Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 04:46 PM EDT

PDB ID	:	7LEP
EMDB ID	:	EMD-23292
Title	:	The composite LBD-TMD structure combined from all hippocampal AMPAR subtypes at 3.25 Angstrom resolution
Authors	:	Yu, J.; Rao, P.; Gouaux, E.
Deposited on	:	2021-01-14
Resolution	:	3.25 Å(reported)

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:

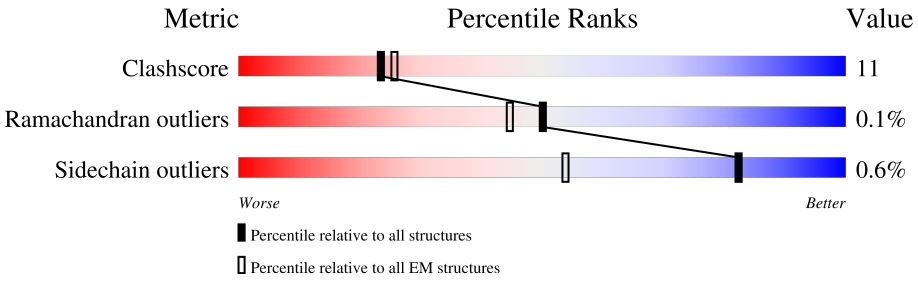
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.25 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	414	5% 79% 18%
2	B	424	6% 72% 22% 5%
2	D	424	6% 74% 21% 5%
3	C	413	5% 77% 20%
4	E	159	17% 72% 16% 11%
4	F	159	16% 67% 21% 11%
5	G	215	62% 14% 24%
5	H	215	63% 13% 24%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16559 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 Mix of AMPAR subunits (GluA1, GluA3, and GluA4).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	403	Total	C	N	O	S	1	0
			2844	1852	462	512	18		

- Molecule 2 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	403	Total	C	N	O	S	0	0
			2929	1905	474	531	19		
2	D	403	Total	C	N	O	S	0	0
			2921	1898	474	530	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	756	GLU	GLN	conflict	UNP C9K0Z0
D	756	GLU	GLN	conflict	UNP C9K0Z0

- Molecule 3 is a protein called Mix of AMPAR subunits (GluA1, GluA3, and GluAX).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	403	Total	C	N	O	S	0	0
			2855	1860	460	517	18		

- Molecule 4 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	141	Total	C	N	O	S	0	0
			1092	741	165	175	11		
4	F	141	Total	C	N	O	S	0	0
			1096	743	165	177	11		

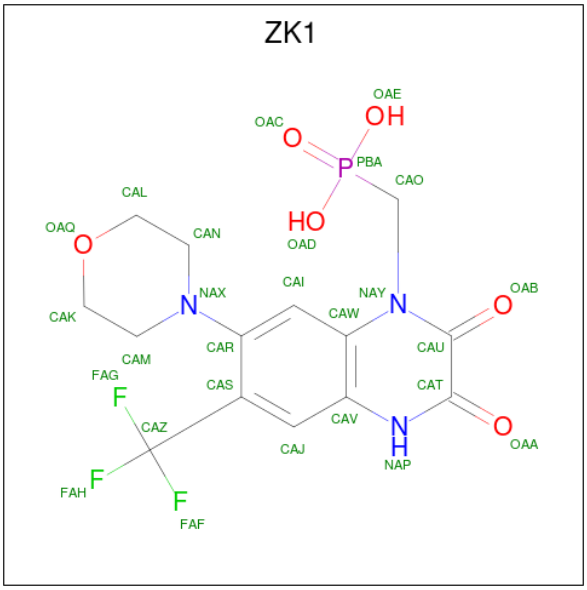
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	100	THR	TYR	conflict	UNP O35089
F	100	THR	TYR	conflict	UNP O35089

- Molecule 5 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

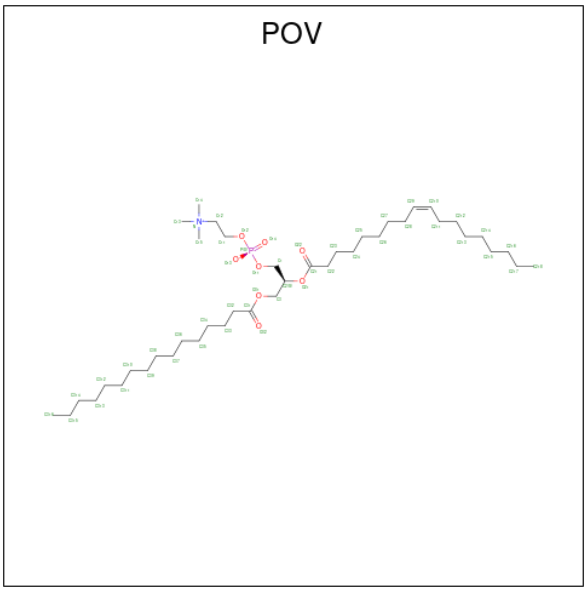
Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	164	Total	C	N	O	S	0	0
			1144	757	184	198	5		
5	H	164	Total	C	N	O	S	0	0
			1144	757	184	198	5		

- Molecule 6 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
6	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
6	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
6	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



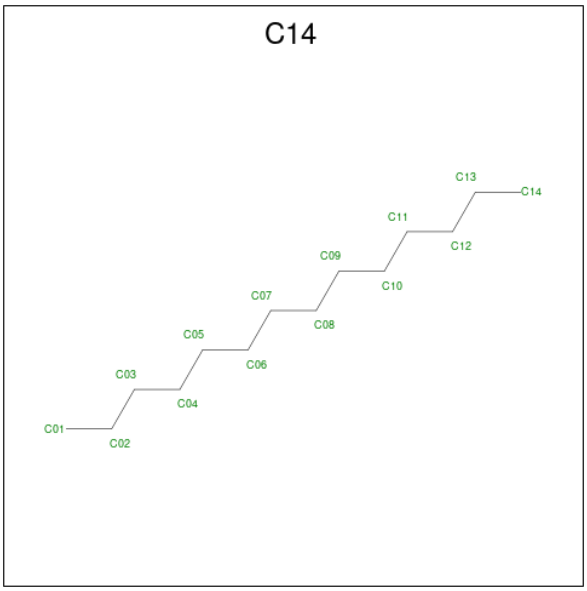
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C 6 6	0
7	A	1	Total C 11 11	0
7	A	1	Total C 12 12	0
7	A	1	Total C 7 7	0
7	A	1	Total C 10 10	0
7	A	1	Total C 8 8	0
7	A	1	Total C 8 8	0
7	A	1	Total C 5 5	0
7	B	1	Total C N O P 41 31 1 8 1	0
7	B	1	Total C 8 8	0
7	B	1	Total C 8 8	0
7	B	1	Total C 11 11	0
7	B	1	Total C 8 8	0
7	C	1	Total C 10 10	0

Continued on next page...

Continued from previous page...

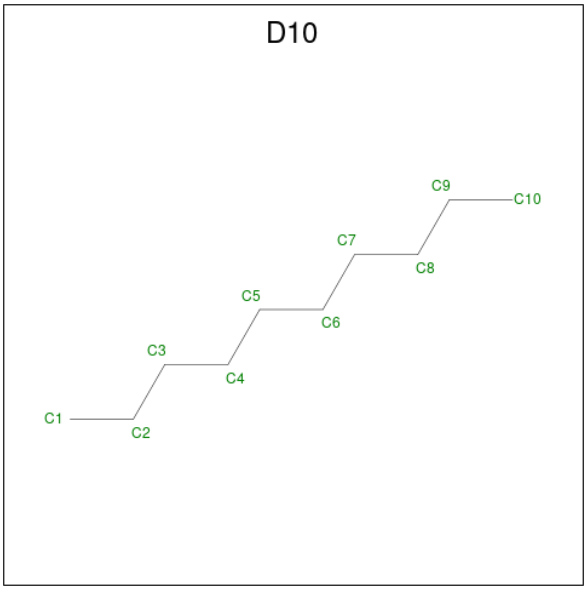
Mol	Chain	Residues	Atoms	AltConf
7	C	1	Total C 6 6	0
7	C	1	Total C 8 8	0
7	C	1	Total C 6 6	0
7	C	1	Total C 8 8	0
7	C	1	Total C 12 12	0
7	C	1	Total C 7 7	0
7	D	1	Total C N O P 41 31 1 8 1	0
7	D	1	Total C 8 8	0
7	D	1	Total C 11 11	0
7	D	1	Total C 9 9	0
7	D	1	Total C 7 7	0
7	D	1	Total C 8 8	0
7	E	1	Total C 8 8	0
7	F	1	Total C 8 8	0
7	G	1	Total C 9 9	0
7	H	1	Total C 9 9	0

- Molecule 8 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



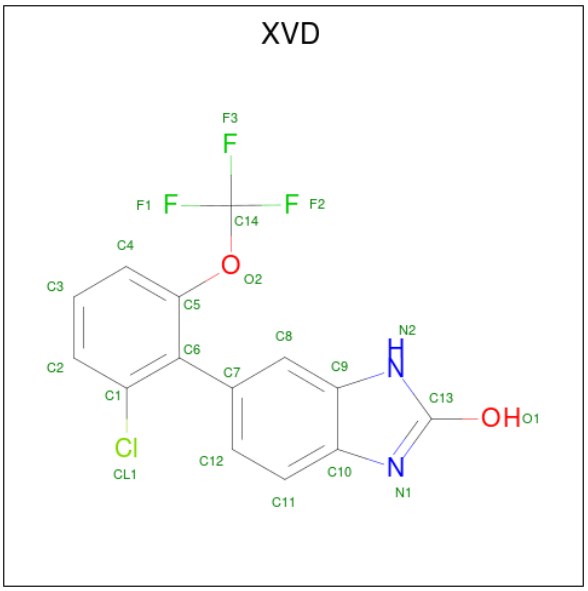
Mol	Chain	Residues	Atoms	AltConf
8	B	1	Total C 14 14	0

- Molecule 9 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



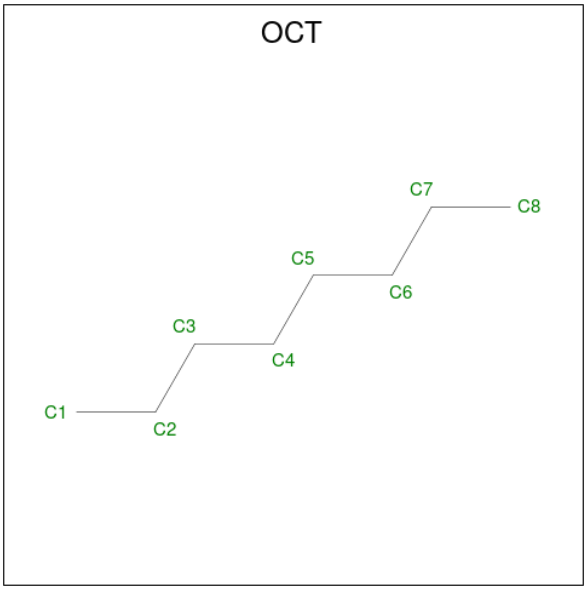
Mol	Chain	Residues	Atoms	AltConf
9	C	1	Total C 10 10	0

- Molecule 10 is 6-[2-chloro-6-(trifluoromethoxy)phenyl]-1H-benzimidazol-2-ol (three-letter code: XVD) (formula: $C_{14}H_8ClF_3N_2O_2$) (labeled as "Ligand of Interest" by depositor).



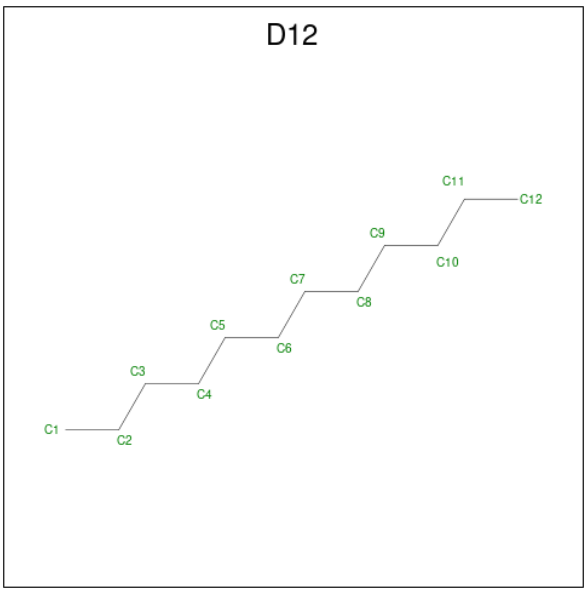
Mol	Chain	Residues	Atoms						AltConf
10	G	1	Total	C	Cl	F	N	O	0
			22	14	1	3	2	2	
10	H	1	Total	C	Cl	F	N	O	0
			22	14	1	3	2	2	

- Molecule 11 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms		AltConf
11	G	1	Total	C	0
			8	8	
11	H	1	Total	C	0
			8	8	

- Molecule 12 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



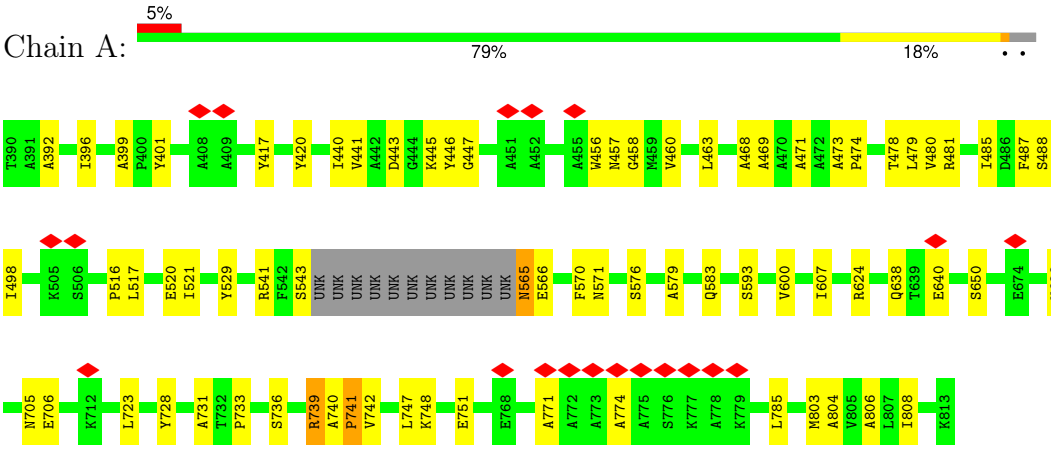
Mol	Chain	Residues	Atoms	AltConf
12	G	1	Total C 12 12	0
12	H	1	Total C 12 12	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

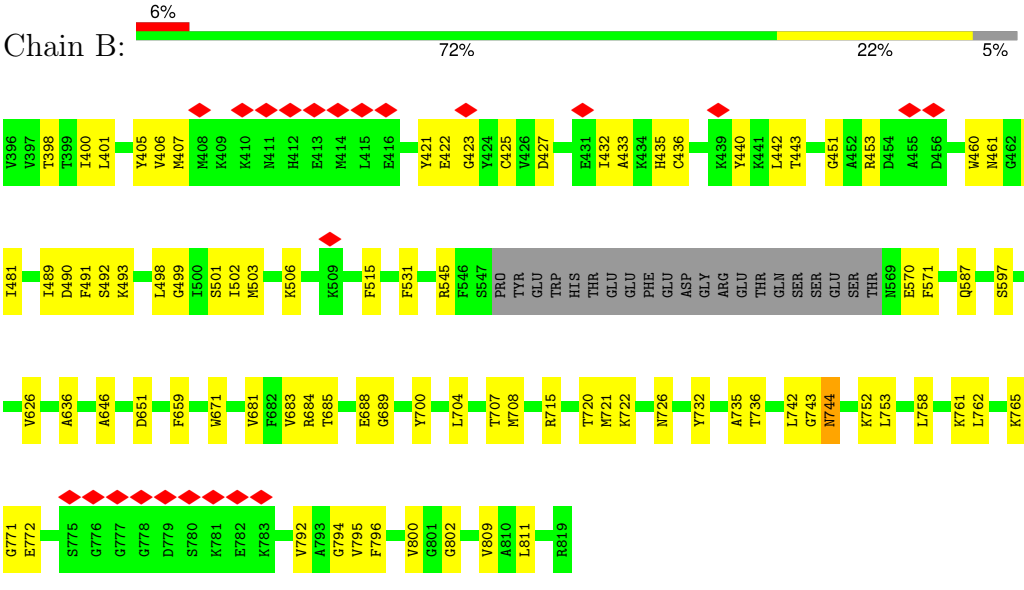
• Molecule 1: Mix of AMPAR subunits (GluA1, GluA3, and GluA4)

Chain A:



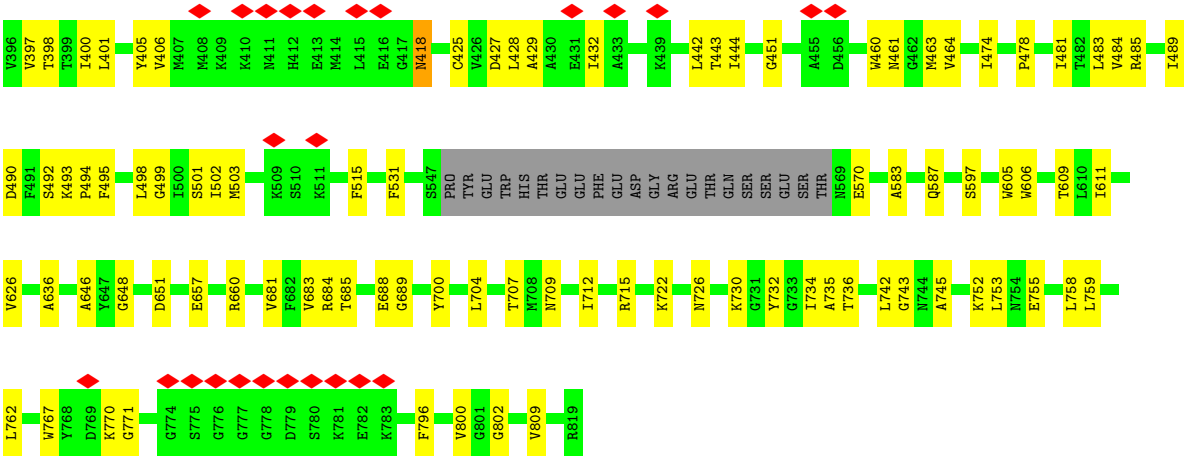
• Molecule 2: Glutamate receptor 2

Chain B:

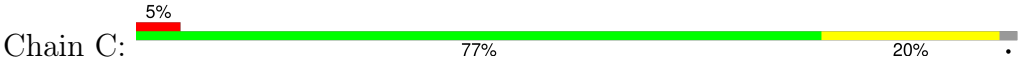


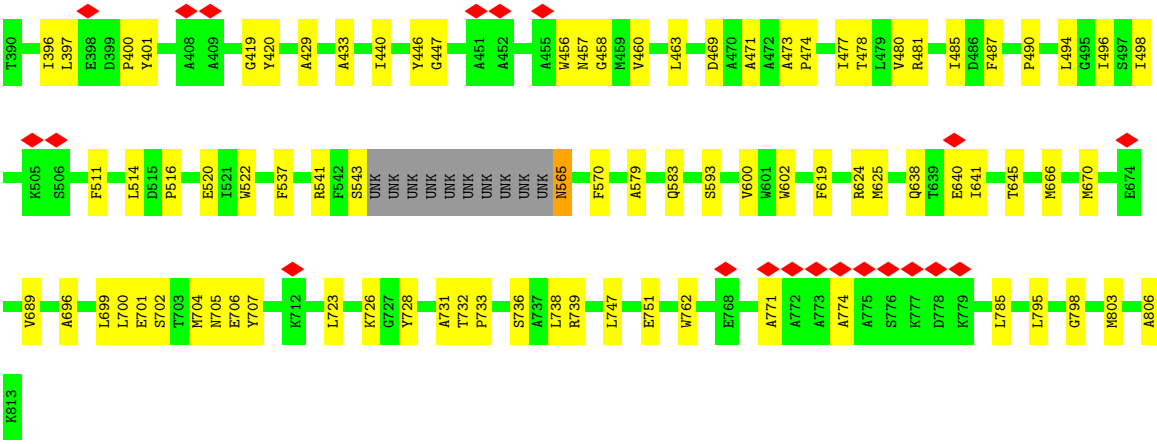
• Molecule 2: Glutamate receptor 2

Chain D:

