Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:53 PM UTC

PDB ID	:	9OLL / pdb_00009oll
EMDB ID	:	EMD-70596
Title	:	Structure of human TRPC3 T573A mutant
Authors	:	Bell, B.; Baker, M.L.; Cordero-Morales, J.F.
Deposited on	:	2025-05-12
Resolution	:	3.10 Å(reported)
Based on initial model	:	9OLK

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:

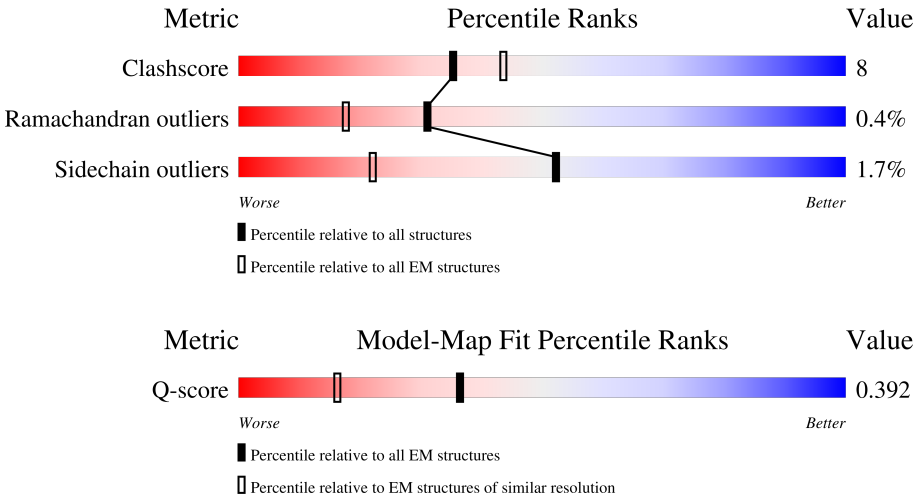
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	848	19% 73% 13% • 12%
1	B	848	18% 72% 14% • 12%
1	C	848	19% 72% 14% • 12%
1	D	848	19% 72% 14% • 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24564 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.

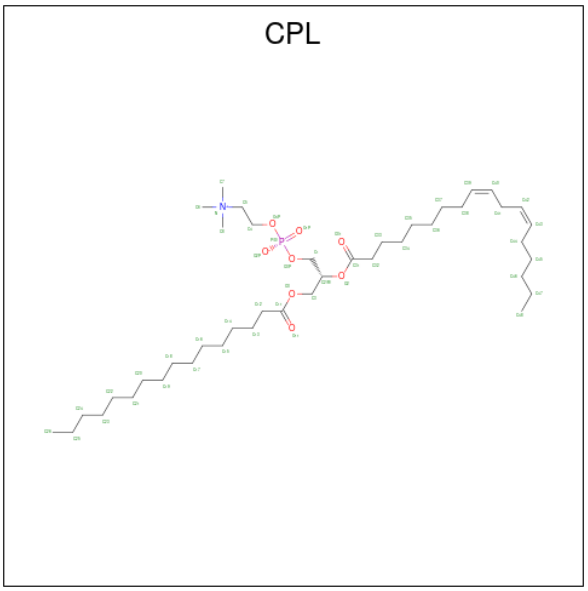
- Molecule 1 is a protein called Short transient receptor potential channel 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	745	Total	C	N	O	S	0	0
			6001	3900	970	1098	33		
1	B	745	Total	C	N	O	S	0	0
			6001	3900	970	1098	33		
1	C	745	Total	C	N	O	S	0	0
			6001	3900	970	1098	33		
1	D	745	Total	C	N	O	S	0	0
			6001	3900	970	1098	33		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	ALA	THR	engineered mutation	UNP Q13507
B	573	ALA	THR	engineered mutation	UNP Q13507
C	573	ALA	THR	engineered mutation	UNP Q13507
D	573	ALA	THR	engineered mutation	UNP Q13507

- Molecule 2 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: $C_{42}H_{80}NO_8P$).

