Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 08:14 AM EST

PDB ID	:	8TI1
EMDB ID	:	EMD-41277
Title	:	Cryo-EM structure of a SUR1/Kir6.2-Q52R ATP-sensitive potassium channel in the presence of PIP2 in the open conformation
Authors	:	Driggers, C.M.; Shyng, S.-L.
Deposited on	:	2023-07-18
Resolution	:	2.90 Å(reported)
Based on initial model	:	6BAA

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 ⓘ 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:

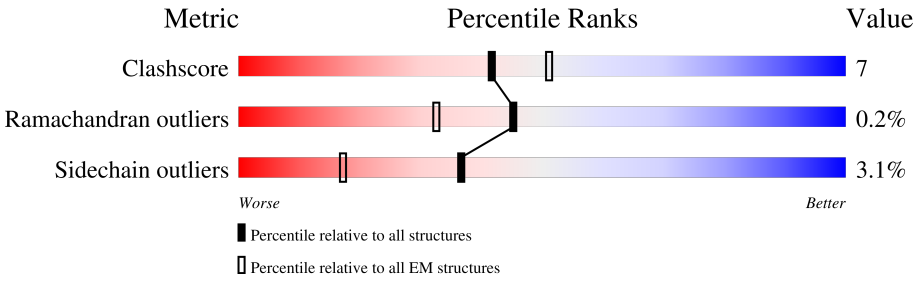
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.90 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	390	70% 12% 18%
1	B	390	70% 12% 18%
1	C	390	70% 13% 18%
1	D	390	70% 13% 18%
2	E	1582	7% 59% 12% • 28%
2	F	1582	7% 59% 13% • 28%
2	G	1582	7% 59% 13% • 28%
2	H	1582	7% 59% 13% • 28%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 45034 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	1	0
			2528	1629	435	447	17		
1	B	321	Total	C	N	O	S	1	0
			2528	1629	435	447	17		
1	C	321	Total	C	N	O	S	1	0
			2528	1629	435	447	17		
1	D	321	Total	C	N	O	S	1	0
			2528	1629	435	447	17		

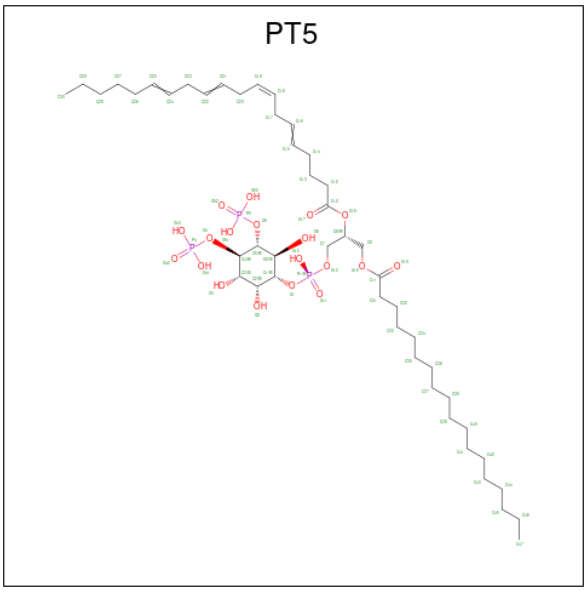
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ARG	GLN	engineered mutation	UNP P70673
B	52	ARG	GLN	engineered mutation	UNP P70673
C	52	ARG	GLN	engineered mutation	UNP P70673
D	52	ARG	GLN	engineered mutation	UNP P70673

- Molecule 2 is a protein called SUR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1141	Total	C	N	O	S	1	0
			8450	5508	1426	1481	35		
2	H	1141	Total	C	N	O	S	1	0
			8450	5508	1426	1481	35		
2	G	1141	Total	C	N	O	S	1	0
			8450	5508	1426	1481	35		
2	F	1141	Total	C	N	O	S	1	0
			8450	5508	1426	1481	35		

- Molecule 3 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: $C_{47}H_{85}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).

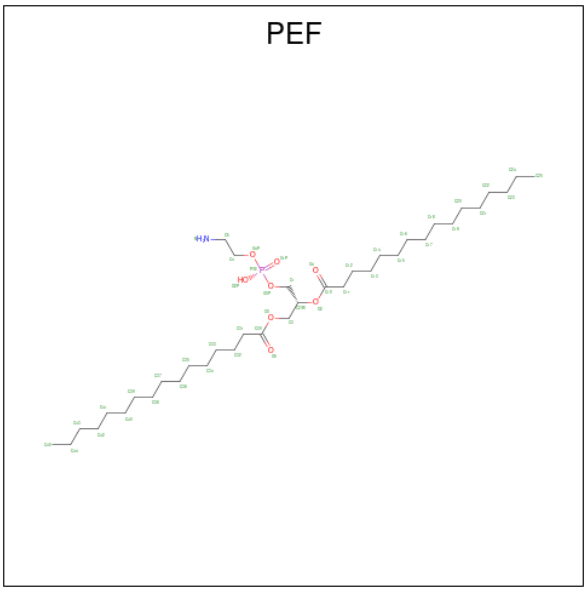


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			69	47	19	3	
3	E	1	Total	C	O	P	0
			69	47	19	3	
3	B	1	Total	C	O	P	0
			69	47	19	3	
3	C	1	Total	C	O	P	0
			69	47	19	3	
3	D	1	Total	C	O	P	0
			69	47	19	3	
3	H	1	Total	C	O	P	0
			69	47	19	3	
3	G	1	Total	C	O	P	0
			69	47	19	3	
3	F	1	Total	C	O	P	0
			69	47	19	3	

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

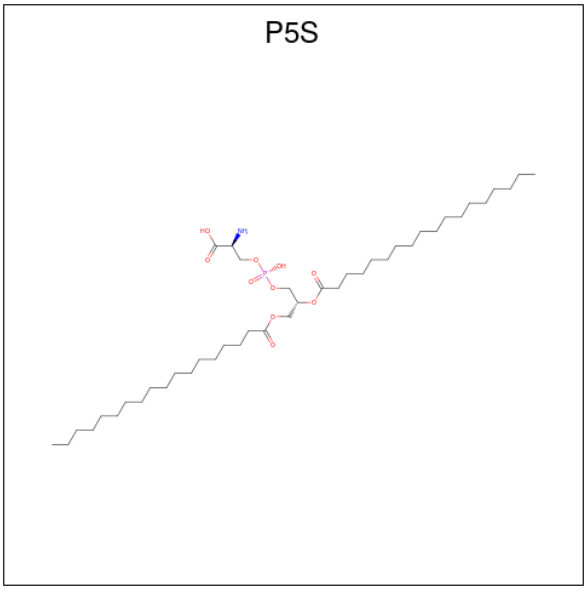
Mol	Chain	Residues	Atoms		AltConf
4	A	4	Total	K	0
			4	4	

- Molecule 5 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



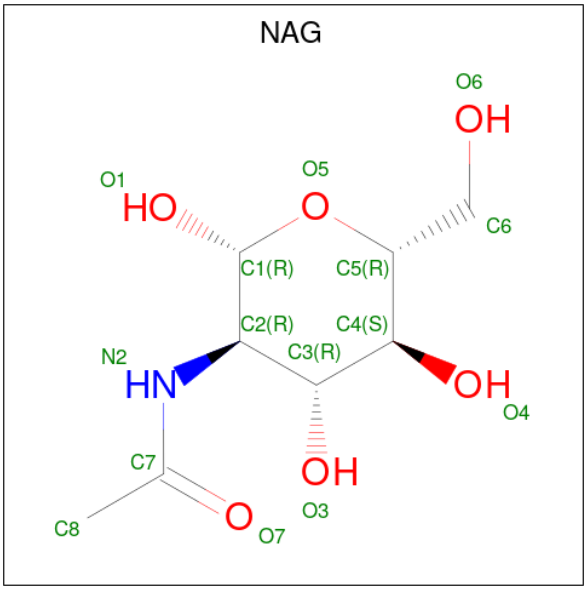
Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			28	18	1	8	1	
5	H	1	Total	C	N	O	P	0
			28	18	1	8	1	
5	G	1	Total	C	N	O	P	0
			28	18	1	8	1	
5	F	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
6	E	1	Total	C	N	O	P	0
			50	38	1	10	1	
6	E	1	Total	C	N	O	P	0
			46	34	1	10	1	
6	H	1	Total	C	N	O	P	0
			50	38	1	10	1	
6	H	1	Total	C	N	O	P	0
			46	34	1	10	1	
6	G	1	Total	C	N	O	P	0
			50	38	1	10	1	
6	G	1	Total	C	N	O	P	0
			46	34	1	10	1	
6	F	1	Total	C	N	O	P	0
			50	38	1	10	1	
6	F	1	Total	C	N	O	P	0
			46	34	1	10	1	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	H	1	Total	C	N	O	0
			14	8	1	5	
7	G	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
7	F	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is water.

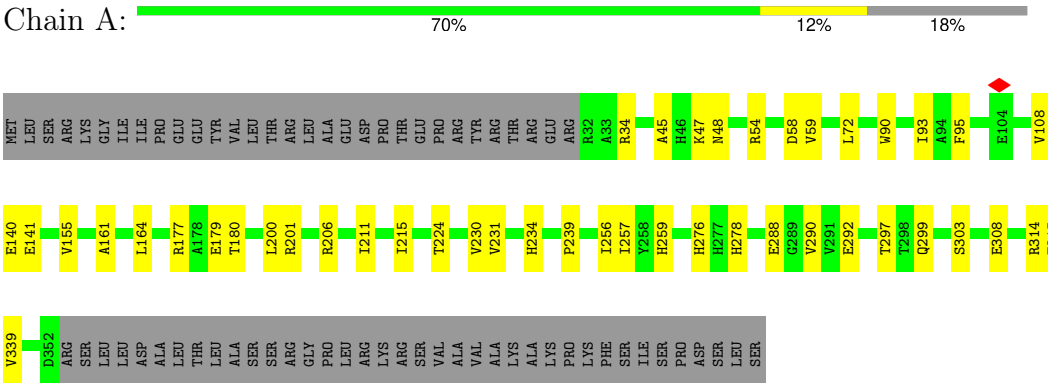
Mol	Chain	Residues	Atoms		AltConf
8	A	4	Total	O	0
			4	4	
8	B	3	Total	O	0
			3	3	
8	C	3	Total	O	0
			3	3	
8	D	4	Total	O	0
			4	4	

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.

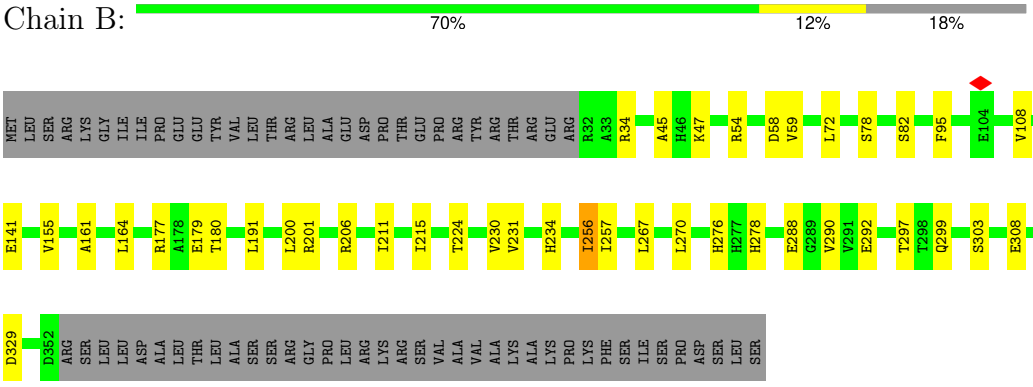
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain A:



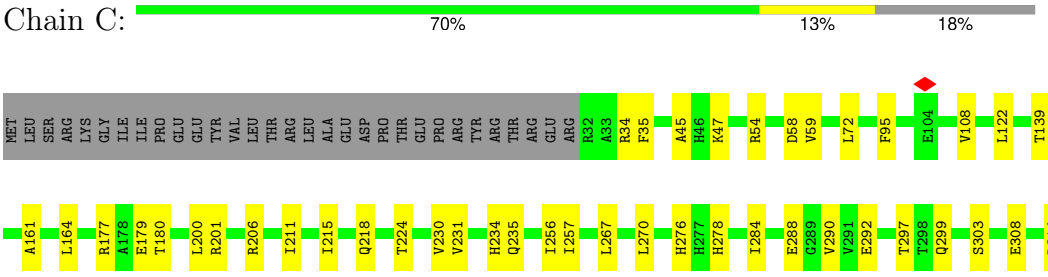
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain B:



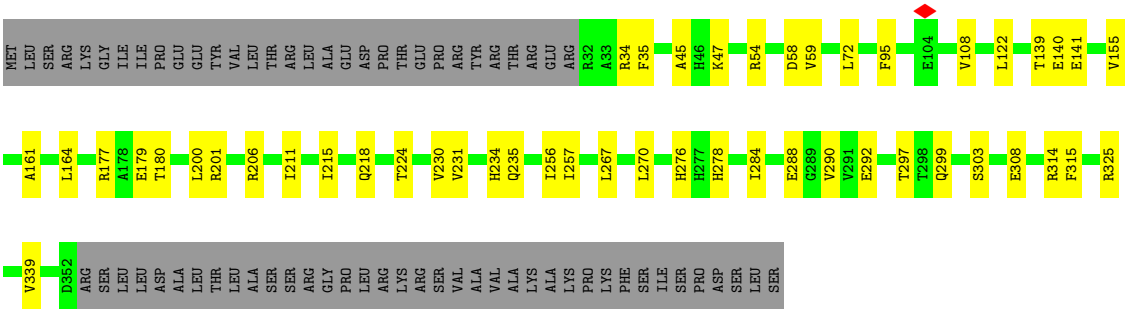
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain C:



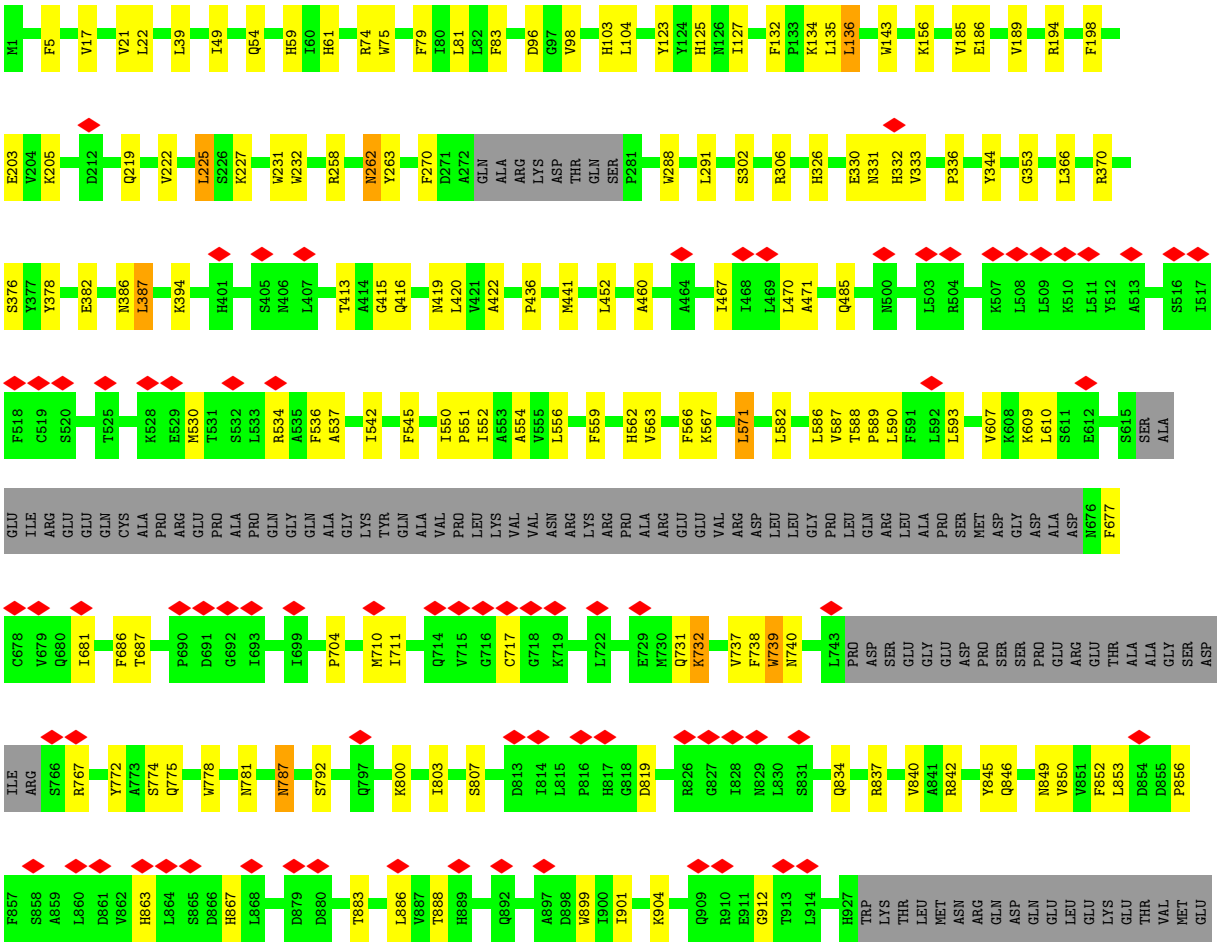
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

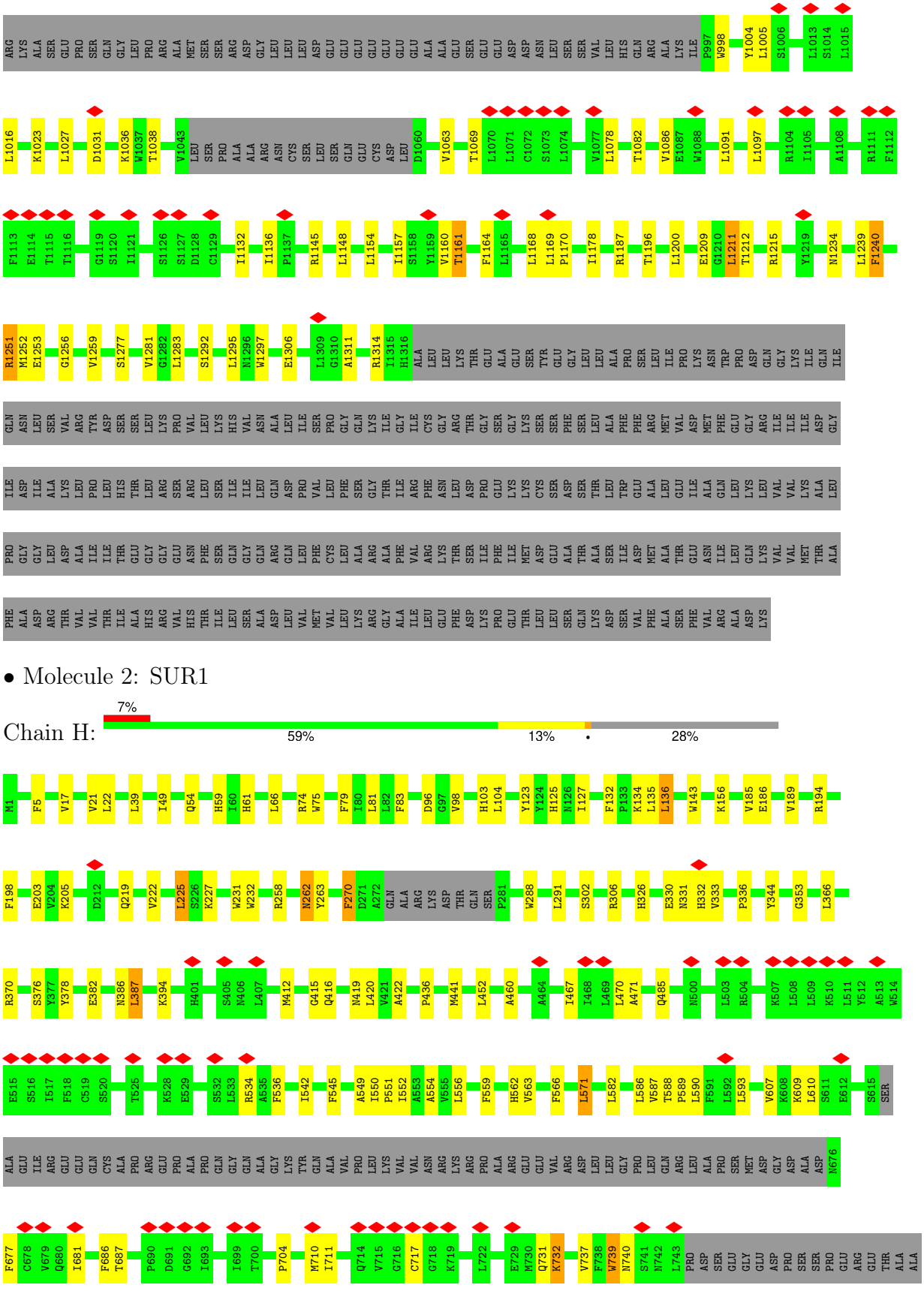
Chain D:



• Molecule 2: SUR1

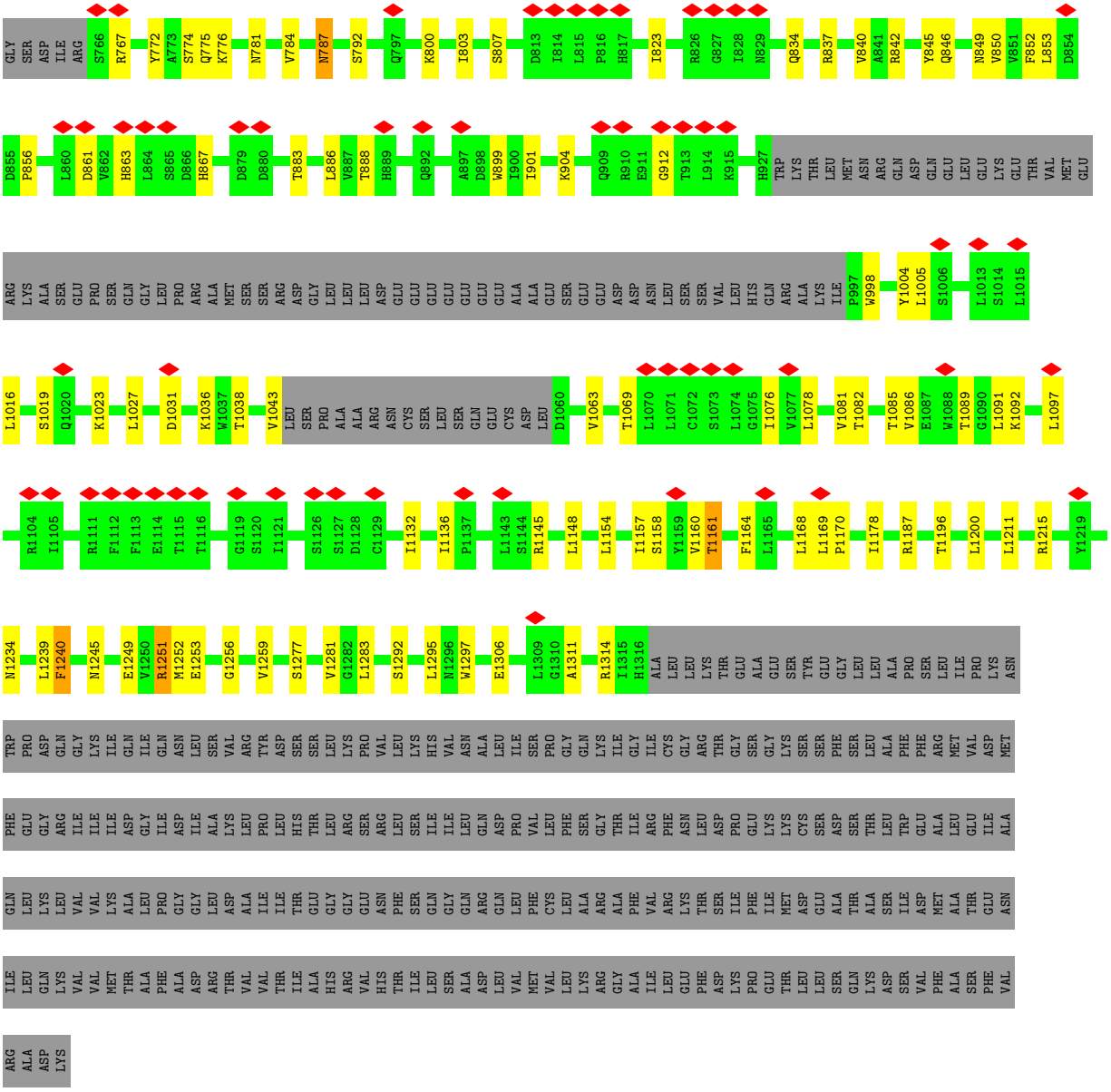
Chain E:





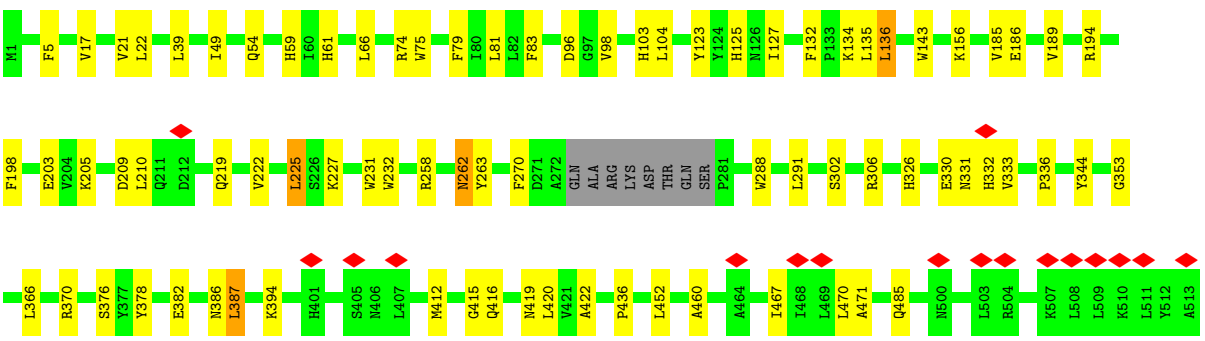
• Molecule 2: SUR1

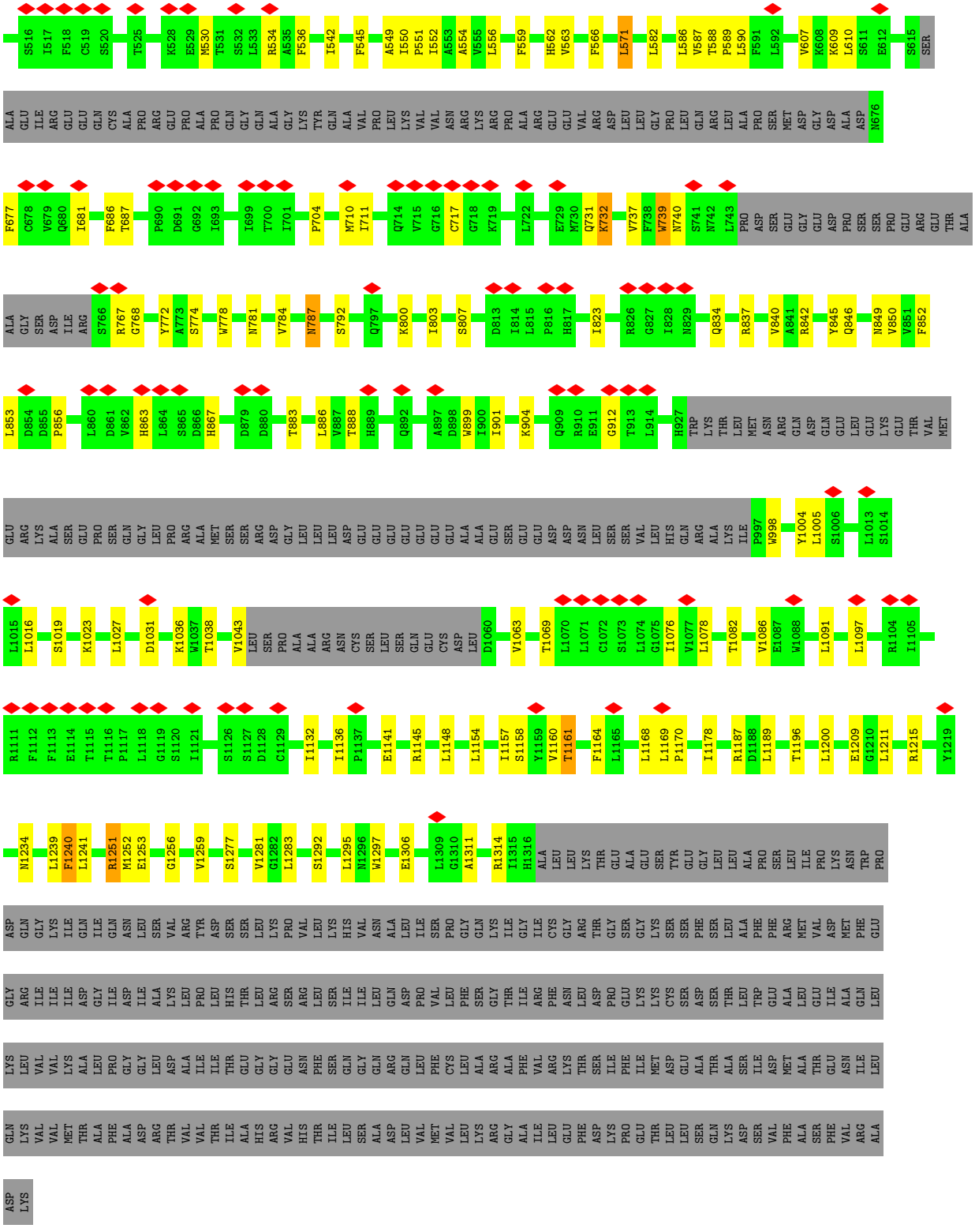
Chain H:



• Molecule 2: SUR1

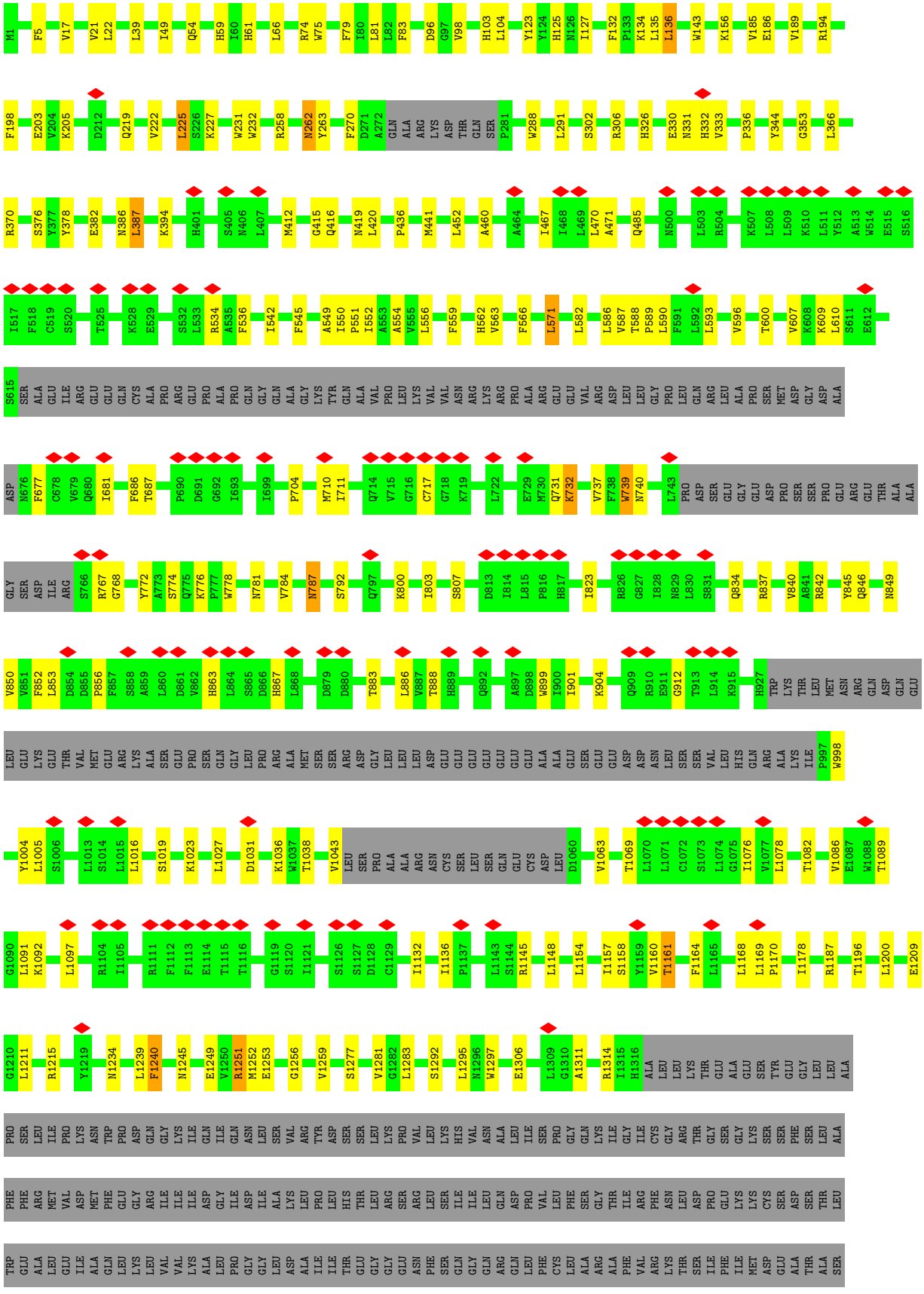
Chain G:





• Molecule 2: SUR1

Chain F:


M1 F5 V17 V21 L22 L39 I49 Q54 H59 I60 H61 L66 R74 W75 F79 I80 L81 L82 F83 D96 G97 V98 H103 L104 Y123 Y124 H125 N126 I127 F132 P133 K134 L135 L136 W143 K156 V185 E186 V189 R194
F198 E203 V204 K205 D212 Q219 V222 L225 S226 K227 W231 W232 R258 N262 Y263 F270 D271 A272 GLN ALA ARG LYS ASP THR GLN SER P281 W288 L291 S302 R306 H326 E330 N331 H332 V333 P336 Y344 G353 L366
R370 S376 Y377 Y378 E382 N386 L387 K394 H401 S405 N406 L407 M412 G415 Q416 N419 L420 P436 M441 L452 A460 A464 T467 T468 L469 L470 A471 Q485 N500 L503 R504 K507 L508 L509 K510 L511 Y512 A513 W514 E515 S516
I517 F518 C519 S520 T525 K528 E529 S532 L533 R534 A535 F536 I542 F545 A549 I550 P551 I552 A553 A554 V555 L556 F559 H562 V563 F566 L571 L582 L586 V587 T588 P589 L590 F591 L592 L593 V596 T600 V607 K608 K609 L610 S611 E612
S615 SER ALA GLU ILE ARG GLU GLU GLN CYS ALA PRO ARG GLU PRO ALA PRO GLN GLY GLN ALA GLY LYS TYR GLN ALA VAL PRO LEU LYS VAL VAL ASN ARG LYS ARG PRO ALA ARG GLU GLU VAL ARG ASP LEU LEU GLY PRO LEU GLN ARG LEU ALA PRO SER MET ASP GLY ASP ALA
ASP N676 F677 C678 V679 Q680 I681 F686 T687 P690 D691 G692 I693 I699 P704 M710 I711 Q714 V715 G716 C717 G718 K719 L722 E729 M730 Q731 K732 V737 F738 W739 N740 L743 PRO ASP SER GLU GLY GLU ASP PRO SER SER PRO GLU ARG GLU THR ALA ALA
GLY SER ASP ILE ARG S766 R767 G768 Y772 A773 S774 Q775 K776 P777 W778 N781 V784 N787 S792 Q797 K800 I803 S807 D813 I814 L815 P816 H817 I823 R826 G827 I828 N829 L830 S831 Q834 R837 V840 A841 R842 Y845 Q846 N849
V850 V851 F852 L853 D854 D855 P856 F857 S858 A859 L860 D861 V862 H863 L864 S865 D866 H867 L868 D879 D880 T883 L886 V887 T888 H889 Q892 A897 D898 W899 I900 I901 K904 Q909 R910 E911 G912 T913 L914 K915 H927 TRP LYS THR LEU MET ASN ARG GLN ASP GLN GLU
LEU GLU LYS GLU THR VAL MET GLU ARG LYS ALA SER GLU PRO SER GLN GLY LEU PRO ARG ALA MET SER SER ARG ASP GLY LEU LEU LEU ASP GLU GLU GLU GLU GLU GLU GLU GLU ALA ALA GLU SER GLU GLU ASP ASP ASN LEU SER SER VAL LEU HIS GLN ARG ALA LYS ILE P997 W998
Y1004 L1005 S1006 L1013 S1014 L1015 L1016 S1019 K1023 L1027 D1031 K1036 W1037 T1038 V1043 LEU SER PRO ALA ALA ARG ASN CYS SER LEU SER GLN GLU CYS ASP LEU D1060 V1063 T1069 L1070 L1071 C1072 S1073 L1074 G1075 I1076 V1077 L1078 T1082 V1086 E1087 W1088 T1089
G1090 L1091 K1092 L1097 R1104 I1105 R1111 F1112 F1113 E1114 T1115 T1116 G1119 S1120 I1121 S1126 S1127 D1128 C1129 I1132 I1136 P1137 L1143 S1144 R1145 L1148 L1154 I1157 S1158 Y1159 V1160 T1161 F1164 L1165 L1168 L1169 P1170 I1178 R1187 T1196 L1200 E1209
G1210 L1211 R1215 Y1219 N1234 L1239 F1240 N1245 E1249 V1250 R1251 M1252 E1253 G1256 V1259 S1277 V1281 G1282 L1283 S1292 L1295 N1296 W1297 E1306 L1309 G1310 A1311 R1314 I1315 H1316 ALA LEU LEU LYS THR GLU ALA GLU LYS GLY LEU LEU ALA
PRO SER LEU ILE PRO LYS ASN TRP PRO ASP GLN GLY LYS ILE GLN ILE GLN ASN LEU SER VAL ARG TYR ASP SER SER LEU LYS PRO VAL LEU LYS HIS VAL ASN ALA LEU ILE SER PRO GLY GLN LYS ILE GLY ILE ILE CYS GLY ARG THR GLY SER GLY LYS SER SER PHE SER LEU ALA
PHE PHE ARG MET VAL ASP MET PHE GLU GLY ARG ILE ILE ILE ASP GLY ILE ASP ILE ALA LYS LEU PRO LEU HIS THR LEU ARG SER ARG LEU SER ILE ILE LEU GLN GLN ASP PRO VAL LEU PHE SER GLY THR ILE ARG PHE ASN LEU ASP PRO SER ILE LYS LYS CYS SER ASP SER THR LEU
TRP GLU ALA LEU GLU ILE ALA GLN LEU LYS LEU VAL VAL LYS ALA LEU PRO GLY GLY LEU ASP ALA ILE THR GLU GLY GLY GLU ASN PHE SER GLN GLY GLN ARG GLN LEU PHE CYS LEU ALA ARG ALA PHE VAL ARG ASN LYS THR SER ILE PHE ILE MET ASP GLU ALA THR ALA SER


ILE ASP MET ALA THR GLU ASN ILE LEU GLN LYS VAL VAL MET THR ALA PHE ALA ASP ARG THR VAL VAL THR ILE ALA HIS ARG VAL HIS THR ILE LEU SER ALA ASP LEU VAL MET VAL LEU LYS ARG GLY ALA ILE LEU GLU PHE ASP LYS PRO GLU THR LEU LEU SER GLN LYS ASP

SER VAL PHE ALA SER PHE VAL ARG ALA ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	14115	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.644	Depositor
Minimum map value	-0.269	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	495.59998, 495.59998, 495.59998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P5S, K, PEF, PT5, 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	0.27	0/2589	0.47	0/3519
1	B	0.27	0/2589	0.47	0/3519
1	C	0.27	0/2589	0.47	0/3519
1	D	0.27	0/2589	0.47	0/3519
2	E	0.24	0/8639	0.42	0/11809
2	F	0.24	0/8639	0.42	0/11809
2	G	0.24	0/8639	0.42	0/11809
2	H	0.24	0/8639	0.42	0/11809
All	All	0.25	0/44912	0.43	0/61312

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	2528	0	2566	34	0
1	B	2528	0	2566	34	0
1	C	2528	0	2566	33	0
1	D	2528	0	2566	33	0
2	E	8450	0	8159	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	8450	0	8159	117	0
2	G	8450	0	8159	117	0
2	H	8450	0	8159	119	0
3	A	69	0	80	4	0
3	B	69	0	80	4	0
3	C	69	0	80	4	0
3	D	69	0	80	4	0
3	E	69	0	80	6	0
3	F	69	0	80	7	0
3	G	69	0	80	6	0
3	H	69	0	80	7	0
4	A	4	0	0	0	0
5	E	28	0	29	1	0
5	F	28	0	29	2	0
5	G	28	0	29	2	0
5	H	28	0	29	1	0
6	E	96	0	127	3	0
6	F	96	0	127	3	0
6	G	96	0	127	3	0
6	H	96	0	127	3	0
7	E	14	0	13	0	0
7	F	14	0	13	0	0
7	G	14	0	13	0	0
7	H	14	0	13	0	0
8	A	4	0	0	0	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	4	0	0	0	0
All	All	45034	0	44216	586	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 7.