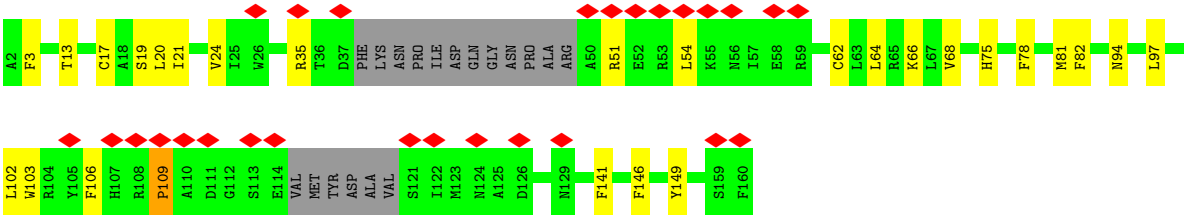


• Molecule 3: Mix of AMPAR subunits (GluA1, GluA3, and GluAX)

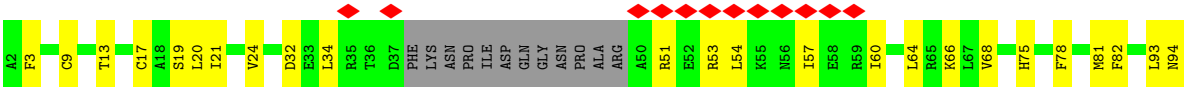


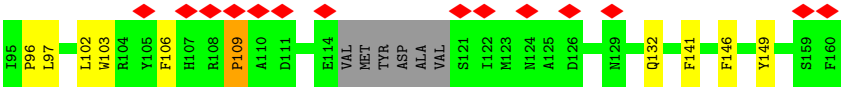


• Molecule 4: Protein cornichon homolog 2



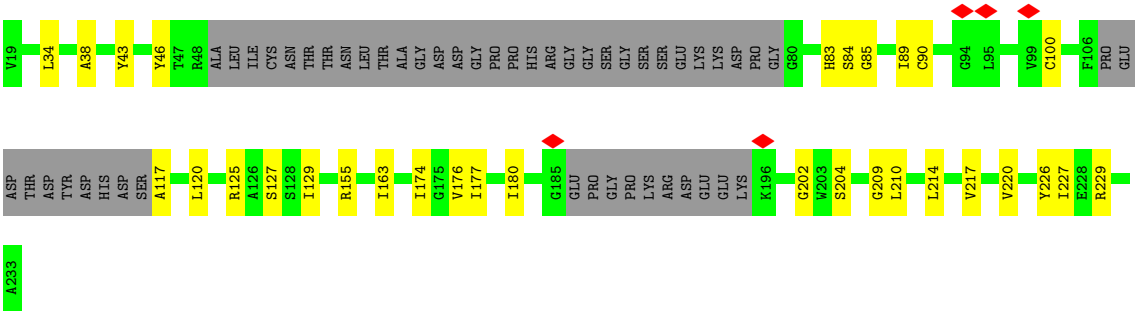
• Molecule 4: Protein cornichon homolog 2





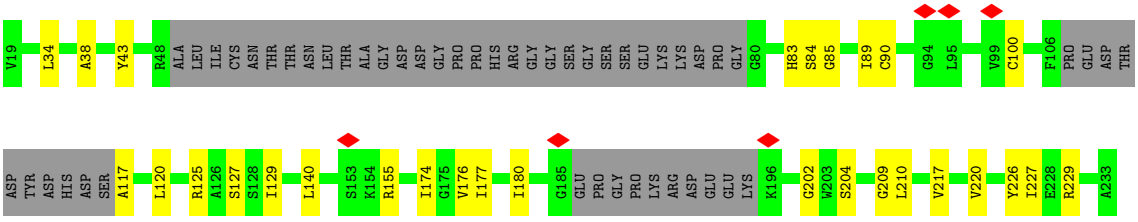
• Molecule 5: Voltage-dependent calcium channel gamma-8 subunit

Chain G:



• Molecule 5: Voltage-dependent calcium channel gamma-8 subunit

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116710	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.191	Depositor
Minimum map value	-0.787	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.156	Depositor
Map size (Å)	441.4, 441.4, 441.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1035, 1.1035, 1.1035	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, D10, D12, C14, OCT, ZK1, XVD

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	0.47	0/2911	0.51	0/3971
2	B	0.43	0/2993	0.50	0/4073
2	D	0.42	0/2984	0.49	0/4060
3	C	0.46	0/2918	0.51	0/3981
4	E	0.36	0/1123	0.49	1/1531 (0.1%)
4	F	0.37	0/1127	0.49	1/1536 (0.1%)
5	G	0.46	0/1164	0.51	0/1588
5	H	0.46	0/1164	0.51	0/1588
All	All	0.44	0/16384	0.50	2/22328 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	109	PRO	N-CA-CB	5.70	110.14	103.30
4	E	109	PRO	N-CA-CB	5.68	110.12	103.30