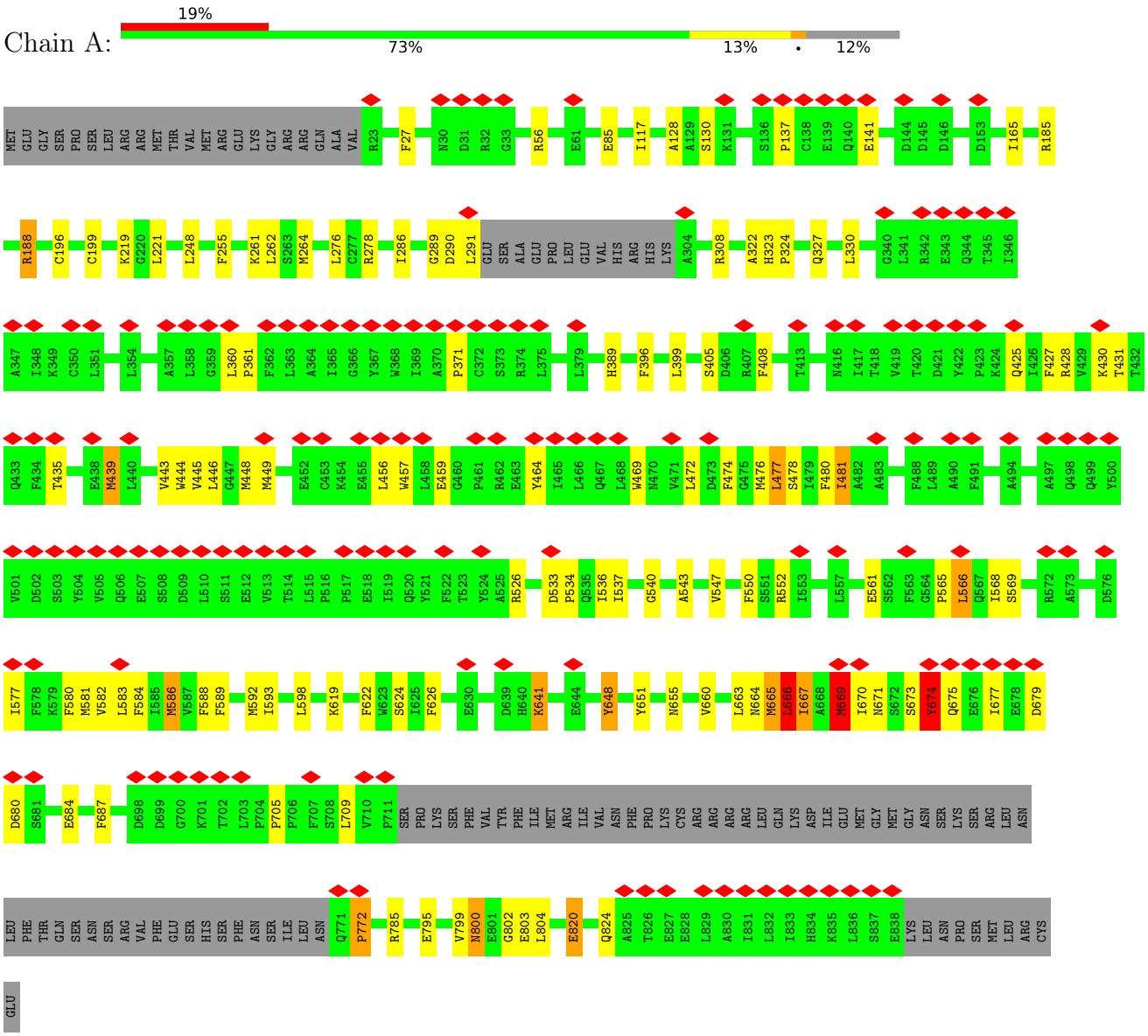


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
2	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
2	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
2	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
2	C	1	Total	C	N	O	P	0
			50	40	1	8	1	
2	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
2	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
2	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
2	D	1	Total	C	N	O	P	0
			50	40	1	8	1	