All (586) 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)
2:F:1023:LYS:HE2	2:F:1078:LEU:HB3	1.68	0.76
2:E:1023:LYS:HE2	2:E:1078:LEU:HB3	1.68	0.76
2:H:1023:LYS:HE2	2:H:1078:LEU:HB3	1.68	0.76
2:G:1023:LYS:HE2	2:G:1078:LEU:HB3	1.68	0.75
2:E:1160:VAL:HG23	2:E:1161:THR:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:856:PRO:HD2	2:G:888:THR:HB	1.72	0.71
2:F:1160:VAL:HG23	2:F:1161:THR:HG22	1.72	0.71
2:H:856:PRO:HD2	2:H:888:THR:HB	1.72	0.70
2:E:856:PRO:HD2	2:E:888:THR:HB	1.73	0.70
2:G:1160:VAL:HG23	2:G:1161:THR:HG22	1.72	0.70
2:F:74:ARG:HH21	2:F:185:VAL:HG12	1.57	0.70
2:H:1160:VAL:HG23	2:H:1161:THR:HG22	1.72	0.70
2:E:1031:ASP:HB3	2:E:1283:LEU:HD21	1.74	0.69
2:H:74:ARG:HH21	2:H:185:VAL:HG12	1.57	0.69
2:E:74:ARG:HH21	2:E:185:VAL:HG12	1.57	0.69
2:F:856:PRO:HD2	2:F:888:THR:HB	1.72	0.69
2:G:551:PRO:HG3	2:G:587:VAL:HG11	1.75	0.69
2:F:551:PRO:HG3	2:F:587:VAL:HG11	1.75	0.69
2:E:551:PRO:HG3	2:E:587:VAL:HG11	1.74	0.68
3:E:1601:PT5:H38	3:B:401:PT5:H28	1.75	0.68
2:G:74:ARG:HH21	2:G:185:VAL:HG12	1.58	0.68
3:A:401:PT5:H28	3:H:1601:PT5:H38	1.76	0.68
2:H:470:LEU:HD22	2:H:550:ILE:HG12	1.76	0.68
3:C:401:PT5:H28	3:F:1601:PT5:H38	1.76	0.68
2:H:551:PRO:HG3	2:H:587:VAL:HG11	1.75	0.68
3:D:401:PT5:H28	3:G:1601:PT5:H38	1.76	0.67
2:F:470:LEU:HD22	2:F:550:ILE:HG12	1.76	0.67
2:G:470:LEU:HD22	2:G:550:ILE:HG12	1.76	0.67
2:F:1031:ASP:HB3	2:F:1283:LEU:HD21	1.77	0.66
2:H:1031:ASP:HB3	2:H:1283:LEU:HD21	1.77	0.66
2:E:470:LEU:HD22	2:E:550:ILE:HG12	1.78	0.66
2:G:1031:ASP:HB3	2:G:1283:LEU:HD21	1.77	0.65
1:A:180:THR:HG21	1:A:206:ARG:HH11	1.62	0.63
2:F:61:HIS:HA	6:F:1603:P5S:HN	1.63	0.63
2:E:262:ASN:N	2:E:262:ASN:OD1	2.31	0.63
2:F:452:LEU:HB3	2:F:460:ALA:HB1	1.81	0.63
2:E:452:LEU:HB3	2:E:460:ALA:HB1	1.82	0.62
2:H:452:LEU:HB3	2:H:460:ALA:HB1	1.81	0.62
2:G:452:LEU:HB3	2:G:460:ALA:HB1	1.81	0.62
2:G:61:HIS:HA	6:G:1603:P5S:HN	1.64	0.62
2:H:262:ASN:N	2:H:262:ASN:OD1	2.31	0.62
2:F:262:ASN:OD1	2:F:262:ASN:N	2.31	0.62
1:B:290:VAL:HG22	1:B:297:THR:HG22	1.82	0.62
2:G:262:ASN:OD1	2:G:262:ASN:N	2.31	0.62
1:C:288:GLU:OE2	1:C:299:GLN:NE2	2.33	0.62
1:D:288:GLU:OE2	1:D:299:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:VAL:HG22	1:D:297:THR:HG22	1.81	0.61
2:F:1256:GLY:HA3	2:F:1292:SER:HB2	1.82	0.61
2:G:1256:GLY:HA3	2:G:1292:SER:HB2	1.82	0.61
2:E:1256:GLY:HA3	2:E:1292:SER:HB2	1.82	0.61
2:H:61:HIS:HA	6:H:1603:P5S:HN	1.63	0.61
1:A:290:VAL:HG22	1:A:297:THR:HG22	1.83	0.61
1:A:108:VAL:HB	1:A:141:GLU:HG3	1.83	0.61
1:C:34:ARG:NH1	1:C:308:GLU:OE2	2.34	0.61
1:C:108:VAL:HB	1:C:141:GLU:HG3	1.83	0.61
2:H:1256:GLY:HA3	2:H:1292:SER:HB2	1.83	0.61
1:B:108:VAL:HB	1:B:141:GLU:HG3	1.83	0.61
2:E:61:HIS:HA	6:E:1603:P5S:HN	1.64	0.61
1:D:108:VAL:HB	1:D:141:GLU:HG3	1.83	0.61
1:B:288:GLU:OE2	1:B:299:GLN:NE2	2.33	0.60
1:D:34:ARG:NH1	1:D:308:GLU:OE2	2.34	0.60
2:H:767:ARG:NH2	2:H:849:ASN:OD1	2.34	0.60
2:F:717:CYS:HB3	2:F:904:LYS:HA	1.83	0.60
2:E:767:ARG:NH2	2:E:849:ASN:OD1	2.34	0.60
2:G:717:CYS:HB3	2:G:904:LYS:HA	1.83	0.60
2:F:767:ARG:NH2	2:F:849:ASN:OD1	2.35	0.60
2:E:717:CYS:HB3	2:E:904:LYS:HA	1.83	0.60
2:G:125:HIS:ND1	6:G:1603:P5S:O18	2.35	0.60
1:A:288:GLU:OE2	1:A:299:GLN:NE2	2.34	0.60
1:C:290:VAL:HG22	1:C:297:THR:HG22	1.82	0.60
2:H:717:CYS:HB3	2:H:904:LYS:HA	1.84	0.60
2:F:125:HIS:ND1	6:F:1603:P5S:O18	2.35	0.60
2:G:1004:TYR:HE1	2:G:1097:LEU:HD11	1.67	0.60
2:E:1311:ALA:HA	2:E:1314:ARG:HH21	1.67	0.60
2:H:1311:ALA:HA	2:H:1314:ARG:HH21	1.66	0.59
2:G:767:ARG:NH2	2:G:849:ASN:OD1	2.35	0.59
2:E:125:HIS:ND1	6:E:1603:P5S:O18	2.35	0.59
2:H:125:HIS:ND1	6:H:1603:P5S:O18	2.35	0.59
2:F:1004:TYR:HE1	2:F:1097:LEU:HD11	1.67	0.59
2:E:1277:SER:HB3	2:E:1281:VAL:HG23	1.85	0.59
2:F:559:PHE:O	2:F:562:HIS:ND1	2.36	0.59
2:E:559:PHE:O	2:E:562:HIS:ND1	2.36	0.59
1:C:45:ALA:HB2	1:D:325:ARG:HD3	1.86	0.58
2:G:559:PHE:O	2:G:562:HIS:ND1	2.36	0.58
2:G:1311:ALA:HA	2:G:1314:ARG:HH21	1.66	0.58
2:F:1311:ALA:HA	2:F:1314:ARG:HH21	1.67	0.58
2:E:534:ARG:HD3	2:E:1091:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1004:TYR:HE1	2:H:1097:LEU:HD11	1.68	0.58
1:B:45:ALA:HB2	1:C:325:ARG:HD3	1.85	0.58
2:H:559:PHE:O	2:H:562:HIS:ND1	2.36	0.58
2:H:1277:SER:HB3	2:H:1281:VAL:HG23	1.86	0.58
2:F:534:ARG:HD3	2:F:1091:LEU:HD13	1.85	0.57
2:E:686:PHE:HA	2:E:732:LYS:HA	1.86	0.57
1:B:34:ARG:NH1	1:B:308:GLU:OE2	2.38	0.57
2:G:1277:SER:HB3	2:G:1281:VAL:HG23	1.86	0.57
2:G:83:PHE:HB2	6:G:1604:P5S:H53	1.86	0.57
2:E:1004:TYR:HE1	2:E:1097:LEU:HD11	1.68	0.57
2:H:534:ARG:HD3	2:H:1091:LEU:HD13	1.85	0.57
2:F:1277:SER:HB3	2:F:1281:VAL:HG23	1.86	0.57
1:B:34:ARG:NH2	1:B:303:SER:OG	2.37	0.57
2:G:686:PHE:HA	2:G:732:LYS:HA	1.87	0.57
2:G:1253:GLU:OE1	2:G:1292:SER:OG	2.22	0.57
2:F:686:PHE:HA	2:F:732:LYS:HA	1.87	0.57
1:A:34:ARG:NH2	1:A:303:SER:OG	2.37	0.57
1:A:45:ALA:HB2	1:B:325:ARG:HD3	1.86	0.57
2:F:83:PHE:HB2	6:F:1604:P5S:H53	1.87	0.57
2:H:552:ILE:HD11	2:H:1027:LEU:HD21	1.87	0.57
2:G:534:ARG:HD3	2:G:1091:LEU:HD13	1.86	0.56
2:F:552:ILE:HD11	2:F:1027:LEU:HD21	1.87	0.56
2:H:686:PHE:HA	2:H:732:LYS:HA	1.86	0.56
3:H:1601:PT5:O41	3:H:1601:PT5:O6	2.20	0.56
2:F:1253:GLU:OE1	2:F:1292:SER:OG	2.22	0.56
2:E:83:PHE:HB2	6:E:1604:P5S:H53	1.86	0.56
2:H:134:LYS:HB3	3:H:1601:PT5:H20	1.88	0.56
2:G:552:ILE:HD11	2:G:1027:LEU:HD21	1.87	0.56
2:E:1253:GLU:OE1	2:E:1292:SER:OG	2.22	0.56
2:H:83:PHE:HB2	6:H:1604:P5S:H53	1.87	0.56
2:E:787:ASN:HD21	2:E:842:ARG:HH11	1.54	0.55
2:G:134:LYS:HB3	3:G:1601:PT5:H20	1.88	0.55
1:A:177:ARG:NH1	1:A:180:THR:OG1	2.40	0.55
2:F:96:ASP:OD1	2:F:103:HIS:N	2.37	0.55
2:H:1253:GLU:OE1	2:H:1292:SER:OG	2.21	0.55
2:E:552:ILE:HD11	2:E:1027:LEU:HD21	1.89	0.55
2:E:681:ILE:HA	2:E:737:VAL:HB	1.88	0.55
1:C:34:ARG:NH2	1:C:303:SER:OG	2.38	0.55
2:F:1016:LEU:HD13	2:F:1086:VAL:HG23	1.88	0.55
2:G:1016:LEU:HD13	2:G:1086:VAL:HG23	1.88	0.55
2:E:1016:LEU:HD13	2:E:1086:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1016:LEU:HD13	2:H:1086:VAL:HG23	1.89	0.54
2:G:556:LEU:HD22	2:G:1069:THR:HG23	1.89	0.54
2:F:556:LEU:HD22	2:F:1069:THR:HG23	1.89	0.54
2:F:134:LYS:HB3	3:F:1601:PT5:H20	1.88	0.54
2:E:134:LYS:HB3	3:E:1601:PT5:H20	1.90	0.54
2:H:556:LEU:HD22	2:H:1069:THR:HG23	1.90	0.54
2:G:219:GLN:OE1	2:G:232:TRP:NE1	2.31	0.54
1:A:325:ARG:HD3	1:D:45:ALA:HB2	1.89	0.54
2:E:556:LEU:HD22	2:E:1069:THR:HG23	1.90	0.54
2:H:96:ASP:OD1	2:H:103:HIS:N	2.37	0.54
2:G:96:ASP:OD1	2:G:103:HIS:N	2.37	0.54
2:F:291:LEU:HD22	2:F:387:LEU:HD21	1.89	0.54
2:F:331:ASN:HB3	2:F:333:VAL:HG22	1.90	0.54
2:E:291:LEU:HD22	2:E:387:LEU:HD21	1.89	0.54
2:G:415:GLY:O	2:G:419:ASN:ND2	2.41	0.54
2:E:677:PHE:HA	2:E:704:PRO:HA	1.90	0.54
1:C:231:VAL:HB	1:C:234:HIS:HB2	1.90	0.54
2:G:291:LEU:HD22	2:G:387:LEU:HD21	1.89	0.54
1:A:231:VAL:HB	1:A:234:HIS:HB2	1.90	0.53
2:H:291:LEU:HD22	2:H:387:LEU:HD21	1.89	0.53
2:H:415:GLY:O	2:H:419:ASN:ND2	2.42	0.53
2:E:1154:LEU:HG	2:E:1168:LEU:HD21	1.90	0.53
3:E:1601:PT5:O41	3:E:1601:PT5:O6	2.20	0.53
1:A:164:LEU:HD22	1:D:161:ALA:HB2	1.91	0.53
1:A:34:ARG:NH1	1:A:308:GLU:OE2	2.41	0.53
1:A:47:LYS:HA	2:E:59[A]:HIS:HB3	1.91	0.53
2:H:787:ASN:HD21	2:H:842:ARG:HH11	1.56	0.53
2:G:331:ASN:HB3	2:G:333:VAL:HG22	1.91	0.53
1:A:161:ALA:HB2	1:B:164:LEU:HD22	1.91	0.53
2:E:415:GLY:O	2:E:419:ASN:ND2	2.41	0.53
2:H:331:ASN:HB3	2:H:333:VAL:HG22	1.90	0.53
2:F:415:GLY:O	2:F:419:ASN:ND2	2.41	0.53
2:E:96:ASP:OD1	2:E:103:HIS:N	2.36	0.53
2:H:1154:LEU:HG	2:H:1168:LEU:HD21	1.91	0.53
2:G:681:ILE:HA	2:G:737:VAL:HB	1.90	0.53
1:A:47:LYS:HA	2:E:59[B]:HIS:HB2	1.91	0.53
1:B:231:VAL:HB	1:B:234:HIS:HB2	1.90	0.52
2:H:681:ILE:HA	2:H:737:VAL:HB	1.90	0.52
2:F:787:ASN:HD21	2:F:842:ARG:HH11	1.56	0.52
1:A:59:VAL:HG12	2:E:49:ILE:HG21	1.91	0.52
2:E:330:GLU:O	2:E:332:HIS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ALA:HB2	1:D:164:LEU:HD22	1.91	0.52
1:D:34:ARG:NH2	1:D:303:SER:OG	2.38	0.52
1:D:224:THR:HG22	1:D:230:VAL:HG12	1.91	0.52
2:H:330:GLU:O	2:H:332:HIS:N	2.43	0.52
2:G:1154:LEU:HG	2:G:1168:LEU:HD21	1.91	0.52
2:E:331:ASN:HB3	2:E:333:VAL:HG22	1.92	0.52
2:F:1154:LEU:HG	2:F:1168:LEU:HD21	1.91	0.52
2:E:222:VAL:O	2:E:227:LYS:NZ	2.35	0.52
1:D:231:VAL:HB	1:D:234:HIS:HB2	1.90	0.52
1:C:59:VAL:HG12	2:G:49:ILE:HG21	1.91	0.52
2:F:1023:LYS:NZ	2:F:1082:THR:OG1	2.30	0.52
3:C:401:PT5:H31	3:F:1601:PT5:H38	1.92	0.52
1:D:59:VAL:HG12	2:H:49:ILE:HG21	1.92	0.52
2:G:677:PHE:HA	2:G:704:PRO:HA	1.91	0.52
2:F:681:ILE:HA	2:F:737:VAL:HB	1.90	0.52
1:B:224:THR:HG22	1:B:230:VAL:HG12	1.92	0.51
2:G:787:ASN:HD21	2:G:842:ARG:HH11	1.57	0.51
2:F:677:PHE:HA	2:F:704:PRO:HA	1.91	0.51
1:B:161:ALA:HB2	1:C:164:LEU:HD22	1.91	0.51
2:H:850:VAL:HG12	2:H:883:THR:HB	1.93	0.51
1:D:211:ILE:HD11	1:D:292:GLU:HG3	1.92	0.51
3:D:401:PT5:H31	3:G:1601:PT5:H38	1.92	0.51
2:H:1023:LYS:NZ	2:H:1082:THR:OG1	2.30	0.51
2:H:471:ALA:HB2	2:H:590:LEU:HD11	1.93	0.51
2:G:135:LEU:HD23	3:G:1601:PT5:H21	1.92	0.51
2:F:135:LEU:HD23	3:F:1601:PT5:H21	1.92	0.51
2:F:330:GLU:O	2:F:332:HIS:N	2.42	0.51
2:F:850:VAL:HG12	2:F:883:THR:HB	1.92	0.51
2:E:135:LEU:HD23	3:E:1601:PT5:H21	1.92	0.51
2:H:772:TYR:CE2	2:H:774:SER:HB2	2.46	0.51
2:G:772:TYR:CE2	2:G:774:SER:HB2	2.46	0.51
1:A:211:ILE:HD11	1:A:292:GLU:HG3	1.93	0.51
1:B:211:ILE:HD11	1:B:292:GLU:HG3	1.92	0.51
2:F:471:ALA:HB2	2:F:590:LEU:HD11	1.93	0.51
2:F:772:TYR:HA	2:F:852:PHE:HB2	1.92	0.51
1:A:224:THR:HG22	1:A:230:VAL:HG12	1.93	0.51
3:E:1601:PT5:H38	3:B:401:PT5:H31	1.93	0.51
1:B:59:VAL:HG12	2:F:49:ILE:HG21	1.91	0.51
2:H:219:GLN:OE1	2:H:232:TRP:NE1	2.31	0.51
3:A:401:PT5:H31	3:H:1601:PT5:H38	1.92	0.51
1:C:224:THR:HG22	1:C:230:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:471:ALA:HB2	2:G:590:LEU:HD11	1.93	0.51
1:B:47:LYS:HA	2:F:59[A]:HIS:HB3	1.93	0.51
1:C:211:ILE:HD11	1:C:292:GLU:HG3	1.92	0.51
2:H:677:PHE:HA	2:H:704:PRO:HA	1.92	0.51
2:E:471:ALA:HB2	2:E:590:LEU:HD11	1.92	0.50
2:H:135:LEU:HD23	3:H:1601:PT5:H21	1.92	0.50
2:G:330:GLU:O	2:G:332:HIS:N	2.42	0.50
2:H:222:VAL:O	2:H:227:LYS:NZ	2.36	0.50
2:G:1023:LYS:NZ	2:G:1082:THR:OG1	2.30	0.50
2:F:74:ARG:NH1	2:F:186:GLU:OE2	2.45	0.50
2:E:772:TYR:CE2	2:E:774:SER:HB2	2.47	0.50
2:H:194:ARG:HD3	2:H:198:PHE:CG	2.47	0.50
2:F:781:ASN:OD1	2:F:781:ASN:N	2.44	0.50
2:E:74:ARG:NH1	2:E:186:GLU:OE2	2.45	0.50
1:C:47:LYS:HA	2:G:59[A]:HIS:HB3	1.93	0.50
2:H:772:TYR:HA	2:H:852:PHE:HB2	1.93	0.50
2:G:194:ARG:HD3	2:G:198:PHE:CG	2.47	0.50
2:H:74:ARG:NH1	2:H:186:GLU:OE2	2.44	0.50
2:G:781:ASN:OD1	2:G:781:ASN:N	2.45	0.50
2:G:850:VAL:HG12	2:G:883:THR:HB	1.94	0.50
1:B:58:ASP:OD2	1:C:206:ARG:NH1	2.45	0.50
2:G:222:VAL:O	2:G:227:LYS:NZ	2.36	0.50
2:G:687:THR:N	2:G:731:GLN:O	2.45	0.50
2:F:302:SER:OG	2:F:376:SER:O	2.28	0.50
2:F:687:THR:N	2:F:731:GLN:O	2.45	0.50
1:A:58:ASP:OD2	1:B:206:ARG:NH1	2.45	0.49
2:F:219:GLN:OE1	2:F:232:TRP:NE1	2.31	0.49
2:G:203:GLU:HG3	2:G:205:LYS:H	1.77	0.49
2:F:772:TYR:CE2	2:F:774:SER:HB2	2.46	0.49
3:F:1601:PT5:O41	3:F:1601:PT5:O6	2.20	0.49
2:E:710:MET:HA	2:E:886:LEU:H	1.77	0.49
2:E:194:ARG:HD3	2:E:198:PHE:CG	2.47	0.49
2:E:413:THR:HG22	2:E:416:GLN:H	1.77	0.49
2:H:302:SER:OG	2:H:376:SER:O	2.28	0.49
2:G:74:ARG:NH1	2:G:186:GLU:OE2	2.44	0.49
2:F:79:PHE:HZ	2:F:225:LEU:HG	1.77	0.49
1:B:177:ARG:NH1	1:B:180:THR:OG1	2.46	0.49
2:E:850:VAL:HG12	2:E:883:THR:HB	1.95	0.49
1:C:58:ASP:OD2	1:D:206:ARG:NH1	2.45	0.49
1:D:47:LYS:HA	2:H:59[A]:HIS:HB3	1.93	0.49
2:F:194:ARG:HD3	2:F:198:PHE:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:781:ASN:OD1	2:E:781:ASN:N	2.44	0.49
1:B:47:LYS:HA	2:F:59[B]:HIS:HB2	1.95	0.49
2:E:772:TYR:HA	2:E:852:PHE:HB2	1.95	0.49
2:H:899:TRP:HD1	2:H:912:GLY:HA2	1.78	0.49
2:G:79:PHE:HZ	2:G:225:LEU:HG	1.78	0.49
2:E:1157:ILE:HD13	2:E:1164:PHE:CD2	2.48	0.49
1:B:180:THR:HG21	1:B:206:ARG:HH11	1.78	0.49
1:C:47:LYS:HA	2:G:59[B]:HIS:HB2	1.94	0.49
1:D:47:LYS:HA	2:H:59[B]:HIS:HB2	1.95	0.49
2:H:203:GLU:HG3	2:H:205:LYS:H	1.78	0.49
2:H:807:SER:O	2:H:837:ARG:NH2	2.46	0.49
1:C:177:ARG:NH1	1:C:180:THR:OG1	2.46	0.48
2:G:772:TYR:HA	2:G:852:PHE:HB2	1.93	0.48
1:D:177:ARG:NH1	1:D:180:THR:OG1	2.46	0.48
2:E:306:ARG:HD2	2:E:436:PRO:HB2	1.96	0.48
2:G:1178:ILE:HD13	2:G:1251:ARG:HB3	1.94	0.48
2:E:420:LEU:HD13	2:E:609:LYS:HE2	1.95	0.48
2:E:542:ILE:HA	2:E:545:PHE:CE2	2.49	0.48
2:E:1023:LYS:NZ	2:E:1082:THR:OG1	2.30	0.48
1:C:201:ARG:NH2	1:C:315:PHE:HB3	2.29	0.48
1:A:206:ARG:NH1	1:D:58:ASP:OD2	2.46	0.48
2:E:79:PHE:HZ	2:E:225:LEU:HG	1.77	0.48
2:F:1157:ILE:HD13	2:F:1164:PHE:CD2	2.49	0.48
2:F:203:GLU:HG3	2:F:205:LYS:H	1.77	0.48
1:A:180:THR:HG21	1:A:206:ARG:HD3	1.95	0.48
1:D:201:ARG:NH2	1:D:315:PHE:HB3	2.29	0.48
2:H:79:PHE:HZ	2:H:225:LEU:HG	1.78	0.48
2:G:739:TRP:HD1	2:G:740:ASN:H	1.62	0.48
2:H:739:TRP:HD1	2:H:740:ASN:H	1.62	0.48
2:F:1187:ARG:HE	2:F:1306:GLU:HG2	1.79	0.48
2:F:739:TRP:HD1	2:F:740:ASN:H	1.62	0.48
1:D:180:THR:HG21	1:D:206:ARG:HH11	1.79	0.47
2:H:571:LEU:HD13	2:H:1038:THR:HG22	1.96	0.47
2:F:75:TRP:HZ3	2:F:225:LEU:HD12	1.79	0.47
2:H:687:THR:N	2:H:731:GLN:O	2.45	0.47
2:G:807:SER:O	2:G:837:ARG:NH2	2.47	0.47
2:G:1157:ILE:HD13	2:G:1164:PHE:CD2	2.49	0.47
2:E:219:GLN:OE1	2:E:232:TRP:NE1	2.31	0.47
2:H:1187:ARG:HE	2:H:1306:GLU:HG2	1.80	0.47
2:F:807:SER:O	2:F:837:ARG:NH2	2.47	0.47
2:E:98:VAL:HG21	2:E:336:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1187:ARG:HE	2:E:1306:GLU:HG2	1.79	0.47
2:E:1196:THR:HG21	2:E:1234:ASN:HA	1.96	0.47
2:H:1157:ILE:HD13	2:H:1164:PHE:CD2	2.49	0.47
2:G:420:LEU:HD13	2:G:609:LYS:HE2	1.96	0.47
2:G:899:TRP:HD1	2:G:912:GLY:HA2	1.80	0.47
1:C:180:THR:HG21	1:C:206:ARG:HD3	1.96	0.47
1:D:180:THR:HG21	1:D:206:ARG:HD3	1.96	0.47
2:H:306:ARG:HD2	2:H:436:PRO:HB2	1.96	0.47
2:H:1178:ILE:HD13	2:H:1251:ARG:HB3	1.95	0.47
2:G:306:ARG:HD2	2:G:436:PRO:HB2	1.96	0.47
2:F:899:TRP:HD1	2:F:912:GLY:HA2	1.78	0.47
1:B:201:ARG:NH2	1:B:315:PHE:HB3	2.29	0.47
2:G:136:LEU:HD23	2:G:189:VAL:HG21	1.97	0.47
2:G:1196:THR:HG21	2:G:1234:ASN:HA	1.96	0.47
2:F:288:TRP:HZ2	2:F:607:VAL:HG21	1.80	0.47
2:F:306:ARG:HD2	2:F:436:PRO:HB2	1.96	0.47
2:F:1178:ILE:HD13	2:F:1251:ARG:HB3	1.95	0.47
2:E:75:TRP:HZ3	2:E:225:LEU:HD12	1.79	0.47
2:H:420:LEU:HD13	2:H:609:LYS:HE2	1.97	0.47
2:H:1196:THR:HG21	2:H:1234:ASN:HA	1.96	0.47
2:F:571:LEU:HD13	2:F:1038:THR:HG22	1.97	0.47
2:F:710:MET:HA	2:F:886:LEU:H	1.80	0.47
2:H:75:TRP:HZ3	2:H:225:LEU:HD12	1.79	0.47
2:G:571:LEU:HD13	2:G:1038:THR:HG22	1.97	0.47
2:F:222:VAL:O	2:F:227:LYS:NZ	2.36	0.47
1:A:239:PRO:O	1:A:259:HIS:ND1	2.46	0.46
1:C:180:THR:HG21	1:C:206:ARG:HH11	1.80	0.46
3:H:1601:PT5:H72	3:H:1601:PT5:H78	1.53	0.46
2:E:288:TRP:HZ2	2:E:607:VAL:HG21	1.80	0.46
2:H:781:ASN:OD1	2:H:781:ASN:N	2.44	0.46
2:G:542:ILE:HA	2:G:545:PHE:CE2	2.50	0.46
1:A:276:HIS:NE2	1:A:278:HIS:O	2.48	0.46
2:H:288:TRP:HZ2	2:H:607:VAL:HG21	1.80	0.46
2:H:542:ILE:HA	2:H:545:PHE:CE2	2.50	0.46
2:G:75:TRP:HZ3	2:G:225:LEU:HD12	1.79	0.46
2:G:302:SER:OG	2:G:376:SER:O	2.28	0.46
2:G:1187:ARG:HE	2:G:1306:GLU:HG2	1.80	0.46
2:F:136:LEU:HD23	2:F:189:VAL:HG21	1.97	0.46
2:F:382:GLU:O	2:F:386:ASN:ND2	2.44	0.46
2:F:143:TRP:HD1	2:F:186:GLU:HG3	1.80	0.46
1:A:201:ARG:NH2	1:A:315:PHE:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1178:ILE:HD13	2:E:1251:ARG:HB3	1.96	0.46
2:H:263:TYR:HE2	2:H:394:LYS:HG2	1.81	0.46
2:F:1196:THR:HG21	2:F:1234:ASN:HA	1.97	0.46
2:E:136:LEU:HD23	2:E:189:VAL:HG21	1.97	0.46
2:E:143:TRP:HD1	2:E:186:GLU:HG3	1.80	0.46
2:H:588:THR:HB	2:H:589:PRO:HD3	1.98	0.46
2:G:710:MET:HA	2:G:886:LEU:H	1.80	0.46
2:F:542:ILE:HA	2:F:545:PHE:CE2	2.50	0.46
1:C:218:GLN:OE1	1:C:235:GLN:NE2	2.45	0.46
2:G:263:TYR:HE2	2:G:394:LYS:HG2	1.81	0.46
2:F:416:GLN:HA	2:F:419:ASN:HD21	1.81	0.46
1:B:180:THR:HG21	1:B:206:ARG:HD3	1.97	0.46
3:G:1601:PT5:H78	3:G:1601:PT5:H72	1.53	0.46
2:E:588:THR:HB	2:E:589:PRO:HD3	1.98	0.46
2:H:143:TRP:HD1	2:H:186:GLU:HG3	1.80	0.46
2:H:416:GLN:HA	2:H:419:ASN:HD21	1.81	0.46
2:G:143:TRP:HD1	2:G:186:GLU:HG3	1.80	0.46
2:F:711:ILE:HA	2:F:901:ILE:HG23	1.98	0.46
3:F:1601:PT5:H78	3:F:1601:PT5:H72	1.53	0.46
2:E:807:SER:O	2:E:837:ARG:NH2	2.49	0.46
2:H:840:VAL:HG23	2:H:853:LEU:HD22	1.98	0.46
2:G:288:TRP:HZ2	2:G:607:VAL:HG21	1.80	0.46
2:F:420:LEU:HD13	2:F:609:LYS:HE2	1.97	0.46
2:E:263:TYR:HE2	2:E:394:LYS:HG2	1.80	0.45
1:D:276:HIS:NE2	1:D:278:HIS:O	2.49	0.45
2:H:125:HIS:NE2	5:H:1602:PEF:O2P	2.45	0.45
2:H:136:LEU:HD23	2:H:189:VAL:HG21	1.97	0.45
2:H:1081:VAL:O	2:H:1085:THR:OG1	2.27	0.45
2:F:840:VAL:HG23	2:F:853:LEU:HD22	1.98	0.45
2:E:5:PHE:HA	2:E:104:LEU:HB2	1.99	0.45
2:E:420:LEU:HD11	2:E:610:LEU:HD23	1.98	0.45
2:G:588:THR:HB	2:G:589:PRO:HD3	1.98	0.45
2:E:840:VAL:HG23	2:E:853:LEU:HD22	1.99	0.45
1:C:54:ARG:NE	1:D:179:GLU:O	2.47	0.45
2:H:710:MET:HA	2:H:886:LEU:H	1.81	0.45
2:F:420:LEU:HD11	2:F:610:LEU:HD23	1.98	0.45
2:E:302:SER:OG	2:E:376:SER:O	2.28	0.45
2:G:416:GLN:HA	2:G:419:ASN:HD21	1.81	0.45
2:G:834:GLN:HA	2:G:837:ARG:HD3	1.98	0.45
1:A:48:ASN:ND2	1:B:329:ASP:OD1	2.33	0.45
2:E:127:ILE:HG23	2:E:132:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:382:GLU:O	2:G:386:ASN:ND2	2.44	0.45
2:F:588:THR:HB	2:F:589:PRO:HD3	1.98	0.45
2:E:819:ASP:OD1	2:E:819:ASP:N	2.45	0.45
1:B:78:SER:O	1:B:82:SER:OG	2.28	0.45
2:F:549:ALA:HB1	2:F:1076:ILE:HG13	1.99	0.45
2:E:899:TRP:HD1	2:E:912:GLY:HA2	1.81	0.45
1:D:35:PHE:HD2	1:D:284:ILE:HD11	1.82	0.45
2:G:800:LYS:HA	2:G:803:ILE:HG22	1.99	0.45
2:G:840:VAL:HG23	2:G:853:LEU:HD22	1.98	0.45
2:F:834:GLN:HA	2:F:837:ARG:HD3	1.98	0.45
1:C:276:HIS:NE2	1:C:278:HIS:O	2.49	0.45
2:G:711:ILE:HA	2:G:901:ILE:HG23	1.99	0.45
2:H:800:LYS:HA	2:H:803:ILE:HG22	1.99	0.45
2:F:98:VAL:HG21	2:F:336:PRO:HD3	1.99	0.45
1:D:218:GLN:OE1	1:D:235:GLN:NE2	2.45	0.44
2:G:420:LEU:HD11	2:G:610:LEU:HD23	1.99	0.44
2:F:127:ILE:HG23	2:F:132:PHE:HB2	1.99	0.44
2:F:263:TYR:HE2	2:F:394:LYS:HG2	1.80	0.44
2:E:834:GLN:HA	2:E:837:ARG:HD3	1.99	0.44
2:E:125:HIS:NE2	5:E:1602:PEF:O2P	2.44	0.44
2:E:419:ASN:HA	2:E:422:ALA:HB3	1.99	0.44
2:E:774:SER:OG	2:E:775:GLN:N	2.50	0.44
1:B:276:HIS:NE2	1:B:278:HIS:O	2.50	0.44
2:H:467:ILE:HD11	2:H:554:ALA:HB2	1.99	0.44
2:E:382:GLU:O	2:E:386:ASN:ND2	2.46	0.44
2:H:711:ILE:HA	2:H:901:ILE:HG23	2.00	0.44
2:H:834:GLN:HA	2:H:837:ARG:HD3	1.98	0.44
3:G:1601:PT5:O41	3:G:1601:PT5:O6	2.20	0.44
2:E:416:GLN:HA	2:E:419:ASN:HD21	1.82	0.44
2:F:863:HIS:O	2:F:867:HIS:ND1	2.51	0.44
2:H:420:LEU:HD11	2:H:610:LEU:HD23	1.99	0.44
1:B:256:ILE:H	1:B:256:ILE:HG13	1.67	0.44
2:H:336:PRO:HG2	2:H:344:TYR:HB3	2.00	0.44
3:F:1601:PT5:H62	3:F:1601:PT5:H55	1.76	0.44
2:E:123:TYR:O	2:E:127:ILE:HG12	2.18	0.44
2:E:467:ILE:HD11	2:E:554:ALA:HB2	2.00	0.44
2:E:863:HIS:O	2:E:867:HIS:ND1	2.50	0.44
2:E:1132:ILE:HA	2:E:1136:ILE:HG12	2.00	0.44
2:G:127:ILE:HG23	2:G:132:PHE:HB2	1.99	0.43
2:E:203:GLU:HG3	2:E:205:LYS:H	1.82	0.43
2:E:800:LYS:HA	2:E:803:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1132:ILE:HA	2:F:1136:ILE:HG12	2.00	0.43
2:E:22:LEU:HB3	2:E:156:LYS:HE3	2.00	0.43
2:H:123:TYR:O	2:H:127:ILE:HG12	2.18	0.43
2:H:382:GLU:O	2:H:386:ASN:ND2	2.44	0.43
2:G:326:HIS:CE1	2:G:353:GLY:HA2	2.53	0.43
2:G:863:HIS:O	2:G:867:HIS:ND1	2.51	0.43
2:E:792:SER:OG	2:E:846:GLN:NE2	2.52	0.43
2:H:98:VAL:HG21	2:H:336:PRO:HD3	2.00	0.43
2:H:326:HIS:CE1	2:H:353:GLY:HA2	2.53	0.43
2:H:549:ALA:HB1	2:H:1076:ILE:HG13	2.00	0.43
2:G:549:ALA:HB1	2:G:1076:ILE:HG13	1.98	0.43
2:F:5:PHE:HA	2:F:104:LEU:HB2	2.01	0.43
2:H:127:ILE:HG23	2:H:132:PHE:HB2	2.00	0.43
2:H:863:HIS:O	2:H:867:HIS:ND1	2.51	0.43
2:F:800:LYS:HA	2:F:803:ILE:HG22	1.99	0.43
2:F:326:HIS:CE1	2:F:353:GLY:HA2	2.54	0.43
2:F:336:PRO:HG2	2:F:344:TYR:HB3	2.00	0.43
2:F:467:ILE:HD11	2:F:554:ALA:HB2	1.99	0.43
2:E:1164:PHE:HZ	2:E:1259:VAL:HG13	1.84	0.43
1:B:140:GLU:HG3	1:C:122:LEU:HD12	2.01	0.43
2:H:792:SER:OG	2:H:846:GLN:NE2	2.52	0.43
2:G:5:PHE:HA	2:G:104:LEU:HB2	2.01	0.43
2:G:582:LEU:O	2:G:586:LEU:HB2	2.19	0.43
2:E:739:TRP:HD1	2:E:740:ASN:H	1.66	0.43
2:H:5:PHE:HA	2:H:104:LEU:HB2	2.01	0.43
2:G:336:PRO:HG2	2:G:344:TYR:HB3	2.00	0.43
2:G:792:SER:OG	2:G:846:GLN:NE2	2.51	0.43
2:F:1089:THR:HA	2:F:1092:LYS:HE2	2.01	0.43
2:E:326:HIS:CE1	2:E:353:GLY:HA2	2.54	0.43
2:G:98:VAL:HG21	2:G:336:PRO:HD3	1.99	0.43
2:F:123:TYR:O	2:F:127:ILE:HG12	2.18	0.43
2:F:784:VAL:HG22	2:F:823:ILE:HB	2.00	0.43
2:H:22:LEU:HB3	2:H:156:LYS:HE3	2.01	0.42
2:G:17:VAL:HB	2:G:21:VAL:HG12	2.01	0.42
2:G:562:HIS:CD2	2:G:563:VAL:HG13	2.54	0.42
2:G:1132:ILE:HA	2:G:1136:ILE:HG12	2.01	0.42
2:F:582:LEU:O	2:F:586:LEU:HB2	2.19	0.42
2:E:49:ILE:HD13	2:E:49:ILE:HA	1.90	0.42
2:G:22:LEU:HB3	2:G:156:LYS:HE3	2.01	0.42
1:A:54:ARG:NE	1:B:179:GLU:O	2.47	0.42
2:E:336:PRO:HG2	2:E:344:TYR:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:219:GLN:HG2	2:H:378:TYR:CZ	2.55	0.42
2:G:123:TYR:O	2:G:127:ILE:HG12	2.18	0.42
1:A:140:GLU:HG3	1:B:122:LEU:HD12	2.01	0.42
2:E:17:VAL:HB	2:E:21:VAL:HG12	2.01	0.42
1:D:267:LEU:HD23	1:D:270:LEU:HD22	2.01	0.42
2:E:441:MET:HG3	2:E:593:LEU:HD23	2.02	0.42
2:E:687:THR:N	2:E:731:GLN:O	2.48	0.42
1:C:267:LEU:HD23	1:C:270:LEU:HD22	2.01	0.42
2:H:550:ILE:HG23	2:H:551:PRO:HD3	2.02	0.42
2:H:784:VAL:HG22	2:H:823:ILE:HB	2.01	0.42
2:H:1132:ILE:HA	2:H:1136:ILE:HG12	2.00	0.42
2:G:784:VAL:HG22	2:G:823:ILE:HB	2.02	0.42
2:H:1157:ILE:HA	2:H:1160:VAL:HG22	2.01	0.42
2:F:22:LEU:HB3	2:F:156:LYS:HE3	2.02	0.42
2:E:582:LEU:O	2:E:586:LEU:HB2	2.20	0.42
2:E:1164:PHE:CZ	2:E:1259:VAL:HG13	2.55	0.42
1:B:54:ARG:NE	1:C:179:GLU:O	2.47	0.42
1:B:215:ILE:HG21	1:B:257:ILE:HG21	2.01	0.42
1:C:215:ILE:HG21	1:C:257:ILE:HG21	2.02	0.42
2:H:861:ASP:OD1	2:H:861:ASP:N	2.52	0.42
1:C:72:LEU:HD11	3:C:401:PT5:H16	2.02	0.42
2:H:774:SER:OG	2:H:775:GLN:N	2.53	0.42
3:H:1601:PT5:H62	3:H:1601:PT5:H55	1.76	0.42
2:F:366:LEU:O	2:F:370:ARG:HG2	2.20	0.42
2:F:792:SER:OG	2:F:846:GLN:NE2	2.53	0.42
1:A:179:GLU:O	1:D:54:ARG:NE	2.45	0.42
2:H:366:LEU:O	2:H:370:ARG:HG2	2.20	0.42
2:G:219:GLN:HG2	2:G:378:TYR:CZ	2.55	0.42
2:G:1189:LEU:HD13	2:G:1241:LEU:HA	2.01	0.42
2:F:441:MET:HG3	2:F:593:LEU:HD23	2.02	0.42
2:F:562:HIS:CD2	2:F:563:VAL:HG13	2.55	0.42
2:F:711:ILE:N	2:F:886:LEU:O	2.44	0.42
2:E:366:LEU:O	2:E:370:ARG:HG2	2.20	0.41
2:E:530:MET:HB3	2:E:530:MET:HE2	1.89	0.41
2:E:711:ILE:HA	2:E:901:ILE:HG23	2.02	0.41
1:B:267:LEU:HD23	1:B:270:LEU:HD22	2.01	0.41
1:C:35:PHE:HD2	1:C:284:ILE:HD11	1.85	0.41
2:G:550:ILE:HG23	2:G:551:PRO:HD3	2.02	0.41
2:G:1019:SER:O	2:G:1023:LYS:HG2	2.21	0.41
1:C:140:GLU:HG3	1:D:122:LEU:HD12	2.01	0.41
2:H:582:LEU:O	2:H:586:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:288:TRP:CZ2	2:G:607:VAL:HG21	2.55	0.41
2:G:467:ILE:HD11	2:G:554:ALA:HB2	2.01	0.41
2:G:711:ILE:N	2:G:886:LEU:O	2.43	0.41
1:B:72:LEU:HD11	3:B:401:PT5:H16	2.02	0.41
2:H:288:TRP:CZ2	2:H:607:VAL:HG21	2.56	0.41
2:G:366:LEU:O	2:G:370:ARG:HG2	2.20	0.41
2:F:1019:SER:O	2:F:1023:LYS:HG2	2.21	0.41
2:F:1157:ILE:HA	2:F:1160:VAL:HG22	2.02	0.41
2:E:219:GLN:HG2	2:E:378:TYR:CZ	2.55	0.41
2:G:54:GLN:H	2:G:54:GLN:CD	2.24	0.41
2:F:1239:LEU:HD12	2:F:1240:PHE:N	2.36	0.41
2:E:571:LEU:HD13	2:E:1038:THR:HG22	2.01	0.41
2:E:1157:ILE:HA	2:E:1160:VAL:HG22	2.01	0.41
1:B:155:VAL:HG13	3:C:401:PT5:H24	2.02	0.41
1:D:72:LEU:HD11	3:D:401:PT5:H16	2.02	0.41
2:F:54:GLN:CD	2:F:54:GLN:H	2.24	0.41
2:F:1157:ILE:HD12	2:F:1158:SER:N	2.35	0.41
2:E:288:TRP:CZ2	2:E:607:VAL:HG21	2.55	0.41
2:H:441:MET:HG3	2:H:593:LEU:HD23	2.02	0.41
2:H:562:HIS:CD2	2:H:563:VAL:HG13	2.55	0.41
2:H:1019:SER:O	2:H:1023:LYS:HG2	2.21	0.41
2:H:1089:THR:HA	2:H:1092:LYS:HE2	2.02	0.41
2:H:1239:LEU:HD12	2:H:1240:PHE:N	2.36	0.41
2:G:1157:ILE:HD12	2:G:1158:SER:N	2.36	0.41
2:G:1239:LEU:HD12	2:G:1240:PHE:N	2.36	0.41
2:F:219:GLN:HG2	2:F:378:TYR:CZ	2.55	0.41
2:F:222:VAL:HG11	2:F:232:TRP:HB3	2.02	0.41
1:A:155:VAL:HG13	3:B:401:PT5:H24	2.02	0.41
2:E:222:VAL:HG11	2:E:232:TRP:HB3	2.03	0.41
2:E:537:ALA:HB2	2:E:1091:LEU:HD21	2.03	0.41
2:E:1211:LEU:HD12	2:E:1212:THR:H	1.85	0.41
2:H:1157:ILE:H	2:H:1157:ILE:HG13	1.65	0.41
2:G:485:GLN:HB2	2:G:536:PHE:CE1	2.56	0.41
2:G:530:MET:HE2	2:G:530:MET:HB3	1.94	0.41
1:A:90:TRP:CE3	1:A:93:ILE:HD11	2.56	0.41
1:A:290:VAL:HA	1:A:297:THR:HA	2.03	0.41
1:D:215:ILE:HG21	1:D:257:ILE:HG21	2.02	0.41
2:H:222:VAL:HG11	2:H:232:TRP:HB3	2.03	0.41
2:H:1157:ILE:HD12	2:H:1158:SER:N	2.35	0.41
2:H:1245:ASN:O	2:H:1249:GLU:HG2	2.21	0.41
2:G:1157:ILE:HA	2:G:1160:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1164:PHE:CZ	2:F:1259:VAL:HG13	2.56	0.41
1:A:122:LEU:HD12	1:D:140:GLU:HG3	2.01	0.41
2:E:1169:LEU:HB2	2:E:1170:PRO:HD3	2.03	0.41
3:E:1601:PT5:H55	3:E:1601:PT5:H62	1.76	0.41
1:D:314:ARG:CZ	1:D:339:VAL:HG11	2.51	0.41
2:H:711:ILE:N	2:H:886:LEU:O	2.44	0.41
2:H:1169:LEU:HB2	2:H:1170:PRO:HD3	2.03	0.41
2:G:419:ASN:HA	2:G:422:ALA:HB3	2.02	0.41
2:G:1164:PHE:HZ	2:G:1259:VAL:HG13	1.86	0.41
2:F:125:HIS:NE2	5:F:1602:PEF:O2P	2.45	0.41
2:F:288:TRP:CZ2	2:F:607:VAL:HG21	2.55	0.41
2:F:596:VAL:O	2:F:600:THR:N	2.51	0.41
2:E:54:GLN:H	2:E:54:GLN:CD	2.23	0.41
2:E:485:GLN:HB2	2:E:536:PHE:CE1	2.56	0.41
2:E:562:HIS:CD2	2:E:563:VAL:HG13	2.56	0.41
2:E:1239:LEU:HD12	2:E:1240:PHE:N	2.36	0.41
1:C:155:VAL:HG13	3:D:401:PT5:H24	2.02	0.41
2:H:17:VAL:HB	2:H:21:VAL:HG12	2.02	0.41
2:G:125:HIS:NE2	5:G:1602:PEF:O2P	2.45	0.41
2:G:767:ARG:HG2	2:G:768:GLY:H	1.86	0.41
2:G:1169:LEU:HB2	2:G:1170:PRO:HD3	2.03	0.41
2:F:1169:LEU:HB2	2:F:1170:PRO:HD3	2.03	0.41
2:E:778:TRP:NE1	2:E:1209:GLU:O	2.54	0.40
1:A:215:ILE:HG21	1:A:257:ILE:HG21	2.03	0.40
1:A:314:ARG:CZ	1:A:339:VAL:HG11	2.50	0.40
3:A:401:PT5:H24	1:D:155:VAL:HG13	2.02	0.40
2:H:270:PHE:HD1	2:H:270:PHE:HA	1.82	0.40
2:H:485:GLN:HB2	2:H:536:PHE:CE1	2.56	0.40
2:G:222:VAL:HG11	2:G:232:TRP:HB3	2.03	0.40
2:F:767:ARG:HG2	2:F:768:GLY:H	1.86	0.40
2:H:1164:PHE:HZ	2:H:1259:VAL:HG13	1.86	0.40
2:F:550:ILE:HG23	2:F:551:PRO:HD3	2.04	0.40
2:F:778:TRP:NE1	2:F:1209:GLU:O	2.55	0.40
1:A:72:LEU:HD11	3:A:401:PT5:H16	2.03	0.40
1:C:314:ARG:CZ	1:C:339:VAL:HG11	2.51	0.40
2:H:1164:PHE:CZ	2:H:1259:VAL:HG13	2.56	0.40
2:G:225:LEU:HD22	5:G:1602:PEF:H141	2.04	0.40
2:G:1086:VAL:HG11	2:G:1141:GLU:HG3	2.04	0.40
2:F:17:VAL:HB	2:F:21:VAL:HG12	2.03	0.40
2:F:485:GLN:HB2	2:F:536:PHE:CE1	2.57	0.40
2:F:1245:ASN:O	2:F:1249:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.97	0.40
2:H:54:GLN:H	2:H:54:GLN:CD	2.24	0.40
2:H:419:ASN:HA	2:H:422:ALA:HB3	2.02	0.40
2:G:209:ASP:OD1	2:G:210:LEU:N	2.47	0.40
2:G:778:TRP:NE1	2:G:1209:GLU:O	2.55	0.40
2:F:49:ILE:HD13	2:F:49:ILE:HA	1.90	0.40
2:F:225:LEU:HD22	5:F:1602:PEF:H141	2.04	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	320/390 (82%)	311 (97%)	9 (3%)	0	100	100
1	B	320/390 (82%)	307 (96%)	13 (4%)	0	100	100
1	C	320/390 (82%)	307 (96%)	13 (4%)	0	100	100
1	D	320/390 (82%)	307 (96%)	13 (4%)	0	100	100
2	E	1130/1582 (71%)	1071 (95%)	57 (5%)	2 (0%)	44	73
2	F	1130/1582 (71%)	1075 (95%)	52 (5%)	3 (0%)	37	66
2	G	1130/1582 (71%)	1078 (95%)	50 (4%)	2 (0%)	44	73
2	H	1130/1582 (71%)	1077 (95%)	50 (4%)	3 (0%)	37	66
All	All	5800/7888 (74%)	5533 (95%)	257 (4%)	10 (0%)	45	73