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	2844	0	2752	69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2929	0	2778	77	0
2	D	2921	0	2767	68	0
3	C	2855	0	2753	77	0
4	E	1092	0	1039	21	0
4	F	1096	0	1043	26	0
5	G	1144	0	1103	26	0
5	H	1144	0	1103	25	0
6	A	27	0	13	1	0
6	B	27	0	13	0	0
6	C	27	0	13	3	0
6	D	27	0	13	4	0
7	A	67	0	102	6	0
7	B	76	0	108	2	0
7	C	57	0	86	16	0
7	D	84	0	120	1	0
7	E	8	0	12	0	0
7	F	8	0	12	0	0
7	G	9	0	14	0	0
7	H	9	0	14	0	0
8	B	14	0	30	0	0
9	C	10	0	22	3	0
10	G	22	0	0	4	0
10	H	22	0	0	4	0
11	G	8	0	18	0	0
11	H	8	0	18	0	0
12	G	12	0	26	0	0
12	H	12	0	26	0	0
All	All	16559	0	15998	353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:485:ARG:NH2	6:D:901:ZK1:OAA	1.74	1.21
3:C:570:PHE:HE1	7:C:909:POV:C21	1.58	1.15
3:C:570:PHE:CE1	7:C:909:POV:C21	2.32	1.12
3:C:570:PHE:HE1	7:C:909:POV:C22	1.64	1.10
2:D:485:ARG:CZ	6:D:901:ZK1:OAA	2.12	0.98
2:D:485:ARG:NH1	6:D:901:ZK1:OAA	1.97	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:570:PHE:CE1	7:C:909:POV:H22	1.99	0.97
3:C:570:PHE:HE1	7:C:909:POV:H22	1.28	0.95
3:C:570:PHE:CE1	7:C:909:POV:C22	2.54	0.90
1:A:485:ILE:HD11	1:A:733:PRO:HA	1.58	0.85
2:B:489:ILE:HG21	2:B:735:ALA:HB1	1.59	0.85
3:C:565:ASN:N	3:C:565:ASN:HD22	1.75	0.84
2:D:489:ILE:HG21	2:D:735:ALA:HB1	1.59	0.84
3:C:514:LEU:HD11	7:C:908:POV:H33	1.61	0.81
1:A:565:ASN:N	1:A:565:ASN:HD22	1.82	0.78
2:B:570:GLU:HG2	2:B:571:PHE:H	1.50	0.76
1:A:498:ILE:O	1:A:705:ASN:ND2	2.19	0.75
2:D:485:ARG:HH22	6:D:901:ZK1:CAT	1.97	0.75
3:C:397:LEU:HD11	3:C:440:ILE:HD13	1.68	0.75
3:C:498:ILE:O	3:C:705:ASN:ND2	2.21	0.73
3:C:485:ILE:HD11	3:C:733:PRO:HA	1.71	0.71
5:H:125:ARG:O	5:H:125:ARG:NH1	2.23	0.70
5:G:125:ARG:O	5:G:125:ARG:NH1	2.23	0.69
3:C:511:PHE:CD1	7:C:908:POV:H32A	2.28	0.68
2:B:715:ARG:NH2	2:B:770:LYS:O	2.27	0.68
3:C:701:GLU:HG3	6:C:901:ZK1:HAM	1.77	0.66
1:A:396:ILE:HG12	1:A:446:TYR:HE1	1.60	0.66
3:C:447:GLY:HA3	3:C:460:VAL:HG12	1.77	0.66
3:C:570:PHE:CD2	7:C:906:POV:C26	2.79	0.66
2:B:499:GLY:HA3	2:B:726:ASN:HB3	1.79	0.65
9:C:902:D10:H22	7:C:908:POV:H33A	1.80	0.64
2:B:545:ARG:NH2	2:B:570:GLU:O	2.31	0.64
4:E:103:TRP:HA	4:E:106:PHE:HD1	1.64	0.63
1:A:566:GLU:O	1:A:571:ASN:ND2	2.28	0.63
4:F:20:LEU:HD22	4:F:78:PHE:HE2	1.64	0.62
3:C:543:SER:O	5:H:226:TYR:OH	2.17	0.62
1:A:624:ARG:NH2	2:D:626:VAL:O	2.33	0.61
4:E:20:LEU:HD22	4:E:78:PHE:HE2	1.64	0.61
3:C:522:TRP:HB3	9:C:902:D10:H42	1.83	0.60
1:A:593:SER:HB3	2:B:809:VAL:HG23	1.84	0.60
1:A:541:ARG:HB3	5:G:227:ILE:HD11	1.83	0.60
3:C:638:GLN:NE2	3:C:640:GLU:HG3	2.17	0.60
2:B:623:PHE:HA	3:C:624:ARG:NH2	2.17	0.60
2:B:765:LYS:HE3	2:B:766:TRP:CD1	2.37	0.60
4:E:94:ASN:ND2	4:E:149:TYR:OH	2.27	0.59
1:A:751:GLU:OE2	2:D:730:LYS:NZ	2.23	0.59
4:E:13:THR:HG22	4:E:78:PHE:HD1	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:HD21	1:A:728:TYR:CZ	2.38	0.59
3:C:456:TRP:HH2	3:C:480:VAL:HG12	1.67	0.59
1:A:457:ASN:OD1	1:A:458:GLY:N	2.35	0.59
3:C:638:GLN:HE22	3:C:641:ILE:H	1.51	0.59
2:D:704:LEU:HD21	2:D:709:ASN:HB2	1.84	0.59
4:F:103:TRP:HA	4:F:106:PHE:HD1	1.67	0.59
1:A:570:PHE:HB2	7:A:908:POV:H26A	1.84	0.58
3:C:537:PHE:CE2	5:H:220:VAL:HG23	2.38	0.58
1:A:447:GLY:HA3	1:A:460:VAL:HG12	1.86	0.58
1:A:565:ASN:N	1:A:565:ASN:ND2	2.51	0.58
2:B:753:LEU:HD22	2:B:758:LEU:HD23	1.84	0.58
1:A:747:LEU:O	1:A:751:GLU:HG2	2.04	0.58
2:B:685:THR:HG23	2:B:688:GLU:H	1.69	0.58
4:E:62:CYS:O	4:E:66:LYS:HG3	2.05	0.57
5:G:127:SER:O	5:G:129:ILE:N	2.38	0.57
3:C:771:ALA:HB1	3:C:774:ALA:HB2	1.87	0.57
1:A:456:TRP:HH2	1:A:480:VAL:HG12	1.68	0.57
3:C:463:LEU:HD11	3:C:471:ALA:HB2	1.86	0.57
5:H:127:SER:O	5:H:129:ILE:N	2.38	0.56
2:B:432:ILE:O	2:B:436:CYS:N	2.37	0.56
4:E:13:THR:HG22	4:E:78:PHE:CD1	2.39	0.56
3:C:520:GLU:HG2	5:H:180:ILE:HG21	1.86	0.56
2:D:685:THR:HG23	2:D:688:GLU:H	1.70	0.56
2:D:753:LEU:HD22	2:D:758:LEU:HD23	1.87	0.56
1:A:748:LYS:HG2	2:D:483:LEU:HD22	1.87	0.56
4:F:13:THR:HG22	4:F:78:PHE:CD1	2.41	0.56
1:A:441:VAL:HG21	1:A:458:GLY:HA2	1.87	0.55
2:D:405:TYR:HD1	2:D:478:PRO:HD3	1.72	0.55
2:B:407:MET:N	2:B:422:GLU:O	2.30	0.55
2:D:648:GLY:HA3	2:D:681:VAL:HG12	1.89	0.55
1:A:487:PHE:CD1	1:A:731:ALA:HB2	2.43	0.54
3:C:469:ASP:O	3:C:733:PRO:HD3	2.08	0.54
2:D:495:PHE:HB2	2:D:759:LEU:HD11	1.90	0.54
2:B:606:TRP:CD1	3:C:583:GLN:HG3	2.43	0.54
4:E:75:HIS:NE2	4:E:94:ASN:OD1	2.40	0.54
2:D:498:LEU:HD21	2:D:732:TYR:CZ	2.43	0.54
4:F:75:HIS:NE2	4:F:94:ASN:OD1	2.40	0.54
4:F:94:ASN:ND2	4:F:149:TYR:OH	2.40	0.54
3:C:565:ASN:N	3:C:565:ASN:ND2	2.48	0.54
3:C:666:MET:O	3:C:670:MET:HG3	2.08	0.54
2:B:501:SER:OG	2:B:722:LYS:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:626:VAL:HG21	3:C:625:MET:HB3	1.89	0.53
1:A:529:TYR:HD1	1:A:576:SER:HG	1.56	0.53
3:C:457:ASN:OD1	3:C:458:GLY:N	2.41	0.53
2:D:605:TRP:O	2:D:609:THR:HG23	2.08	0.53
2:B:400:ILE:HG13	2:B:401:LEU:H	1.72	0.53
2:D:796:PHE:HB3	5:H:177:ILE:HD13	1.91	0.53
2:B:796:PHE:HB3	5:G:177:ILE:HD13	1.91	0.53
2:B:400:ILE:O	2:B:406:VAL:HB	2.09	0.53
4:F:97:LEU:HD22	4:F:141:PHE:CE2	2.44	0.53
5:G:209:GLY:HA3	10:G:501:XVD:CL1	2.46	0.52
5:H:209:GLY:HA3	10:H:501:XVD:CL1	2.46	0.52
2:B:570:GLU:N	2:B:570:GLU:OE1	2.42	0.52
2:B:761:LYS:NZ	2:B:765:LYS:HB2	2.25	0.52
3:C:638:GLN:NE2	3:C:641:ILE:HG12	2.24	0.52
1:A:401:TYR:O	1:A:420:TYR:N	2.43	0.52
1:A:579:ALA:HA	2:B:587:GLN:HE22	1.75	0.52
3:C:593:SER:HB3	2:D:809:VAL:HG23	1.92	0.51
2:D:489:ILE:HG22	2:D:490:ASP:N	2.25	0.51
2:B:683:VAL:HG11	2:B:689:GLY:N	2.25	0.51
1:A:570:PHE:HB2	7:A:908:POV:H24	1.92	0.51
2:D:651:ASP:OD2	2:D:684:ARG:HA	2.10	0.51
3:C:494:LEU:HD21	3:C:728:TYR:CZ	2.46	0.51
2:D:499:GLY:HA3	2:D:726:ASN:HB3	1.92	0.51
2:B:604:VAL:HG21	3:C:798:GLY:HA3	1.93	0.51
2:D:736:THR:HG21	2:D:743:GLY:HA2	1.93	0.51
1:A:771:ALA:HB1	1:A:774:ALA:HB2	1.92	0.50
3:C:638:GLN:HE22	3:C:641:ILE:N	2.09	0.50
5:G:155:ARG:HA	5:G:229:ARG:CZ	2.41	0.50
2:B:425:CYS:SG	2:B:477:ALA:HA	2.51	0.50
2:B:515:PHE:HZ	7:B:902:POV:H33	1.76	0.50
2:D:742:LEU:HD12	2:D:745:ALA:HB3	1.94	0.50
2:D:400:ILE:HG13	2:D:401:LEU:H	1.75	0.50
3:C:400:PRO:HG3	3:C:707:TYR:CD2	2.46	0.50
2:B:398:THR:HA	2:B:443:THR:O	2.10	0.50
3:C:514:LEU:CD1	7:C:908:POV:H33	2.39	0.50
1:A:543:SER:O	5:G:226:TYR:OH	2.25	0.50
2:D:444:ILE:H	2:D:444:ILE:HD12	1.77	0.50
2:B:453:ARG:HD2	2:B:460:TRP:CZ2	2.47	0.49
5:H:155:ARG:HA	5:H:229:ARG:CZ	2.41	0.49
2:B:405:TYR:HE1	2:B:767:TRP:HZ2	1.60	0.49
4:F:13:THR:HG22	4:F:78:PHE:HD1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:646:ALA:O	2:D:700:TYR:HA	2.12	0.49
3:C:429:ALA:O	3:C:433:ALA:N	2.39	0.49
3:C:447:GLY:HA3	3:C:460:VAL:CG1	2.42	0.49
5:G:38:ALA:O	5:G:204:SER:OG	2.30	0.49
2:B:736:THR:HG21	2:B:743:GLY:HA2	1.95	0.49
3:C:689:VAL:HA	3:C:696:ALA:HB3	1.94	0.49
2:D:397:VAL:HG12	2:D:474:ILE:HG12	1.95	0.49
2:D:657:GLU:HA	2:D:660:ARG:HG2	1.94	0.49
4:F:54:LEU:O	4:F:57:ILE:HG12	2.12	0.49
1:A:479:LEU:HD22	2:D:752:LYS:HG3	1.94	0.48
3:C:487:PHE:CD1	3:C:731:ALA:HB2	2.47	0.48
2:B:715:ARG:HA	2:B:715:ARG:NE	2.28	0.48
9:C:902:D10:C2	7:C:908:POV:H33A	2.43	0.48
2:D:683:VAL:HG11	2:D:689:GLY:N	2.27	0.48
5:H:38:ALA:O	5:H:204:SER:OG	2.30	0.48
5:H:89:ILE:O	5:H:100:CYS:HB2	2.13	0.48
5:H:176:VAL:HG21	10:H:501:XVD:C13	2.44	0.48
4:F:53:ARG:O	4:F:57:ILE:HG23	2.12	0.48
5:G:176:VAL:HG21	10:G:501:XVD:C13	2.44	0.48
2:B:651:ASP:OD2	2:B:684:ARG:HA	2.13	0.48
2:D:715:ARG:HH12	2:D:771:GLY:HA2	1.78	0.48
5:G:89:ILE:O	5:G:100:CYS:HB2	2.13	0.48
1:A:494:LEU:HD21	1:A:728:TYR:CE1	2.48	0.48
2:B:435:HIS:NE2	2:B:752:LYS:HD2	2.28	0.48
4:F:34:LEU:HG	4:F:60:ILE:HG21	1.96	0.48
1:A:689:VAL:HA	1:A:696:ALA:HB3	1.95	0.48
2:B:792:VAL:O	2:B:795:VAL:HG12	2.13	0.48
2:D:515:PHE:HZ	7:D:902:POV:H33	1.78	0.48
1:A:473:ALA:HB1	1:A:474:PRO:HD2	1.96	0.48
3:C:645:THR:HG22	3:C:699:LEU:HB2	1.95	0.48
2:D:460:TRP:CE3	2:D:464:VAL:HG11	2.48	0.48
4:F:51:ARG:HA	4:F:54:LEU:HD13	1.96	0.48
1:A:520:GLU:HG2	5:G:180:ILE:HG21	1.95	0.48
2:B:715:ARG:NH2	2:B:771:GLY:HA2	2.29	0.48
2:D:501:SER:OG	2:D:722:LYS:HG3	2.13	0.48
5:G:90:CYS:HA	5:G:100:CYS:CB	2.44	0.47
2:B:427:ASP:OD1	2:B:762:LEU:HD11	2.15	0.47
4:E:13:THR:HG21	4:E:82:PHE:CZ	2.48	0.47
1:A:541:ARG:HH22	1:A:565:ASN:N	2.12	0.47
3:C:638:GLN:HE22	3:C:641:ILE:HG12	1.80	0.47
2:D:481:ILE:HD12	2:D:494:PRO:HG3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:732:THR:HG21	3:C:738:LEU:O	2.15	0.47
4:F:13:THR:HG21	4:F:82:PHE:CZ	2.50	0.47
2:D:451:GLY:HA2	2:D:461:ASN:O	2.15	0.47
2:D:570:GLU:OE1	2:D:570:GLU:N	2.45	0.47
1:A:740:ALA:HB3	1:A:741:PRO:HD3	1.96	0.47
3:C:473:ALA:HB1	3:C:474:PRO:HD2	1.96	0.47
7:C:905:POV:C28	7:C:906:POV:C21	2.93	0.47
3:C:570:PHE:HD2	7:C:906:POV:C26	2.25	0.47
2:B:421:TYR:CD2	2:B:442:LEU:HD22	2.49	0.47
4:E:97:LEU:HD22	4:E:141:PHE:CE2	2.49	0.47
5:H:90:CYS:HA	5:H:100:CYS:CB	2.44	0.47
4:E:35:ARG:HG2	4:E:35:ARG:HH11	1.80	0.47
1:A:570:PHE:CE2	7:A:909:POV:C25	2.97	0.46
1:A:739:ARG:O	1:A:739:ARG:NH1	2.40	0.46
4:F:54:LEU:O	4:F:57:ILE:N	2.48	0.46
2:D:800:VAL:HB	5:H:174:ILE:HD11	1.98	0.46
2:B:498:LEU:HD21	2:B:732:TYR:CZ	2.51	0.46
5:G:90:CYS:HA	5:G:100:CYS:HB2	1.97	0.46
2:B:400:ILE:HG13	2:B:401:LEU:N	2.31	0.46
1:A:481:ARG:O	1:A:485:ILE:HG22	2.16	0.46
1:A:747:LEU:HD23	1:A:747:LEU:HA	1.77	0.46
2:D:715:ARG:NH1	2:D:771:GLY:HA2	2.30	0.46
5:G:84:SER:OG	5:G:85:GLY:N	2.46	0.46
2:B:406:VAL:HA	2:B:423:GLY:HA3	1.97	0.46
5:H:90:CYS:HA	5:H:100:CYS:HB2	1.97	0.46
2:B:707:THR:HB	2:B:767:TRP:HH2	1.81	0.46
3:C:516:PRO:HA	3:C:619:PHE:HE2	1.81	0.46
5:G:43:TYR:O	5:G:202:GLY:HA3	2.16	0.46
1:A:443:ASP:OD1	1:A:457:ASN:ND2	2.47	0.45
1:A:463:LEU:HD11	1:A:471:ALA:HB2	1.98	0.45
3:C:481:ARG:O	3:C:485:ILE:HG22	2.16	0.45
4:E:17:CYS:HB3	4:E:146:PHE:HD1	1.81	0.45
2:B:479:LEU:O	2:B:732:TYR:HA	2.16	0.45
3:C:446:TYR:HE1	6:C:901:ZK1:CAV	2.29	0.45
2:B:646:ALA:O	2:B:700:TYR:HA	2.17	0.45
2:B:800:VAL:HB	5:G:174:ILE:HD11	1.97	0.45
3:C:638:GLN:HE21	3:C:640:GLU:HG3	1.79	0.45
3:C:747:LEU:O	3:C:751:GLU:HG2	2.16	0.45
2:D:429:ALA:HA	2:D:432:ILE:HG22	1.99	0.45
1:A:445:LYS:HE2	1:A:457:ASN:ND2	2.32	0.45
2:D:405:TYR:HE2	2:D:767:TRP:HZ2	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:TRP:CH2	1:A:480:VAL:HG12	2.48	0.45
1:A:702:SER:O	1:A:706:GLU:HG3	2.17	0.45
2:B:400:ILE:HB	2:B:463:MET:HE1	1.98	0.45
3:C:803:MET:CE	4:F:19:SER:HB3	2.47	0.45
5:H:43:TYR:O	5:H:202:GLY:HA3	2.16	0.45
1:A:445:LYS:O	1:A:458:GLY:HA3	2.17	0.45
2:B:704:LEU:H	2:B:704:LEU:HD23	1.82	0.45
2:D:398:THR:HA	2:D:443:THR:O	2.16	0.45
4:F:20:LEU:HD12	4:F:20:LEU:HA	1.72	0.45
1:A:440:ILE:HD12	1:A:440:ILE:H	1.83	0.44
2:B:597:SER:OG	3:C:806:ALA:HB2	2.17	0.44
2:D:715:ARG:NH1	2:D:770:LYS:O	2.50	0.44
2:B:481:ILE:HG22	2:B:491:PHE:CD1	2.52	0.44
2:B:715:ARG:HH21	2:B:772:GLU:H	1.65	0.44
2:B:765:LYS:O	2:B:769:ASP:HB2	2.17	0.44
2:B:811:LEU:HD11	5:G:163:ILE:HD13	2.00	0.44
3:C:541:ARG:HB3	5:H:227:ILE:HD11	2.00	0.44
5:H:84:SER:OG	5:H:85:GLY:N	2.46	0.44
2:B:464:VAL:O	2:B:468:VAL:HG12	2.17	0.44
5:G:176:VAL:HG21	10:G:501:XVD:C10	2.48	0.44
1:A:733:PRO:HG2	1:A:736:SER:HB2	1.98	0.44
1:A:804:ALA:O	1:A:808:ILE:HG12	2.17	0.44
4:E:103:TRP:HA	4:E:106:PHE:CD1	2.50	0.44
2:D:429:ALA:O	2:D:432:ILE:HG22	2.17	0.44
2:B:421:TYR:HD2	2:B:442:LEU:HD22	1.81	0.44
2:B:433:ALA:HB2	2:B:440:TYR:HE1	1.83	0.44
4:F:32:ASP:OD1	4:F:132:GLN:NE2	2.48	0.44
5:G:217:VAL:O	5:G:220:VAL:HG12	2.18	0.44
5:H:176:VAL:HG21	10:H:501:XVD:C10	2.48	0.44
2:D:707:THR:HB	2:D:767:TRP:HH2	1.81	0.44
1:A:446:TYR:HE2	6:A:901:ZK1:CAJ	2.31	0.43
3:C:570:PHE:CE2	7:C:906:POV:C26	3.01	0.43
2:D:418:ASN:O	2:D:418:ASN:ND2	2.49	0.43
1:A:638:GLN:HE21	1:A:640:GLU:HB3	1.83	0.43
2:B:460:TRP:CE3	2:B:464:VAL:HG11	2.53	0.43
3:C:700:LEU:HD12	3:C:704:MET:HB3	2.00	0.43
5:H:176:VAL:HG21	10:H:501:XVD:N1	2.33	0.43
1:A:570:PHE:CD2	7:A:909:POV:C25	3.02	0.43
1:A:806:ALA:HB2	2:D:597:SER:OG	2.18	0.43
3:C:702:SER:O	3:C:706:GLU:HG3	2.18	0.43
3:C:803:MET:HE3	4:F:19:SER:HB3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:83:HIS:O	5:G:83:HIS:CG	2.71	0.43
5:H:83:HIS:O	5:H:83:HIS:CG	2.71	0.43
3:C:471:ALA:O	3:C:473:ALA:N	2.50	0.43
3:C:733:PRO:HG2	3:C:736:SER:HB2	2.01	0.43
2:D:398:THR:OG1	2:D:463:MET:HG2	2.18	0.43
4:E:102:LEU:HA	4:E:102:LEU:HD23	1.83	0.43
5:G:176:VAL:HG21	10:G:501:XVD:N1	2.33	0.43
1:A:570:PHE:HB2	7:A:908:POV:C26	2.49	0.43
3:C:485:ILE:CD1	3:C:733:PRO:HA	2.45	0.43
3:C:490:PRO:HA	3:C:728:TYR:O	2.18	0.43
2:D:502:ILE:HD11	2:D:636:ALA:HB2	1.99	0.43
2:B:681:VAL:O	2:B:700:TYR:OH	2.33	0.43
1:A:583:GLN:HG3	2:D:606:TRP:CD1	2.53	0.43
2:B:481:ILE:HG22	2:B:491:PHE:CE1	2.54	0.43
3:C:446:TYR:CE1	6:C:901:ZK1:CAV	3.02	0.43
2:D:406:VAL:HG23	2:D:425:CYS:HB2	2.00	0.43
4:F:102:LEU:HA	4:F:102:LEU:HD23	1.78	0.43
1:A:417:TYR:CE2	1:A:440:ILE:HD13	2.54	0.43
2:B:503:MET:HE3	2:B:720:THR:HG21	2.00	0.43
2:B:704:LEU:HD12	2:B:708:MET:HB3	2.01	0.43
3:C:396:ILE:HG13	3:C:397:LEU:H	1.84	0.43
4:F:54:LEU:HA	4:F:57:ILE:HG12	2.01	0.43
4:F:21:ILE:O	4:F:24:VAL:HG12	2.19	0.42
2:B:604:VAL:CG1	3:C:795:LEU:HA	2.49	0.42
2:D:503:MET:HE1	2:D:712:ILE:HG21	2.00	0.42
2:D:704:LEU:HD23	2:D:704:LEU:H	1.85	0.42
5:H:217:VAL:O	5:H:220:VAL:HG12	2.18	0.42
5:G:117:ALA:HB1	5:G:120:LEU:HD13	2.01	0.42
1:A:399:ALA:HB1	1:A:401:TYR:HD2	1.83	0.42
1:A:488:SER:O	2:D:493:LYS:NZ	2.53	0.42
1:A:803:MET:CE	4:E:19:SER:HB3	2.50	0.42
2:B:744:ASN:O	2:B:744:ASN:ND2	2.40	0.42
3:C:785:LEU:HG	4:F:3:PHE:HD2	1.85	0.42
1:A:517:LEU:HD13	1:A:521:ILE:HG21	2.01	0.42
2:B:435:HIS:CD2	2:B:752:LYS:HD2	2.54	0.42
3:C:419:GLY:HA2	3:C:762:TRP:CH2	2.55	0.42
2:D:730:LYS:HA	2:D:730:LYS:HD3	1.89	0.42
4:E:21:ILE:O	4:E:24:VAL:HG12	2.20	0.42
5:H:117:ALA:HB1	5:H:120:LEU:HD13	2.01	0.42
1:A:607:ILE:HD13	1:A:607:ILE:HA	1.83	0.42
3:C:496:ILE:O	3:C:723:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:418:ASN:HA	2:D:442:LEU:HD12	2.01	0.42
2:D:428:LEU:HD21	2:D:734:ILE:HD11	2.02	0.42
2:D:492:SER:OG	2:D:493:LYS:N	2.53	0.42
1:A:740:ALA:O	1:A:742:VAL:N	2.53	0.42
2:B:400:ILE:HB	2:B:463:MET:CE	2.50	0.42
2:B:531:PHE:CE1	4:F:81:MET:HG2	2.54	0.42
2:B:570:GLU:HG2	2:B:571:PHE:N	2.27	0.42
2:B:792:VAL:O	2:B:794:GLY:N	2.52	0.42
2:B:502:ILE:HD11	2:B:636:ALA:HB2	2.01	0.42
2:B:506:LYS:HZ3	2:B:721:MET:HB3	1.84	0.42
2:D:427:ASP:HB2	2:D:762:LEU:HD21	2.02	0.41
5:G:34:LEU:HD12	5:G:210:LEU:HD22	2.01	0.41
2:B:766:TRP:CD1	2:B:766:TRP:N	2.88	0.41
5:H:34:LEU:HD12	5:H:210:LEU:HD22	2.01	0.41
2:B:570:GLU:H	2:B:570:GLU:CD	2.23	0.41
2:D:489:ILE:HG22	2:D:490:ASP:H	1.85	0.41
4:F:17:CYS:HB3	4:F:146:PHE:HD1	1.86	0.41
2:B:659:PHE:HB3	2:B:671:TRP:HB2	2.02	0.41
5:G:214:LEU:HD12	5:G:214:LEU:HA	1.85	0.41
1:A:440:ILE:HD12	1:A:440:ILE:N	2.35	0.41
1:A:447:GLY:HA3	1:A:460:VAL:CG1	2.50	0.41
1:A:785:LEU:HG	4:E:3:PHE:CD2	2.56	0.41
2:B:742:LEU:HD12	2:B:742:LEU:HA	1.89	0.41
3:C:478:THR:OG1	3:C:481:ARG:NH1	2.53	0.41
1:A:478:THR:OG1	2:D:755:GLU:OE1	2.22	0.41
2:B:506:LYS:NZ	2:B:721:MET:HB3	2.36	0.41
3:C:570:PHE:HB2	7:C:905:POV:H24	2.01	0.41
3:C:600:VAL:HG21	2:D:802:GLY:HA3	2.02	0.41
3:C:602:TRP:CD1	2:D:587:GLN:HG3	2.56	0.41
1:A:469:ALA:O	1:A:733:PRO:HD3	2.20	0.41
1:A:516:PRO:O	1:A:517:LEU:HD23	2.21	0.41
2:B:451:GLY:HA2	2:B:461:ASN:O	2.20	0.41
2:B:489:ILE:HG22	2:B:490:ASP:N	2.36	0.41
3:C:477:ILE:HA	3:C:487:PHE:CE2	2.55	0.41
4:E:62:CYS:HB3	4:E:66:LYS:NZ	2.36	0.41
4:E:64:LEU:O	4:E:68:VAL:HG23	2.20	0.41
5:H:34:LEU:CD1	5:H:210:LEU:HD22	2.51	0.41
1:A:496:ILE:O	1:A:723:LEU:HG	2.21	0.41
7:A:908:POV:C28	7:A:909:POV:C21	2.99	0.41
7:B:902:POV:H11A	7:B:902:POV:H14A	1.85	0.41
2:D:531:PHE:CE1	4:E:81:MET:HG2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:GLN:HE22	2:D:583:ALA:HA	1.85	0.40
1:A:600:VAL:HG21	2:B:802:GLY:HA3	2.03	0.40
3:C:401:TYR:O	3:C:420:TYR:N	2.54	0.40
2:D:611:ILE:HD13	2:D:611:ILE:HA	1.91	0.40
4:E:51:ARG:HA	4:E:54:LEU:HD12	2.02	0.40
4:F:9:CYS:O	4:F:13:THR:HG23	2.21	0.40
5:G:34:LEU:CD1	5:G:210:LEU:HD22	2.51	0.40
1:A:396:ILE:HD12	1:A:396:ILE:HA	1.83	0.40
4:E:97:LEU:HD12	4:E:97:LEU:HA	1.91	0.40
4:F:93:LEU:O	4:F:96:PRO:HD2	2.22	0.40
2:B:501:SER:OG	2:B:502:ILE:N	2.54	0.40
2:D:715:ARG:HA	2:D:715:ARG:HD3	1.87	0.40
5:H:140:LEU:HD23	5:H:140:LEU:HA	1.84	0.40
1:A:392:ALA:O	1:A:468:ALA:HB1	2.22	0.40
3:C:494:LEU:HD11	3:C:726:LYS:HD2	2.04	0.40
2:B:492:SER:OG	2:B:493:LYS:N	2.54	0.40
3:C:579:ALA:HA	2:D:587:GLN:HE22	1.86	0.40
4:F:64:LEU:O	4:F:68:VAL:HG23	2.21	0.40
5:G:46:TYR:HE1	5:G:83:HIS:HB2	1.87	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	400/414 (97%)	375 (94%)	24 (6%)	1 (0%)	37 66
2	B	399/424 (94%)	378 (95%)	21 (5%)	0	100 100
2	D	399/424 (94%)	378 (95%)	21 (5%)	0	100 100
3	C	399/413 (97%)	372 (93%)	27 (7%)	0	100 100
4	E	135/159 (85%)	131 (97%)	3 (2%)	1 (1%)	19 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	F	135/159 (85%)	131 (97%)	3 (2%)	1 (1%)	19 49
5	G	156/215 (73%)	148 (95%)	8 (5%)	0	100 100
5	H	156/215 (73%)	148 (95%)	8 (5%)	0	100 100
All	All	2179/2423 (90%)	2061 (95%)	115 (5%)	3 (0%)	50 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	109	PRO
4	F	109	PRO
1	A	741	PRO