3 Residue-property plots (i)

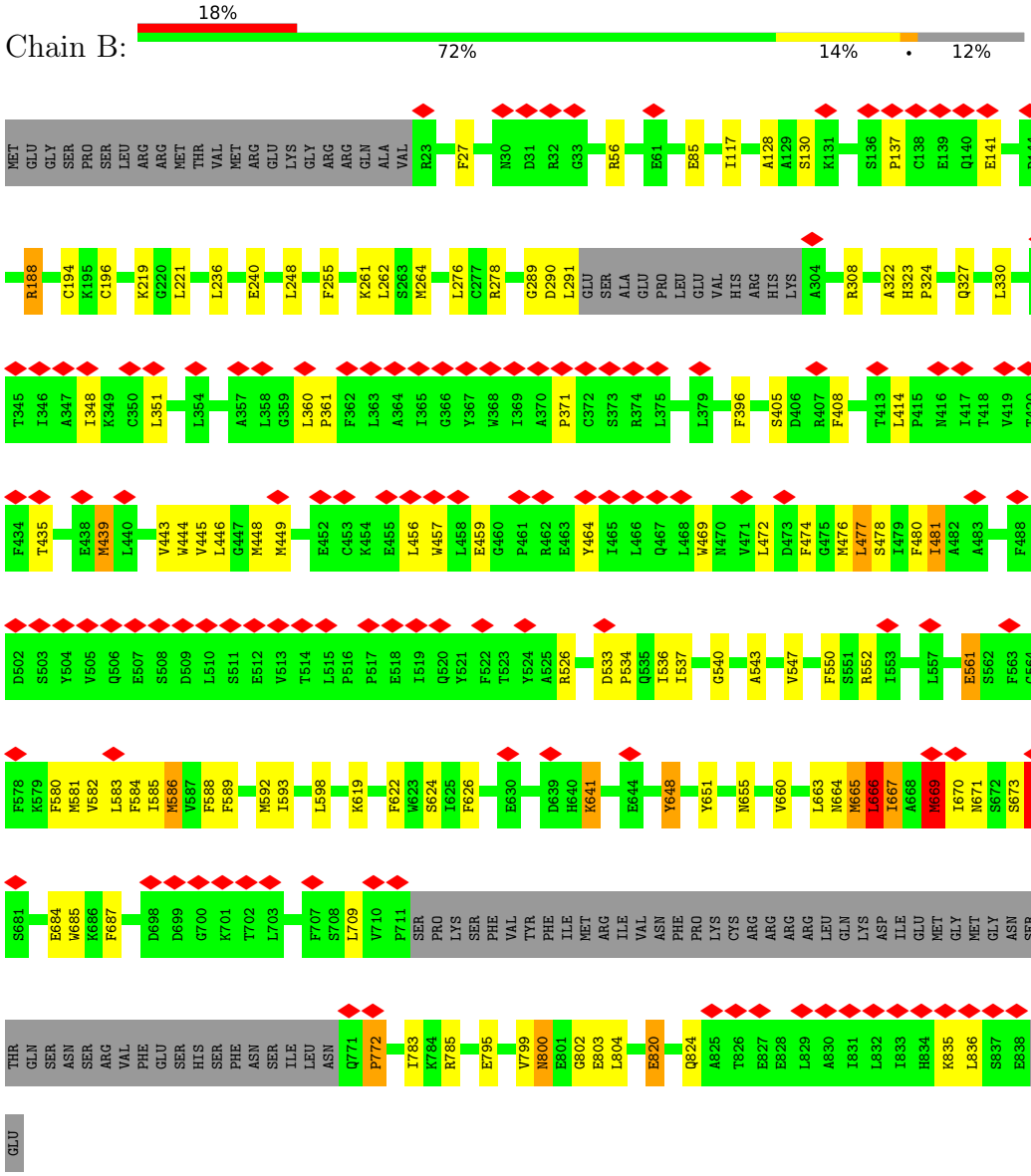
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Short transient receptor potential channel 3



