1104



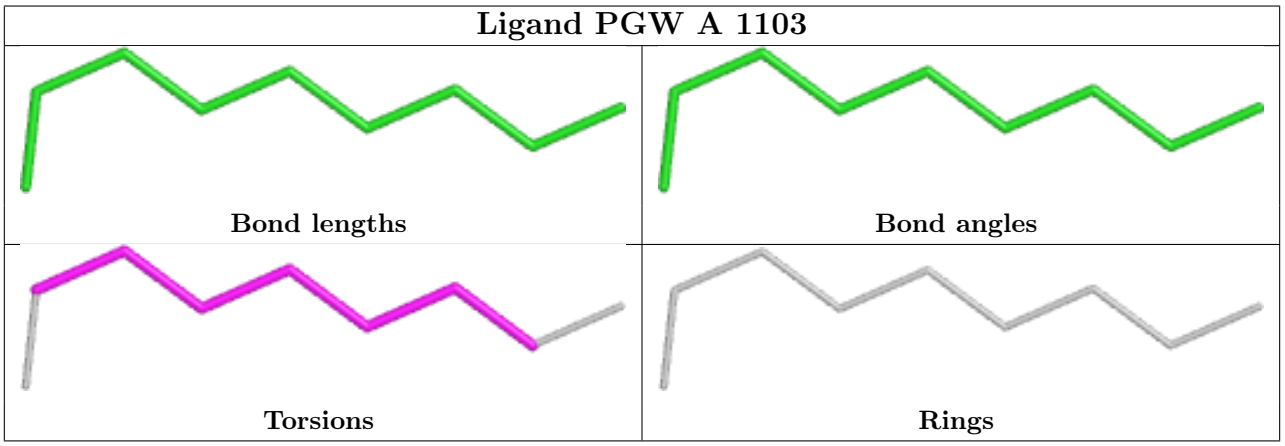
Ligand PGW C 1104



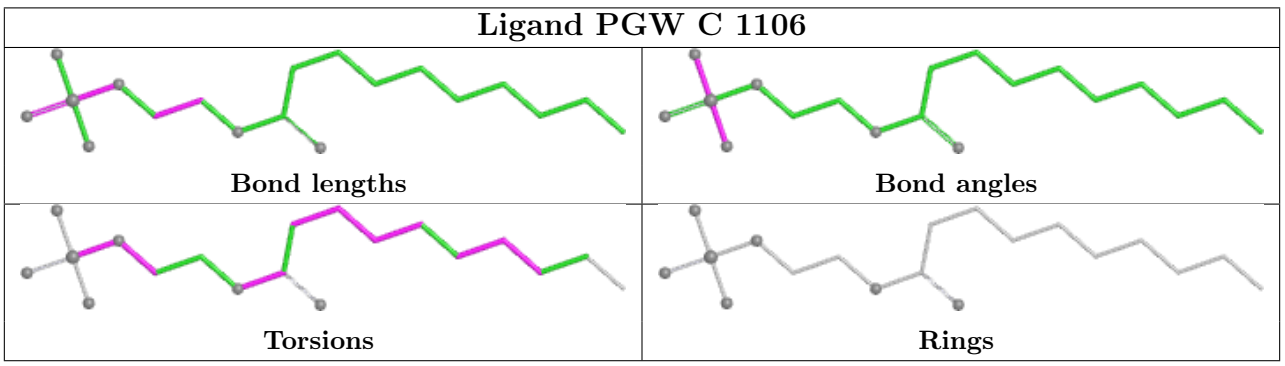
Ligand PGW D 1103



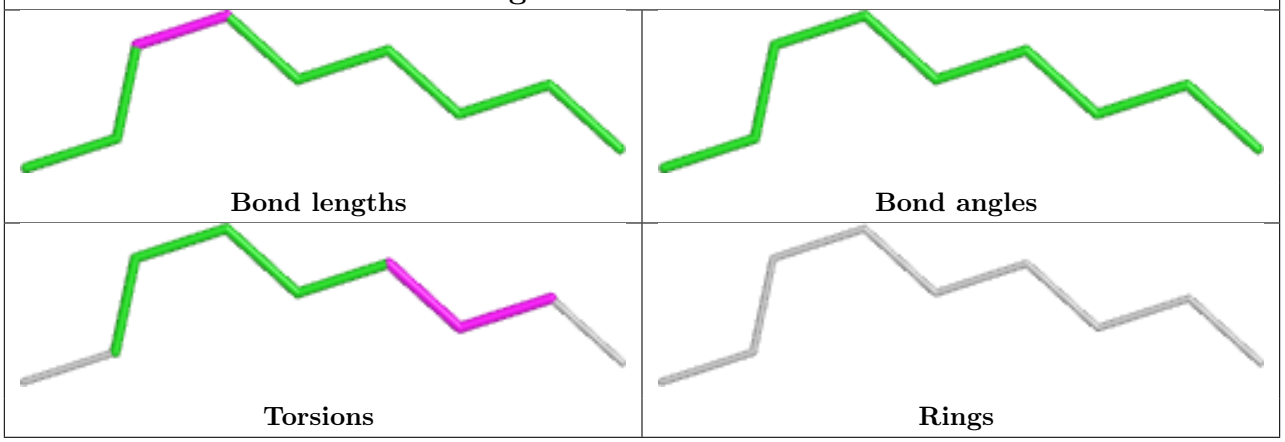
Ligand PGW A 1103



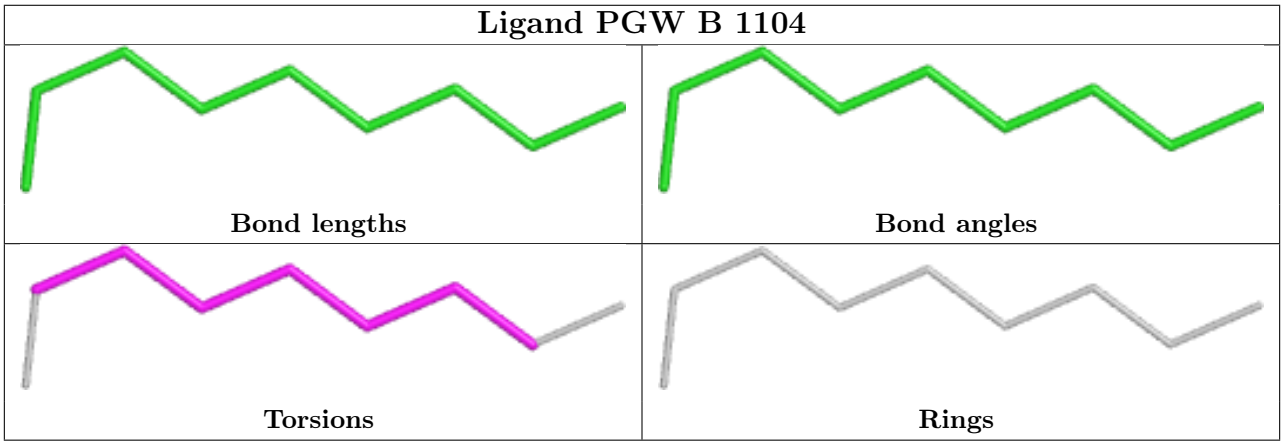