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	254/293 (87%)	250 (98%)	4 (2%)	58 74
2	B	280/357 (78%)	279 (100%)	1 (0%)	89 92
2	D	279/357 (78%)	277 (99%)	2 (1%)	81 87
3	C	256/296 (86%)	254 (99%)	2 (1%)	79 86
4	E	106/142 (75%)	106 (100%)	0	100 100
4	F	107/142 (75%)	106 (99%)	1 (1%)	75 84
5	G	105/173 (61%)	105 (100%)	0	100 100
5	H	105/173 (61%)	105 (100%)	0	100 100
All	All	1492/1933 (77%)	1482 (99%)	10 (1%)	82 87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	ASN
1	A	650[A]	SER
1	A	650[B]	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	739	ARG
2	B	744	ASN
3	C	565	ASN
3	C	739	ARG
2	D	418	ASN
2	D	484	VAL
4	F	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	638	GLN
3	C	638	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	POV	C	905	-	7,7,51	0.28	0	6,6,59	0.33	0
7	POV	C	903	-	9,9,51	0.27	0	8,8,59	0.34	0
7	POV	C	906	-	5,5,51	0.32	0	4,4,59	0.22	0
11	OCT	H	502	-	7,7,7	0.30	0	6,6,6	0.26	0
6	ZK1	D	901	-	29,29,29	3.46	9 (31%)	45,45,45	1.78	12 (26%)
7	POV	B	902	-	40,40,51	1.18	3 (7%)	46,48,59	1.14	3 (6%)
7	POV	B	905	-	7,7,51	0.23	0	6,6,59	0.45	0
7	POV	F	201	-	7,7,51	0.29	0	6,6,59	0.34	0
6	ZK1	A	901	-	29,29,29	3.45	10 (34%)	45,45,45	1.42	8 (17%)
7	POV	A	907	-	7,7,51	0.28	0	6,6,59	0.37	0
7	POV	D	906	-	6,6,51	0.22	0	5,5,59	0.41	0
7	POV	A	906	-	9,9,51	0.29	0	8,8,59	0.27	0
7	POV	C	904	-	5,5,51	0.30	0	4,4,59	0.29	0
10	XVD	H	501	-	23,24,24	1.21	2 (8%)	27,36,36	0.91	1 (3%)
6	ZK1	C	901	-	29,29,29	3.44	10 (34%)	45,45,45	1.44	9 (20%)
7	POV	A	909	-	4,4,51	0.33	0	3,3,59	0.27	0
7	POV	B	904	-	7,7,51	0.27	0	6,6,59	0.31	0
11	OCT	G	502	-	7,7,7	0.29	0	6,6,6	0.25	0
7	POV	A	904	-	11,11,51	0.27	0	10,10,59	0.48	0
7	POV	A	903	-	10,10,51	0.25	0	9,9,59	0.35	0
7	POV	C	907	-	7,7,51	0.28	0	6,6,59	0.36	0
7	POV	D	902	-	40,40,51	1.18	3 (7%)	46,48,59	1.13	3 (6%)
7	POV	G	504	-	8,8,51	0.27	0	7,7,59	0.36	0
9	D10	C	902	-	9,9,9	0.29	0	8,8,8	0.28	0
7	POV	C	908	-	11,11,51	0.27	0	10,10,59	0.48	0
7	POV	H	504	-	8,8,51	0.27	0	7,7,59	0.30	0
7	POV	D	903	-	7,7,51	0.28	0	6,6,59	0.31	0
6	ZK1	B	901	-	29,29,29	3.43	10 (34%)	45,45,45	1.73	12 (26%)
7	POV	A	908	-	7,7,51	0.28	0	6,6,59	0.30	0
7	POV	A	905	-	6,6,51	0.25	0	5,5,59	0.34	0
8	C14	B	903	-	13,13,13	0.27	0	12,12,12	0.34	0
7	POV	B	906	-	10,10,51	0.27	0	9,9,59	0.29	0
7	POV	A	902	-	5,5,51	0.30	0	4,4,59	0.29	0
7	POV	B	907	-	7,7,51	0.28	0	6,6,59	0.36	0
7	POV	D	907	-	7,7,51	0.28	0	6,6,59	0.35	0
7	POV	E	201	-	7,7,51	0.29	0	6,6,59	0.33	0
12	D12	G	503	-	11,11,11	0.25	0	10,10,10	0.39	0
7	POV	D	905	-	8,8,51	0.30	0	7,7,59	0.28	0
10	XVD	G	501	-	23,24,24	1.21	2 (8%)	27,36,36	0.91	1 (3%)
7	POV	C	909	-	6,6,51	0.25	0	5,5,59	0.34	0
7	POV	D	904	-	10,10,51	0.27	0	9,9,59	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	D12	H	503	-	11,11,11	0.24	0	10,10,10	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POV	C	905	-	-	3/5/5/55	-
7	POV	C	903	-	-	1/7/7/55	-
7	POV	C	906	-	-	1/3/3/55	-
11	OCT	H	502	-	-	3/5/5/5	-
6	ZK1	D	901	-	-	10/13/23/23	0/3/3/3
7	POV	B	902	-	-	22/44/44/55	-
7	POV	B	905	-	-	3/5/5/55	-
7	POV	F	201	-	-	1/5/5/55	-
6	ZK1	A	901	-	-	5/13/23/23	0/3/3/3
7	POV	A	907	-	-	0/5/5/55	-
7	POV	D	906	-	-	0/4/4/55	-
7	POV	A	906	-	-	1/7/7/55	-
7	POV	C	904	-	-	0/3/3/55	-
10	XVD	H	501	-	-	3/9/9/9	0/3/3/3
6	ZK1	C	901	-	-	5/13/23/23	0/3/3/3
7	POV	A	909	-	-	1/2/2/55	-
7	POV	B	904	-	-	2/5/5/55	-
11	OCT	G	502	-	-	3/5/5/5	-
7	POV	A	904	-	-	0/9/9/55	-
7	POV	A	903	-	-	2/8/8/55	-
7	POV	C	907	-	-	0/5/5/55	-
7	POV	D	902	-	-	21/44/44/55	-
7	POV	G	504	-	-	0/6/6/55	-
9	D10	C	902	-	-	4/7/7/7	-
7	POV	C	908	-	-	0/9/9/55	-
7	POV	H	504	-	-	0/6/6/55	-
7	POV	D	903	-	-	2/5/5/55	-
6	ZK1	B	901	-	-	8/13/23/23	0/3/3/3
7	POV	A	908	-	-	2/5/5/55	-
7	POV	A	905	-	-	2/4/4/55	-
8	C14	B	903	-	-	2/11/11/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POV	B	906	-	-	5/8/8/55	-
7	POV	A	902	-	-	0/3/3/55	-
7	POV	B	907	-	-	2/5/5/55	-
7	POV	D	907	-	-	2/5/5/55	-
7	POV	E	201	-	-	2/5/5/55	-
12	D12	G	503	-	-	6/9/9/9	-
7	POV	D	905	-	-	0/6/6/55	-
10	XVD	G	501	-	-	3/9/9/9	0/3/3/3
7	POV	C	909	-	-	2/4/4/55	-
7	POV	D	904	-	-	5/8/8/55	-
12	D12	H	503	-	-	7/9/9/9	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	901	ZK1	CAU-CAT	-10.63	1.38	1.53
6	D	901	ZK1	CAU-CAT	-10.60	1.38	1.53
6	C	901	ZK1	CAU-CAT	-10.59	1.38	1.53
6	B	901	ZK1	CAU-CAT	-10.51	1.38	1.53
6	D	901	ZK1	OAA-CAT	8.95	1.40	1.23
6	C	901	ZK1	OAA-CAT	8.73	1.40	1.23
6	A	901	ZK1	OAA-CAT	8.72	1.40	1.23
6	B	901	ZK1	OAA-CAT	8.61	1.39	1.23
6	C	901	ZK1	OAB-CAU	8.41	1.40	1.23
6	A	901	ZK1	OAB-CAU	8.40	1.40	1.23
6	D	901	ZK1	OAB-CAU	8.32	1.40	1.23
6	B	901	ZK1	OAB-CAU	8.31	1.40	1.23
6	D	901	ZK1	CAU-NAY	-3.89	1.31	1.38
6	B	901	ZK1	CAU-NAY	-3.71	1.31	1.38
6	B	901	ZK1	CAV-CAW	-3.60	1.36	1.40
6	D	901	ZK1	CAW-NAY	-3.55	1.35	1.41
6	D	901	ZK1	CAV-CAW	-3.49	1.36	1.40
6	B	901	ZK1	CAW-NAY	-3.43	1.35	1.41
6	C	901	ZK1	CAU-NAY	-3.42	1.32	1.38
6	A	901	ZK1	CAU-NAY	-3.40	1.32	1.38
6	B	901	ZK1	CAR-NAX	3.38	1.48	1.41
6	D	901	ZK1	CAR-NAX	3.36	1.48	1.41
6	C	901	ZK1	CAV-CAW	-3.31	1.36	1.40
6	A	901	ZK1	CAV-CAW	-3.30	1.36	1.40
6	C	901	ZK1	CAR-NAX	3.29	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	901	ZK1	CAR-NAX	3.27	1.48	1.41
6	B	901	ZK1	CAV-NAP	-3.25	1.34	1.39
6	A	901	ZK1	CAV-NAP	-3.18	1.34	1.39
6	C	901	ZK1	CAV-NAP	-3.05	1.34	1.39
6	C	901	ZK1	CAW-NAY	-3.02	1.35	1.41
6	A	901	ZK1	CAW-NAY	-2.98	1.36	1.41
6	D	901	ZK1	CAV-NAP	-2.84	1.35	1.39
6	A	901	ZK1	CAT-NAP	-2.75	1.32	1.35
7	D	902	POV	O31-C31	2.74	1.41	1.33
7	B	902	POV	O31-C31	2.74	1.41	1.33
7	D	902	POV	O21-C2	-2.73	1.40	1.46
7	B	902	POV	O21-C2	-2.73	1.40	1.46
6	C	901	ZK1	CAT-NAP	-2.70	1.32	1.35
7	B	902	POV	O21-C21	2.54	1.41	1.34
7	D	902	POV	O21-C21	2.53	1.41	1.34
10	G	501	XVD	C13-N2	-2.41	1.31	1.34
10	H	501	XVD	C13-N2	-2.41	1.31	1.34
6	B	901	ZK1	CAT-NAP	-2.33	1.32	1.35
6	D	901	ZK1	PBA-CAO	2.29	1.86	1.81
6	B	901	ZK1	PBA-CAO	2.28	1.86	1.81
6	A	901	ZK1	PBA-CAO	2.06	1.86	1.81
6	C	901	ZK1	PBA-CAO	2.06	1.86	1.81
10	H	501	XVD	C1-CL1	2.02	1.78	1.73
10	G	501	XVD	C1-CL1	2.01	1.78	1.73

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	901	ZK1	CAI-CAR-NAX	-4.35	116.25	122.59
6	B	901	ZK1	CAI-CAR-NAX	-4.16	116.53	122.59
6	D	901	ZK1	CAN-NAX-CAM	4.05	120.68	111.57
7	B	902	POV	C15-N-C14	4.03	119.56	108.98
7	D	902	POV	C15-N-C14	3.96	119.39	108.98
6	B	901	ZK1	CAN-NAX-CAM	3.80	120.11	111.57
7	B	902	POV	O21-C21-C22	3.79	119.67	111.48
7	D	902	POV	O21-C21-C22	3.78	119.66	111.48
6	D	901	ZK1	CAS-CAR-NAX	3.70	124.16	119.92
6	A	901	ZK1	CAN-NAX-CAM	3.57	119.60	111.57
6	C	901	ZK1	CAN-NAX-CAM	3.54	119.52	111.57
6	B	901	ZK1	CAO-NAY-CAU	3.51	120.12	116.55
6	B	901	ZK1	CAS-CAR-NAX	3.40	123.82	119.92
6	B	901	ZK1	CAV-NAP-CAT	-3.31	120.18	124.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	901	ZK1	CAV-NAP-CAT	-3.26	120.26	124.82
6	D	901	ZK1	CAO-NAY-CAU	3.23	119.84	116.55
6	B	901	ZK1	CAU-CAT-NAP	3.00	120.53	117.46
6	D	901	ZK1	CAV-CAW-NAY	2.88	121.27	118.01
6	C	901	ZK1	CAV-NAP-CAT	-2.85	120.83	124.82
7	D	902	POV	O31-C31-C32	2.78	120.31	111.83
7	B	902	POV	O31-C31-C32	2.77	120.29	111.83
6	B	901	ZK1	CAV-CAW-NAY	2.77	121.15	118.01
6	A	901	ZK1	CAI-CAR-NAX	-2.72	118.63	122.59
6	B	901	ZK1	CAW-NAY-CAU	-2.70	119.52	122.84
6	C	901	ZK1	CAT-CAU-NAY	2.65	120.29	117.41
6	D	901	ZK1	CAL-CAN-NAX	2.63	114.91	109.93
6	C	901	ZK1	CAW-NAY-CAU	-2.63	119.60	122.84
6	D	901	ZK1	CAW-NAY-CAU	-2.62	119.62	122.84
6	A	901	ZK1	CAV-NAP-CAT	-2.58	121.21	124.82
6	D	901	ZK1	CAU-CAT-NAP	2.55	120.06	117.46
6	A	901	ZK1	CAT-CAU-NAY	2.55	120.18	117.41
6	D	901	ZK1	CAT-CAU-NAY	2.53	120.16	117.41
6	A	901	ZK1	CAW-NAY-CAU	-2.52	119.74	122.84
6	D	901	ZK1	FAG-CAZ-CAS	-2.46	108.29	112.65
6	D	901	ZK1	CAI-CAW-NAY	-2.44	118.58	121.85
6	C	901	ZK1	CAI-CAR-NAX	-2.42	119.07	122.59
10	H	501	XVD	C5-C6-C1	2.35	120.40	117.74
6	B	901	ZK1	FAF-CAZ-CAS	-2.33	108.51	112.65
10	G	501	XVD	C5-C6-C1	2.33	120.38	117.74
6	C	901	ZK1	CAU-CAT-NAP	2.31	119.82	117.46
6	C	901	ZK1	FAG-CAZ-CAS	-2.28	108.60	112.65
6	C	901	ZK1	FAF-CAZ-CAS	-2.25	108.66	112.65
6	A	901	ZK1	FAF-CAZ-CAS	-2.21	108.72	112.65
6	A	901	ZK1	FAG-CAZ-CAS	-2.19	108.77	112.65
6	A	901	ZK1	CAU-CAT-NAP	2.16	119.66	117.46
6	C	901	ZK1	CAO-NAY-CAU	2.15	118.73	116.55
6	B	901	ZK1	CAT-CAU-NAY	2.12	119.72	117.41
6	B	901	ZK1	CAI-CAW-NAY	-2.09	119.04	121.85
6	B	901	ZK1	CAL-CAN-NAX	2.02	113.76	109.93

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	901	ZK1	NAY-CAO-PBA-OAD
6	D	901	ZK1	NAY-CAO-PBA-OAE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	902	POV	O12-C11-C12-N
7	D	902	POV	O12-C11-C12-N
7	B	902	POV	O32-C31-O31-C3
7	D	902	POV	O32-C31-O31-C3
7	B	902	POV	C32-C31-O31-C3
7	D	902	POV	C32-C31-O31-C3
11	G	502	OCT	C3-C4-C5-C6
11	H	502	OCT	C3-C4-C5-C6
7	B	902	POV	C31-C32-C33-C34
7	D	902	POV	C31-C32-C33-C34
7	D	902	POV	C32-C33-C34-C35
7	B	902	POV	C32-C33-C34-C35
9	C	902	D10	C5-C6-C7-C8
7	B	902	POV	C37-C38-C39-C310
7	B	906	POV	C33-C34-C35-C36
7	D	902	POV	C37-C38-C39-C310
7	D	904	POV	C33-C34-C35-C36
12	G	503	D12	C5-C6-C7-C8
7	B	902	POV	C22-C21-O21-C2
7	D	902	POV	C22-C21-O21-C2
7	B	902	POV	O22-C21-O21-C2
7	D	902	POV	O22-C21-O21-C2
7	B	902	POV	C34-C35-C36-C37
12	H	503	D12	C5-C6-C7-C8
7	D	902	POV	C34-C35-C36-C37
7	A	908	POV	C23-C24-C25-C26
6	A	901	ZK1	CAI-CAR-NAX-CAM
7	B	905	POV	C25-C26-C27-C28
6	D	901	ZK1	CAR-CAS-CAZ-FAG
12	H	503	D12	C4-C5-C6-C7
7	B	902	POV	C36-C37-C38-C39
7	B	906	POV	C311-C310-C39-C38
7	B	902	POV	C33-C34-C35-C36
7	D	902	POV	C33-C34-C35-C36
7	D	902	POV	C36-C37-C38-C39
7	E	201	POV	C22-C23-C24-C25
6	D	901	ZK1	CAR-CAS-CAZ-FAF
7	A	908	POV	C25-C26-C27-C28
6	D	901	ZK1	CAR-CAS-CAZ-FAH
7	D	904	POV	C311-C310-C39-C38
11	H	502	OCT	C5-C6-C7-C8
11	G	502	OCT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	G	503	D12	C4-C5-C6-C7
9	C	902	D10	C7-C8-C9-C10
9	C	902	D10	C1-C2-C3-C4
7	D	904	POV	C36-C37-C38-C39
7	B	902	POV	O11-C1-C2-O21
7	D	902	POV	O11-C1-C2-O21
12	H	503	D12	C3-C4-C5-C6
6	C	901	ZK1	CAI-CAR-NAX-CAM
7	F	201	POV	C22-C23-C24-C25
7	D	904	POV	C37-C38-C39-C310
9	C	902	D10	C2-C3-C4-C5
7	D	902	POV	C25-C26-C27-C28
6	B	901	ZK1	CAR-CAS-CAZ-FAH
6	A	901	ZK1	NAY-CAO-PBA-OAD
6	A	901	ZK1	NAY-CAO-PBA-OAE
6	B	901	ZK1	NAY-CAO-PBA-OAD
6	B	901	ZK1	NAY-CAO-PBA-OAE
6	C	901	ZK1	NAY-CAO-PBA-OAD
6	C	901	ZK1	NAY-CAO-PBA-OAE
6	D	901	ZK1	NAY-CAO-PBA-OAC
7	B	902	POV	C25-C26-C27-C28
7	D	904	POV	C35-C36-C37-C38
7	B	907	POV	C25-C26-C27-C28
7	B	906	POV	C35-C36-C37-C38
6	B	901	ZK1	CAI-CAR-NAX-CAM
7	B	906	POV	C37-C38-C39-C310
10	G	501	XVD	F2-C14-O2-C5
10	H	501	XVD	F2-C14-O2-C5
7	B	906	POV	C36-C37-C38-C39
7	D	902	POV	C24-C25-C26-C27
7	D	902	POV	C35-C36-C37-C38
7	B	902	POV	C24-C25-C26-C27
7	B	902	POV	C35-C36-C37-C38
12	G	503	D12	C1-C2-C3-C4
6	D	901	ZK1	CAI-CAR-NAX-CAM
6	B	901	ZK1	CAR-CAS-CAZ-FAF
7	B	902	POV	O11-C1-C2-C3
7	D	902	POV	O11-C1-C2-C3
7	C	905	POV	C23-C24-C25-C26
12	H	503	D12	C9-C10-C11-C12
12	G	503	D12	C3-C4-C5-C6
7	C	909	POV	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	905	POV	C24-C25-C26-C27
12	G	503	D12	C9-C10-C11-C12
7	B	902	POV	C22-C23-C24-C25
6	B	901	ZK1	CAR-CAS-CAZ-FAG
7	A	909	POV	C21-C22-C23-C24
7	D	902	POV	C22-C23-C24-C25
11	G	502	OCT	C2-C3-C4-C5
11	H	502	OCT	C2-C3-C4-C5
7	A	903	POV	C34-C35-C36-C37
6	A	901	ZK1	CAS-CAR-NAX-CAM
7	C	905	POV	C22-C23-C24-C25
7	C	909	POV	C22-C23-C24-C25
7	A	905	POV	C23-C24-C25-C26
7	D	907	POV	C24-C25-C26-C27
8	B	903	C14	C05-C06-C07-C08
7	C	905	POV	C25-C26-C27-C28
7	B	902	POV	O21-C2-C3-O31
7	D	902	POV	O21-C2-C3-O31
7	B	902	POV	C11-C12-N-C15
7	B	904	POV	C21-C22-C23-C24
7	B	902	POV	C311-C310-C39-C38
6	D	901	ZK1	CAJ-CAS-CAZ-FAF
7	D	903	POV	C25-C26-C27-C28
7	A	906	POV	C33-C34-C35-C36
6	A	901	ZK1	NAY-CAO-PBA-OAC
6	B	901	ZK1	NAY-CAO-PBA-OAC
6	C	901	ZK1	NAY-CAO-PBA-OAC
7	A	903	POV	C37-C38-C39-C310
7	B	905	POV	C24-C25-C26-C27
8	B	903	C14	C03-C04-C05-C06
7	D	907	POV	C21-C22-C23-C24
7	D	902	POV	C311-C310-C39-C38
6	D	901	ZK1	CAJ-CAS-CAZ-FAG
6	D	901	ZK1	CAJ-CAS-CAZ-FAH
6	C	901	ZK1	CAS-CAR-NAX-CAM
7	C	906	POV	C23-C24-C25-C26
12	H	503	D12	C1-C2-C3-C4
10	G	501	XVD	F3-C14-O2-C5
10	H	501	XVD	F3-C14-O2-C5
7	B	905	POV	C23-C24-C25-C26
12	G	503	D12	C7-C8-C9-C10
7	D	902	POV	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	H	503	D12	C7-C8-C9-C10
7	B	902	POV	O21-C21-C22-C23
12	H	503	D12	C6-C7-C8-C9
7	D	903	POV	C23-C24-C25-C26
6	B	901	ZK1	CAS-CAR-NAX-CAM
7	B	904	POV	C23-C24-C25-C26
7	E	201	POV	C21-C22-C23-C24
7	C	903	POV	C32-C33-C34-C35
10	G	501	XVD	F1-C14-O2-C5
10	H	501	XVD	F1-C14-O2-C5
7	B	907	POV	C22-C23-C24-C25
7	B	902	POV	O22-C21-C22-C23
7	D	902	POV	O22-C21-C22-C23

There are no ring outliers.