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	412	MET
2	G	412	MET
2	F	412	MET

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Mol	Chain	Res	Type
2	E	258	ARG
2	E	738	PHE
2	H	258	ARG
2	G	258	ARG
2	F	258	ARG
2	H	776	LYS
2	F	776	LYS

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	281/341 (82%)	277 (99%)	4 (1%)	62	86
1	B	281/341 (82%)	277 (99%)	4 (1%)	62	86
1	C	281/341 (82%)	277 (99%)	4 (1%)	62	86
1	D	281/341 (82%)	277 (99%)	4 (1%)	62	86
2	E	829/1371 (60%)	799 (96%)	30 (4%)	30	65
2	F	829/1371 (60%)	798 (96%)	31 (4%)	29	64
2	G	829/1371 (60%)	798 (96%)	31 (4%)	29	64
2	H	829/1371 (60%)	798 (96%)	31 (4%)	29	64
All	All	4440/6848 (65%)	4301 (97%)	139 (3%)	37	70

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	PHE
1	A	139	THR
1	A	200	LEU
1	A	256	ILE
2	E	39	LEU
2	E	81	LEU
2	E	136	LEU
2	E	225	LEU

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Mol	Chain	Res	Type
2	E	231	TRP
2	E	262	ASN
2	E	270	PHE
2	E	387	LEU
2	E	566	PHE
2	E	567	LYS
2	E	571	LEU
2	E	732	LYS
2	E	739	TRP
2	E	787	ASN
2	E	845	TYR
2	E	998	TRP
2	E	1005	LEU
2	E	1036	LYS
2	E	1063	VAL
2	E	1145	ARG
2	E	1148	LEU
2	E	1161	THR
2	E	1200	LEU
2	E	1211	LEU
2	E	1215	ARG
2	E	1240	PHE
2	E	1251	ARG
2	E	1252	MET
2	E	1295	LEU
2	E	1297	TRP
1	B	95	PHE
1	B	139	THR
1	B	200	LEU
1	B	256	ILE
1	C	95	PHE
1	C	139	THR
1	C	200	LEU
1	C	256	ILE
1	D	95	PHE
1	D	139	THR
1	D	200	LEU
1	D	256	ILE
2	H	39	LEU
2	H	66	LEU
2	H	81	LEU
2	H	136	LEU

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Mol	Chain	Res	Type
2	H	225	LEU
2	H	231	TRP
2	H	262	ASN
2	H	270	PHE
2	H	387	LEU
2	H	566	PHE
2	H	571	LEU
2	H	732	LYS
2	H	739	TRP
2	H	787	ASN
2	H	845	TYR
2	H	998	TRP
2	H	1005	LEU
2	H	1036	LYS
2	H	1043	VAL
2	H	1063	VAL
2	H	1145	ARG
2	H	1148	LEU
2	H	1161	THR
2	H	1200	LEU
2	H	1211	LEU
2	H	1215	ARG
2	H	1240	PHE
2	H	1251	ARG
2	H	1252	MET
2	H	1295	LEU
2	H	1297	TRP
2	G	39	LEU
2	G	66	LEU
2	G	81	LEU
2	G	136	LEU
2	G	225	LEU
2	G	231	TRP
2	G	262	ASN
2	G	270	PHE
2	G	387	LEU
2	G	566	PHE
2	G	571	LEU
2	G	732	LYS
2	G	739	TRP
2	G	787	ASN
2	G	845	TYR

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Mol	Chain	Res	Type
2	G	998	TRP
2	G	1005	LEU
2	G	1036	LYS
2	G	1043	VAL
2	G	1063	VAL
2	G	1145	ARG
2	G	1148	LEU
2	G	1161	THR
2	G	1200	LEU
2	G	1211	LEU
2	G	1215	ARG
2	G	1240	PHE
2	G	1251	ARG
2	G	1252	MET
2	G	1295	LEU
2	G	1297	TRP
2	F	39	LEU
2	F	66	LEU
2	F	81	LEU
2	F	136	LEU
2	F	225	LEU
2	F	231	TRP
2	F	262	ASN
2	F	270	PHE
2	F	387	LEU
2	F	566	PHE
2	F	571	LEU
2	F	732	LYS
2	F	739	TRP
2	F	787	ASN
2	F	845	TYR
2	F	998	TRP
2	F	1005	LEU
2	F	1036	LYS
2	F	1043	VAL
2	F	1063	VAL
2	F	1145	ARG
2	F	1148	LEU
2	F	1161	THR
2	F	1200	LEU
2	F	1211	LEU
2	F	1215	ARG

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Mol	Chain	Res	Type
2	F	1240	PHE
2	F	1251	ARG
2	F	1252	MET
2	F	1295	LEU
2	F	1297	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	P5S	G	1604	-	44,45,53	0.57	0	46,52,60	0.99	1 (2%)
6	P5S	F	1604	-	44,45,53	0.58	0	46,52,60	0.99	1 (2%)
5	PEF	H	1602	-	27,27,46	1.20	3 (11%)	30,32,51	1.14	2 (6%)
6	P5S	H	1603	-	48,49,53	0.55	0	50,56,60	0.75	1 (2%)
7	NAG	F	1605	2	14,14,15	0.45	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	G	1605	2	14,14,15	0.46	0	17,19,21	0.41	0
5	PEF	F	1602	-	27,27,46	1.21	3 (11%)	30,32,51	1.14	2 (6%)
3	PT5	B	401	-	69,69,69	1.19	6 (8%)	84,87,87	1.44	9 (10%)
3	PT5	E	1601	-	69,69,69	1.21	6 (8%)	84,87,87	1.33	8 (9%)
7	NAG	E	1605	2	14,14,15	0.46	0	17,19,21	0.40	0
3	PT5	H	1601	-	69,69,69	1.21	6 (8%)	84,87,87	1.33	8 (9%)
6	P5S	E	1603	-	48,49,53	0.55	0	50,56,60	0.76	1 (2%)
3	PT5	D	401	-	69,69,69	1.20	6 (8%)	84,87,87	1.44	9 (10%)
5	PEF	E	1602	-	27,27,46	1.21	3 (11%)	30,32,51	1.13	2 (6%)
3	PT5	A	401	-	69,69,69	1.20	6 (8%)	84,87,87	1.44	9 (10%)
6	P5S	F	1603	-	48,49,53	0.55	0	50,56,60	0.75	1 (2%)
6	P5S	E	1604	-	44,45,53	0.57	0	46,52,60	0.99	1 (2%)
5	PEF	G	1602	-	27,27,46	1.21	3 (11%)	30,32,51	1.14	2 (6%)
6	P5S	G	1603	-	48,49,53	0.55	0	50,56,60	0.75	1 (2%)
6	P5S	H	1604	-	44,45,53	0.57	0	46,52,60	0.99	1 (2%)
7	NAG	H	1605	2	14,14,15	0.45	0	17,19,21	0.41	0
3	PT5	C	401	-	69,69,69	1.20	6 (8%)	84,87,87	1.44	9 (10%)
3	PT5	G	1601	-	69,69,69	1.21	6 (8%)	84,87,87	1.33	8 (9%)
3	PT5	F	1601	-	69,69,69	1.22	6 (8%)	84,87,87	1.33	8 (9%)

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
6	P5S	G	1604	-	-	16/51/51/59	-
6	P5S	F	1604	-	-	16/51/51/59	-
5	PEF	H	1602	-	-	11/31/31/50	-
6	P5S	H	1603	-	-	13/55/55/59	-
7	NAG	F	1605	2	-	2/6/23/26	0/1/1/1
7	NAG	G	1605	2	-	2/6/23/26	0/1/1/1
5	PEF	F	1602	-	-	11/31/31/50	-
3	PT5	B	401	-	-	24/66/90/90	0/1/1/1
3	PT5	E	1601	-	-	28/66/90/90	0/1/1/1
7	NAG	E	1605	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PT5	H	1601	-	-	28/66/90/90	0/1/1/1
6	P5S	E	1603	-	-	13/55/55/59	-
3	PT5	D	401	-	-	24/66/90/90	0/1/1/1
5	PEF	E	1602	-	-	11/31/31/50	-
3	PT5	A	401	-	-	24/66/90/90	0/1/1/1
6	P5S	F	1603	-	-	13/55/55/59	-
6	P5S	E	1604	-	-	16/51/51/59	-
5	PEF	G	1602	-	-	11/31/31/50	-
6	P5S	G	1603	-	-	13/55/55/59	-
6	P5S	H	1604	-	-	16/51/51/59	-
7	NAG	H	1605	2	-	2/6/23/26	0/1/1/1
3	PT5	C	401	-	-	24/66/90/90	0/1/1/1
3	PT5	G	1601	-	-	28/66/90/90	0/1/1/1
3	PT5	F	1601	-	-	28/66/90/90	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1601	PT5	P4-O4	4.71	1.67	1.59
3	E	1601	PT5	P4-O4	4.70	1.67	1.59
3	G	1601	PT5	P4-O4	4.70	1.67	1.59
3	F	1601	PT5	P4-O4	4.70	1.67	1.59
3	A	401	PT5	P4-O4	4.47	1.67	1.59
3	C	401	PT5	P4-O4	4.47	1.67	1.59
3	D	401	PT5	P4-O4	4.43	1.67	1.59
3	B	401	PT5	P4-O4	4.40	1.67	1.59
3	G	1601	PT5	P5-O5	4.05	1.66	1.59
3	F	1601	PT5	P5-O5	4.05	1.66	1.59
3	E	1601	PT5	P5-O5	4.02	1.66	1.59
3	H	1601	PT5	P5-O5	3.99	1.66	1.59
3	C	401	PT5	P5-O5	3.95	1.66	1.59
3	A	401	PT5	P5-O5	3.94	1.66	1.59
3	B	401	PT5	P5-O5	3.92	1.66	1.59
3	D	401	PT5	P5-O5	3.92	1.66	1.59
3	B	401	PT5	O18-C11	2.96	1.42	1.33
3	C	401	PT5	O18-C11	2.96	1.42	1.33
3	D	401	PT5	O18-C11	2.96	1.42	1.33
3	H	1601	PT5	O18-C11	2.94	1.41	1.33
3	A	401	PT5	O18-C11	2.93	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1601	PT5	O18-C11	2.92	1.41	1.33
3	F	1601	PT5	O18-C11	2.91	1.41	1.33
3	G	1601	PT5	O18-C11	2.90	1.41	1.33
3	F	1601	PT5	O16-C10	2.84	1.42	1.34
3	E	1601	PT5	O16-C10	2.82	1.42	1.34
3	G	1601	PT5	O16-C10	2.79	1.42	1.34
3	H	1601	PT5	O16-C10	2.79	1.42	1.34
3	D	401	PT5	O16-C10	2.79	1.42	1.34
3	C	401	PT5	O16-C10	2.76	1.42	1.34
3	A	401	PT5	O16-C10	2.76	1.42	1.34
3	B	401	PT5	O16-C10	2.75	1.42	1.34
5	E	1602	PEF	O2-C10	2.65	1.41	1.34
5	G	1602	PEF	O2-C10	2.64	1.41	1.34
5	H	1602	PEF	O2-C10	2.63	1.41	1.34
5	F	1602	PEF	O2-C10	2.63	1.41	1.34
5	H	1602	PEF	O3-C30	2.55	1.40	1.33
5	E	1602	PEF	O3-C30	2.54	1.40	1.33
5	G	1602	PEF	O3-C30	2.54	1.40	1.33
5	F	1602	PEF	O3-C30	2.52	1.40	1.33
5	E	1602	PEF	O3-C3	-2.40	1.39	1.45
3	B	401	PT5	O16-C8	-2.39	1.41	1.46
3	D	401	PT5	O16-C8	-2.39	1.41	1.46
5	G	1602	PEF	O3-C3	-2.39	1.39	1.45
5	F	1602	PEF	O3-C3	-2.39	1.39	1.45
3	A	401	PT5	O16-C8	-2.39	1.41	1.46
3	C	401	PT5	O16-C8	-2.36	1.41	1.46
3	H	1601	PT5	O16-C8	-2.35	1.41	1.46
5	H	1602	PEF	O3-C3	-2.34	1.39	1.45
3	F	1601	PT5	O16-C8	-2.34	1.41	1.46
3	G	1601	PT5	O16-C8	-2.34	1.41	1.46
3	E	1601	PT5	O16-C8	-2.33	1.41	1.46
3	A	401	PT5	P1-O1	2.28	1.66	1.59
3	C	401	PT5	P1-O1	2.27	1.66	1.59
3	B	401	PT5	P1-O1	2.27	1.66	1.59
3	D	401	PT5	P1-O1	2.27	1.66	1.59
3	E	1601	PT5	P1-O1	2.27	1.66	1.59
3	F	1601	PT5	P1-O1	2.26	1.66	1.59
3	H	1601	PT5	P1-O1	2.24	1.66	1.59
3	G	1601	PT5	P1-O1	2.23	1.66	1.59

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	1604	P5S	OG-CB-CA	5.67	113.01	108.06
6	H	1604	P5S	OG-CB-CA	5.65	112.98	108.06
6	F	1604	P5S	OG-CB-CA	5.64	112.98	108.06
6	E	1604	P5S	OG-CB-CA	5.63	112.97	108.06
3	A	401	PT5	C2-C1-C6	4.68	117.35	110.86
3	D	401	PT5	C2-C1-C6	4.65	117.32	110.86
3	C	401	PT5	C2-C1-C6	4.63	117.29	110.86
3	B	401	PT5	C2-C1-C6	4.63	117.28	110.86
3	G	1601	PT5	C20-C19-C18	-4.49	85.66	123.57
3	H	1601	PT5	C20-C19-C18	-4.49	85.67	123.57
3	E	1601	PT5	C20-C19-C18	-4.49	85.70	123.57
3	F	1601	PT5	C20-C19-C18	-4.48	85.71	123.57
3	A	401	PT5	C20-C19-C18	-4.28	87.46	123.57
3	B	401	PT5	C20-C19-C18	-4.28	87.47	123.57
3	C	401	PT5	C20-C19-C18	-4.28	87.48	123.57
3	D	401	PT5	C20-C19-C18	-4.27	87.53	123.57
3	E	1601	PT5	C21-C20-C19	3.94	131.44	112.02
3	F	1601	PT5	C21-C20-C19	3.94	131.42	112.02
3	H	1601	PT5	C21-C20-C19	3.94	131.41	112.02
3	G	1601	PT5	C21-C20-C19	3.93	131.39	112.02
3	H	1601	PT5	O16-C10-C12	3.81	119.72	111.48
3	A	401	PT5	C21-C20-C19	3.81	130.77	112.02
3	C	401	PT5	C21-C20-C19	3.80	130.76	112.02
3	D	401	PT5	C21-C20-C19	3.80	130.75	112.02
6	E	1603	P5S	OG-CB-CA	3.80	111.37	108.06
3	B	401	PT5	C21-C20-C19	3.79	130.71	112.02
3	F	1601	PT5	O16-C10-C12	3.79	119.68	111.48
3	G	1601	PT5	O16-C10-C12	3.78	119.67	111.48
3	E	1601	PT5	O16-C10-C12	3.78	119.65	111.48
3	B	401	PT5	O16-C10-C12	3.77	119.65	111.48
6	G	1603	P5S	OG-CB-CA	3.77	111.34	108.06
3	A	401	PT5	O16-C10-C12	3.77	119.63	111.48
3	C	401	PT5	O16-C10-C12	3.76	119.61	111.48
3	D	401	PT5	O16-C10-C12	3.75	119.60	111.48
6	F	1603	P5S	OG-CB-CA	3.74	111.32	108.06
6	H	1603	P5S	OG-CB-CA	3.72	111.31	108.06
5	F	1602	PEF	O2-C10-C11	3.55	119.17	111.48
3	A	401	PT5	C23-C22-C21	3.55	153.55	123.57
3	C	401	PT5	C23-C22-C21	3.55	153.53	123.57
3	B	401	PT5	C23-C22-C21	3.55	153.53	123.57
3	D	401	PT5	C23-C22-C21	3.55	153.51	123.57
5	G	1602	PEF	O2-C10-C11	3.54	119.15	111.48
3	H	1601	PT5	C17-C16-C15	3.54	153.48	123.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1601	PT5	C17-C16-C15	3.54	153.47	123.57
5	H	1602	PEF	O2-C10-C11	3.54	119.14	111.48
3	F	1601	PT5	C17-C16-C15	3.54	153.45	123.57
3	G	1601	PT5	C17-C16-C15	3.54	153.42	123.57
5	E	1602	PEF	O2-C10-C11	3.53	119.11	111.48
3	E	1601	PT5	C23-C22-C21	3.49	153.00	123.57
3	H	1601	PT5	C23-C22-C21	3.48	152.97	123.57
3	F	1601	PT5	C23-C22-C21	3.48	152.97	123.57
3	G	1601	PT5	C23-C22-C21	3.48	152.96	123.57
3	B	401	PT5	C17-C16-C15	3.16	150.24	123.57
3	A	401	PT5	C17-C16-C15	3.16	150.20	123.57
3	C	401	PT5	C17-C16-C15	3.15	150.16	123.57
3	D	401	PT5	C17-C16-C15	3.15	150.15	123.57
3	B	401	PT5	C5-C6-C1	2.98	115.14	109.11
3	C	401	PT5	C5-C6-C1	2.95	115.09	109.11
3	D	401	PT5	C5-C6-C1	2.95	115.09	109.11
3	A	401	PT5	C5-C6-C1	2.94	115.06	109.11
3	D	401	PT5	C3-C2-C1	2.93	116.33	109.68
3	A	401	PT5	C3-C2-C1	2.92	116.31	109.68
3	B	401	PT5	C3-C2-C1	2.92	116.30	109.68
3	C	401	PT5	C3-C2-C1	2.92	116.30	109.68
3	H	1601	PT5	C2-C1-C6	2.76	114.69	110.86
3	G	1601	PT5	C2-C1-C6	2.75	114.68	110.86
3	E	1601	PT5	C2-C1-C6	2.73	114.65	110.86
3	F	1601	PT5	C2-C1-C6	2.73	114.65	110.86
3	B	401	PT5	O18-C11-C31	2.71	120.08	111.83
3	E	1601	PT5	O18-C11-C31	2.70	120.08	111.83
3	C	401	PT5	O18-C11-C31	2.70	120.08	111.83
3	F	1601	PT5	O18-C11-C31	2.70	120.08	111.83
3	H	1601	PT5	O18-C11-C31	2.70	120.07	111.83
3	G	1601	PT5	O18-C11-C31	2.70	120.06	111.83
3	D	401	PT5	O18-C11-C31	2.69	120.05	111.83
3	A	401	PT5	O18-C11-C31	2.69	120.04	111.83
5	F	1602	PEF	O3-C30-C31	2.65	119.92	111.83
5	H	1602	PEF	O3-C30-C31	2.64	119.88	111.83
5	E	1602	PEF	O3-C30-C31	2.63	119.86	111.83
5	G	1602	PEF	O3-C30-C31	2.63	119.86	111.83
3	E	1601	PT5	C5-C6-C1	2.24	113.64	109.11
3	H	1601	PT5	C5-C6-C1	2.23	113.63	109.11
3	F	1601	PT5	C5-C6-C1	2.22	113.61	109.11
3	G	1601	PT5	C5-C6-C1	2.21	113.58	109.11

There are no chirality outliers.