Ligand PGW C 1106



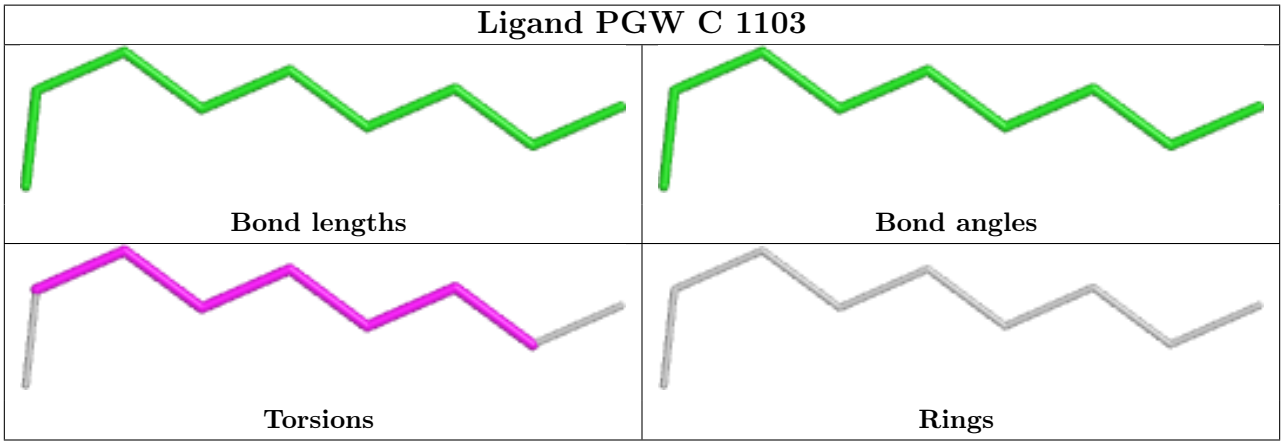
Ligand PGW B 1105



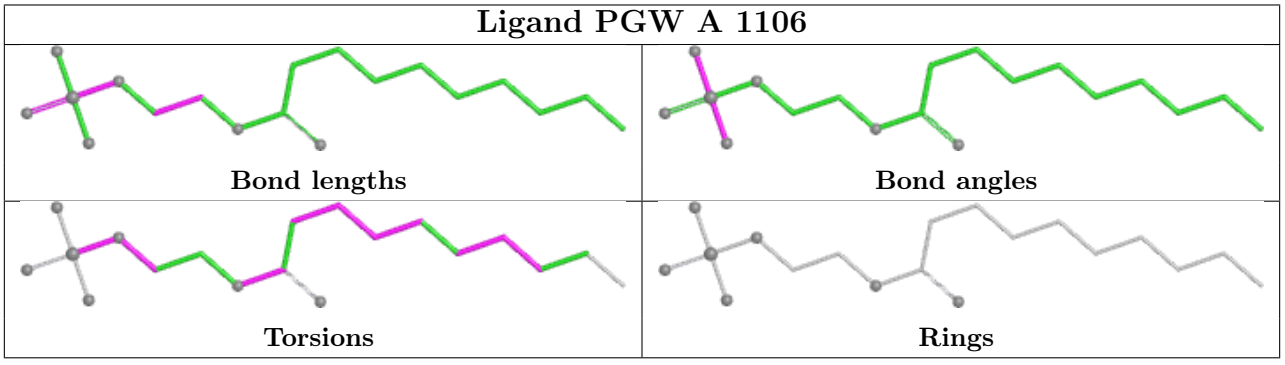
Ligand PGW B 1104



Ligand PGW C 1103



Ligand PGW A 1106



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.