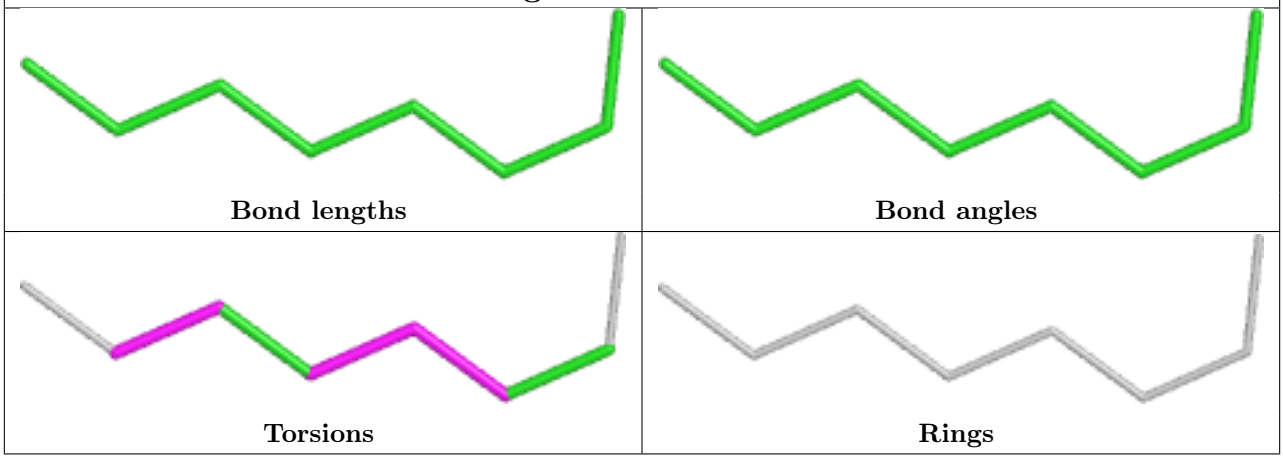
14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	905	POV	2	0
7	C	906	POV	4	0
6	D	901	ZK1	4	0
7	B	902	POV	2	0
6	A	901	ZK1	1	0
10	H	501	XVD	4	0
6	C	901	ZK1	3	0
7	A	909	POV	3	0
7	D	902	POV	1	0
9	C	902	D10	3	0
7	C	908	POV	5	0
7	A	908	POV	4	0
10	G	501	XVD	4	0
7	C	909	POV	6	0

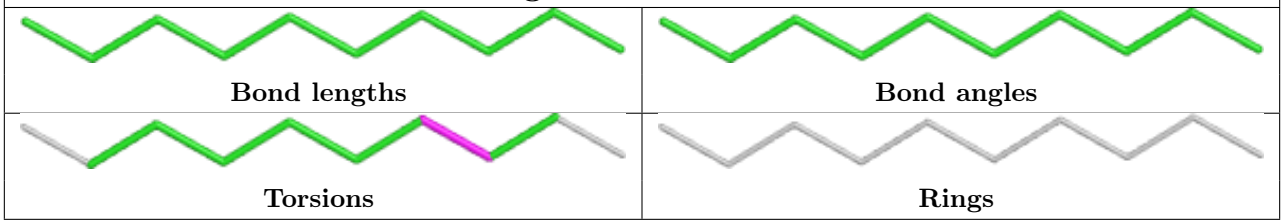
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

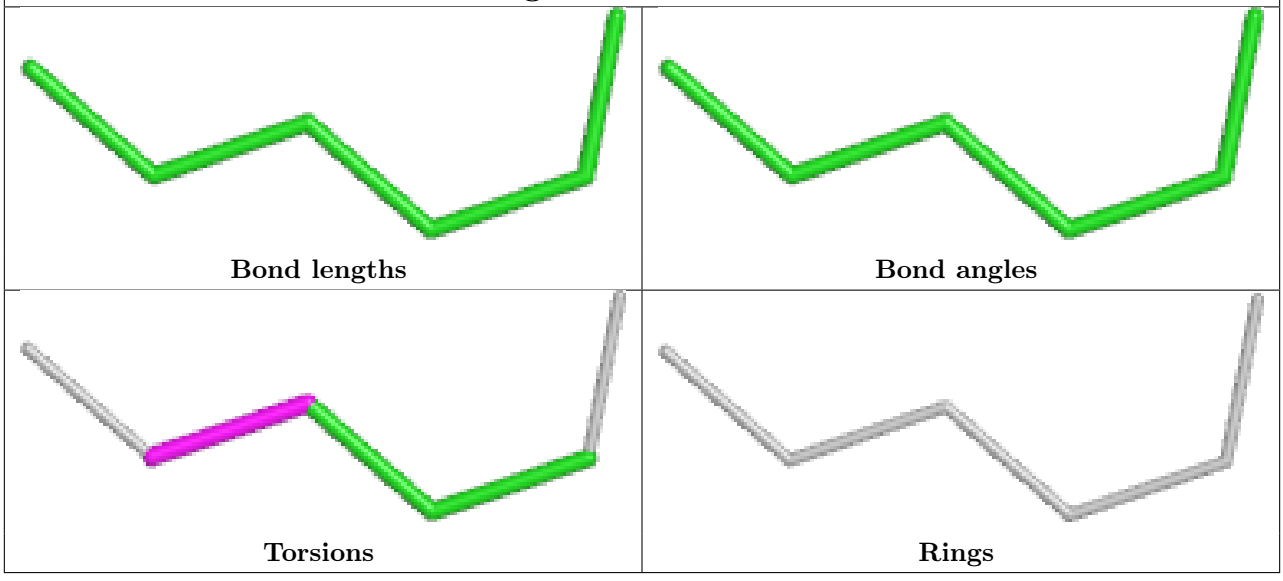
Ligand POV C 905



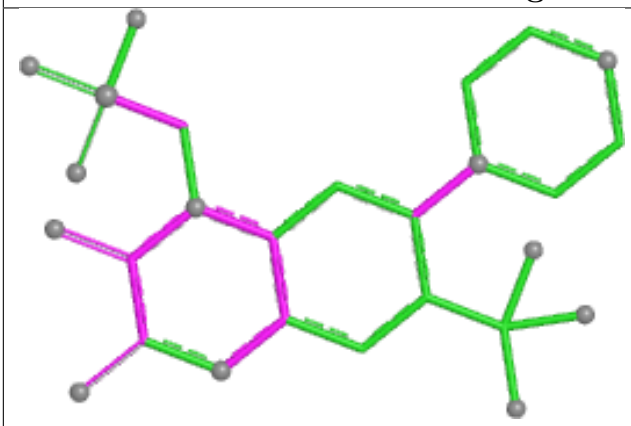
Ligand POV C 903



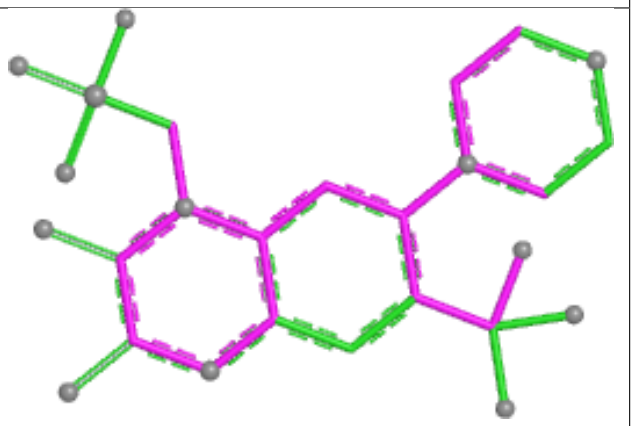
Ligand POV C 906



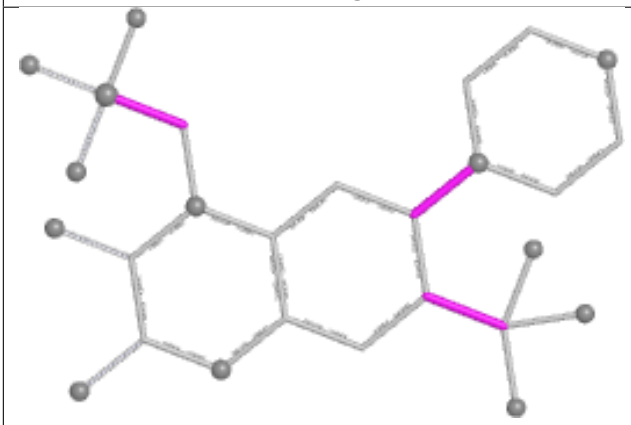
Ligand ZK1 D 901



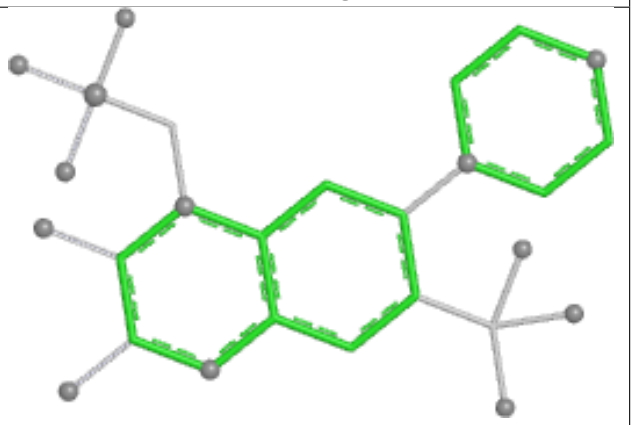
Bond lengths



Bond angles

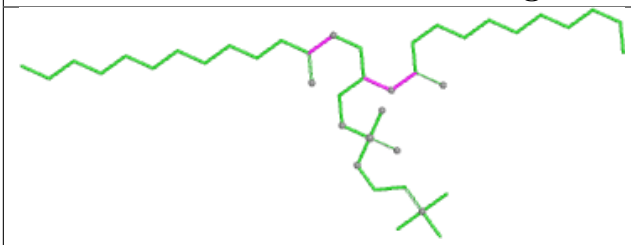


Torsions

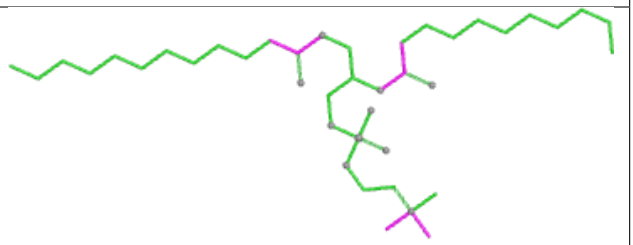


Rings

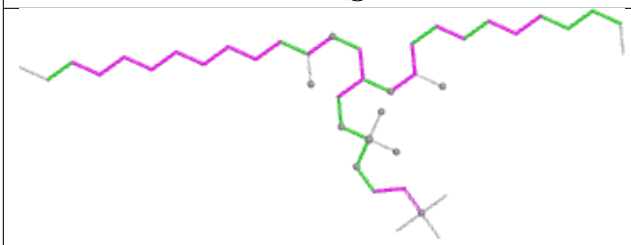
Ligand POV B 902



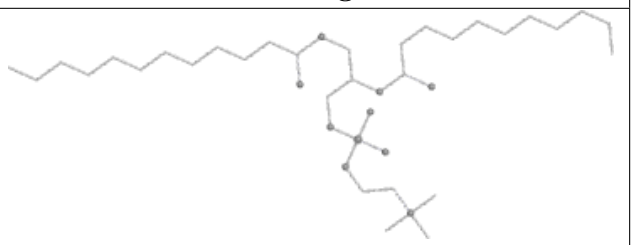
Bond lengths



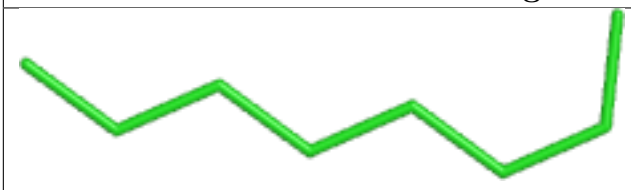
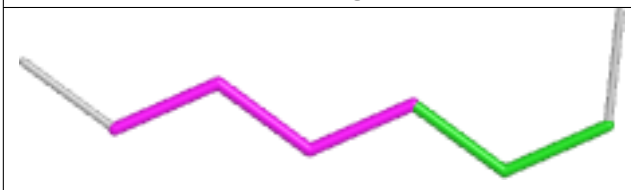
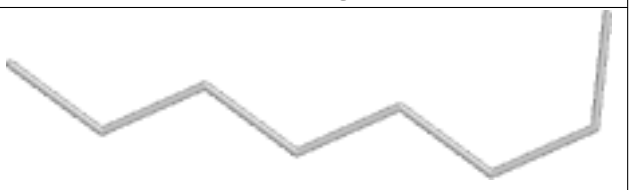
Bond angles

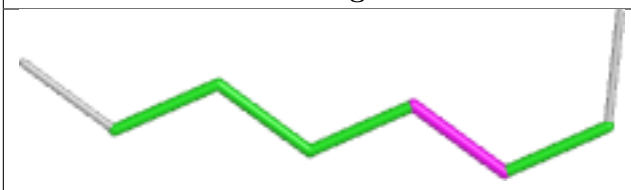
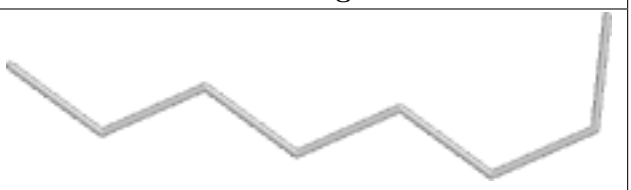


Torsions

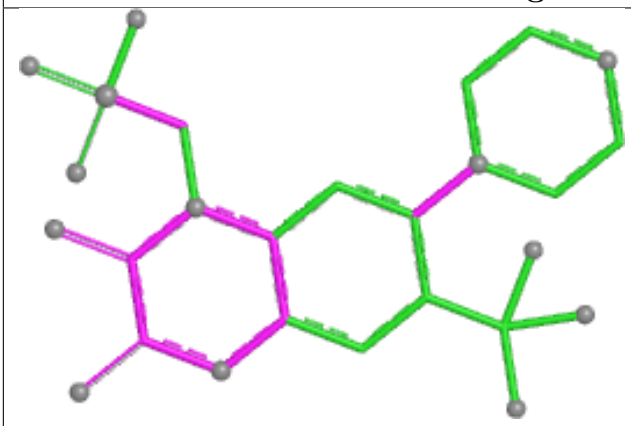


Rings

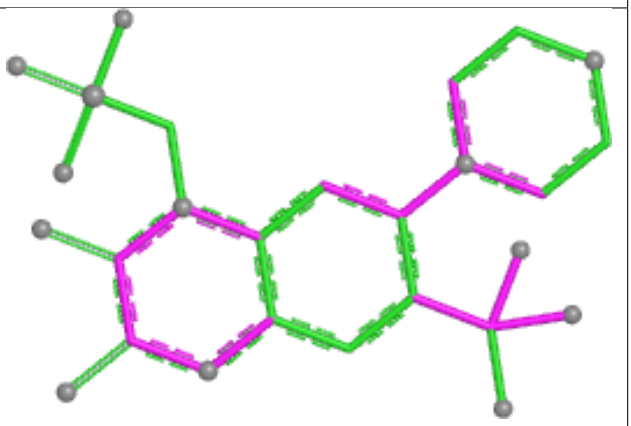
Ligand POV B 905	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV F 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