All (376) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	PT5	C7-O13-P1-O11
3	A	401	PT5	C7-O13-P1-O1
3	A	401	PT5	C1-O1-P1-O12
3	A	401	PT5	C1-O1-P1-O13
3	E	1601	PT5	C1-O1-P1-O12
3	E	1601	PT5	C1-O1-P1-O13
3	E	1601	PT5	C5-C4-O4-P4
3	E	1601	PT5	C6-C5-O5-P5
3	E	1601	PT5	C4-C5-O5-P5
3	B	401	PT5	C7-O13-P1-O11
3	B	401	PT5	C7-O13-P1-O1
3	B	401	PT5	C1-O1-P1-O12
3	B	401	PT5	C1-O1-P1-O13
3	C	401	PT5	C7-O13-P1-O11
3	C	401	PT5	C7-O13-P1-O1
3	C	401	PT5	C1-O1-P1-O12
3	C	401	PT5	C1-O1-P1-O13
3	D	401	PT5	C7-O13-P1-O11
3	D	401	PT5	C7-O13-P1-O1
3	D	401	PT5	C1-O1-P1-O12
3	D	401	PT5	C1-O1-P1-O13
3	H	1601	PT5	C1-O1-P1-O12
3	H	1601	PT5	C1-O1-P1-O13
3	H	1601	PT5	C5-C4-O4-P4
3	H	1601	PT5	C6-C5-O5-P5
3	H	1601	PT5	C4-C5-O5-P5
3	G	1601	PT5	C1-O1-P1-O12
3	G	1601	PT5	C1-O1-P1-O13
3	G	1601	PT5	C5-C4-O4-P4
3	G	1601	PT5	C6-C5-O5-P5
3	G	1601	PT5	C4-C5-O5-P5
3	F	1601	PT5	C1-O1-P1-O12
3	F	1601	PT5	C1-O1-P1-O13
3	F	1601	PT5	C5-C4-O4-P4
3	F	1601	PT5	C6-C5-O5-P5
3	F	1601	PT5	C4-C5-O5-P5
5	E	1602	PEF	C4-O4P-P-O1P
5	E	1602	PEF	C4-O4P-P-O3P
5	H	1602	PEF	C4-O4P-P-O1P
5	H	1602	PEF	C4-O4P-P-O3P
5	G	1602	PEF	C4-O4P-P-O1P
5	G	1602	PEF	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
5	F	1602	PEF	C4-O4P-P-O1P
5	F	1602	PEF	C4-O4P-P-O3P
6	E	1603	P5S	C1-C2-O37-C38
6	E	1603	P5S	C39-C38-O37-C2
6	E	1604	P5S	O-C-CA-N
6	E	1604	P5S	OXT-C-CA-CB
6	E	1604	P5S	O37-C2-C3-O16
6	E	1604	P5S	C-CA-CB-OG
6	E	1604	P5S	N-CA-CB-OG
6	E	1604	P5S	CA-CB-OG-P12
6	H	1603	P5S	C1-C2-O37-C38
6	H	1603	P5S	C39-C38-O37-C2
6	H	1604	P5S	O-C-CA-N
6	H	1604	P5S	O37-C2-C3-O16
6	H	1604	P5S	C-CA-CB-OG
6	H	1604	P5S	N-CA-CB-OG
6	H	1604	P5S	CA-CB-OG-P12
6	G	1603	P5S	O-C-CA-N
6	G	1603	P5S	C1-C2-O37-C38
6	G	1603	P5S	C39-C38-O37-C2
6	G	1604	P5S	O-C-CA-N
6	G	1604	P5S	O37-C2-C3-O16
6	G	1604	P5S	C-CA-CB-OG
6	G	1604	P5S	N-CA-CB-OG
6	G	1604	P5S	CA-CB-OG-P12
6	F	1603	P5S	C1-C2-O37-C38
6	F	1603	P5S	C39-C38-O37-C2
6	F	1604	P5S	O-C-CA-N
6	F	1604	P5S	O37-C2-C3-O16
6	F	1604	P5S	C-CA-CB-OG
6	F	1604	P5S	N-CA-CB-OG
6	F	1604	P5S	CA-CB-OG-P12
6	E	1603	P5S	O47-C38-O37-C2
6	H	1603	P5S	O47-C38-O37-C2
6	G	1603	P5S	O47-C38-O37-C2
6	F	1603	P5S	O47-C38-O37-C2
3	E	1601	PT5	C31-C11-O18-C9
3	H	1601	PT5	C31-C11-O18-C9
3	G	1601	PT5	C31-C11-O18-C9
3	F	1601	PT5	C31-C11-O18-C9
7	H	1605	NAG	O5-C5-C6-O6
7	G	1605	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	F	1605	NAG	O5-C5-C6-O6
7	E	1605	NAG	C4-C5-C6-O6
7	G	1605	NAG	C4-C5-C6-O6
7	E	1605	NAG	O5-C5-C6-O6
7	H	1605	NAG	C4-C5-C6-O6
7	F	1605	NAG	C4-C5-C6-O6
3	H	1601	PT5	O19-C11-O18-C9
3	G	1601	PT5	O19-C11-O18-C9
3	F	1601	PT5	O19-C11-O18-C9
3	E	1601	PT5	O19-C11-O18-C9
6	E	1604	P5S	C17-C20-C21-C22
6	H	1604	P5S	C17-C20-C21-C22
6	G	1604	P5S	C17-C20-C21-C22
6	F	1604	P5S	C17-C20-C21-C22
3	E	1601	PT5	C12-C10-O16-C8
3	H	1601	PT5	C12-C10-O16-C8
3	G	1601	PT5	C12-C10-O16-C8
3	F	1601	PT5	C12-C10-O16-C8
6	E	1604	P5S	OXT-C-CA-N
6	H	1604	P5S	OXT-C-CA-N
6	G	1604	P5S	OXT-C-CA-N
6	F	1604	P5S	OXT-C-CA-N
3	E	1601	PT5	O17-C10-O16-C8
3	H	1601	PT5	O17-C10-O16-C8
3	G	1601	PT5	O17-C10-O16-C8
3	F	1601	PT5	O17-C10-O16-C8
3	A	401	PT5	C31-C11-O18-C9
3	B	401	PT5	C31-C11-O18-C9
3	C	401	PT5	C31-C11-O18-C9
3	D	401	PT5	C31-C11-O18-C9
3	E	1601	PT5	C10-C12-C13-C14
6	H	1603	P5S	C30-C31-C32-C33
6	E	1603	P5S	C30-C31-C32-C33
6	G	1603	P5S	C30-C31-C32-C33
6	F	1603	P5S	C30-C31-C32-C33
6	E	1604	P5S	C39-C38-O37-C2
6	H	1604	P5S	C39-C38-O37-C2
6	G	1604	P5S	C39-C38-O37-C2
6	F	1604	P5S	C39-C38-O37-C2
3	F	1601	PT5	C10-C12-C13-C14
5	E	1602	PEF	C12-C13-C14-C15
5	H	1602	PEF	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
5	G	1602	PEF	C12-C13-C14-C15
5	F	1602	PEF	C12-C13-C14-C15
3	H	1601	PT5	C10-C12-C13-C14
3	G	1601	PT5	C10-C12-C13-C14
5	E	1602	PEF	C30-C31-C32-C33
5	H	1602	PEF	C30-C31-C32-C33
5	G	1602	PEF	C30-C31-C32-C33
5	F	1602	PEF	C30-C31-C32-C33
3	A	401	PT5	O19-C11-O18-C9
3	B	401	PT5	O19-C11-O18-C9
3	D	401	PT5	O19-C11-O18-C9
6	E	1603	P5S	C46-C48-C49-C50
6	H	1603	P5S	C46-C48-C49-C50
6	G	1603	P5S	C46-C48-C49-C50
6	F	1603	P5S	C46-C48-C49-C50
3	C	401	PT5	O19-C11-O18-C9
6	G	1604	P5S	C20-C21-C22-C23
6	E	1604	P5S	C20-C21-C22-C23
6	H	1604	P5S	C20-C21-C22-C23
6	F	1604	P5S	C20-C21-C22-C23
6	E	1604	P5S	O47-C38-O37-C2
6	H	1604	P5S	O47-C38-O37-C2
6	G	1604	P5S	O47-C38-O37-C2
6	F	1604	P5S	O47-C38-O37-C2
6	E	1603	P5S	C22-C23-C24-C25
6	H	1603	P5S	C22-C23-C24-C25
6	G	1603	P5S	C22-C23-C24-C25
6	F	1603	P5S	C22-C23-C24-C25
3	B	401	PT5	C12-C10-O16-C8
3	C	401	PT5	C12-C10-O16-C8
3	D	401	PT5	C12-C10-O16-C8
3	H	1601	PT5	C37-C38-C39-C40
3	E	1601	PT5	C37-C38-C39-C40
3	F	1601	PT5	C37-C38-C39-C40
3	G	1601	PT5	C37-C38-C39-C40
3	A	401	PT5	C12-C10-O16-C8
3	E	1601	PT5	C34-C35-C36-C37
3	H	1601	PT5	C34-C35-C36-C37
3	F	1601	PT5	C34-C35-C36-C37
3	G	1601	PT5	C34-C35-C36-C37
5	E	1602	PEF	O2-C2-C3-O3
5	H	1602	PEF	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	G	1602	PEF	O2-C2-C3-O3
5	F	1602	PEF	O2-C2-C3-O3
5	G	1602	PEF	C11-C12-C13-C14
5	F	1602	PEF	C11-C12-C13-C14
5	E	1602	PEF	C11-C12-C13-C14
5	H	1602	PEF	C11-C12-C13-C14
3	C	401	PT5	C38-C39-C40-C41
3	D	401	PT5	C38-C39-C40-C41
3	A	401	PT5	C38-C39-C40-C41
3	B	401	PT5	C38-C39-C40-C41
6	E	1604	P5S	C1-C2-C3-O16
6	H	1604	P5S	C1-C2-C3-O16
6	G	1604	P5S	C1-C2-C3-O16
6	F	1604	P5S	C1-C2-C3-O16
6	E	1603	P5S	OXT-C-CA-N
6	H	1603	P5S	OXT-C-CA-N
6	G	1603	P5S	OXT-C-CA-N
6	F	1603	P5S	OXT-C-CA-N
3	A	401	PT5	C35-C36-C37-C38
3	D	401	PT5	C35-C36-C37-C38
3	B	401	PT5	C35-C36-C37-C38
3	C	401	PT5	C35-C36-C37-C38
6	E	1603	P5S	O19-C1-C2-C3
6	H	1603	P5S	O19-C1-C2-C3
6	G	1603	P5S	O19-C1-C2-C3
6	F	1603	P5S	O19-C1-C2-C3
3	G	1601	PT5	C41-C42-C43-C44
3	F	1601	PT5	C41-C42-C43-C44
3	E	1601	PT5	C41-C42-C43-C44
3	H	1601	PT5	C41-C42-C43-C44
3	C	401	PT5	C37-C38-C39-C40
3	B	401	PT5	C37-C38-C39-C40
3	A	401	PT5	C37-C38-C39-C40
3	D	401	PT5	C37-C38-C39-C40
3	A	401	PT5	C41-C42-C43-C44
3	B	401	PT5	C41-C42-C43-C44
3	C	401	PT5	C41-C42-C43-C44
3	D	401	PT5	C41-C42-C43-C44
3	A	401	PT5	C31-C32-C33-C34
3	B	401	PT5	C31-C32-C33-C34
3	C	401	PT5	C31-C32-C33-C34
3	D	401	PT5	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
5	E	1602	PEF	C1-C2-C3-O3
5	H	1602	PEF	C1-C2-C3-O3
5	G	1602	PEF	C1-C2-C3-O3
5	F	1602	PEF	C1-C2-C3-O3
6	E	1603	P5S	O-C-CA-N
6	H	1603	P5S	O-C-CA-N
6	F	1603	P5S	O-C-CA-N
3	B	401	PT5	O17-C10-O16-C8
3	C	401	PT5	O17-C10-O16-C8
3	D	401	PT5	O17-C10-O16-C8
3	A	401	PT5	C15-C16-C17-C18
3	A	401	PT5	C22-C23-C24-C25
3	B	401	PT5	C15-C16-C17-C18
3	B	401	PT5	C22-C23-C24-C25
3	C	401	PT5	C15-C16-C17-C18
3	C	401	PT5	C22-C23-C24-C25
3	D	401	PT5	C15-C16-C17-C18
3	D	401	PT5	C22-C23-C24-C25
3	A	401	PT5	O17-C10-O16-C8
6	E	1604	P5S	C43-C44-C45-C46
6	H	1604	P5S	C43-C44-C45-C46
3	E	1601	PT5	O13-C7-C8-C9
3	H	1601	PT5	O13-C7-C8-C9
3	G	1601	PT5	O13-C7-C8-C9
3	F	1601	PT5	O13-C7-C8-C9
6	G	1604	P5S	C43-C44-C45-C46
6	F	1604	P5S	C43-C44-C45-C46
5	H	1602	PEF	C14-C15-C16-C17
6	E	1603	P5S	N-CA-CB-OG
6	H	1603	P5S	N-CA-CB-OG
6	G	1603	P5S	N-CA-CB-OG
6	F	1603	P5S	N-CA-CB-OG
5	F	1602	PEF	C14-C15-C16-C17
5	G	1602	PEF	C14-C15-C16-C17
5	E	1602	PEF	C14-C15-C16-C17
5	E	1602	PEF	C2-C1-O3P-P
5	H	1602	PEF	C2-C1-O3P-P
5	G	1602	PEF	C2-C1-O3P-P
5	F	1602	PEF	C2-C1-O3P-P
3	E	1601	PT5	C5-O5-P5-O52
3	H	1601	PT5	C5-O5-P5-O52
3	G	1601	PT5	C5-O5-P5-O52

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Mol	Chain	Res	Type	Atoms
3	F	1601	PT5	C5-O5-P5-O52
3	H	1601	PT5	O13-C7-C8-O16
3	G	1601	PT5	O13-C7-C8-O16
3	F	1601	PT5	O13-C7-C8-O16
3	A	401	PT5	C36-C37-C38-C39
3	C	401	PT5	C36-C37-C38-C39
3	D	401	PT5	C36-C37-C38-C39
3	B	401	PT5	C36-C37-C38-C39
3	F	1601	PT5	C42-C43-C44-C45
3	G	1601	PT5	C42-C43-C44-C45
3	E	1601	PT5	C42-C43-C44-C45
3	H	1601	PT5	C42-C43-C44-C45
3	A	401	PT5	C7-O13-P1-O12
3	B	401	PT5	C7-O13-P1-O12
3	C	401	PT5	C7-O13-P1-O12
3	D	401	PT5	C7-O13-P1-O12
6	H	1604	P5S	OXT-C-CA-CB
6	G	1604	P5S	OXT-C-CA-CB
6	F	1604	P5S	OXT-C-CA-CB
3	E	1601	PT5	C8-C7-O13-P1
3	H	1601	PT5	C8-C7-O13-P1
3	G	1601	PT5	C8-C7-O13-P1
3	F	1601	PT5	C8-C7-O13-P1
3	B	401	PT5	C10-C12-C13-C14
3	D	401	PT5	C10-C12-C13-C14
3	E	1601	PT5	C7-C8-O16-C10
3	H	1601	PT5	C7-C8-O16-C10
3	G	1601	PT5	C7-C8-O16-C10
3	F	1601	PT5	C7-C8-O16-C10
3	C	401	PT5	C32-C33-C34-C35
3	A	401	PT5	C10-C12-C13-C14
3	C	401	PT5	C10-C12-C13-C14
3	D	401	PT5	C32-C33-C34-C35
3	A	401	PT5	C32-C33-C34-C35
3	B	401	PT5	C32-C33-C34-C35
3	E	1601	PT5	O13-C7-C8-O16
5	E	1602	PEF	C15-C16-C17-C18
5	G	1602	PEF	C15-C16-C17-C18
5	H	1602	PEF	C15-C16-C17-C18
5	F	1602	PEF	C15-C16-C17-C18
3	E	1601	PT5	C3-C4-O4-P4
3	H	1601	PT5	C3-C4-O4-P4

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Mol	Chain	Res	Type	Atoms
3	G	1601	PT5	C3-C4-O4-P4
3	F	1601	PT5	C3-C4-O4-P4
6	G	1604	P5S	C49-C50-C51-C52
6	E	1604	P5S	C49-C50-C51-C52
6	H	1604	P5S	C49-C50-C51-C52
6	F	1604	P5S	C49-C50-C51-C52
5	E	1602	PEF	C1-C2-O2-C10
5	H	1602	PEF	C1-C2-O2-C10
5	G	1602	PEF	C1-C2-O2-C10
5	F	1602	PEF	C1-C2-O2-C10
3	A	401	PT5	C6-C1-O1-P1
3	B	401	PT5	C6-C1-O1-P1
3	C	401	PT5	C6-C1-O1-P1
3	D	401	PT5	C6-C1-O1-P1
6	E	1603	P5S	O19-C1-C2-O37
6	H	1603	P5S	O19-C1-C2-O37
6	G	1603	P5S	O19-C1-C2-O37
6	F	1603	P5S	O19-C1-C2-O37
3	A	401	PT5	C21-C22-C23-C24
3	B	401	PT5	C21-C22-C23-C24
3	C	401	PT5	C21-C22-C23-C24
3	D	401	PT5	C21-C22-C23-C24
3	E	1601	PT5	C4-O4-P4-O42
3	H	1601	PT5	C4-O4-P4-O42
3	G	1601	PT5	C4-O4-P4-O42
3	F	1601	PT5	C4-O4-P4-O42
6	E	1603	P5S	C21-C22-C23-C24
6	G	1603	P5S	C21-C22-C23-C24
6	H	1603	P5S	C21-C22-C23-C24
6	F	1603	P5S	C21-C22-C23-C24
3	H	1601	PT5	C40-C41-C42-C43
3	G	1601	PT5	C40-C41-C42-C43
3	F	1601	PT5	C40-C41-C42-C43
6	F	1603	P5S	C45-C46-C48-C49
6	G	1603	P5S	C45-C46-C48-C49
3	E	1601	PT5	C40-C41-C42-C43
6	E	1603	P5S	C45-C46-C48-C49
6	H	1603	P5S	C45-C46-C48-C49
3	E	1601	PT5	C13-C14-C15-C16
3	H	1601	PT5	C13-C14-C15-C16
3	G	1601	PT5	C13-C14-C15-C16
3	F	1601	PT5	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	E	1601	PT5	C35-C36-C37-C38
3	F	1601	PT5	C35-C36-C37-C38
3	H	1601	PT5	C35-C36-C37-C38
3	G	1601	PT5	C33-C34-C35-C36
3	G	1601	PT5	C35-C36-C37-C38
3	H	1601	PT5	C33-C34-C35-C36
3	F	1601	PT5	C33-C34-C35-C36
3	E	1601	PT5	C33-C34-C35-C36
3	B	401	PT5	C40-C41-C42-C43
3	A	401	PT5	C1-O1-P1-O11
3	E	1601	PT5	C1-O1-P1-O11
3	B	401	PT5	C1-O1-P1-O11
3	C	401	PT5	C1-O1-P1-O11
3	D	401	PT5	C1-O1-P1-O11
3	H	1601	PT5	C1-O1-P1-O11
3	G	1601	PT5	C1-O1-P1-O11
3	F	1601	PT5	C1-O1-P1-O11
3	A	401	PT5	C40-C41-C42-C43
3	D	401	PT5	C40-C41-C42-C43
3	C	401	PT5	C40-C41-C42-C43
3	G	1601	PT5	C32-C33-C34-C35
3	F	1601	PT5	C32-C33-C34-C35
3	H	1601	PT5	C32-C33-C34-C35
3	E	1601	PT5	C32-C33-C34-C35
3	A	401	PT5	C5-O5-P5-O52
3	B	401	PT5	C5-O5-P5-O52
3	C	401	PT5	C5-O5-P5-O52
3	D	401	PT5	C5-O5-P5-O52
6	F	1604	P5S	C23-C24-C25-C26
3	E	1601	PT5	O16-C10-C12-C13
3	H	1601	PT5	O16-C10-C12-C13
6	E	1604	P5S	C23-C24-C25-C26
6	G	1604	P5S	C51-C52-C53-C54
6	H	1604	P5S	C23-C24-C25-C26
6	G	1604	P5S	C23-C24-C25-C26
3	F	1601	PT5	O16-C10-C12-C13
3	G	1601	PT5	O16-C10-C12-C13
6	E	1604	P5S	C51-C52-C53-C54
6	H	1604	P5S	C51-C52-C53-C54
6	F	1604	P5S	C51-C52-C53-C54

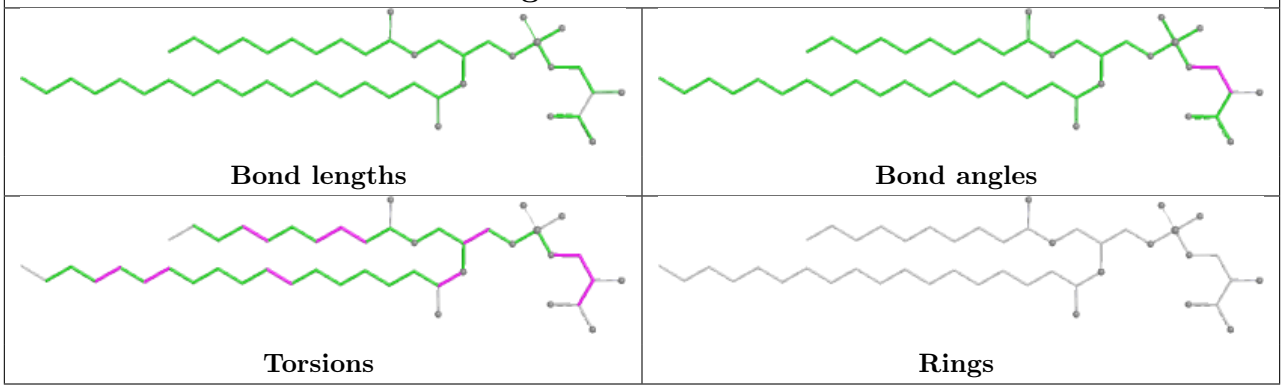
There are no ring outliers.

20 monomers are involved in 52 short contacts:

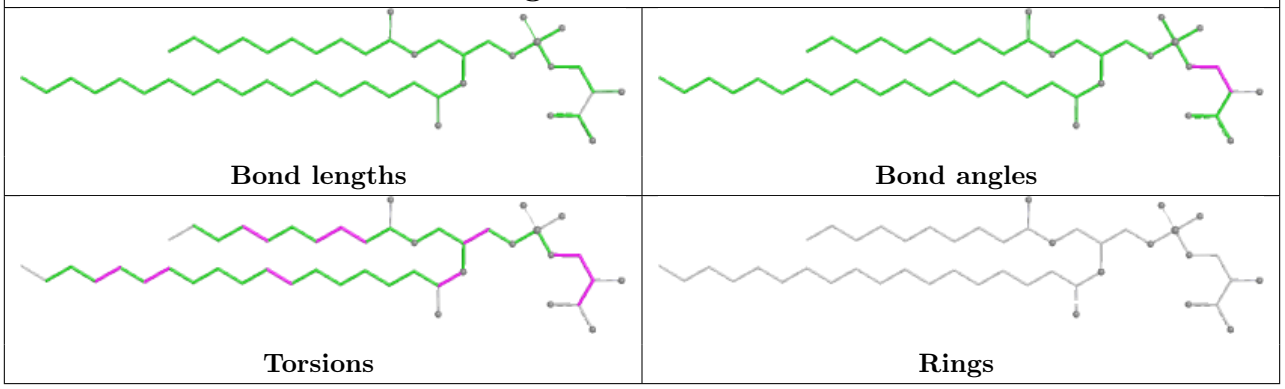
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1604	P5S	1	0
6	F	1604	P5S	1	0
5	H	1602	PEF	1	0
6	H	1603	P5S	2	0
5	F	1602	PEF	2	0
3	B	401	PT5	4	0
3	E	1601	PT5	6	0
3	H	1601	PT5	7	0
6	E	1603	P5S	2	0
3	D	401	PT5	4	0
5	E	1602	PEF	1	0
3	A	401	PT5	4	0
6	F	1603	P5S	2	0
6	E	1604	P5S	1	0
5	G	1602	PEF	2	0
6	G	1603	P5S	2	0
6	H	1604	P5S	1	0
3	C	401	PT5	4	0
3	G	1601	PT5	6	0
3	F	1601	PT5	7	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.