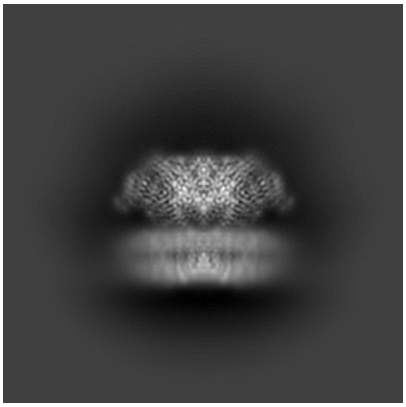
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24493. These allow visual inspection of the internal detail of the map and identification of artifacts.

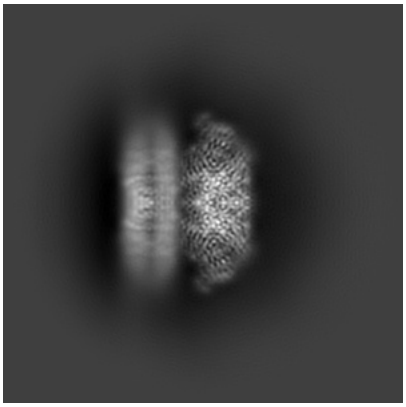
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

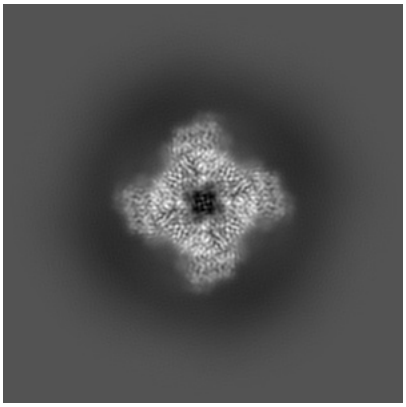
6.1.1 Primary map



X



Y



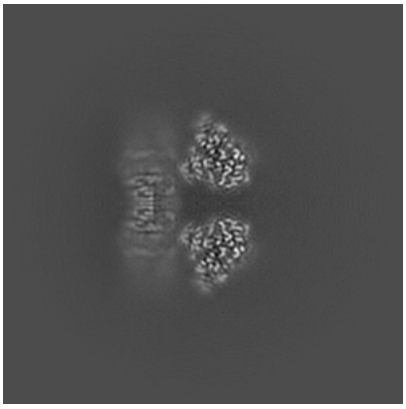
Z

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

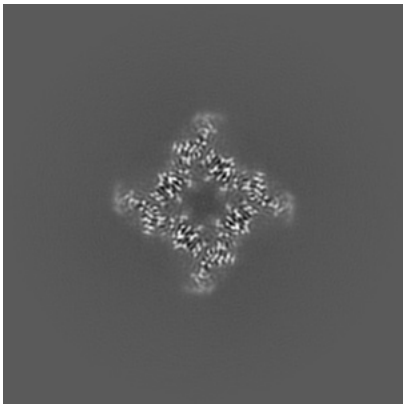
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128



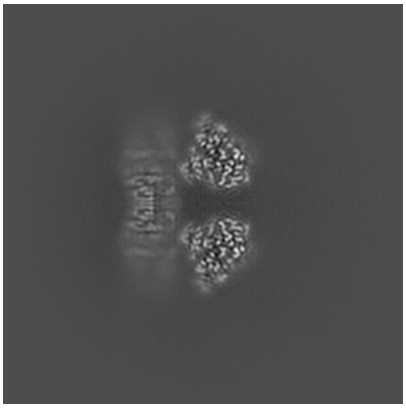
Z Index: 128

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

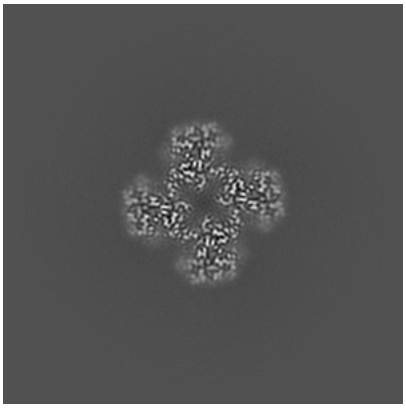
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 128



Y Index: 128

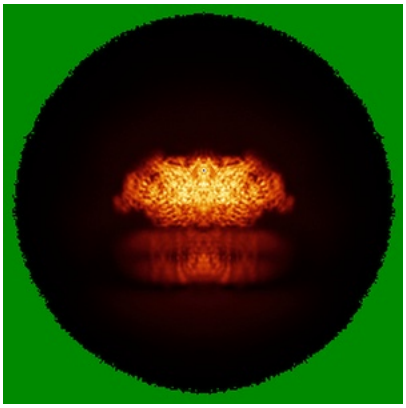


Z Index: 140

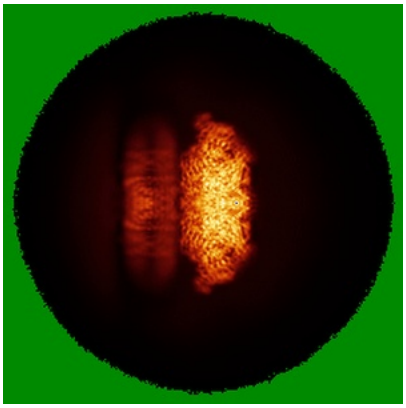
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