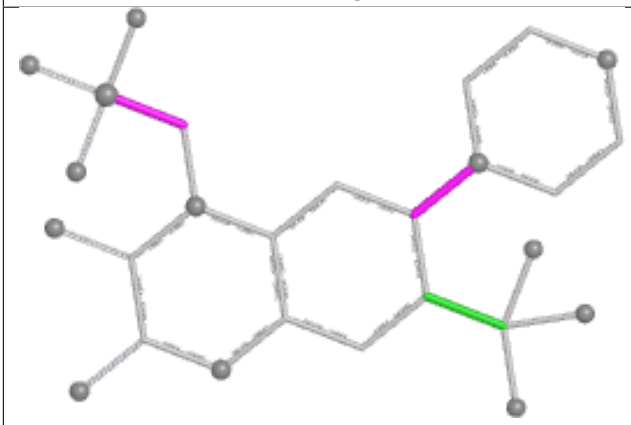
Ligand ZK1 A 901



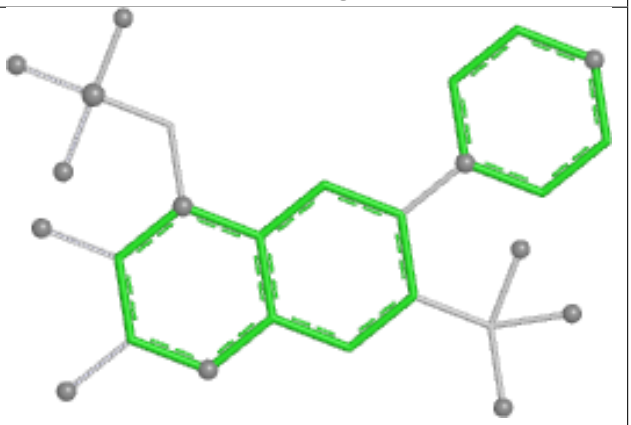
Bond lengths



Bond angles

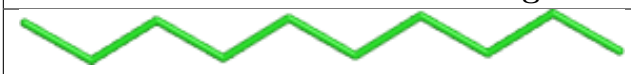


Torsions



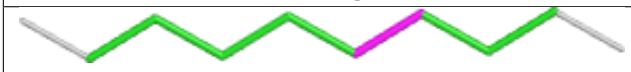
Rings

Ligand POV A 906



Bond lengths

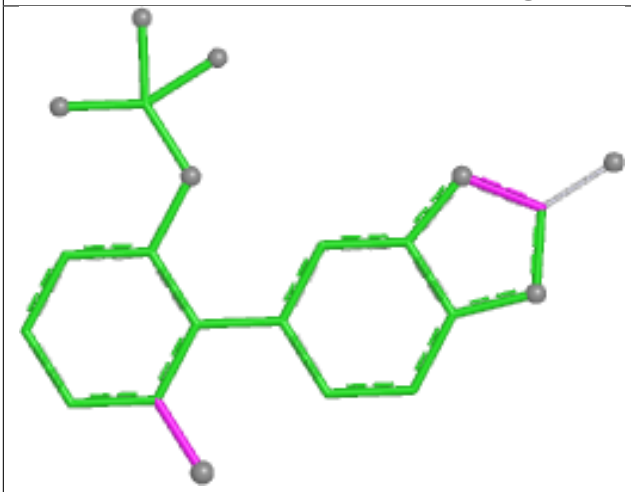
Bond angles



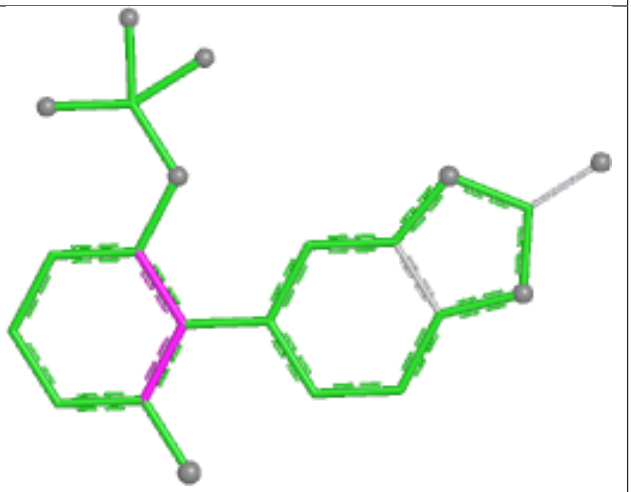
Torsions

Rings

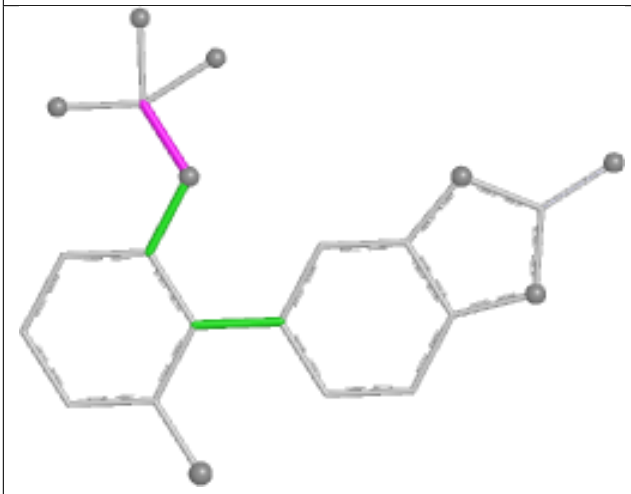
Ligand XVD H 501



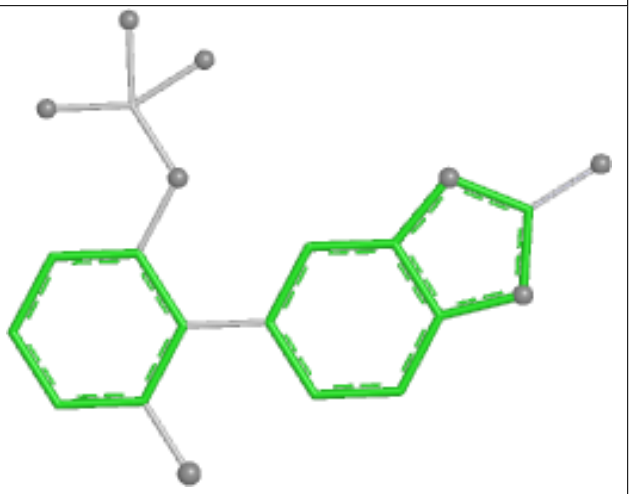
Bond lengths



Bond angles

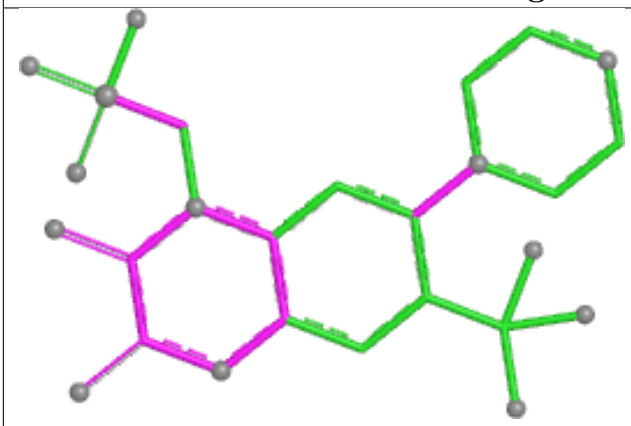


Torsions

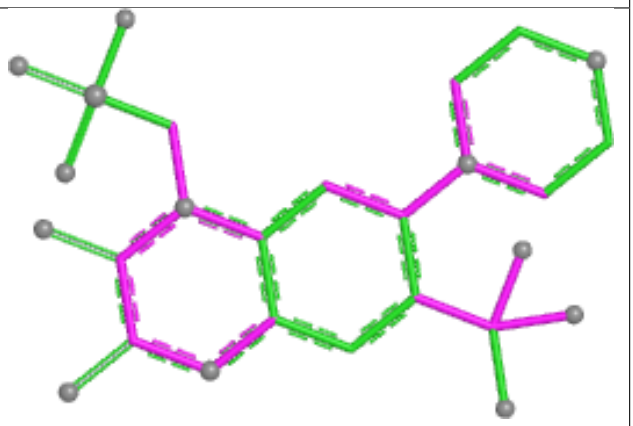


Rings

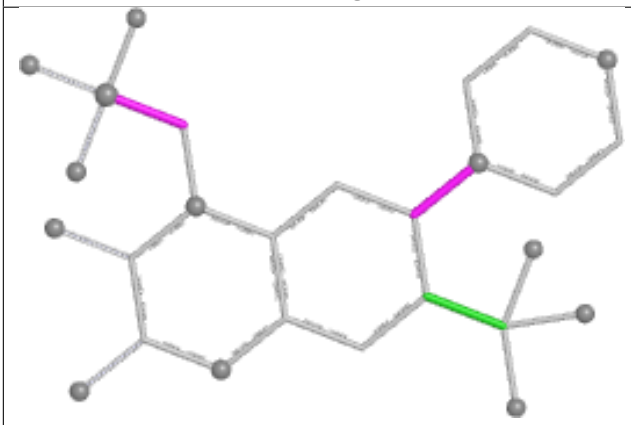
Ligand ZK1 C 901



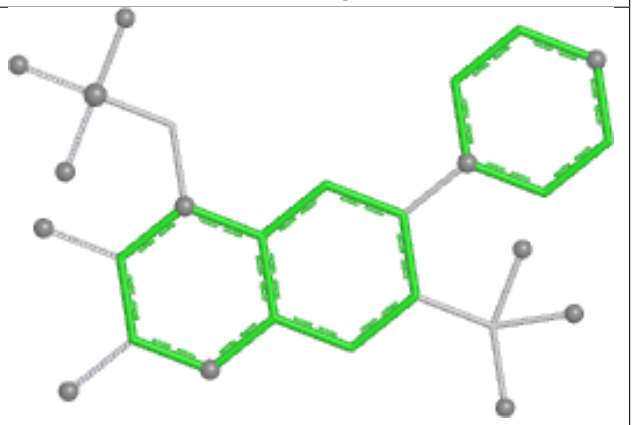
Bond lengths



Bond angles

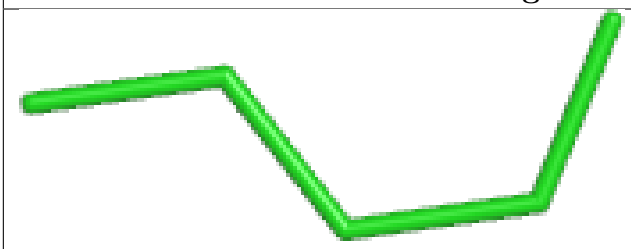


Torsions

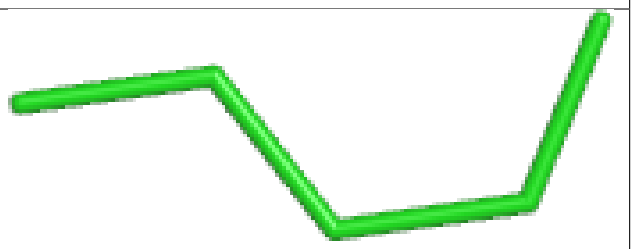


Rings

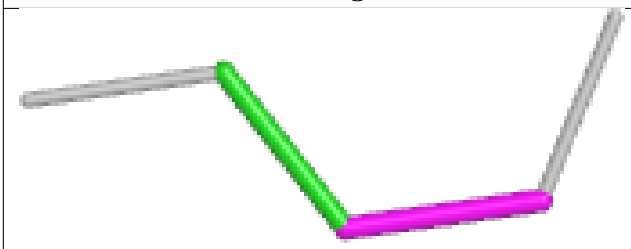
Ligand POV A 909



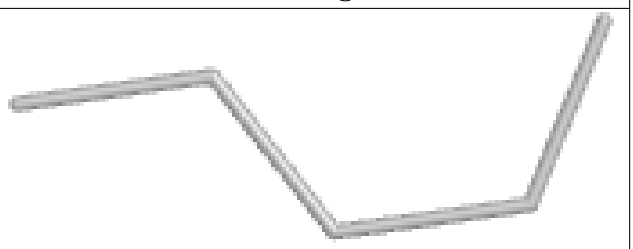
Bond lengths



Bond angles

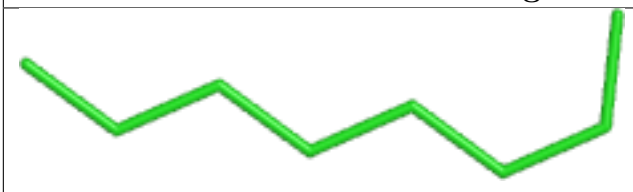


Torsions

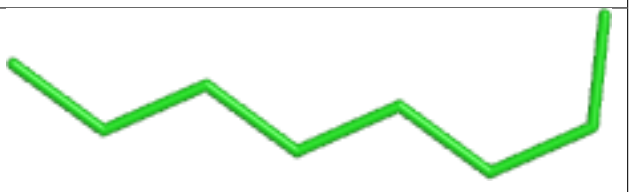


Rings

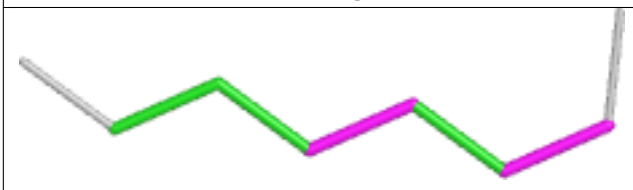
Ligand POV B 904



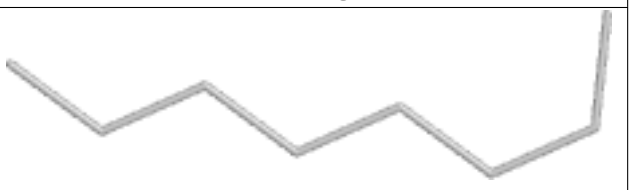
Bond lengths



Bond angles



Torsions



Rings

Ligand POV A 903

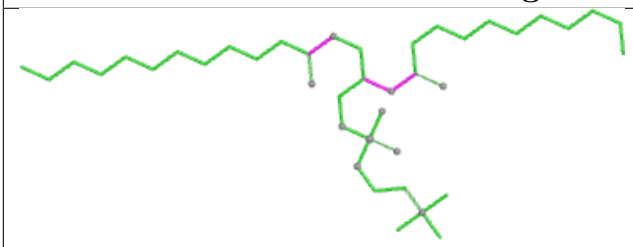
Bond lengths

Bond angles

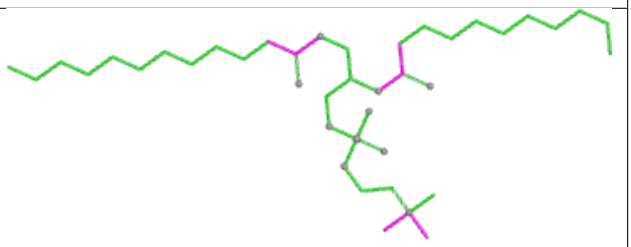
Torsions

Rings

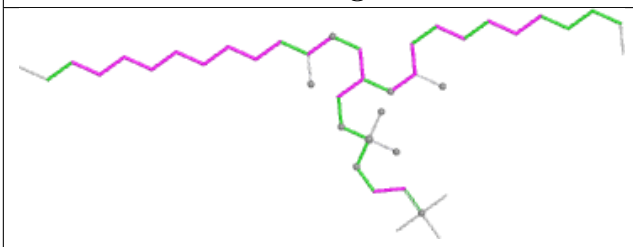
Ligand POV D 902



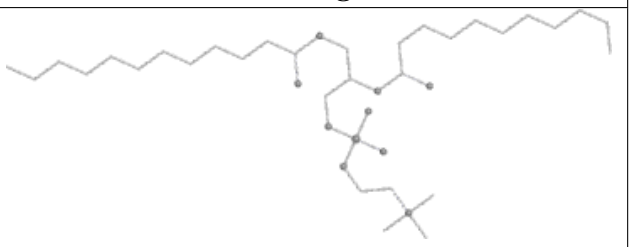
Bond lengths



Bond angles

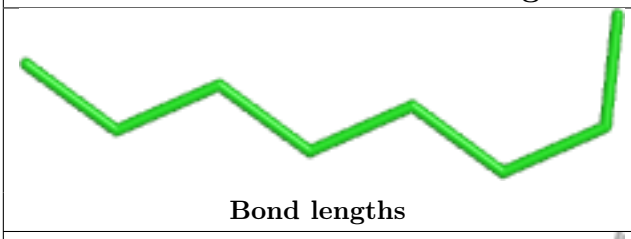


Torsions

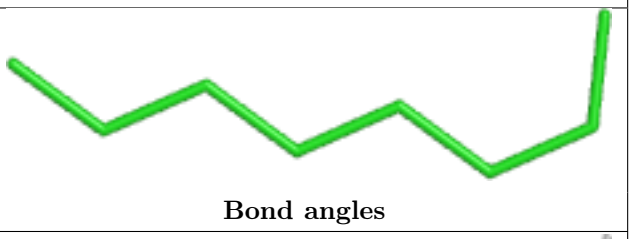


Rings

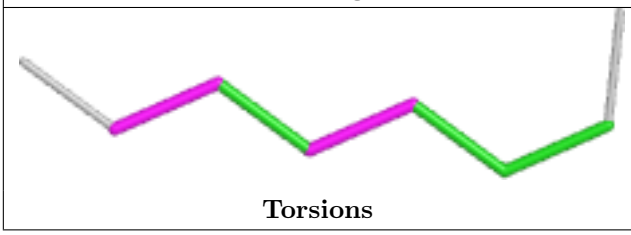
Ligand POV D 903



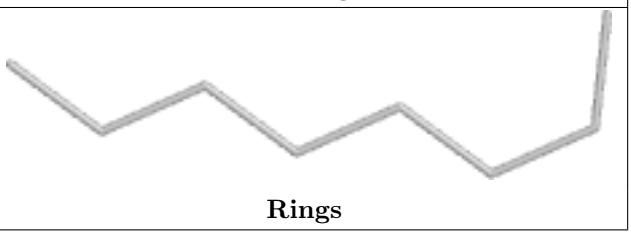
Bond lengths



Bond angles

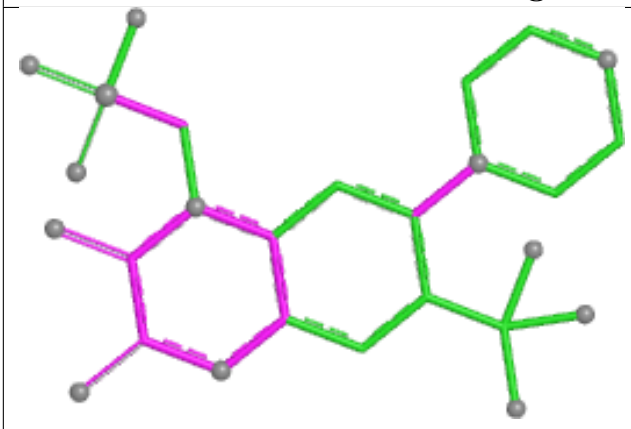


Torsions

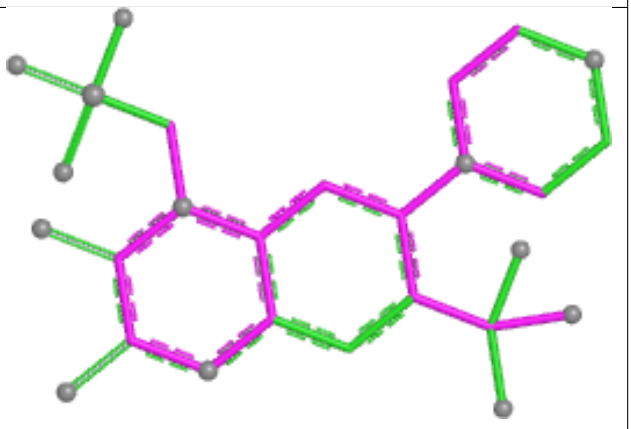


Rings

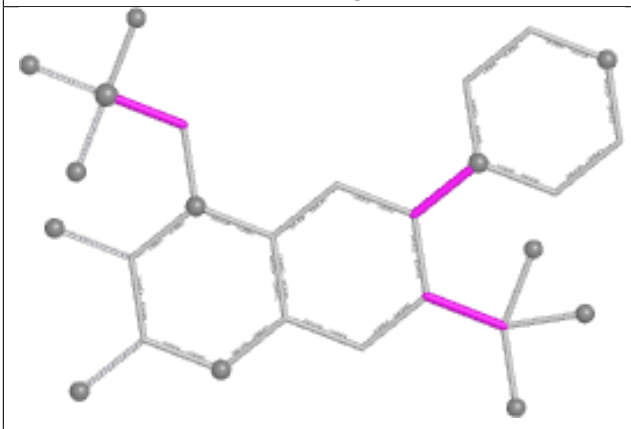
Ligand ZK1 B 901



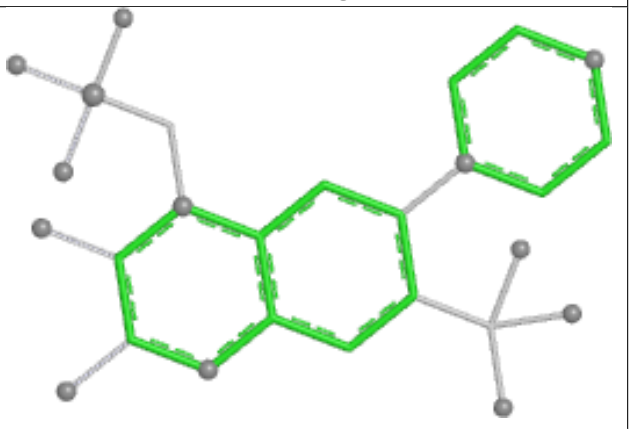
Bond lengths



Bond angles

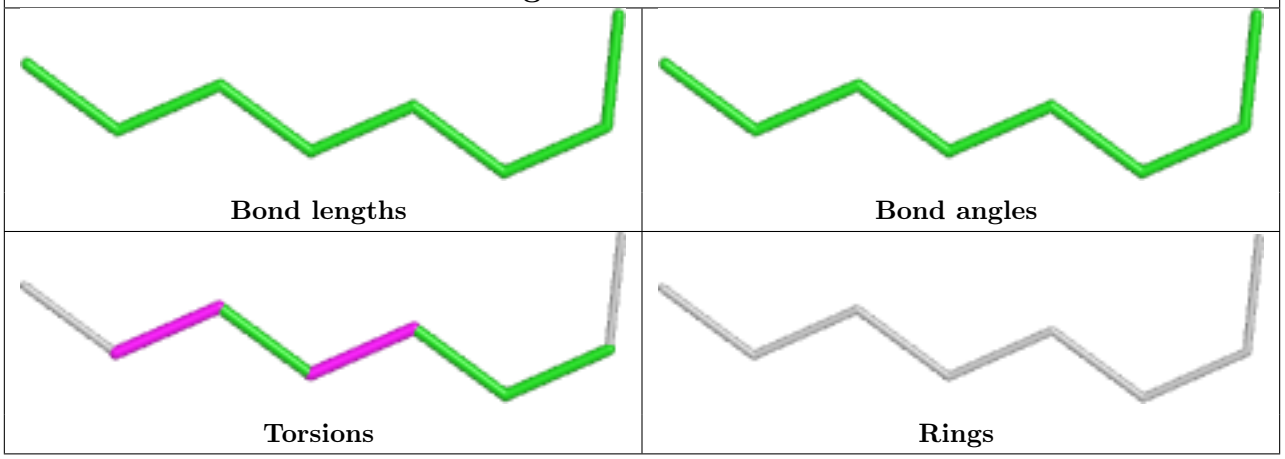


Torsions

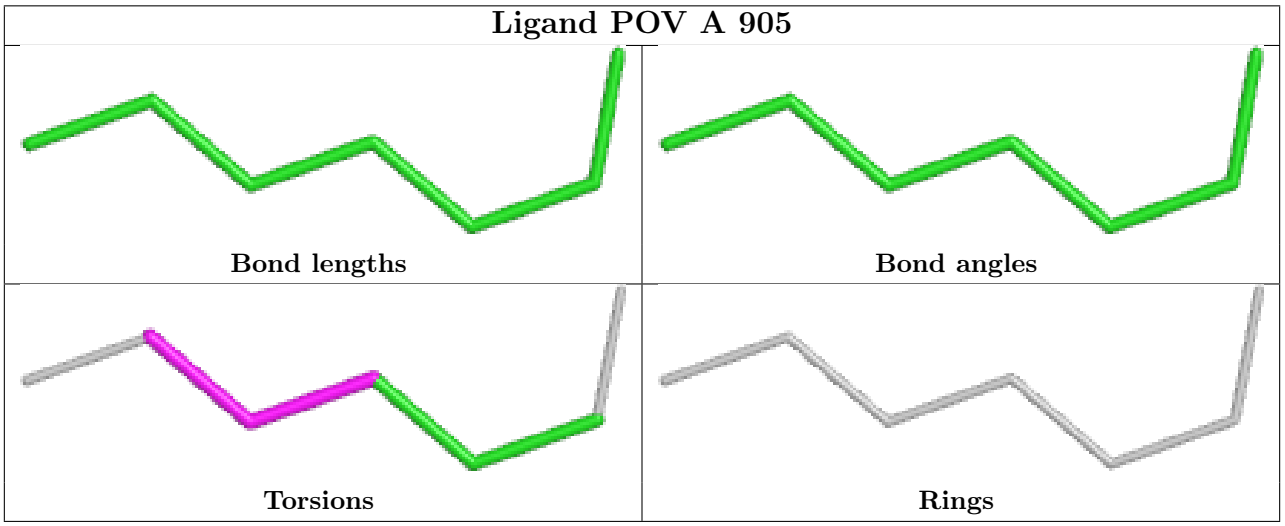


Rings

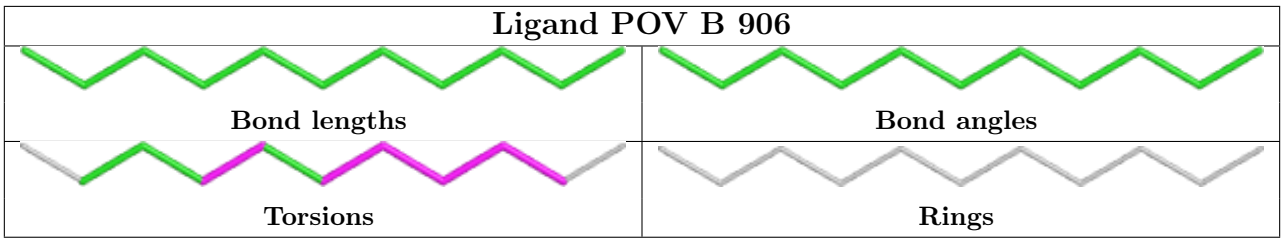