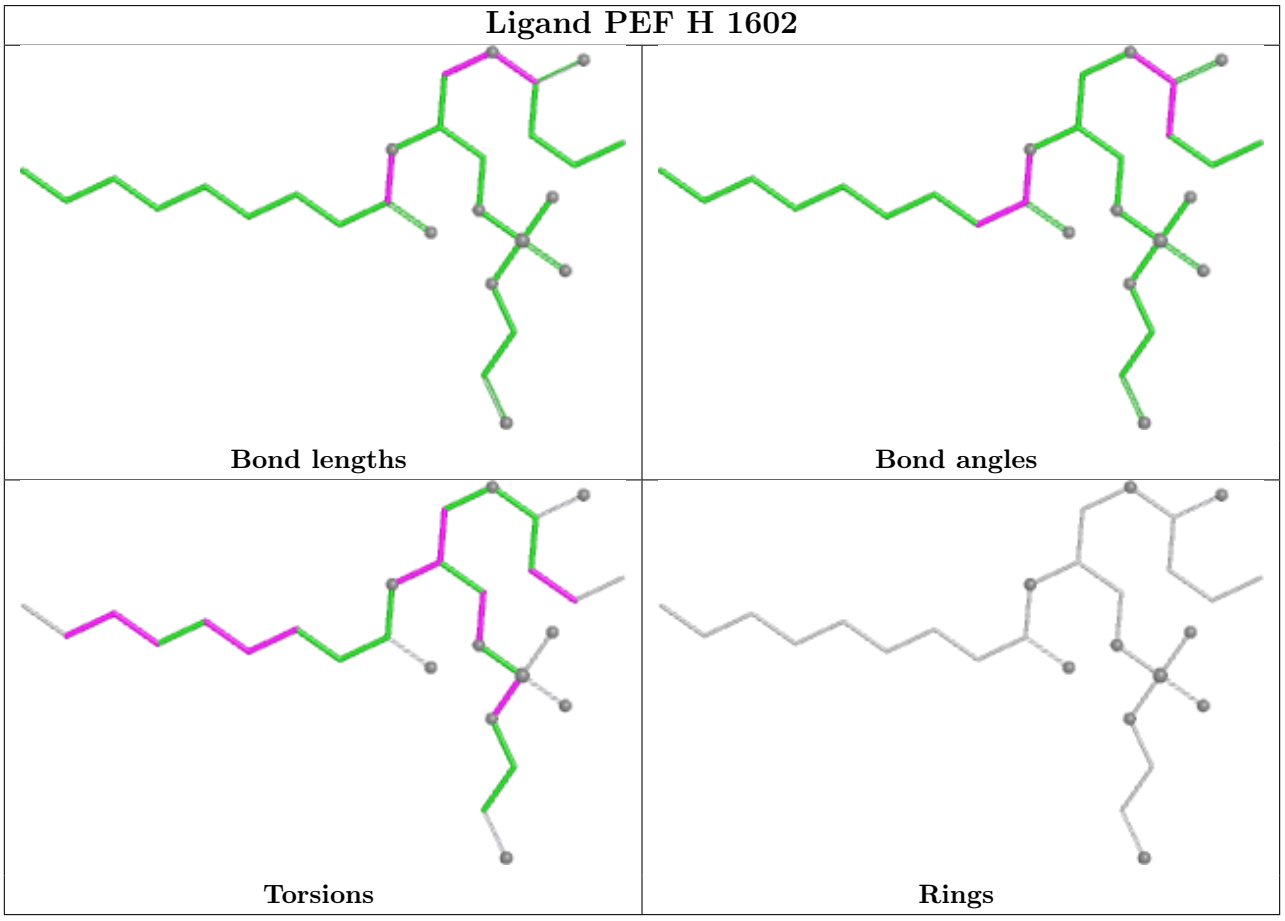
Ligand P5S G 1604



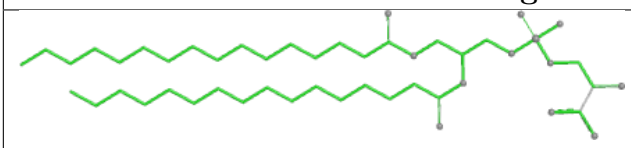
Ligand P5S F 1604



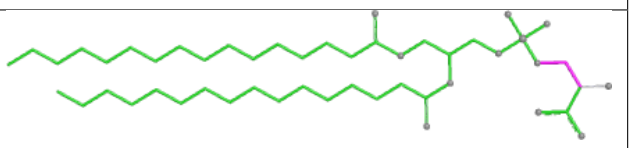
Ligand PEF H 1602



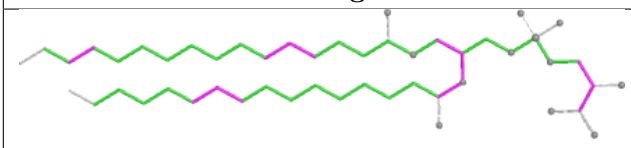
Ligand P5S H 1603



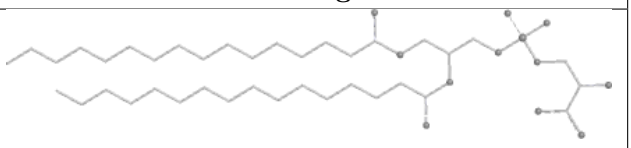
Bond lengths



Bond angles

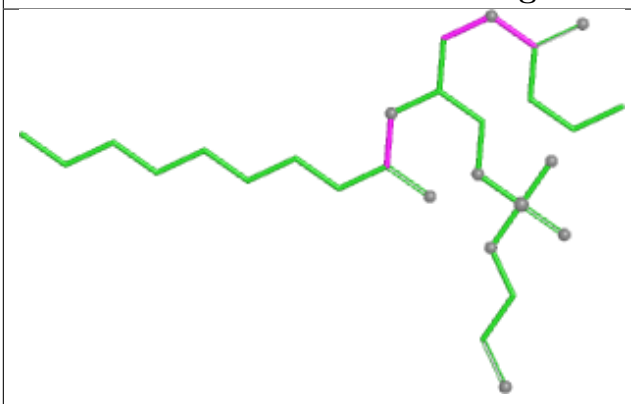


Torsions

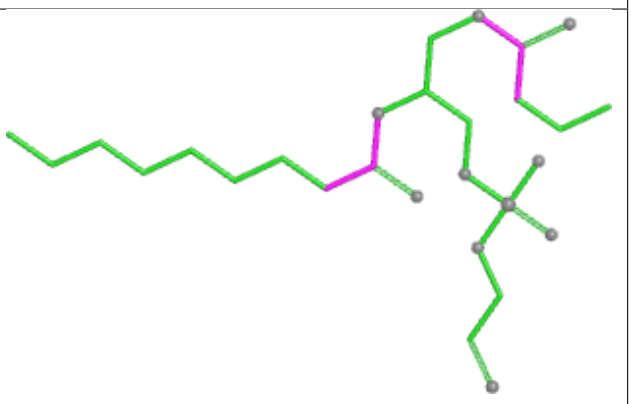


Rings

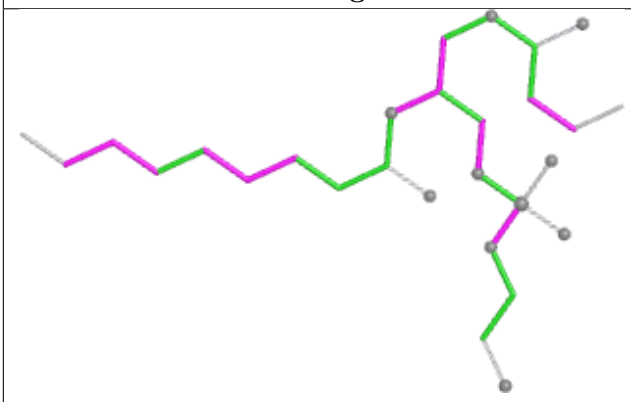
Ligand PEF F 1602



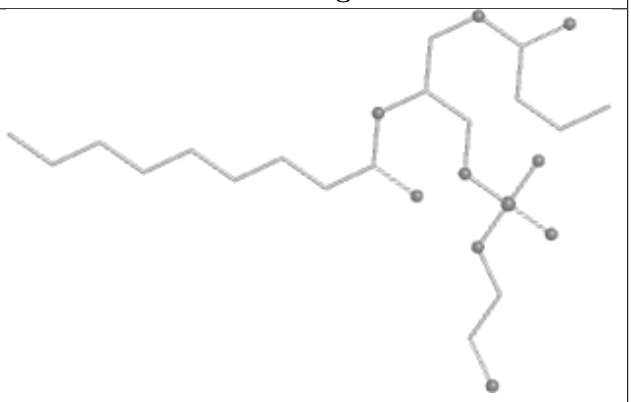
Bond lengths



Bond angles

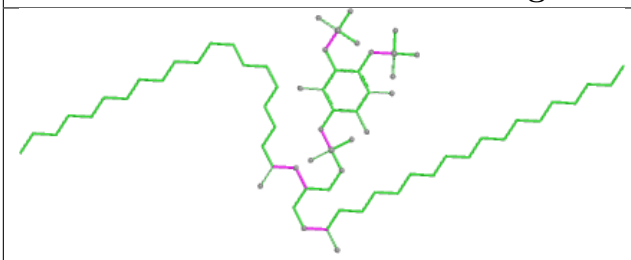


Torsions

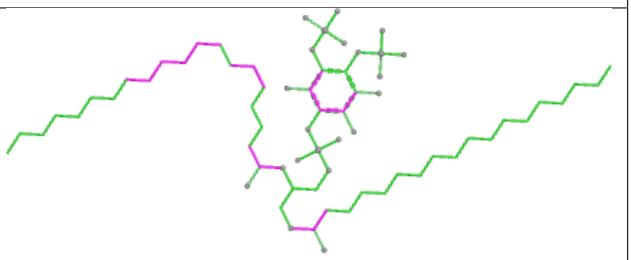


Rings

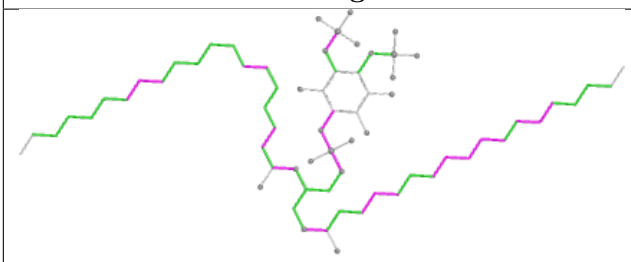
Ligand PT5 B 401



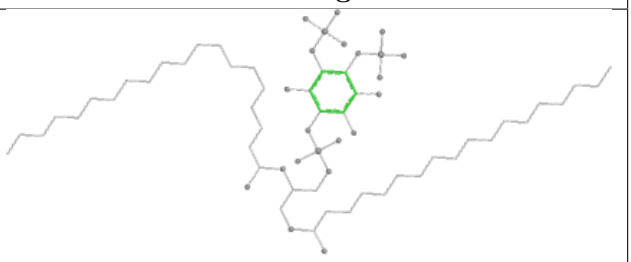
Bond lengths



Bond angles

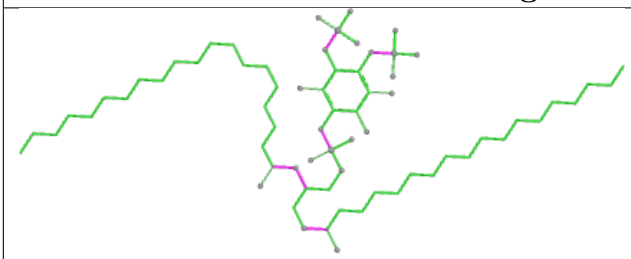


Torsions

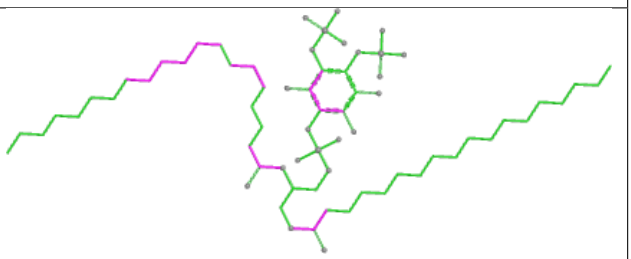


Rings

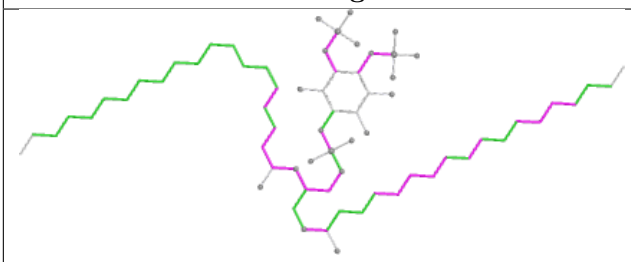
Ligand PT5 E 1601



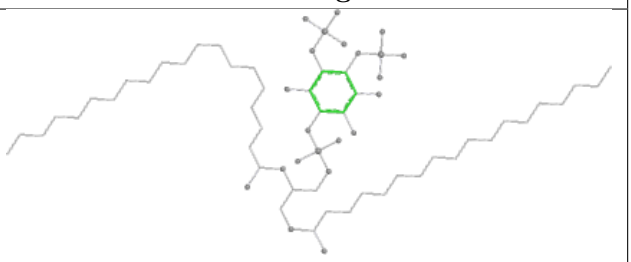
Bond lengths



Bond angles

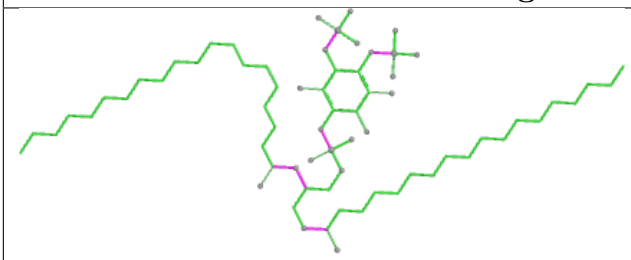


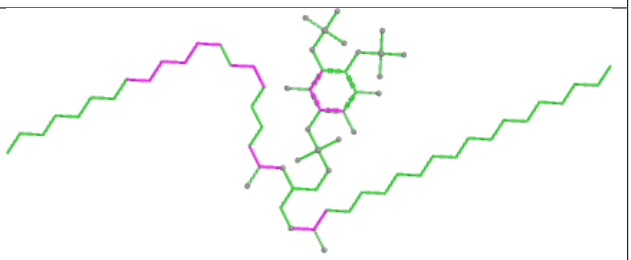
Torsions

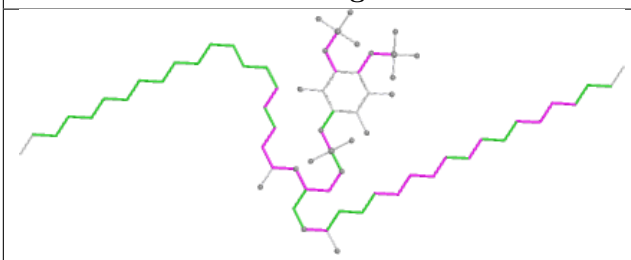


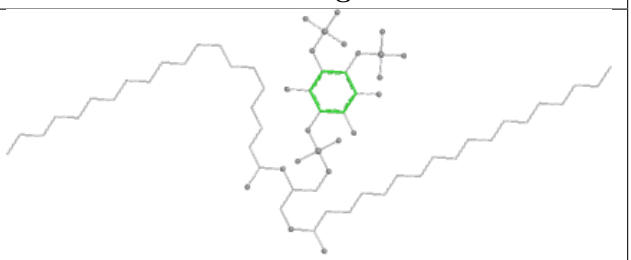
Rings

Ligand PT5 H 1601

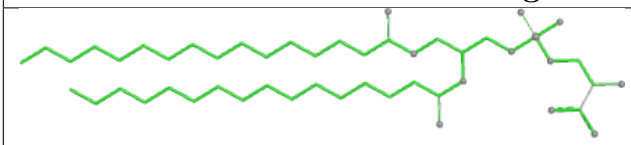

Bond lengths

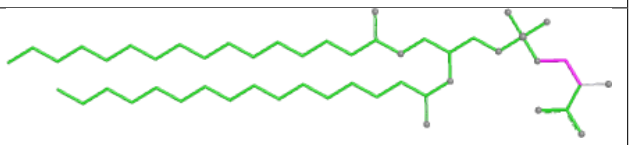

Bond angles

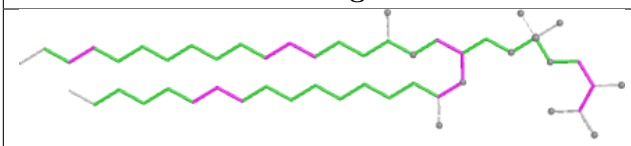

Torsions

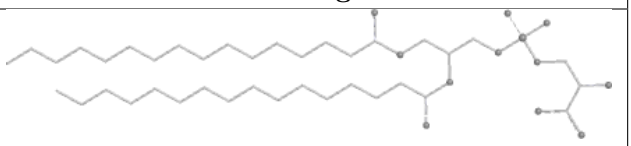

Rings

Ligand P5S E 1603

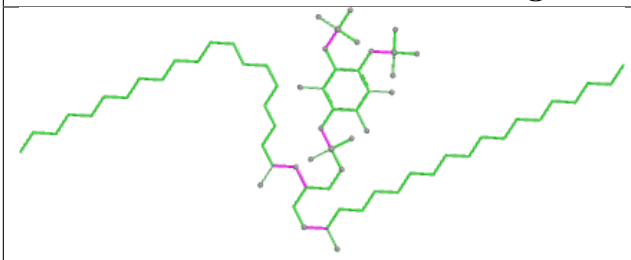

Bond lengths

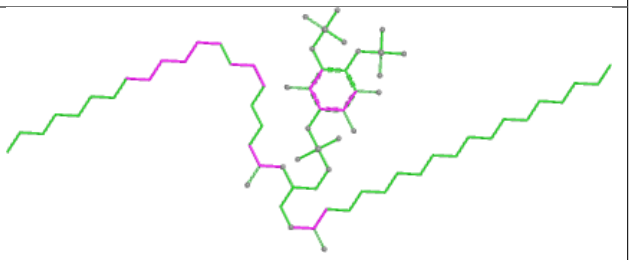

Bond angles

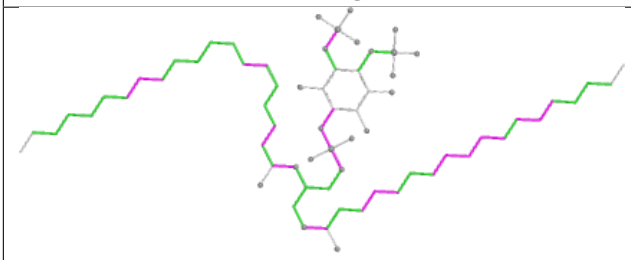

Torsions

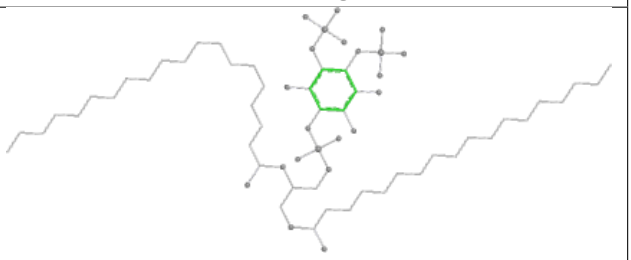

Rings

Ligand PT5 D 401

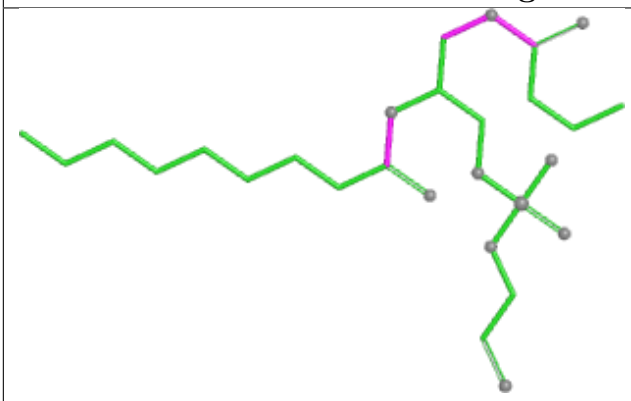

Bond lengths


Bond angles

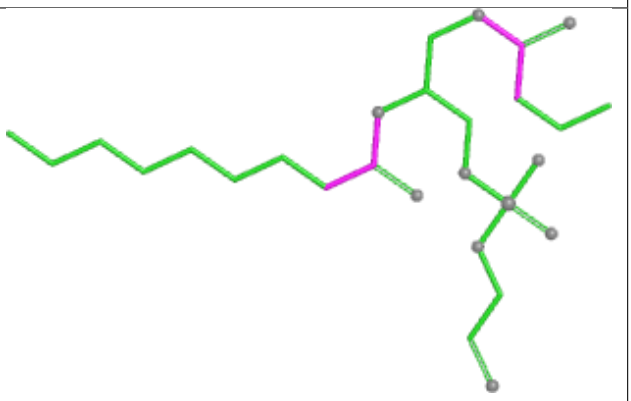

Torsions


Rings

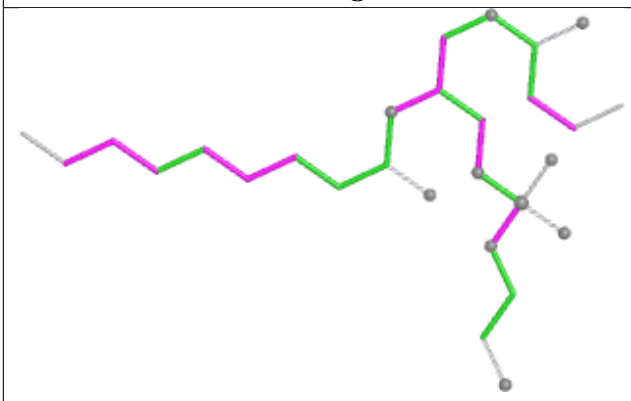
Ligand PEF E 1602



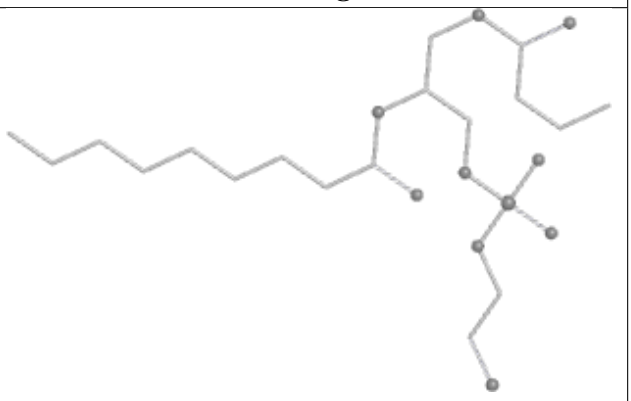
Bond lengths



Bond angles

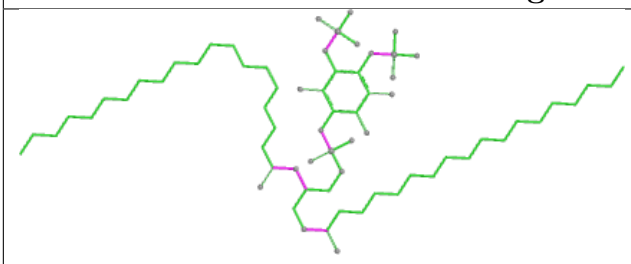


Torsions

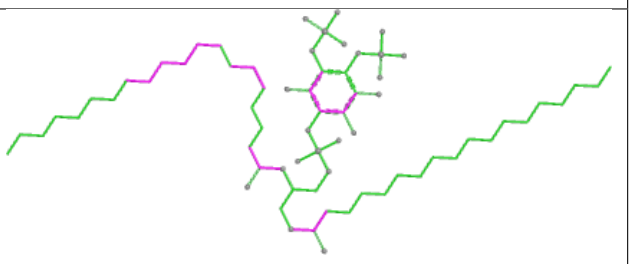


Rings

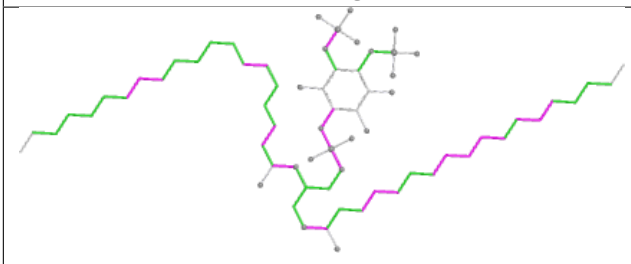
Ligand PT5 A 401



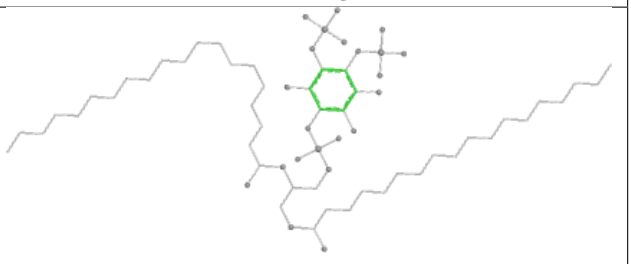
Bond lengths



Bond angles

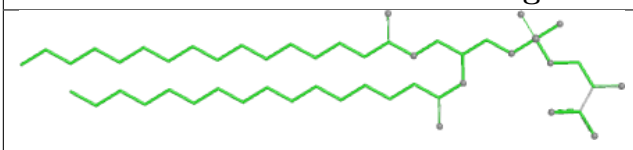


Torsions

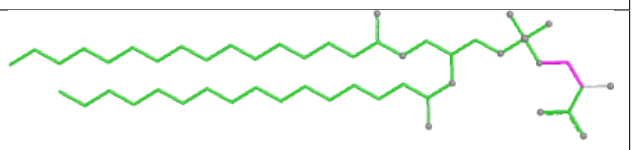


Rings

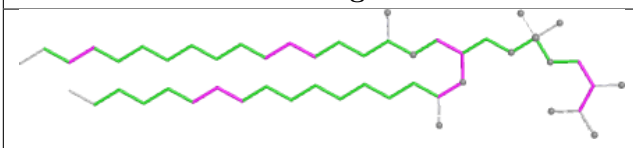
Ligand P5S F 1603



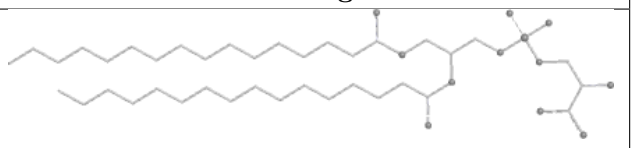
Bond lengths



Bond angles

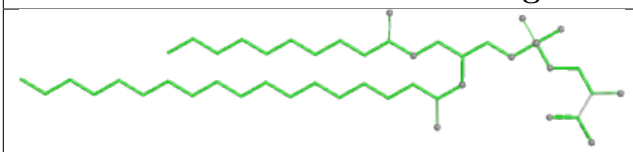


Torsions

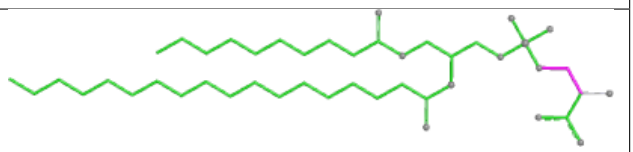


Rings

Ligand P5S E 1604

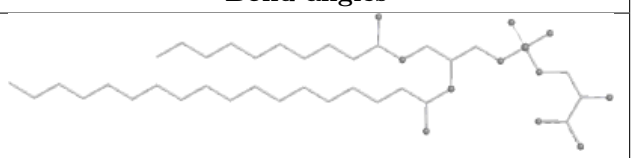


Bond lengths



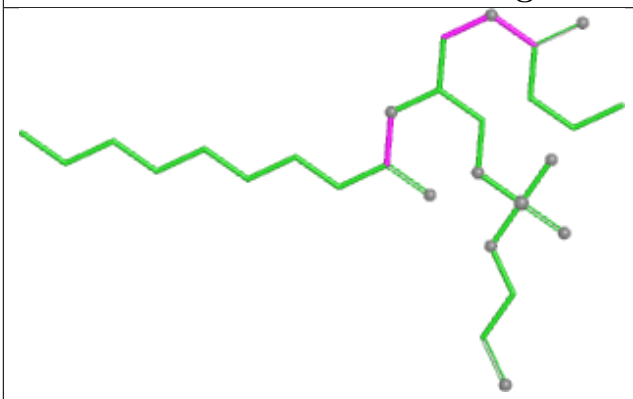