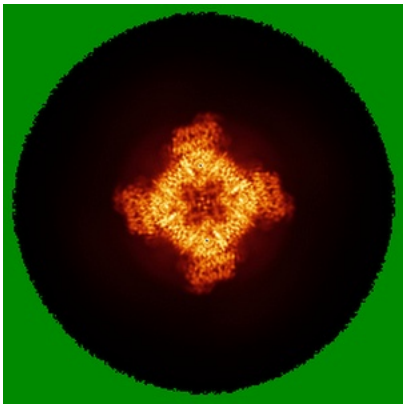
6.4.1 Primary map



X



Y

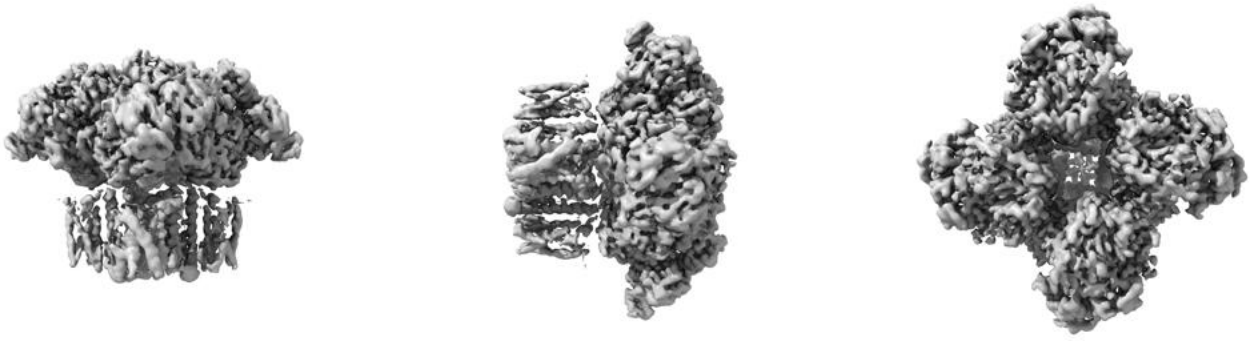


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

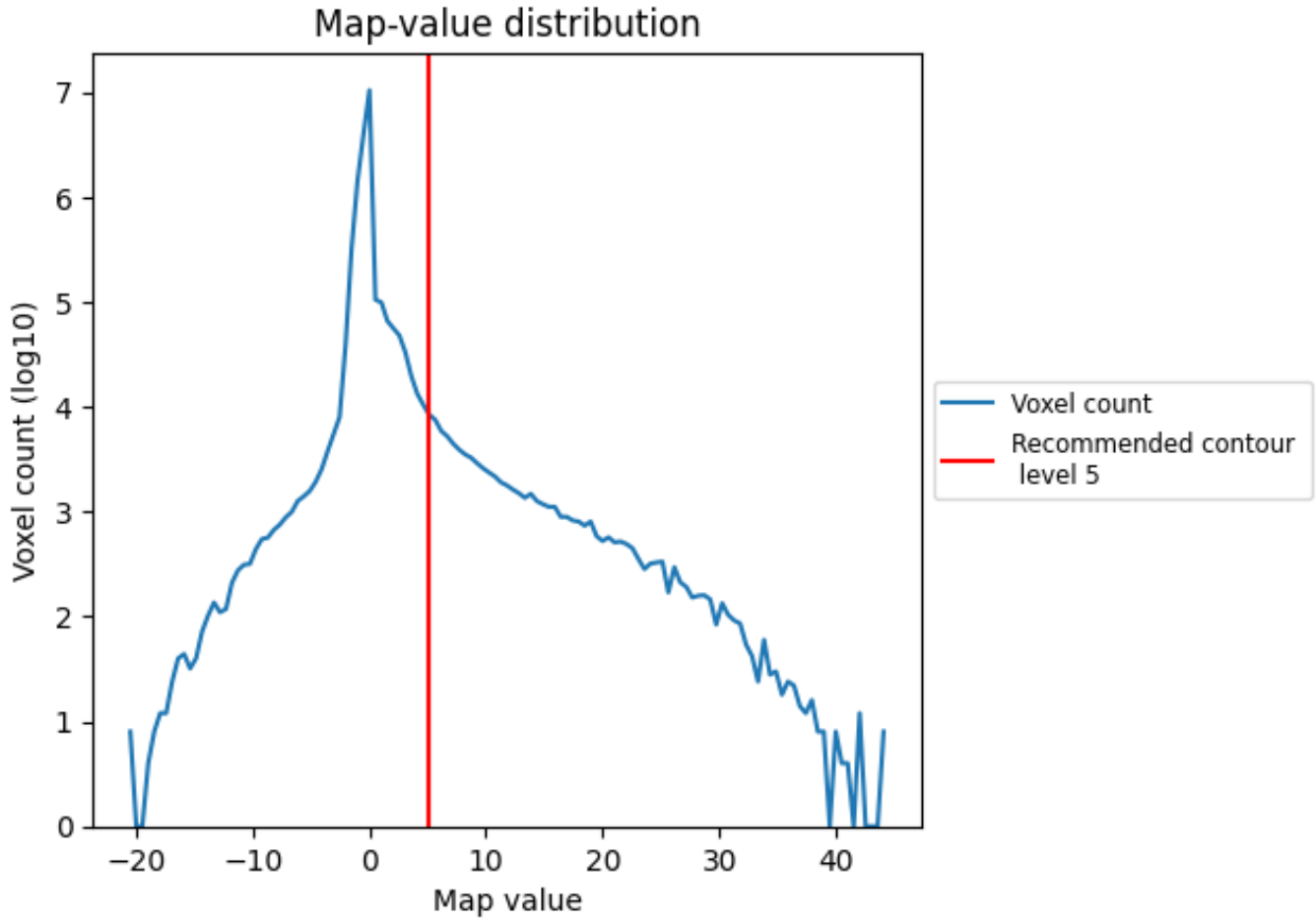
6.6 Mask visualisation (i)