Ligand POV A 908



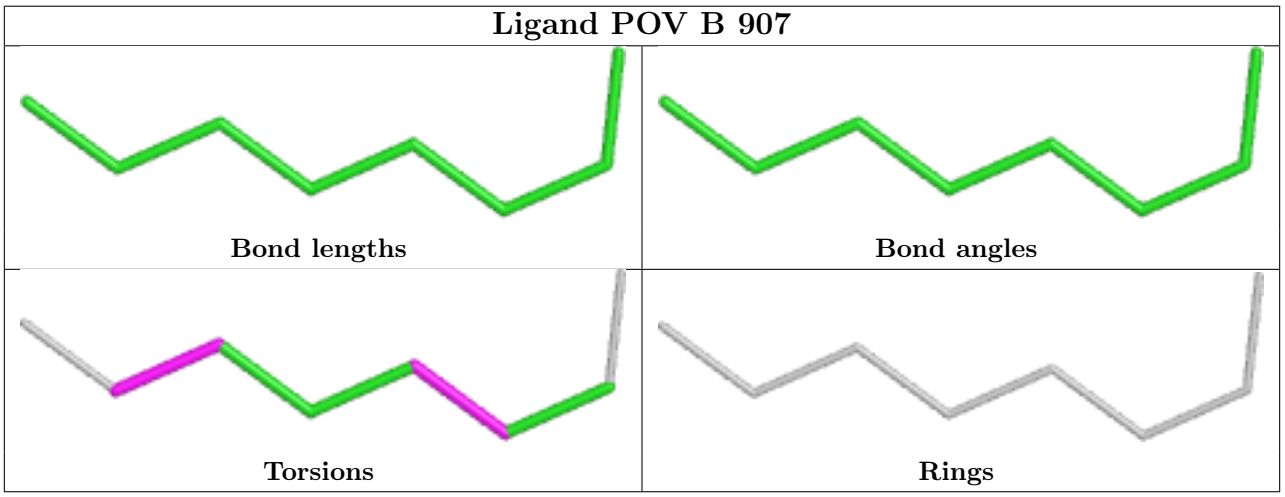
Ligand POV A 905



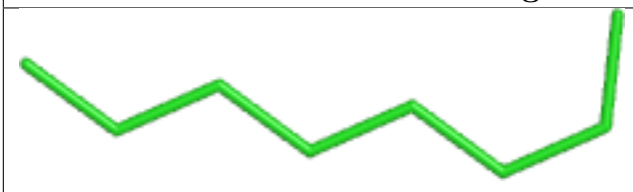
Ligand POV B 906



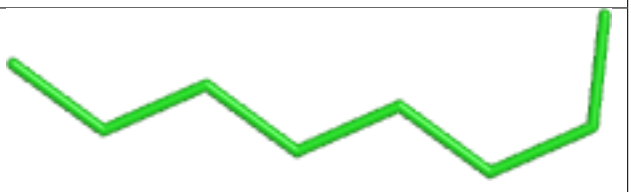
Ligand POV B 907



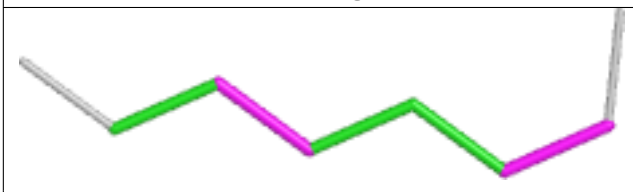
Ligand POV D 907



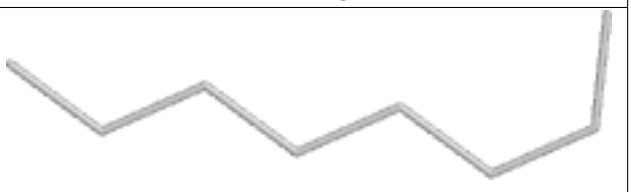
Bond lengths



Bond angles



Torsions

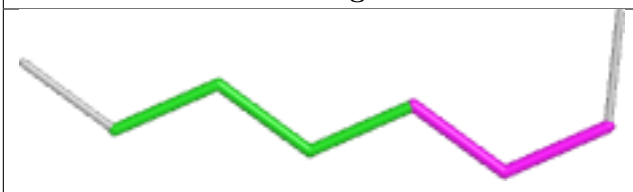


Rings

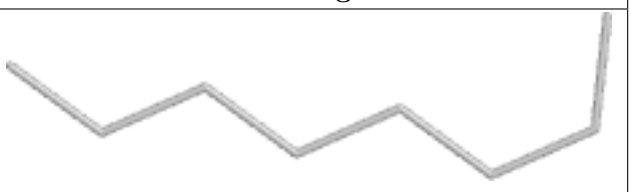
Ligand POV E 201

Bond lengths

Bond angles

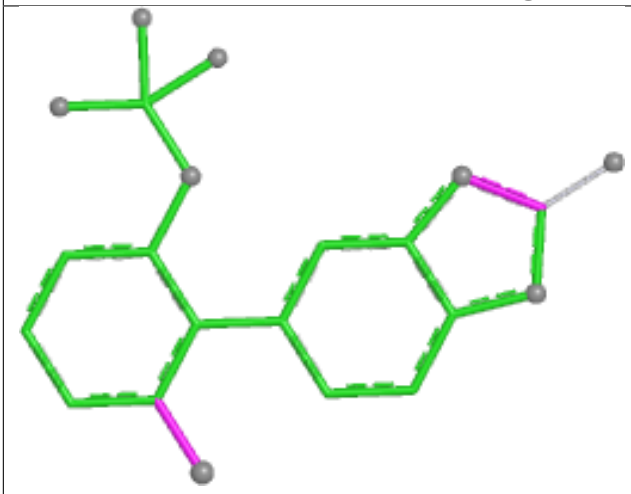


Torsions

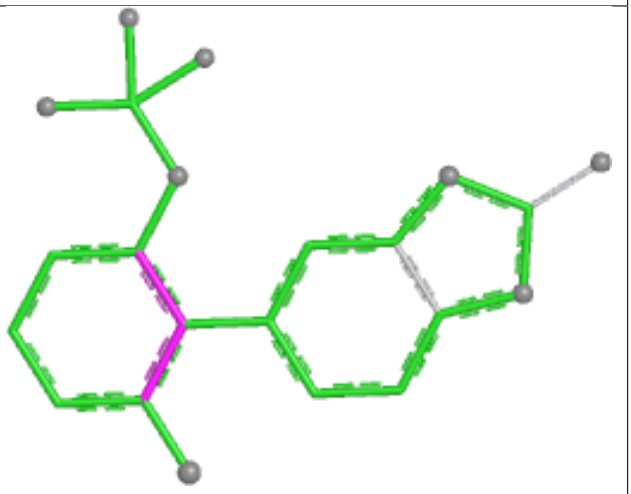


Rings

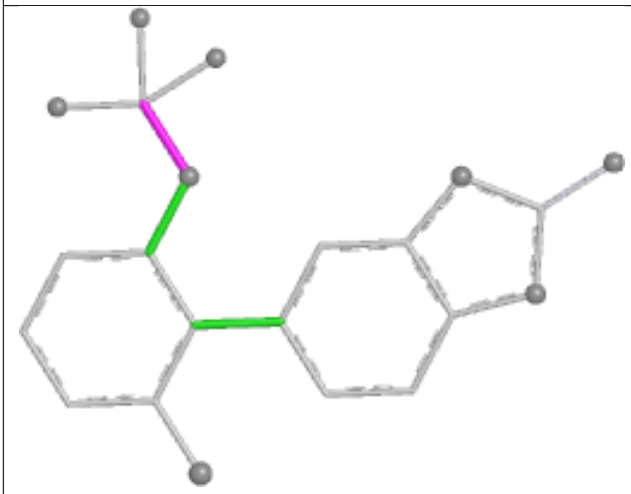
Ligand XVD G 501



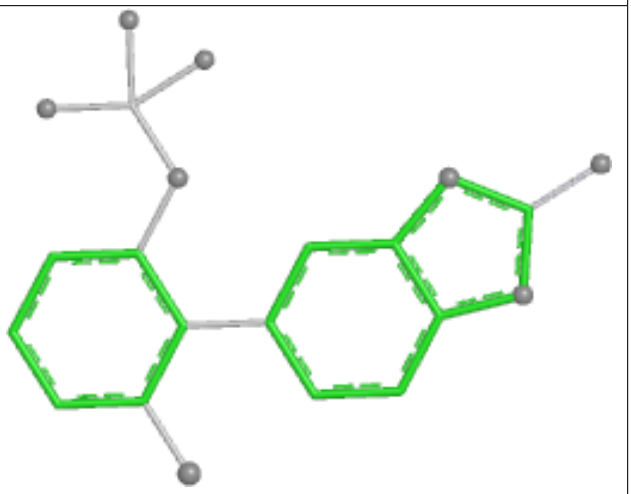
Bond lengths



Bond angles

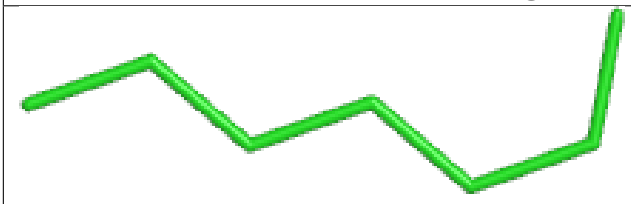


Torsions

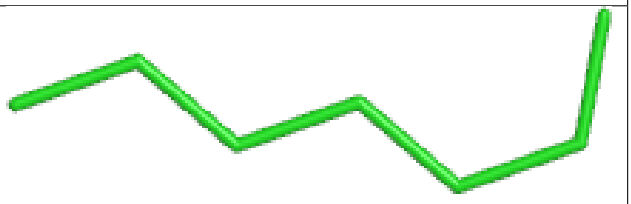


Rings

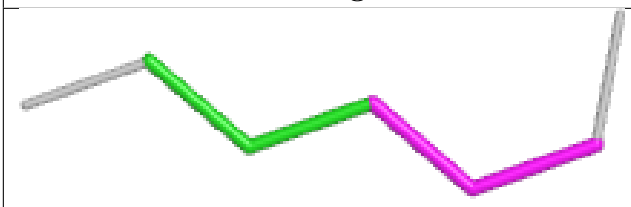
Ligand POV C 909



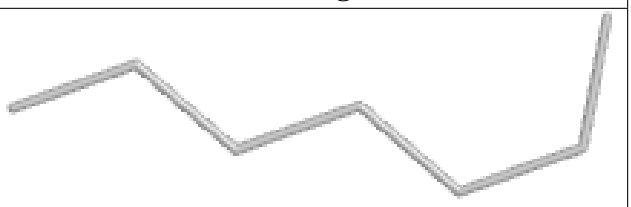
Bond lengths



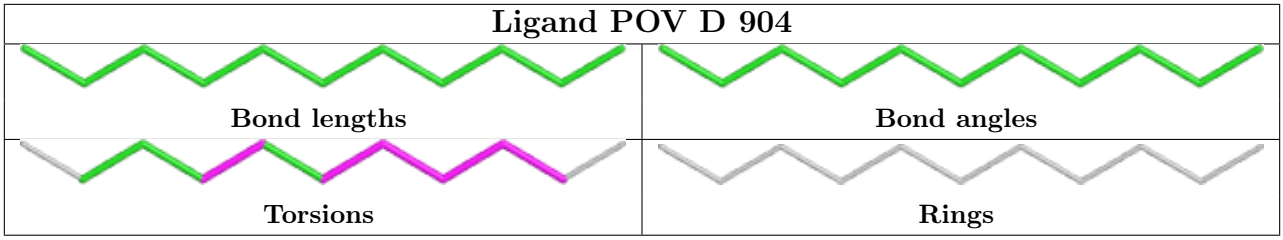
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

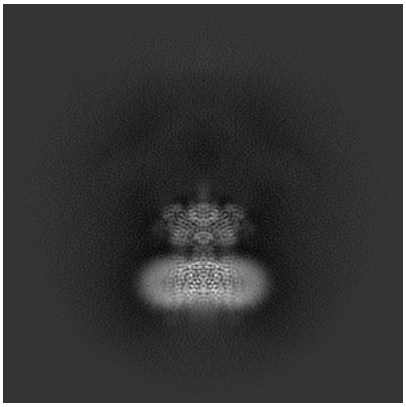
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23292. These allow visual inspection of the internal detail of the map and identification of artifacts.

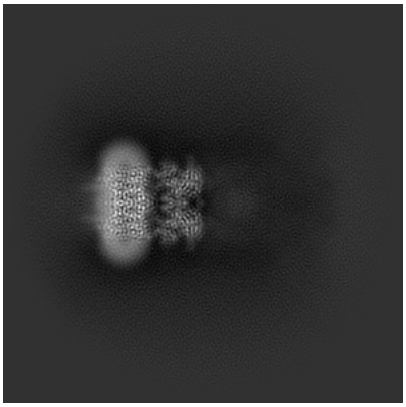
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

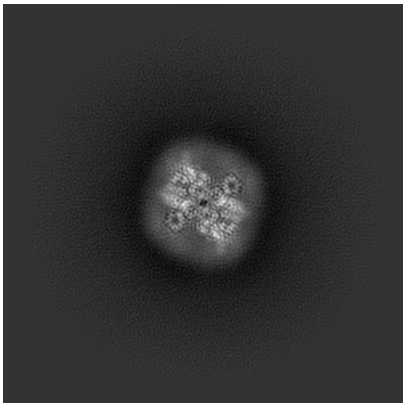
6.1.1 Primary map



X



Y

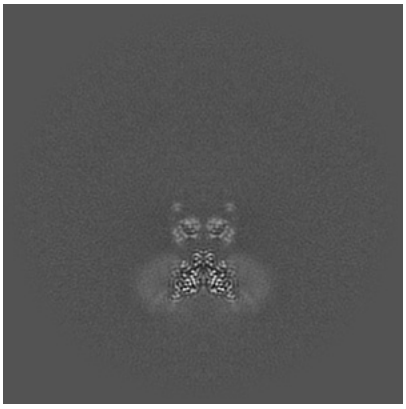


Z

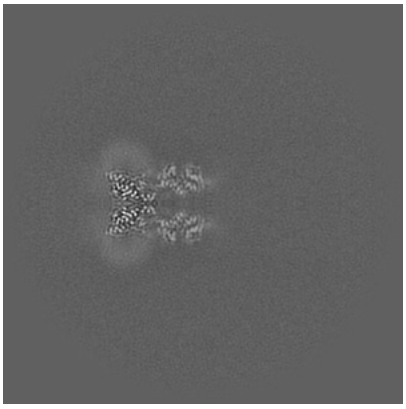
The images above show the map projected in three orthogonal directions.

6.2 Central slices

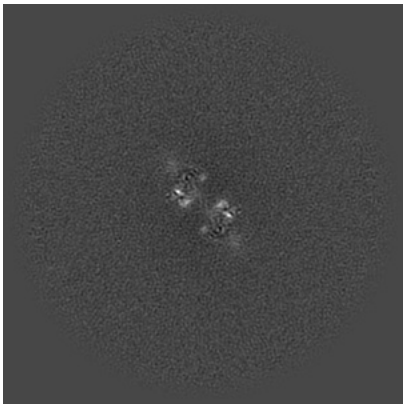
6.2.1 Primary map



X Index: 200



Y Index: 200

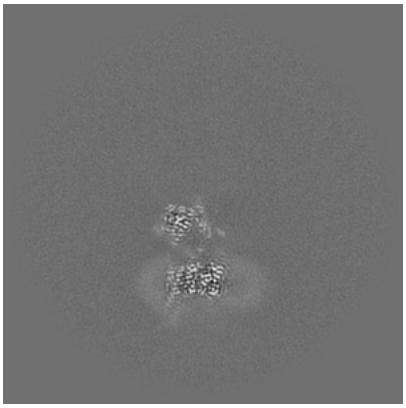


Z Index: 200

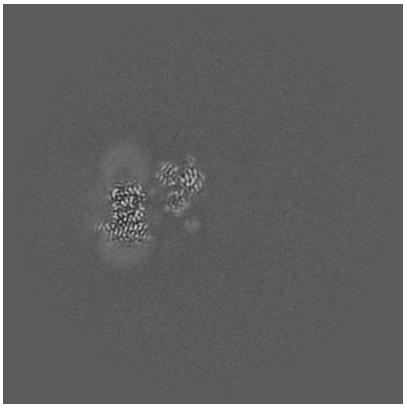
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

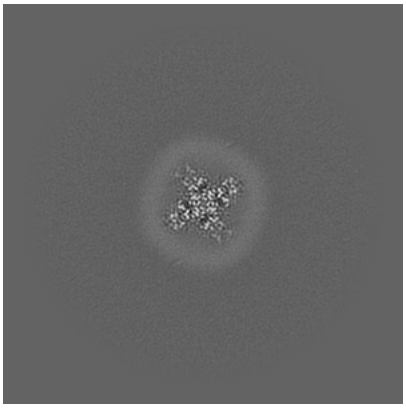
6.3.1 Primary map



X Index: 213



Y Index: 187

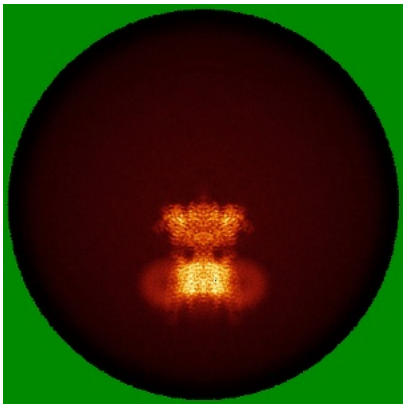


Z Index: 121

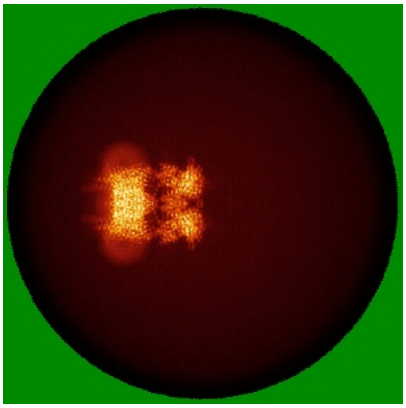
The images above show the largest variance slices of the map in three orthogonal directions.