Bond angles

Torsions

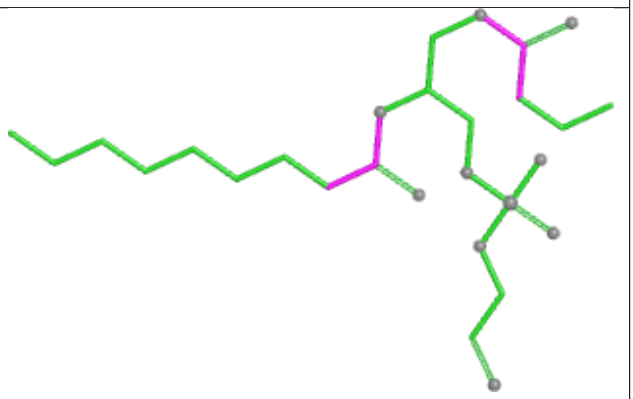


Rings

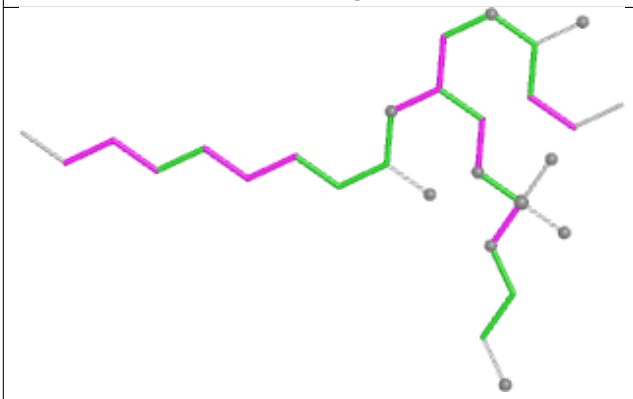
Ligand PEF G 1602



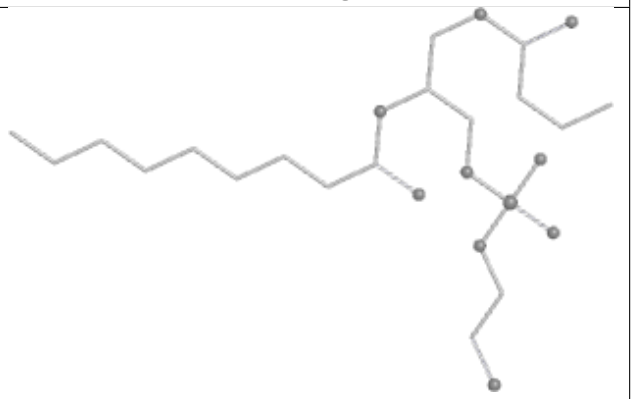
Bond lengths



Bond angles

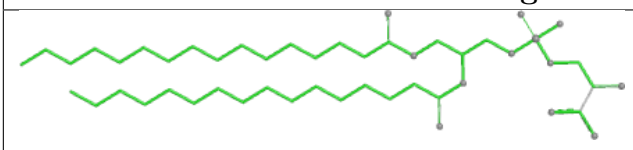


Torsions

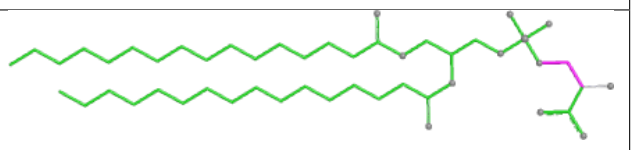


Rings

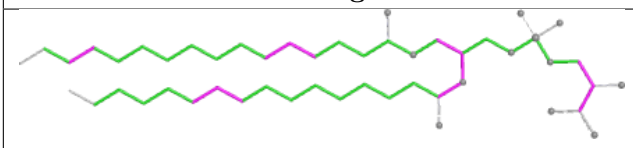
Ligand P5S G 1603



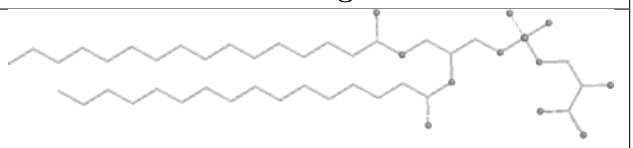
Bond lengths



Bond angles

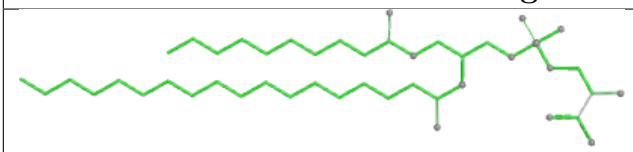


Torsions

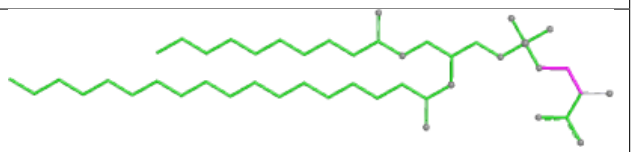


Rings

Ligand P5S H 1604

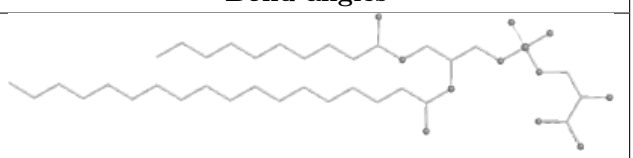


Bond lengths



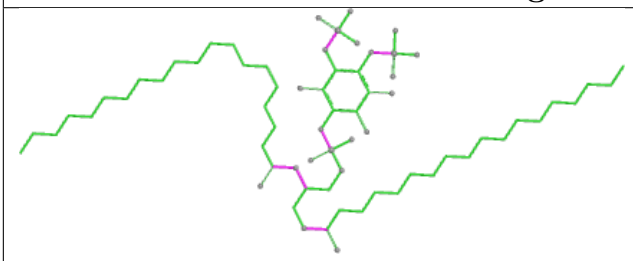
Bond angles

Torsions

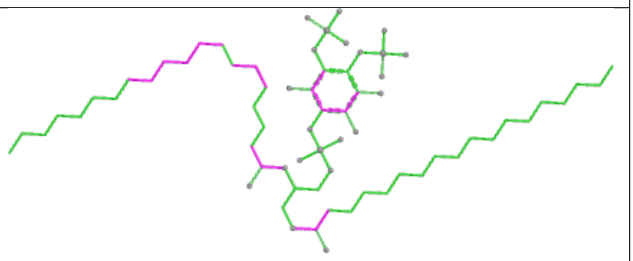


Rings

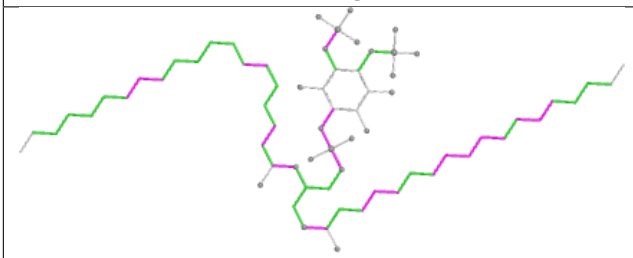
Ligand PT5 C 401



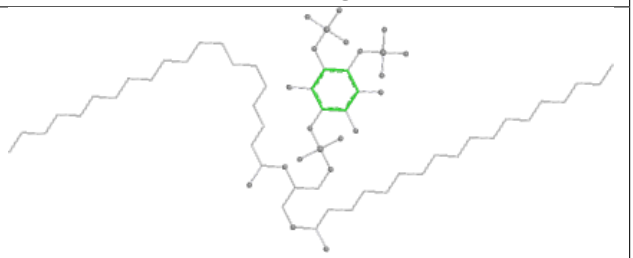
Bond lengths



Bond angles

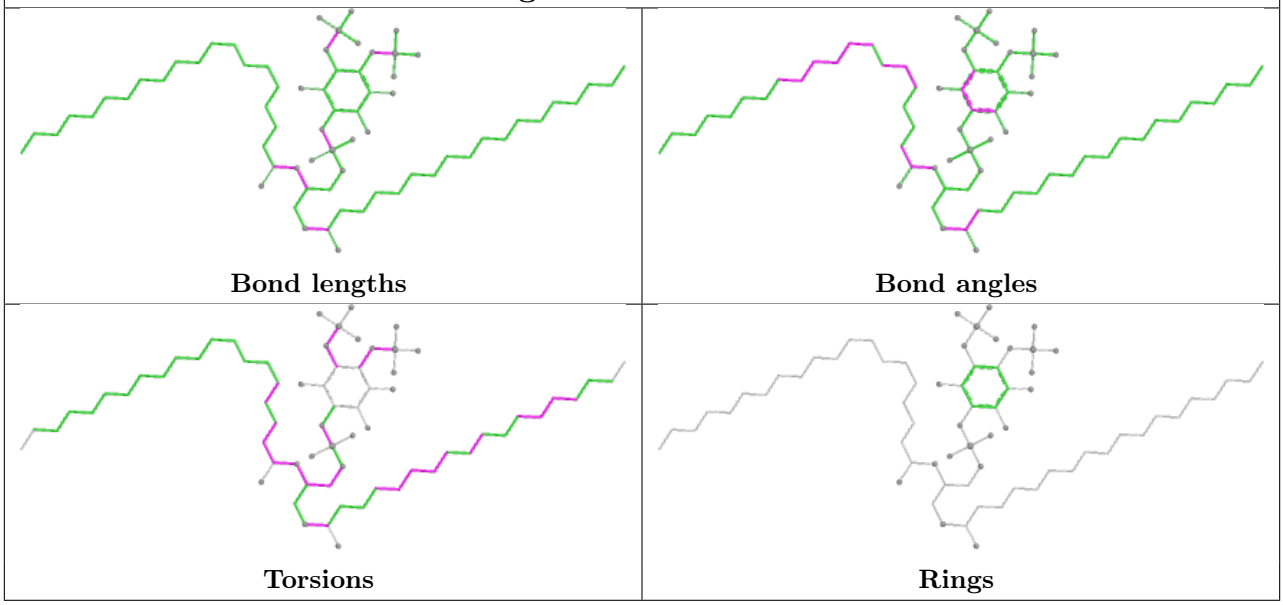


Torsions

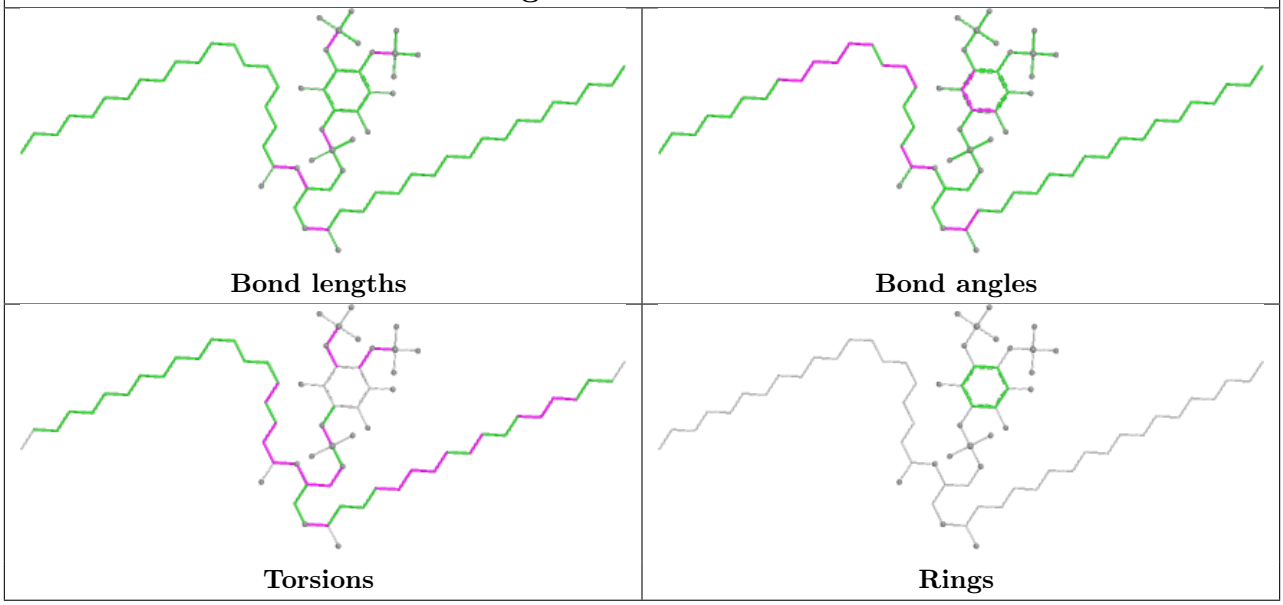


Rings

Ligand PT5 G 1601



Ligand PT5 F 1601



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.

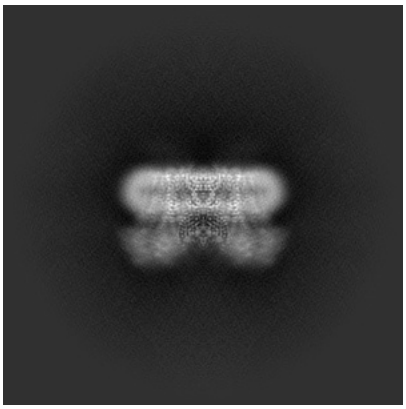
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41277. These allow visual inspection of the internal detail of the map and identification of artifacts.

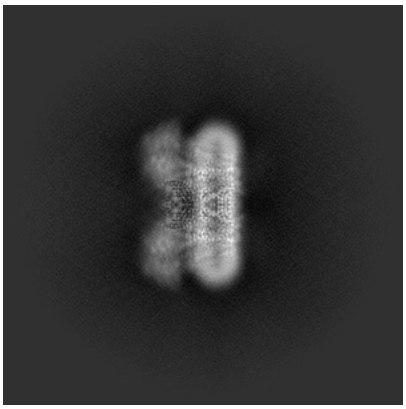
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

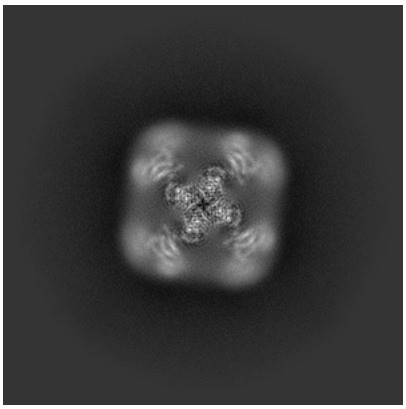
6.1.1 Primary map



X

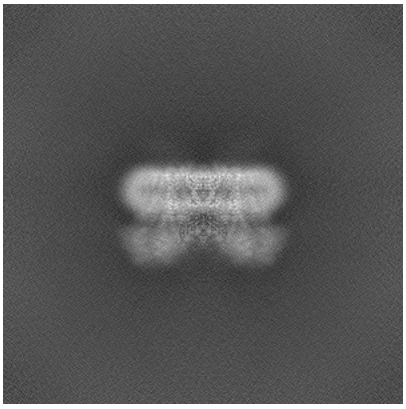


Y

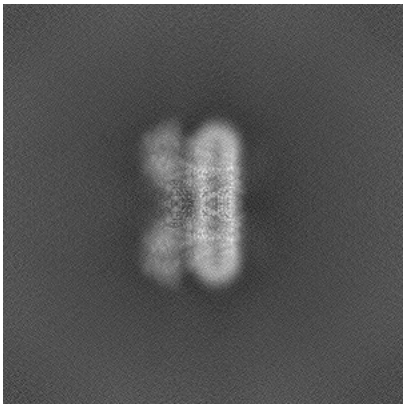


Z

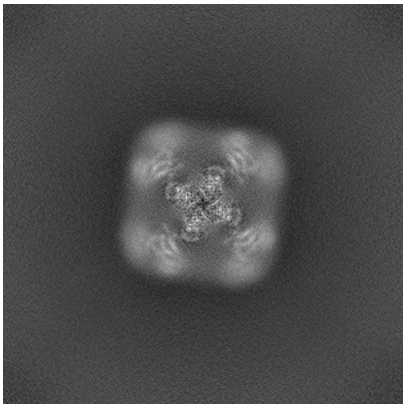
6.1.2 Raw map



X



Y

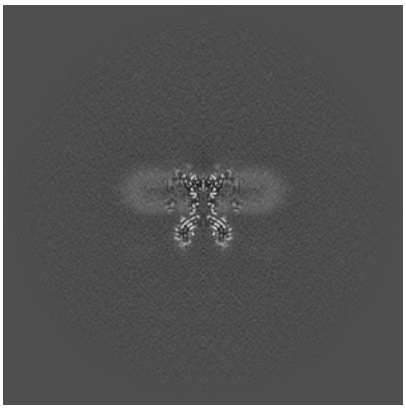


Z

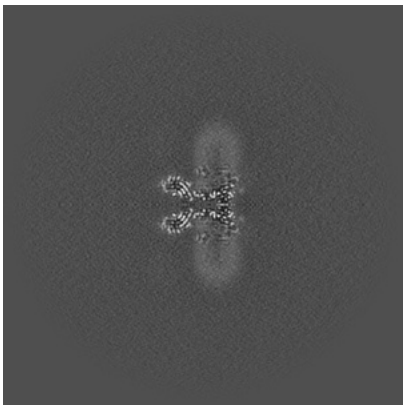
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

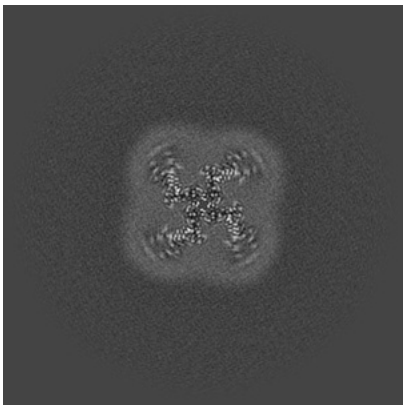
6.2.1 Primary map



X Index: 300

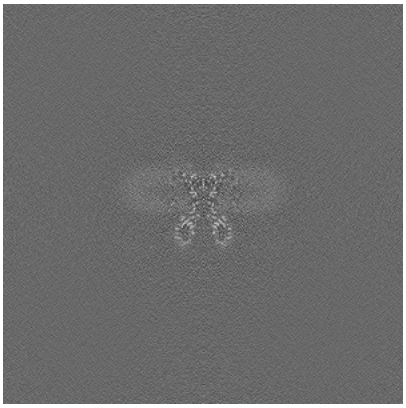


Y Index: 300

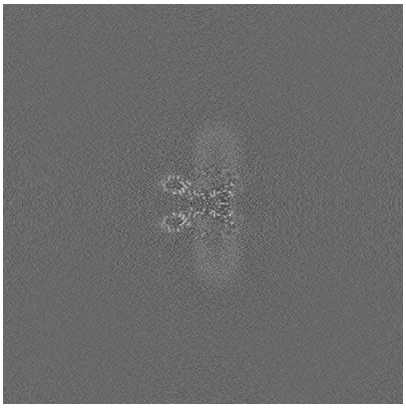


Z Index: 300

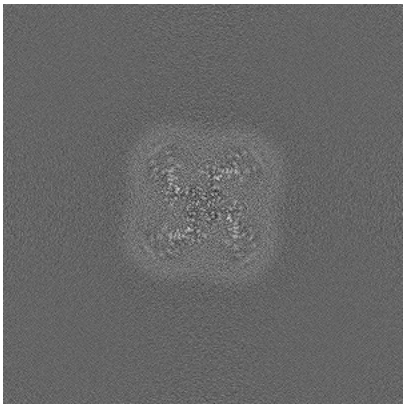
6.2.2 Raw map



X Index: 300



Y Index: 300

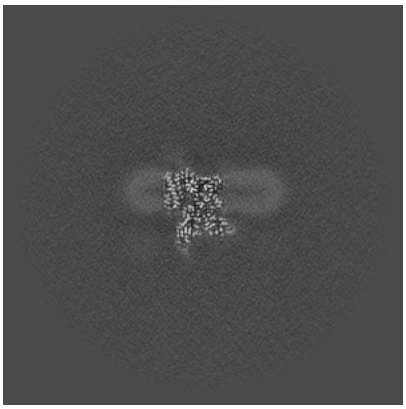


Z Index: 300

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

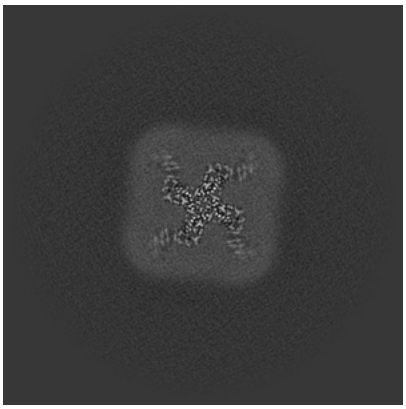
6.3 Largest variance slices (i)

6.3.1 Primary map



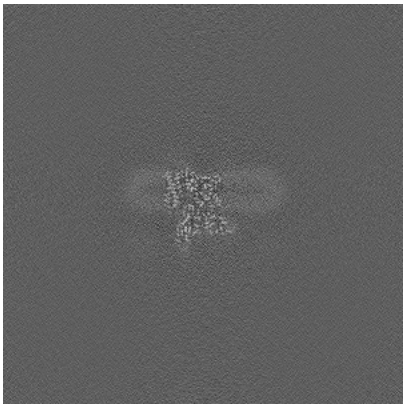
X Index: 290

Y Index: 290

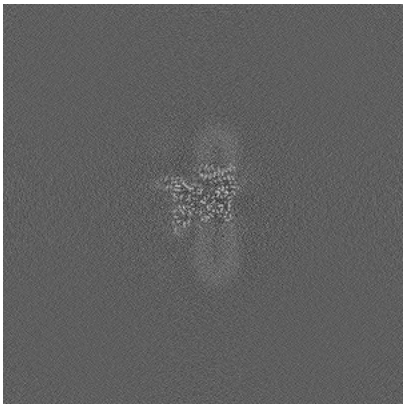


Z Index: 341

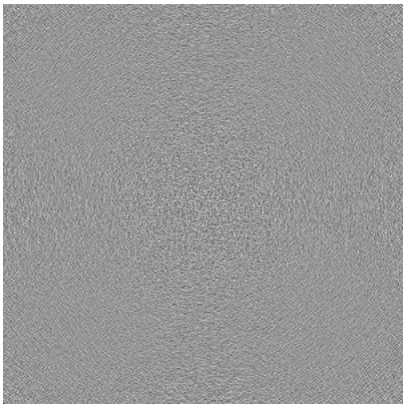
6.3.2 Raw map



X Index: 290



Y Index: 290

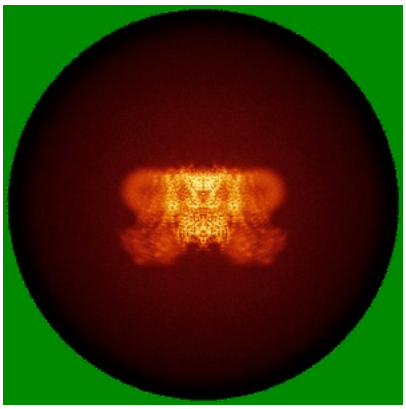


Z Index: 0

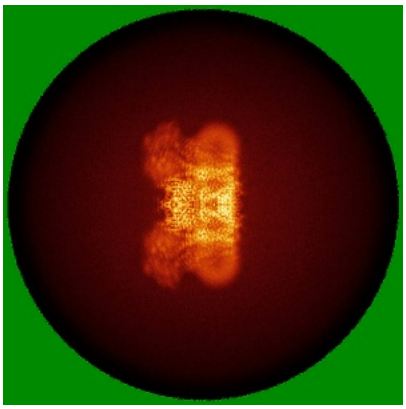
The images above show the largest variance slices of the map in three orthogonal directions.