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

7 Map analysis

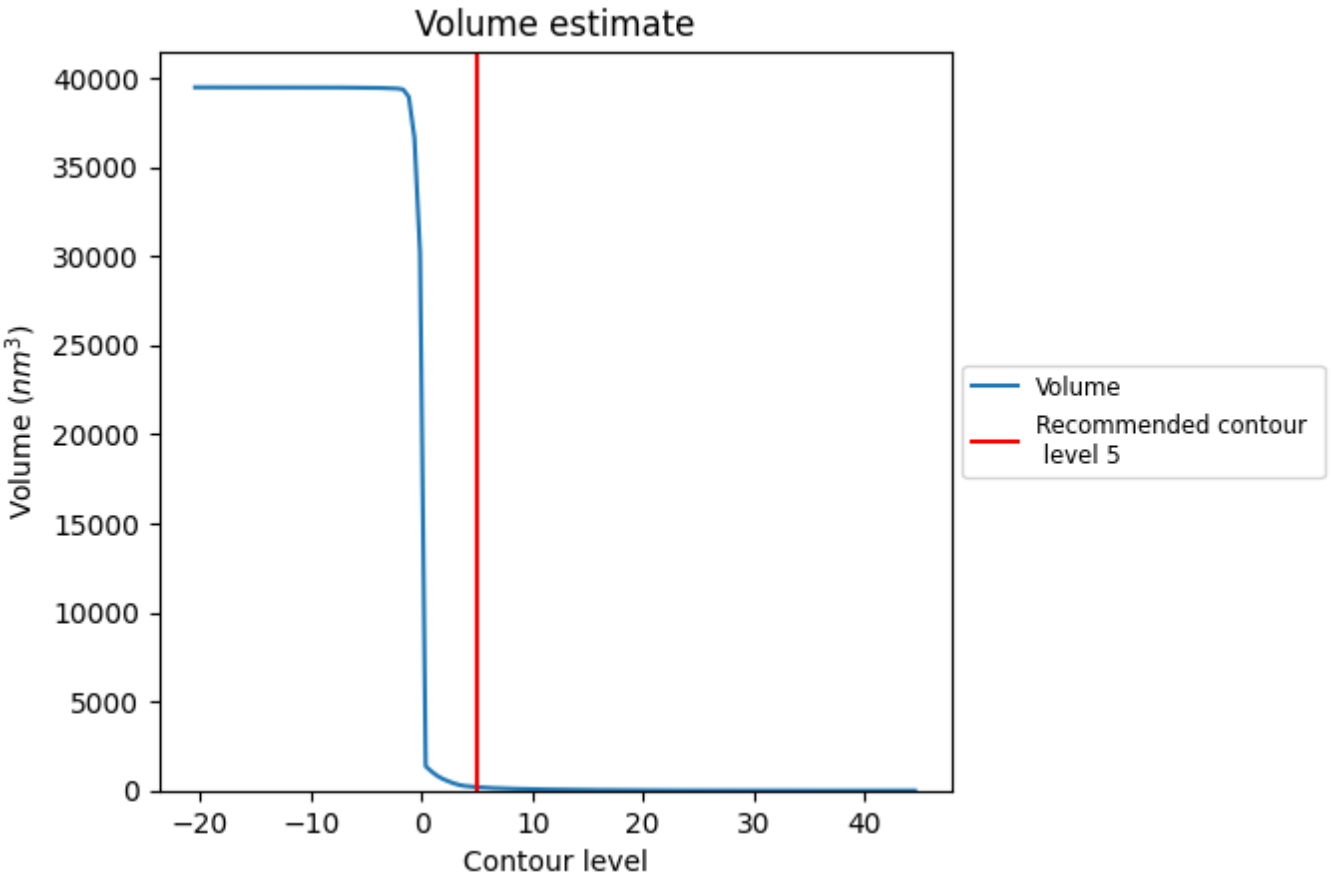
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