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

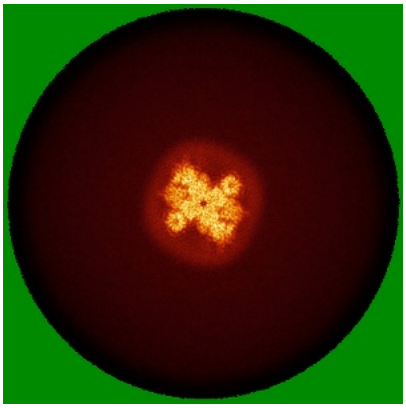
6.4.1 Primary map



X



Y

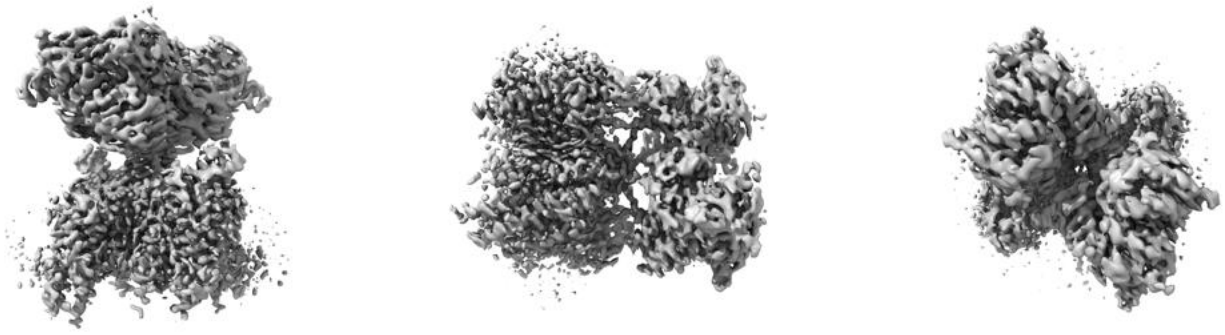


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

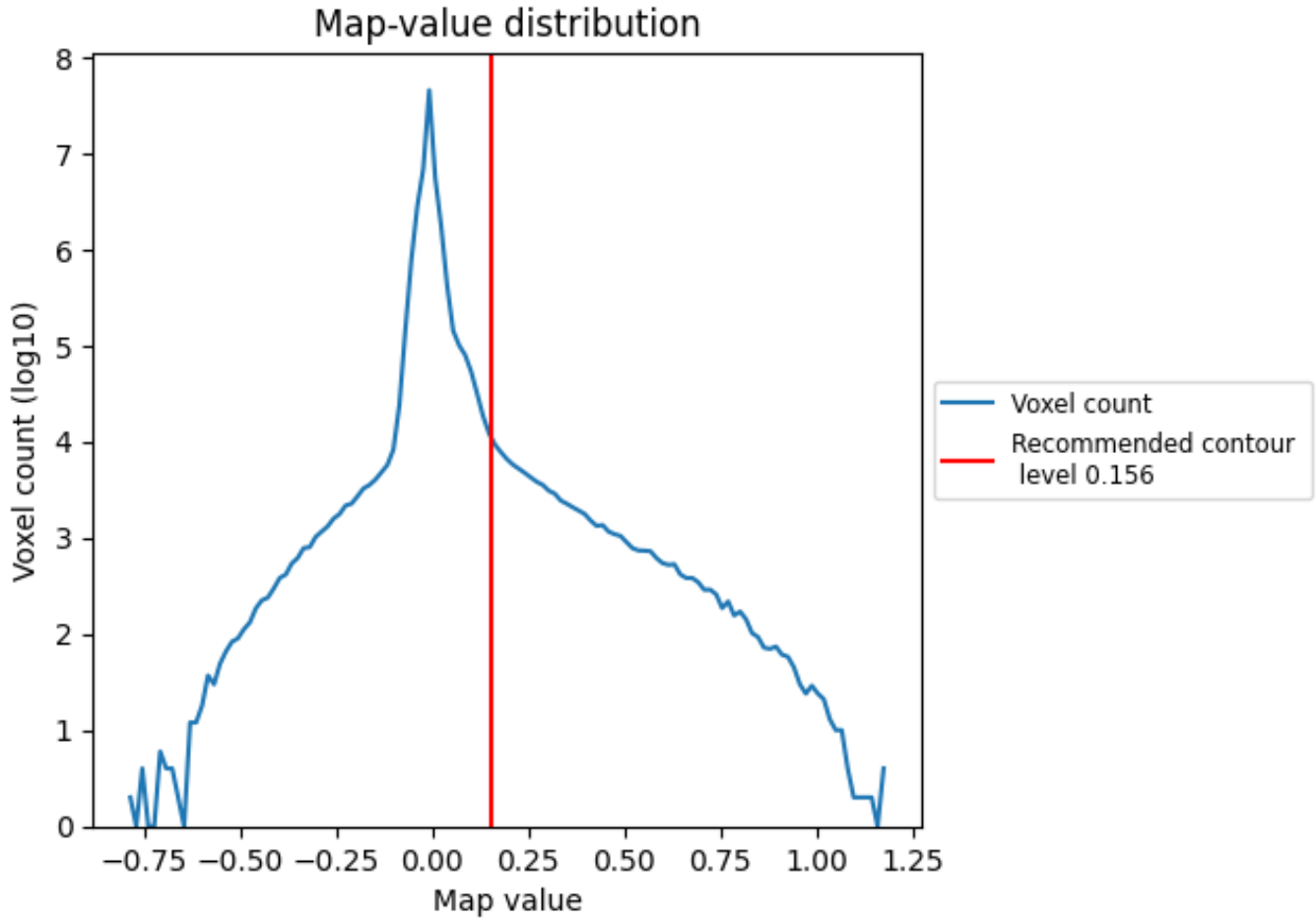
6.6 Mask visualisation (i)

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

7 Map analysis

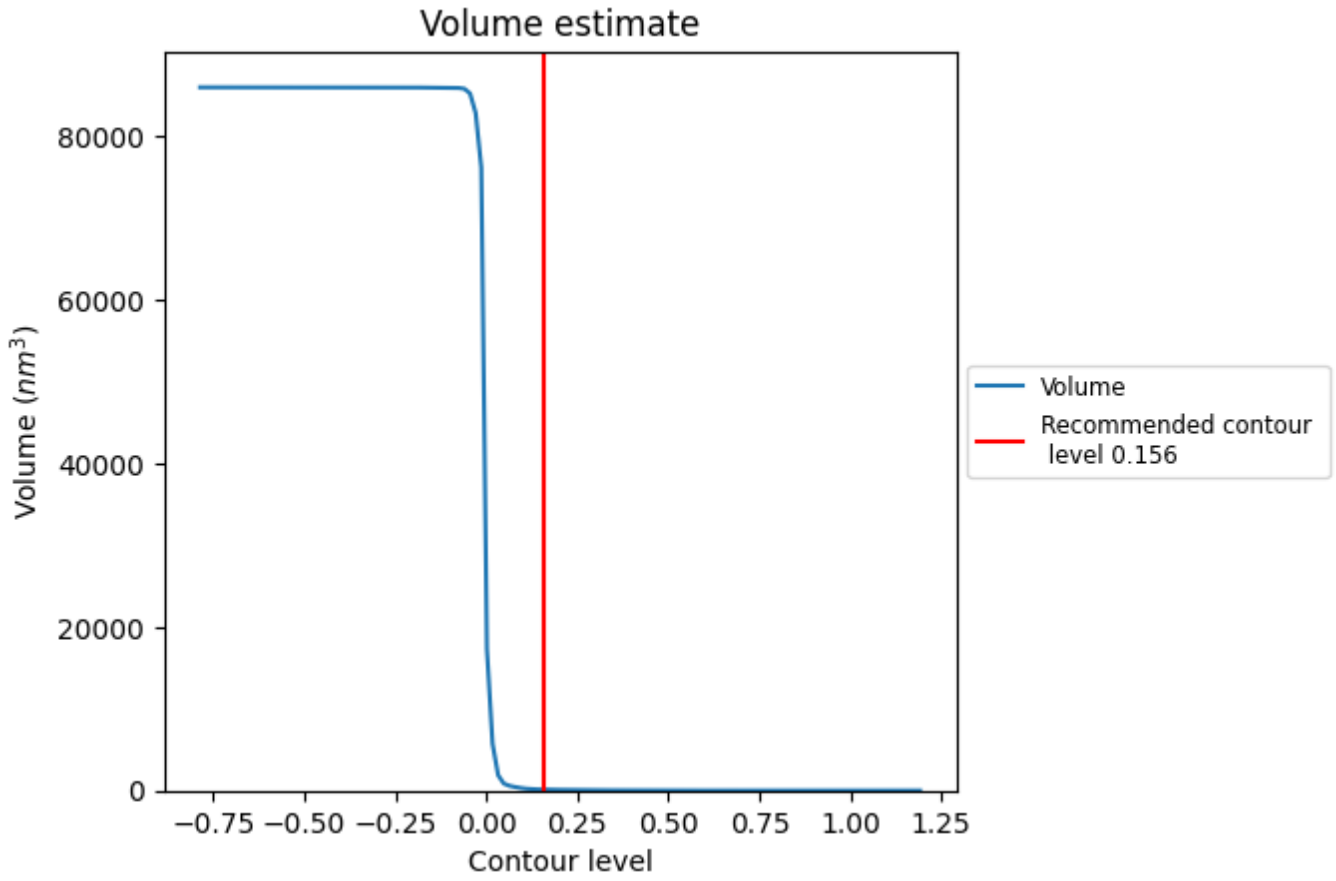
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

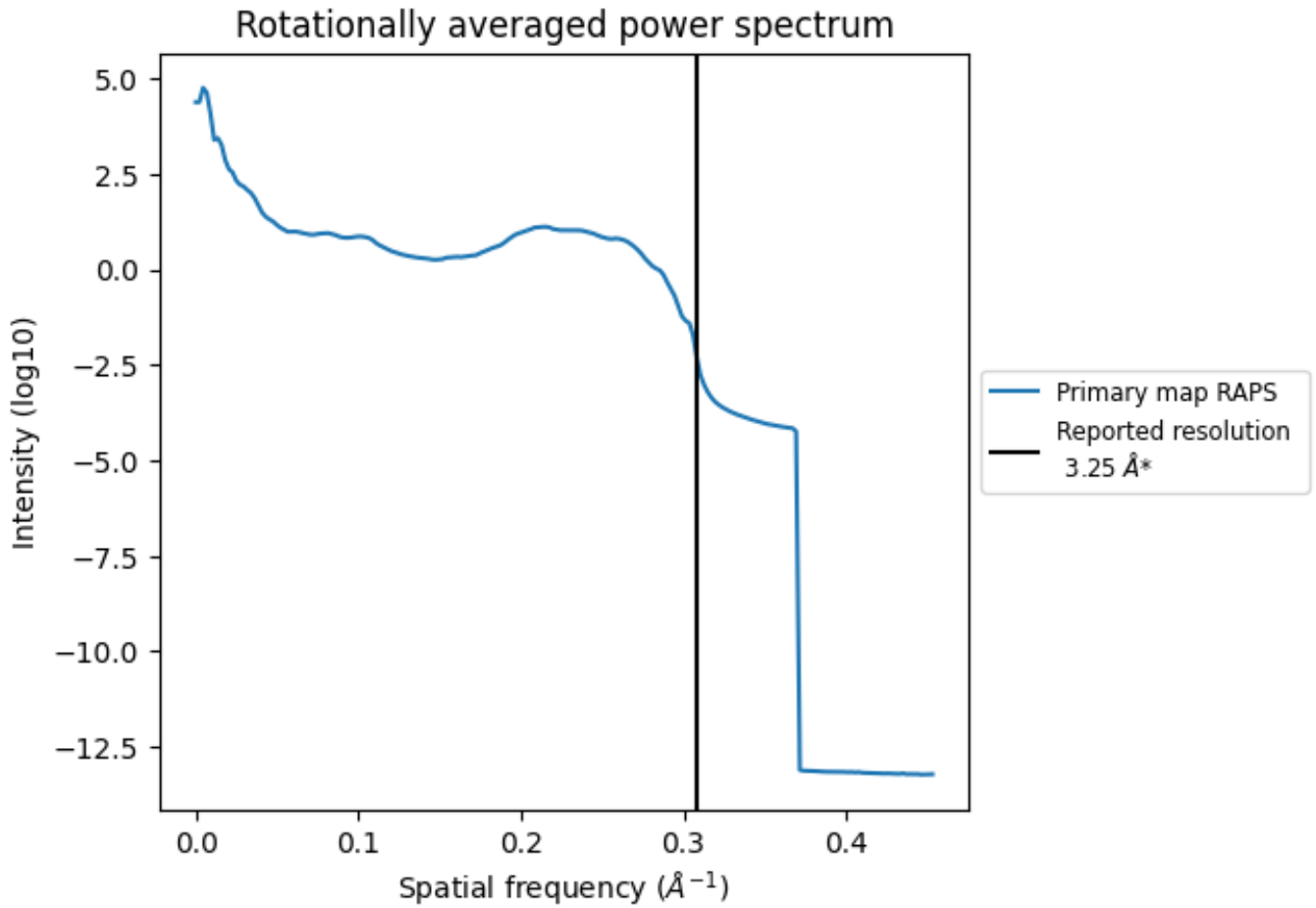
7.2 Volume estimate



The volume at the recommended contour level is 121 nm^3; this corresponds to an approximate mass of 110 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 0.308 $Å^{-1}$

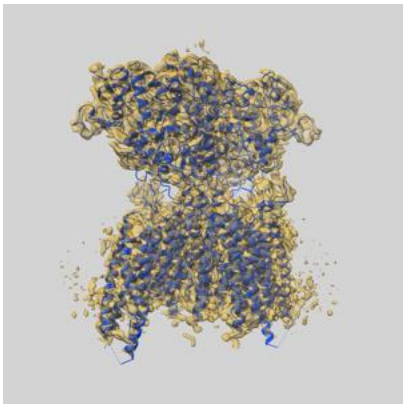
8 Fourier-Shell correlation (i)

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

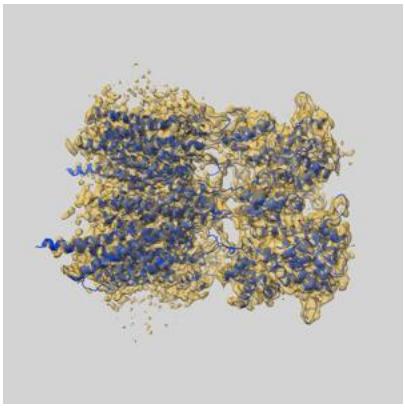
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23292 and PDB model 7LEP. Per-residue inclusion information can be found in section 3 on page 10.

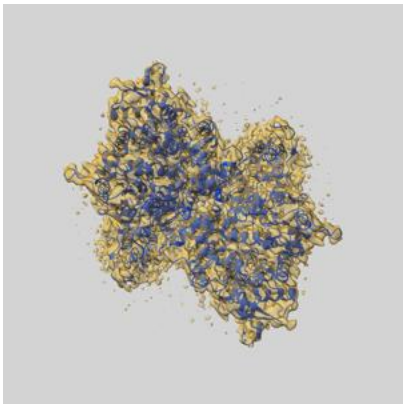
9.1 Map-model overlay



X



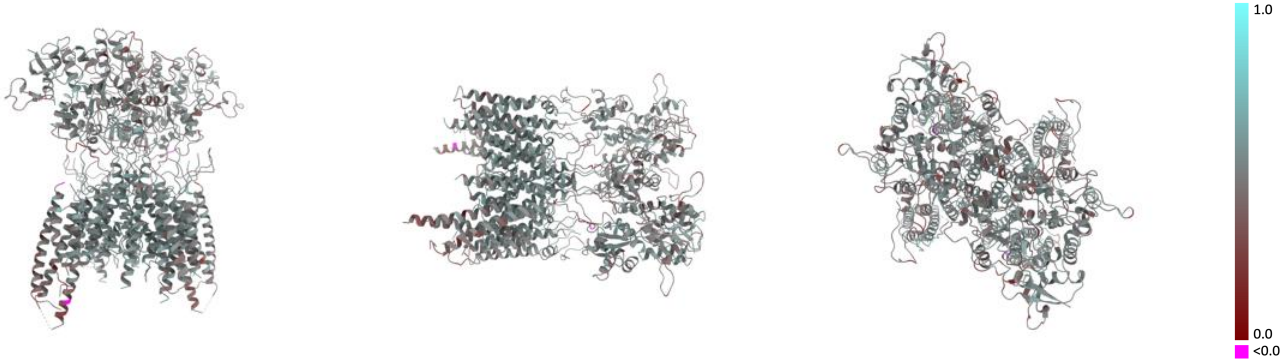
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.156 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.

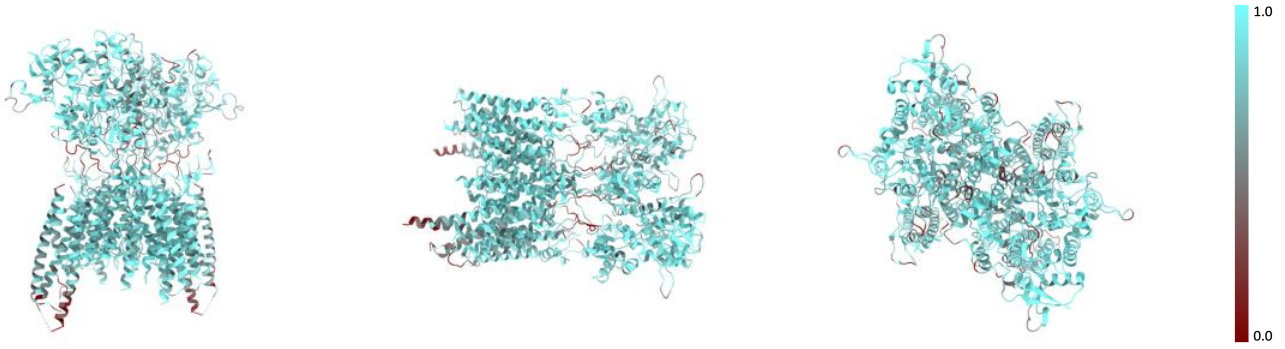
9.2 Q-score mapped to coordinate model (i)



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.

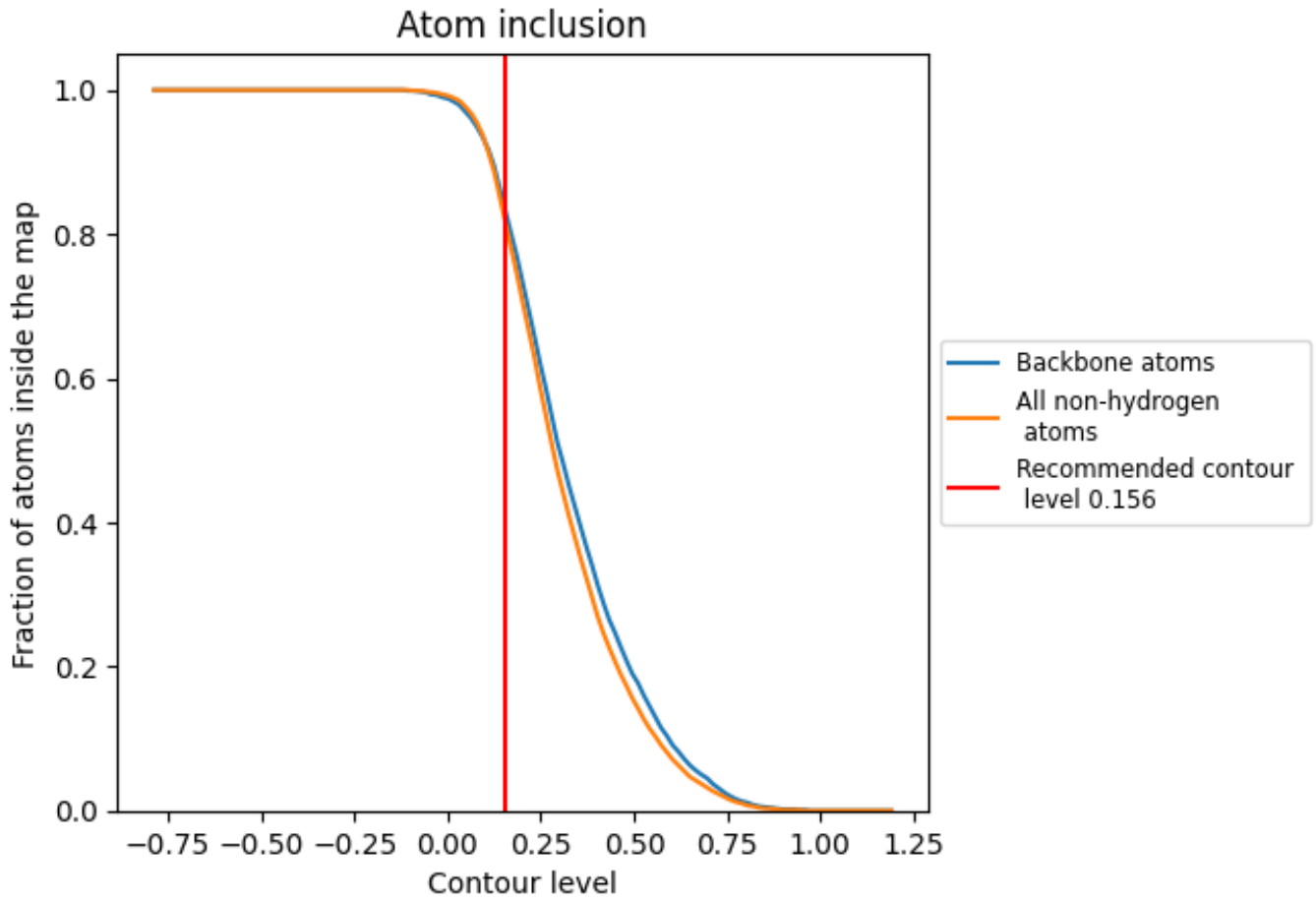
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.156).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.4980
A	0.8460	0.5060
B	0.8330	0.5010
C	0.8500	0.5090
D	0.8270	0.5040
E	0.6600	0.4560
F	0.6610	0.4490
G	0.8460	0.5060
H	0.8410	0.5060