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

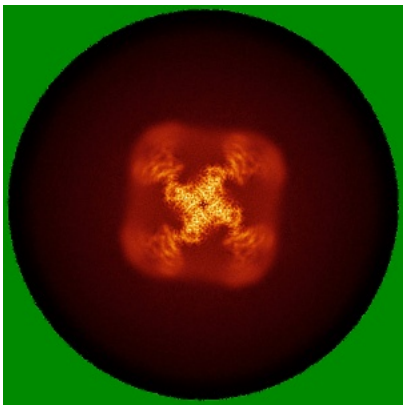
6.4.1 Primary map



X

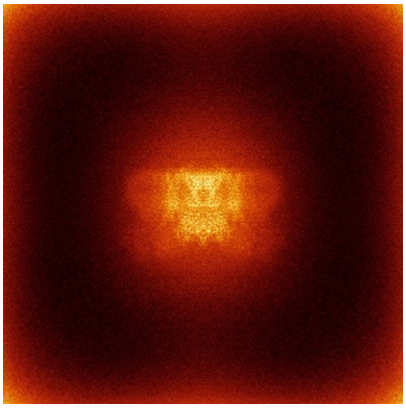


Y

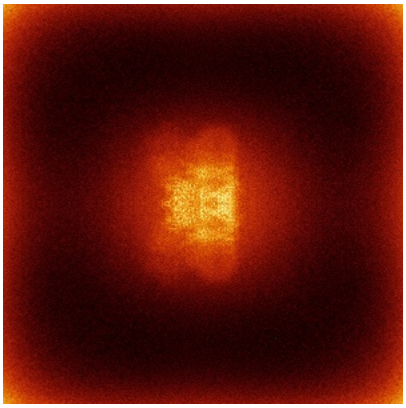


Z

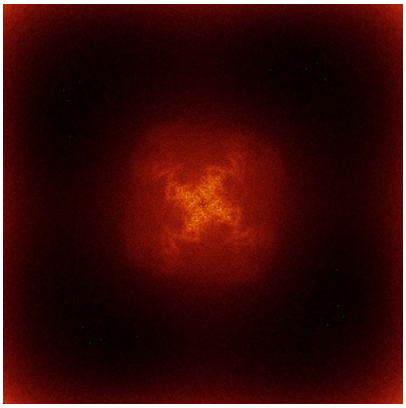
6.4.2 Raw map



X



Y

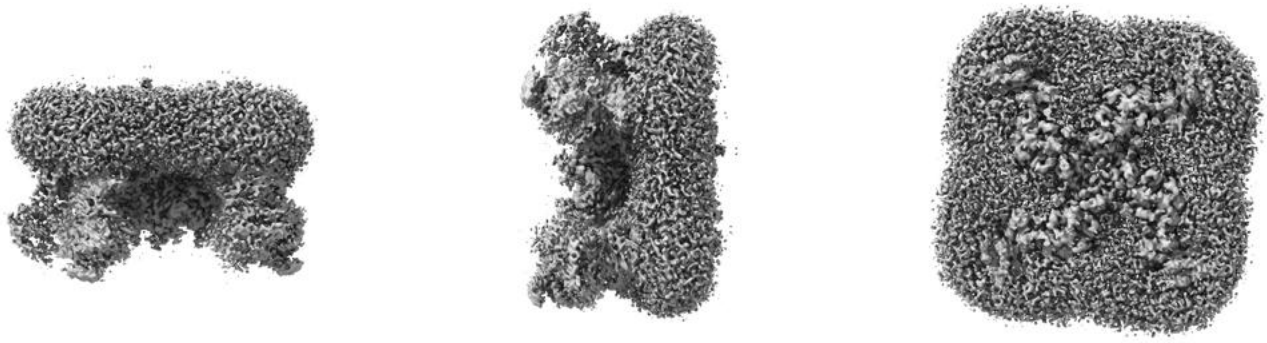


Z

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 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

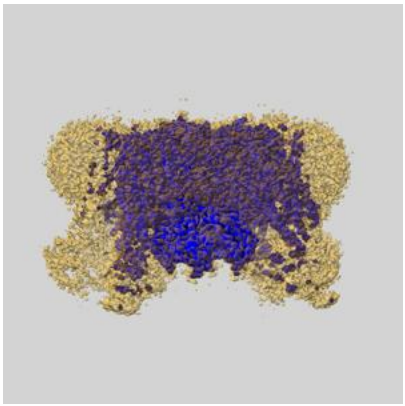
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

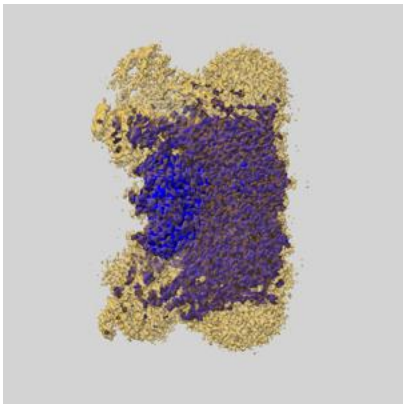
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

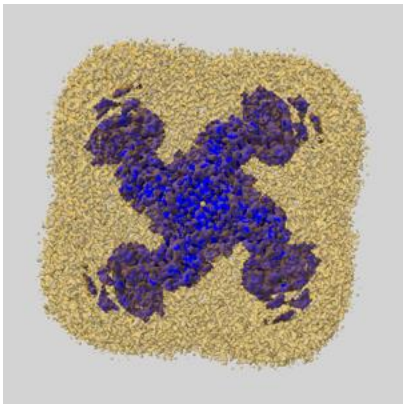
6.6.1 emd_41277_msk_1.map (i)



X



Y

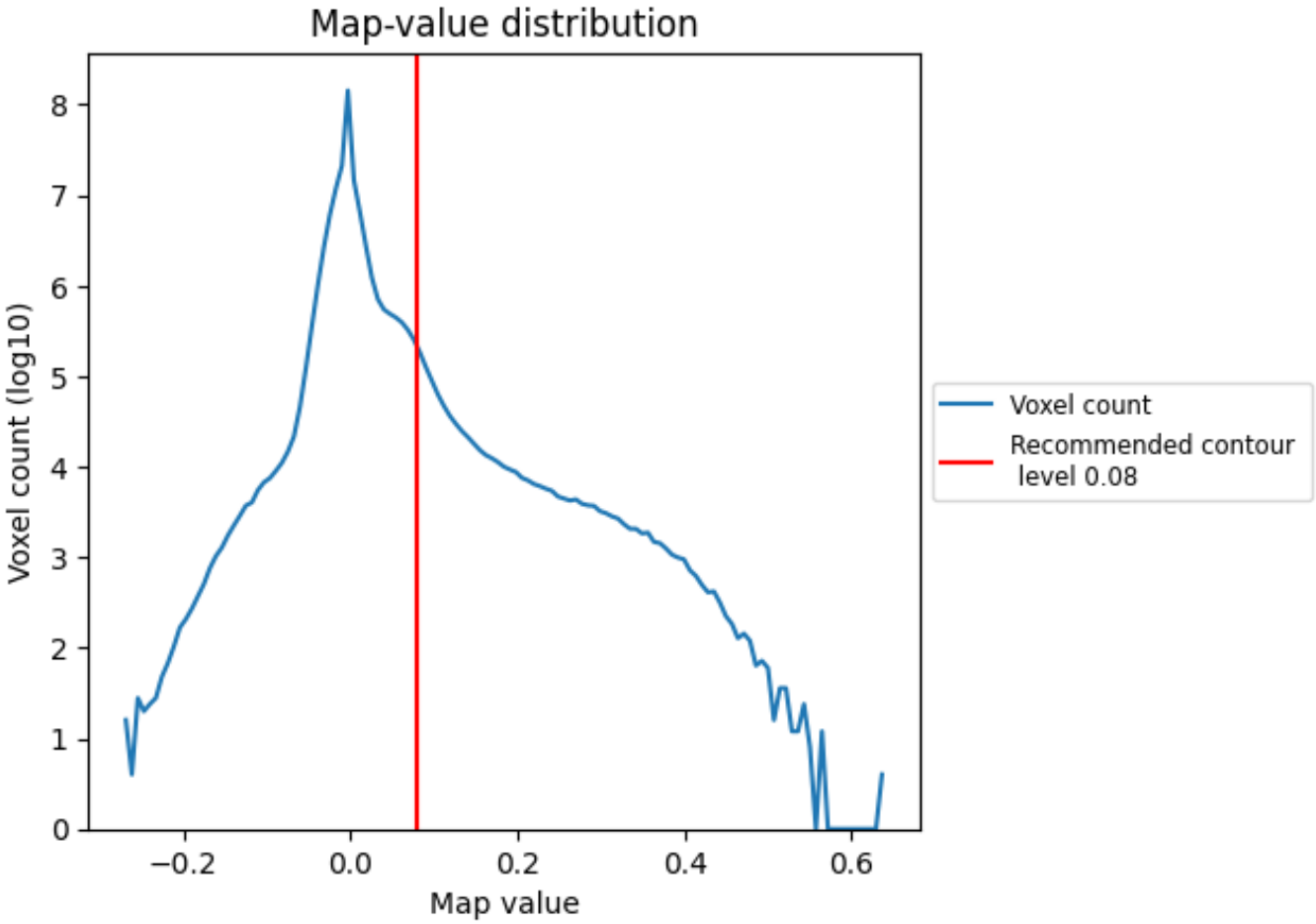


Z

7 Map analysis

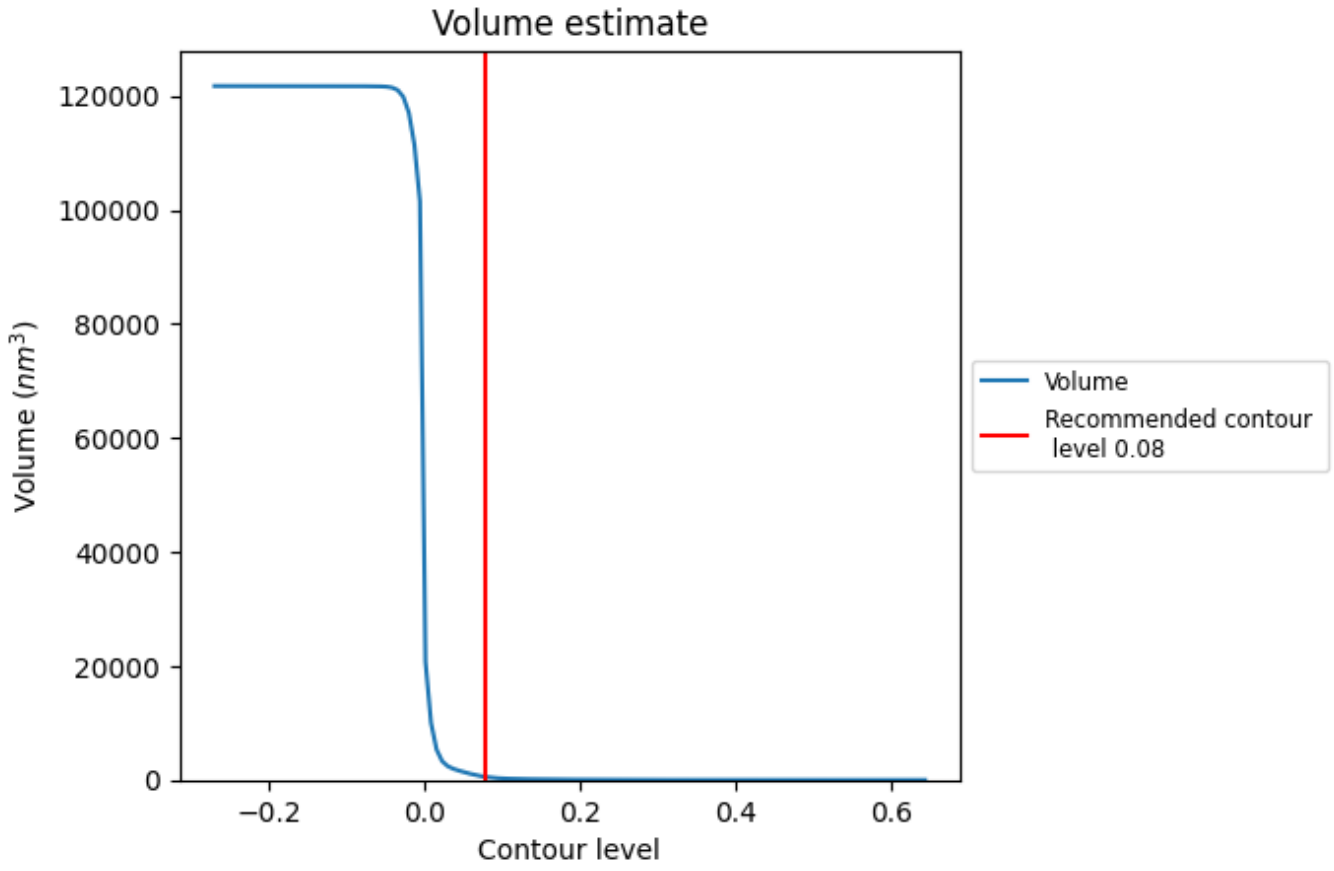
This section contains the results of statistical analysis of the map.

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.

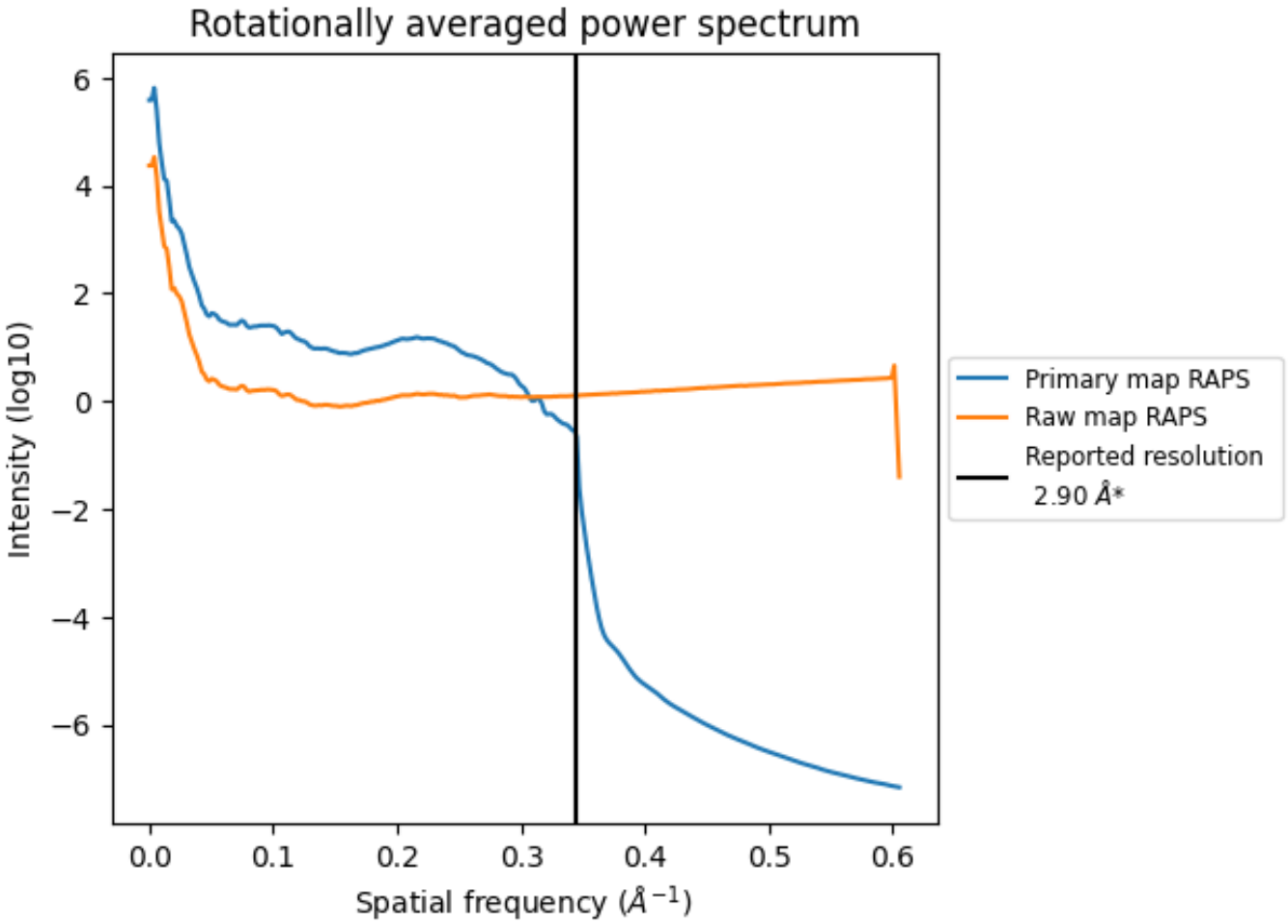
7.2 Volume estimate



The volume at the recommended contour level is 524 nm^3; this corresponds to an approximate mass of 473 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)

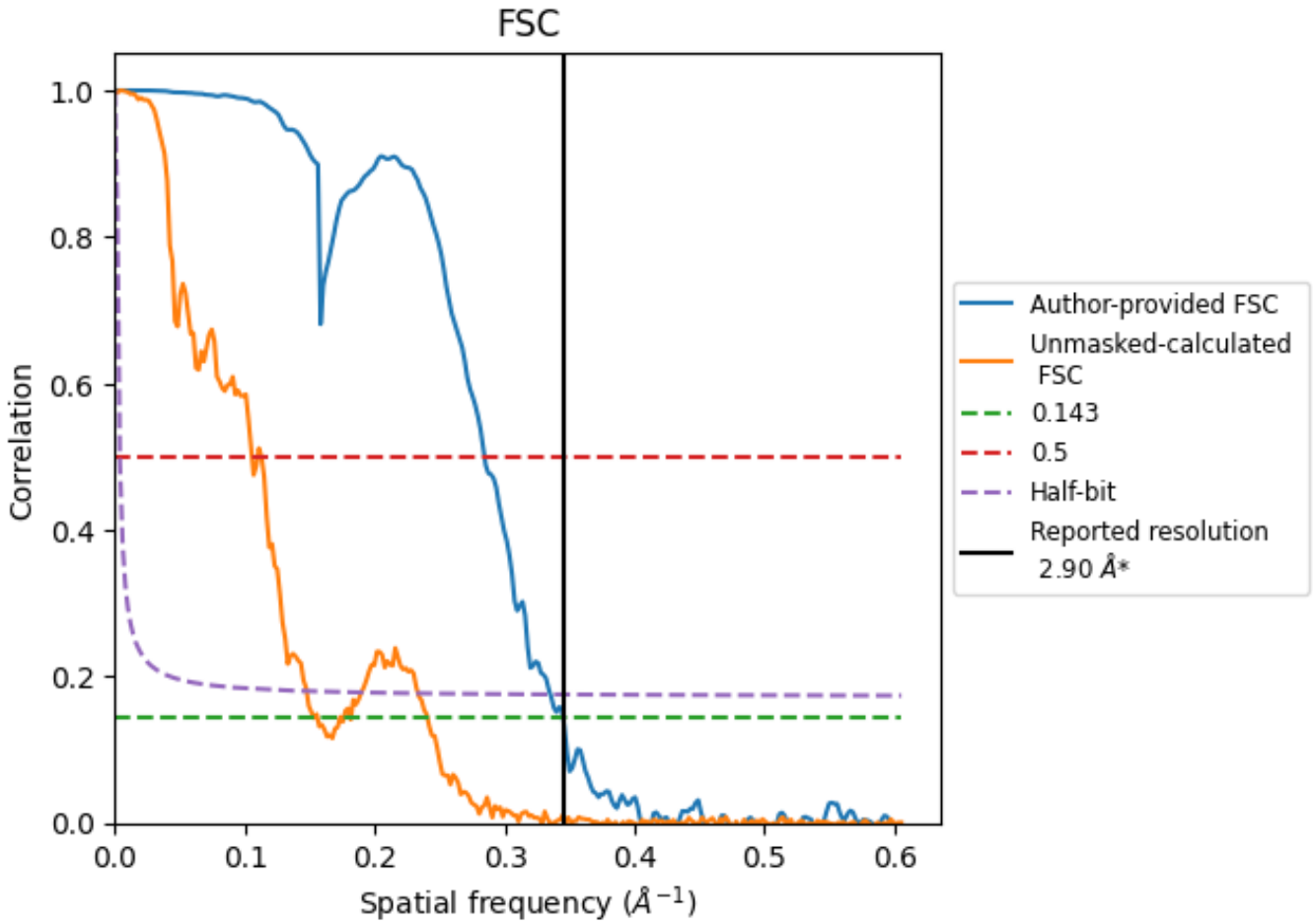


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 $Å^{-1}$

8.2 Resolution estimates (i)

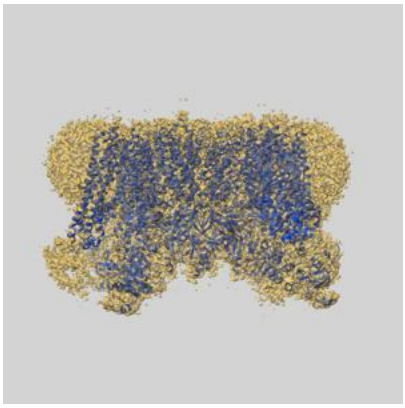
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.51	2.98
Unmasked-calculated*	6.41	9.47	6.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 2.9 by more than 10 %

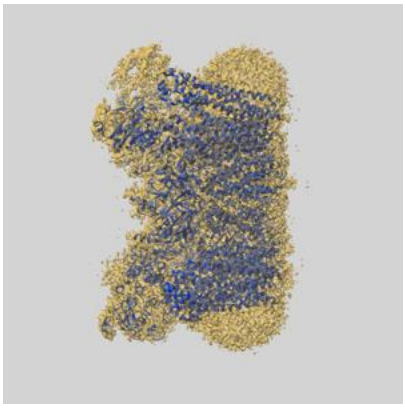
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41277 and PDB model 8TI1. Per-residue inclusion information can be found in section 3 on page 8.

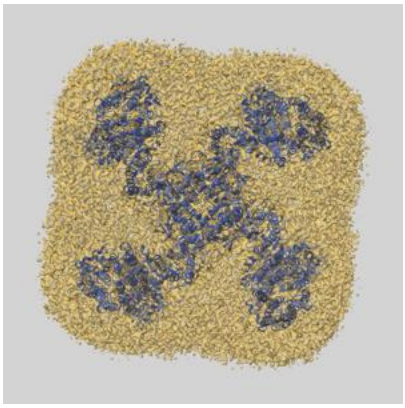
9.1 Map-model overlay



X



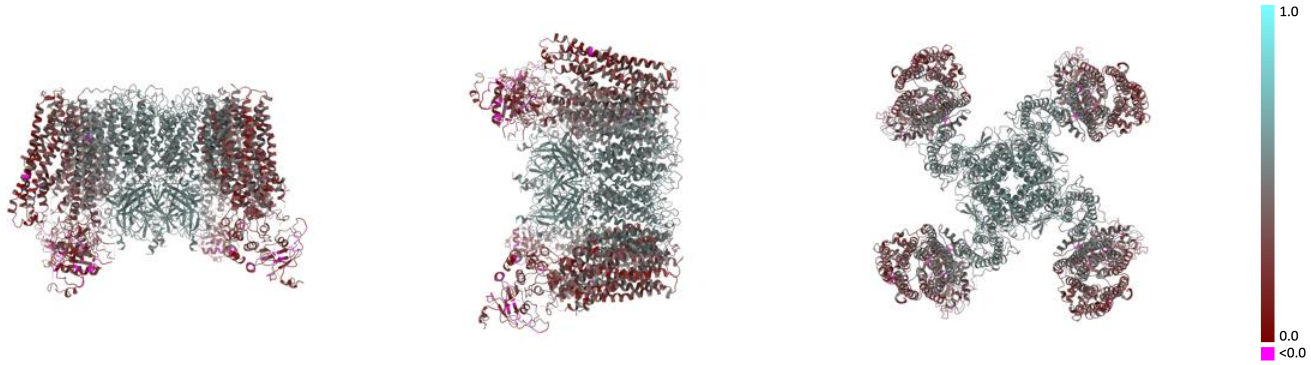
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

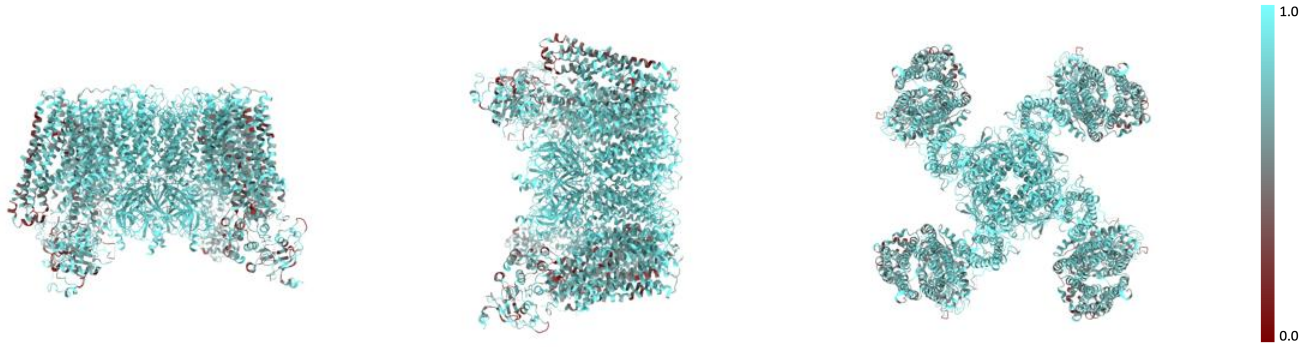
9.2 Q-score mapped to coordinate model (i)



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.

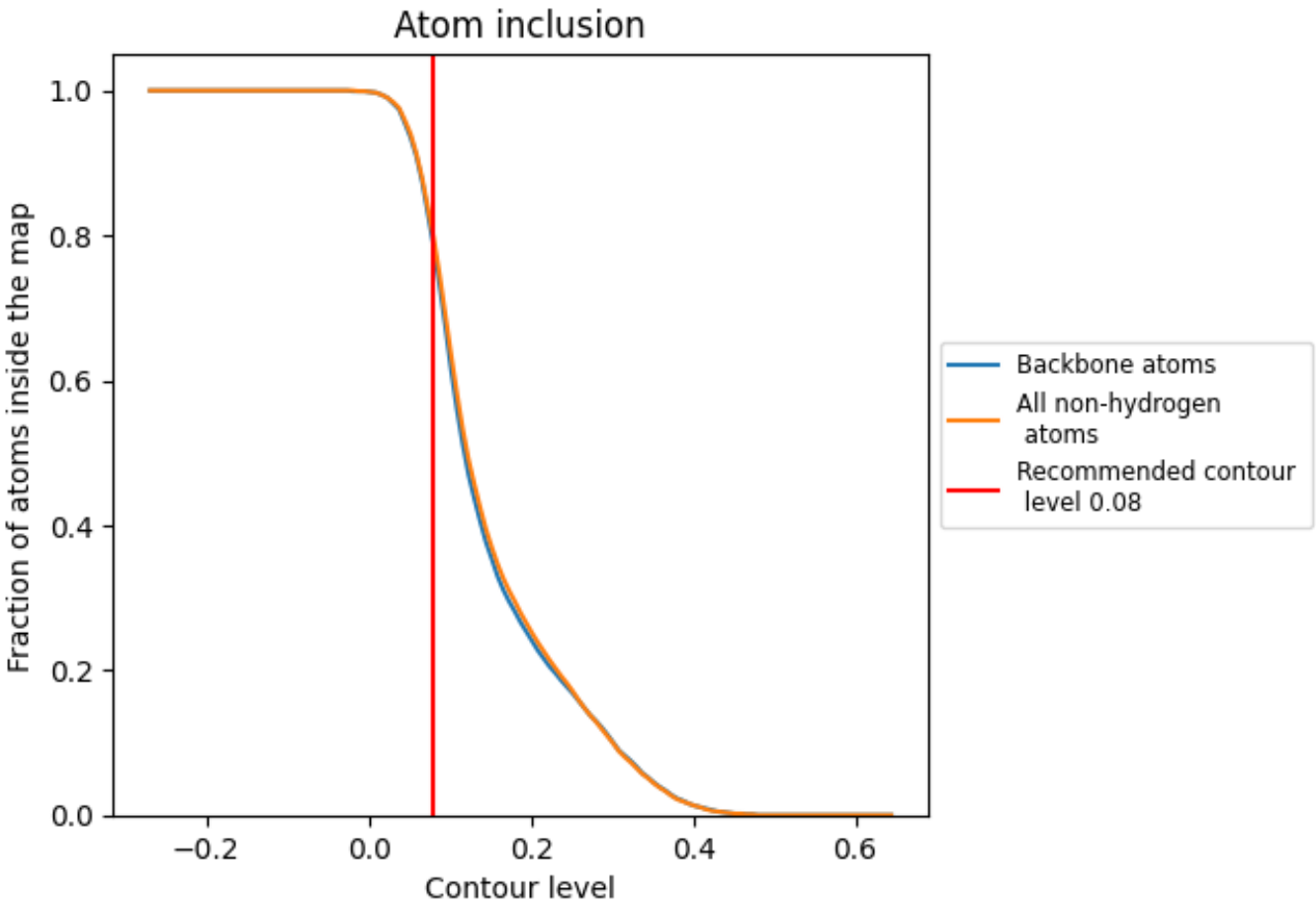
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 80% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.4190
A	0.9290	0.5580
B	0.9280	0.5590
C	0.9280	0.5590
D	0.9270	0.5590
E	0.7660	0.3770
F	0.7650	0.3780
G	0.7650	0.3780
H	0.7660	0.3780