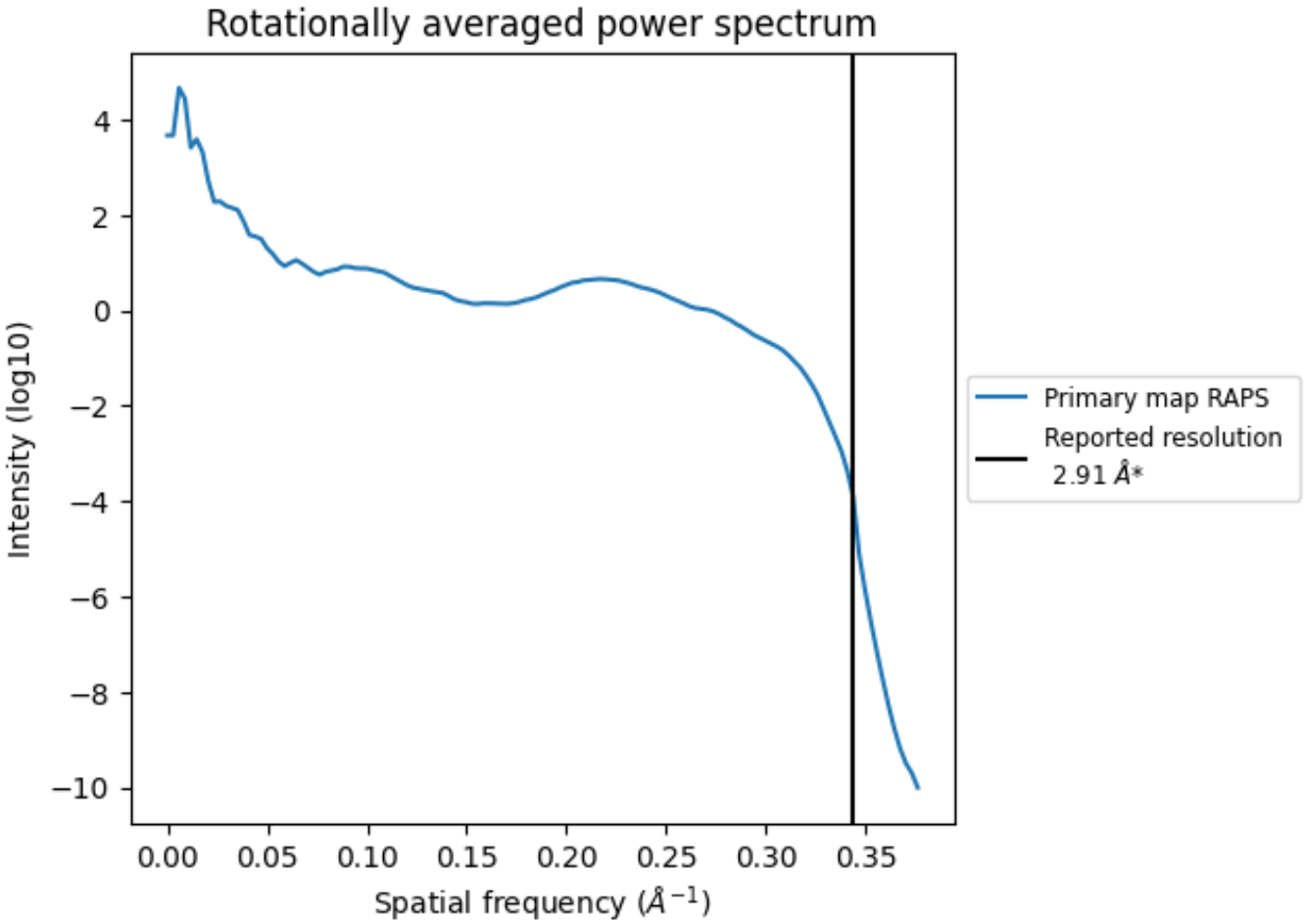
7.2 Volume estimate (i)



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 175 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)

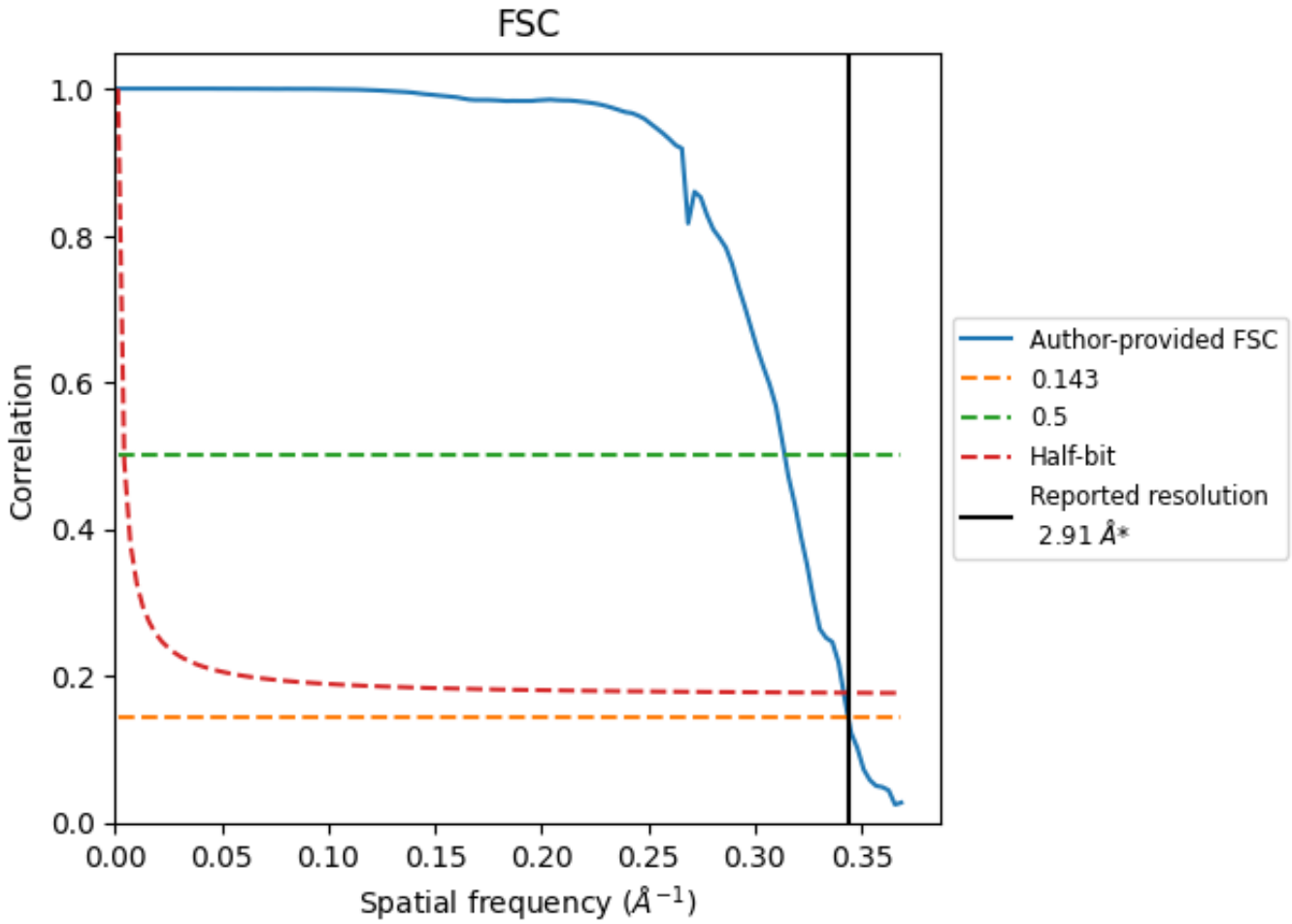


*Reported resolution corresponds to spatial frequency of 0.344 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.344 Å^{-1}

8.2 Resolution estimates (i)

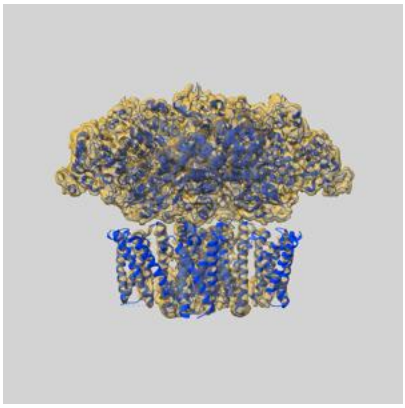
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.18	2.93
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

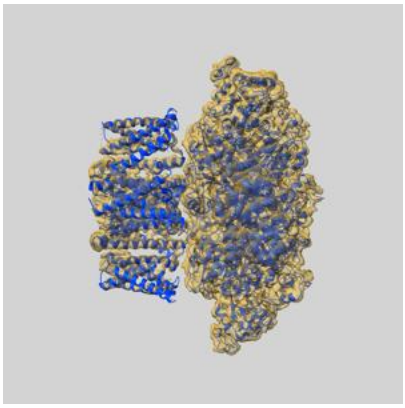
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24493 and PDB model 7RK6. Per-residue inclusion information can be found in section 3 on page 7.

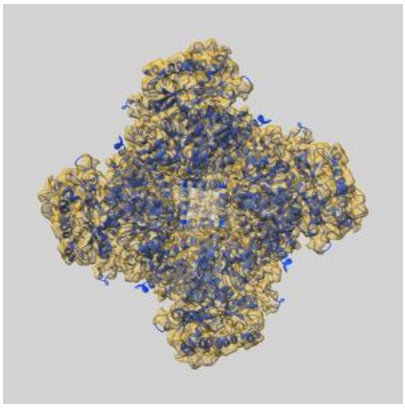
9.1 Map-model overlay



X



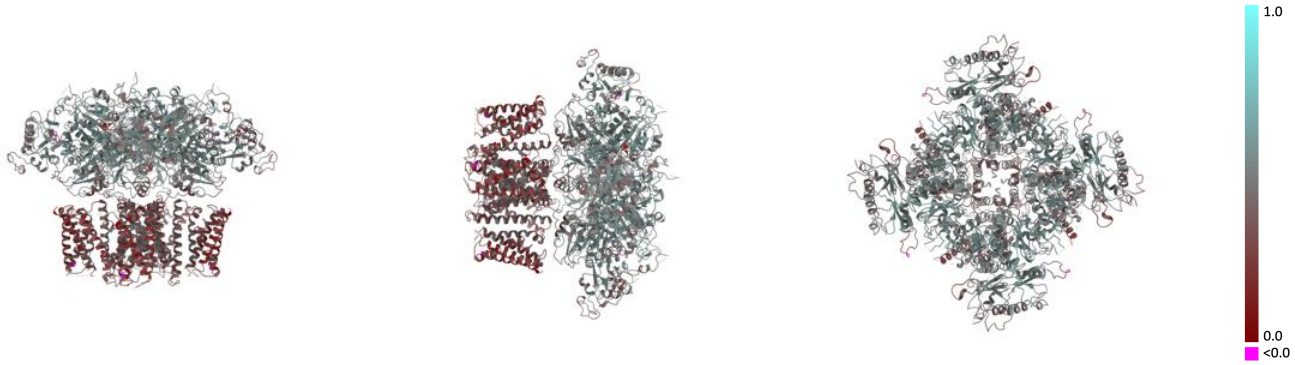
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

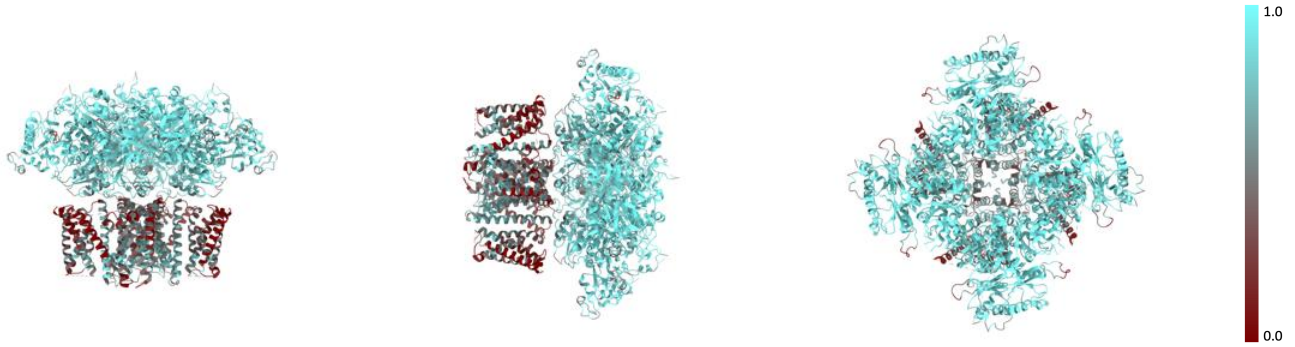
9.2 Q-score mapped to coordinate model (i)



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.

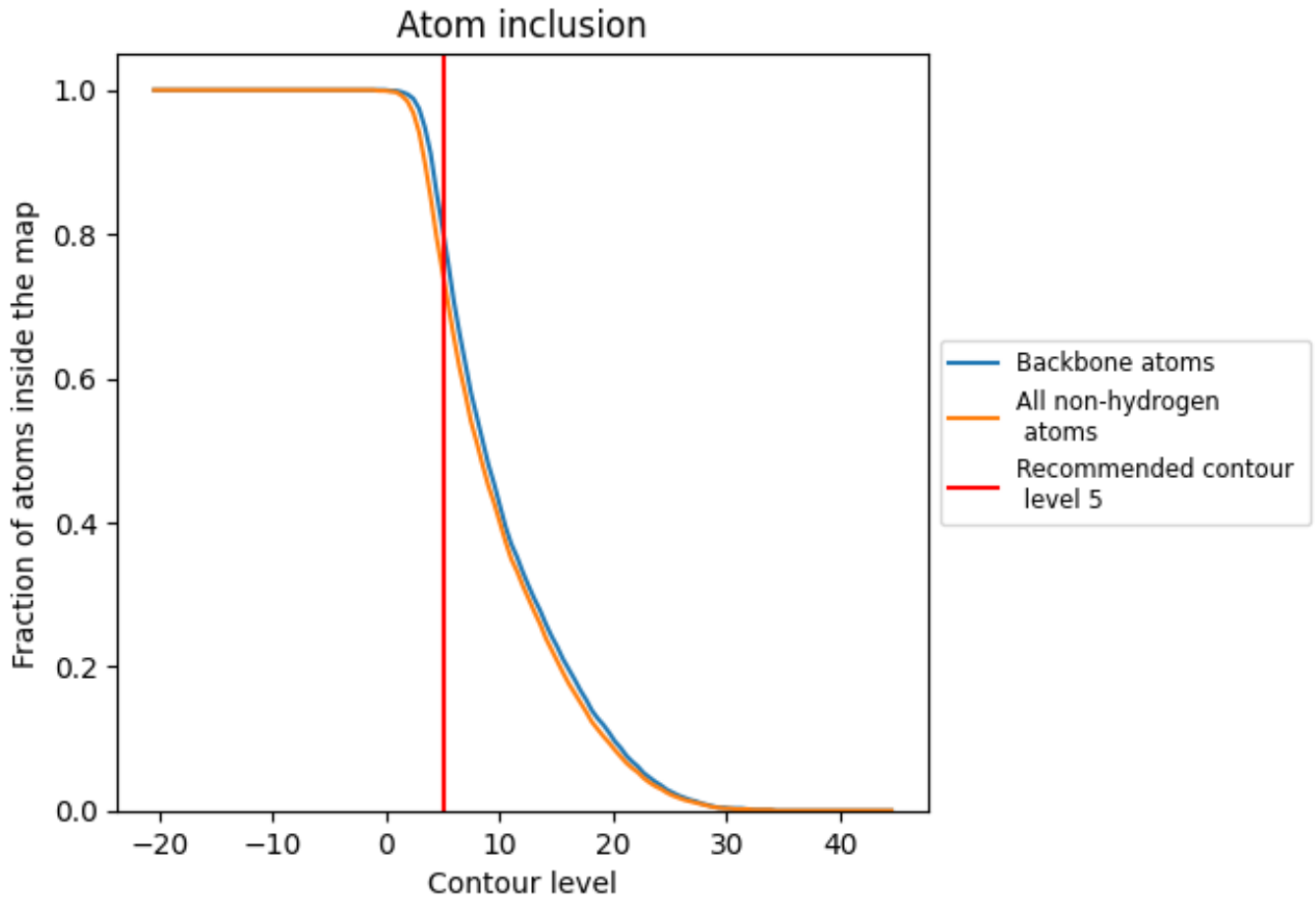
9.3 Atom inclusion mapped to coordinate model (i)



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 (5).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.4470
A	0.7510	0.4470
B	0.7510	0.4470
C	0.7510	0.4470
D	0.7510	0.4470