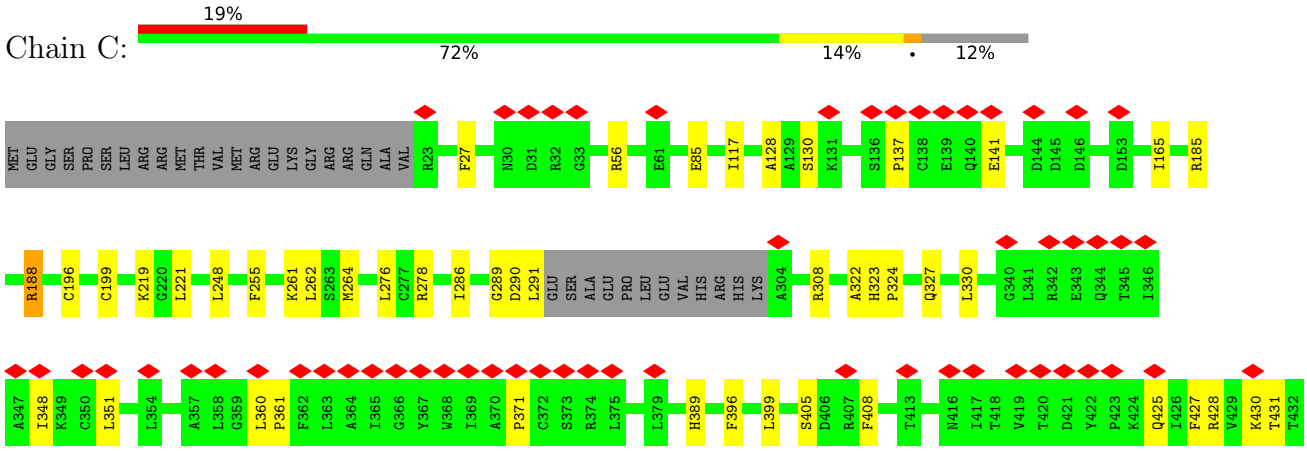
• Molecule 1: Short transient receptor potential channel 3

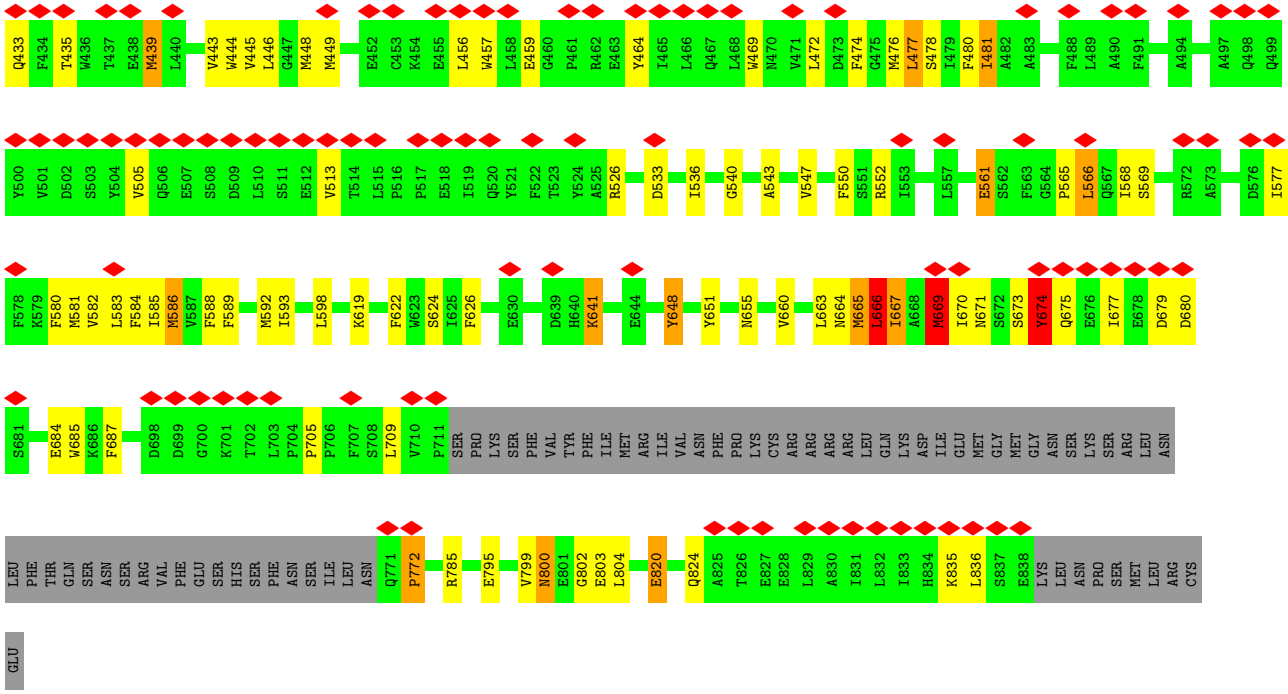
Chain B:



• Molecule 1: Short transient receptor potential channel 3

Chain C:

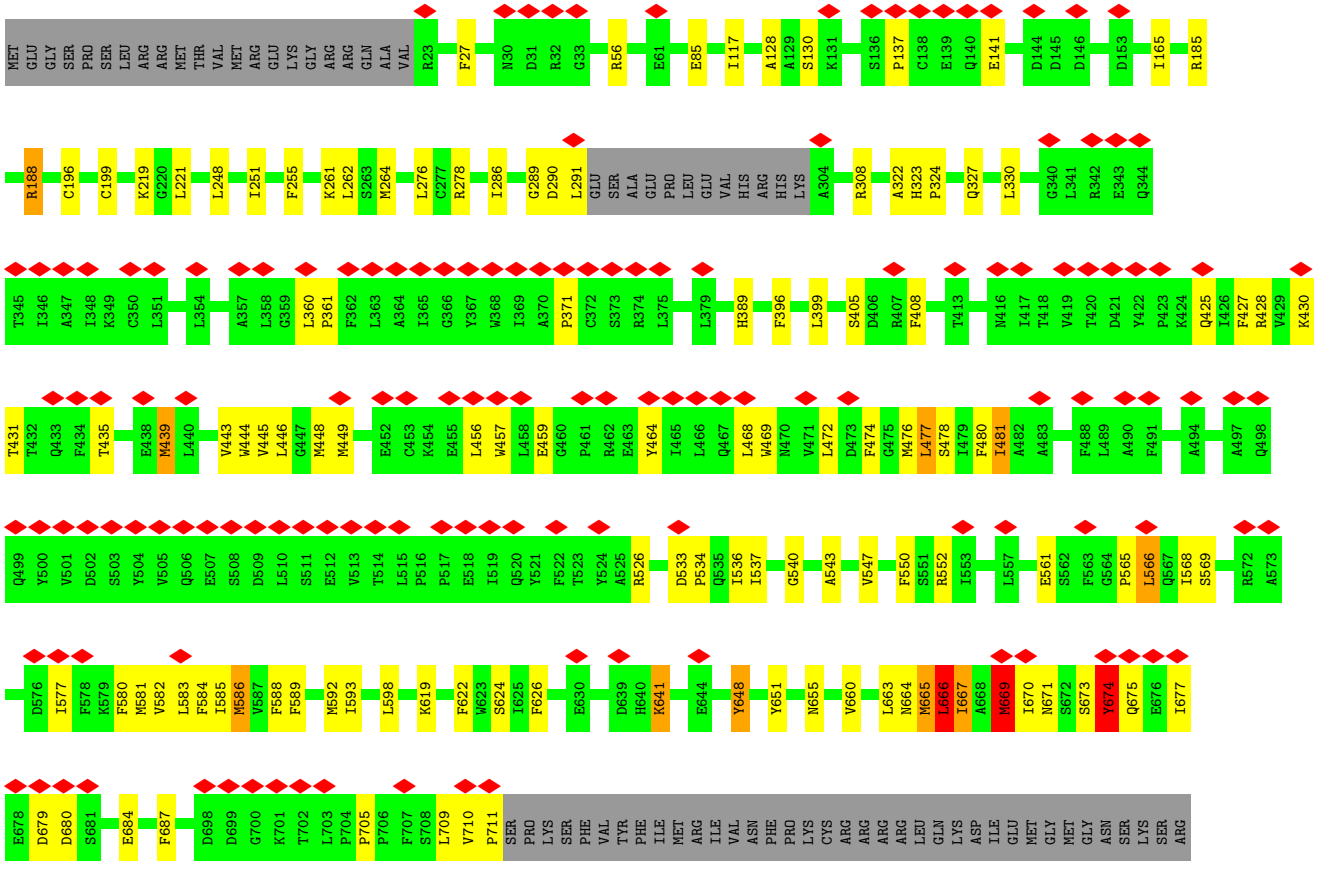


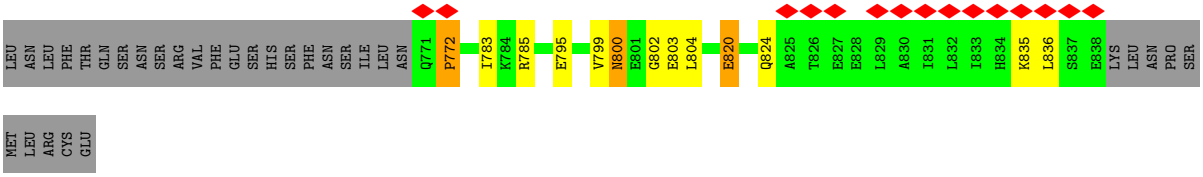


- Molecule 1: Short transient receptor potential channel 3

Chain D:






LEU ASN LEU PHE THR GLN SER ASN SER ARG VAL PHE GLU SER HIS SER PHE ASN SER ILE LEU ASN Q771 P772 I783 K784 R785 E795 V799 N800 E801 G802 E803 L804 E820 Q824 A825 T826 E827 E828 L829 A830 I831 L832 I833 H834 K835 L836 S837 E838 LYS LEU ASN PRO SER
MET LEU ARG CYS GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	57354	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.637	Depositor
Minimum map value	-0.432	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CPL

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	0.73	5/6134 (0.1%)	1.08	28/8305 (0.3%)
1	B	0.73	5/6134 (0.1%)	1.08	28/8305 (0.3%)
1	C	0.73	5/6134 (0.1%)	1.08	28/8305 (0.3%)
1	D	0.73	5/6134 (0.1%)	1.08	28/8305 (0.3%)
All	All	0.73	20/24536 (0.1%)	1.08	112/33220 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	666	LEU	C-O	-6.34	1.16	1.24
1	B	666	LEU	C-O	-6.34	1.16	1.24
1	C	666	LEU	C-O	-6.34	1.16	1.24
1	D	666	LEU	C-O	-6.34	1.16	1.24
1	A	324	PRO	N-CD	-6.24	1.39	1.47
1	B	324	PRO	N-CD	-6.24	1.39	1.47
1	C	324	PRO	N-CD	-6.24	1.39	1.47
1	D	324	PRO	N-CD	-6.24	1.39	1.47
1	A	569	SER	C-O	6.06	1.31	1.24
1	B	569	SER	C-O	6.06	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	569	SER	C-O	6.06	1.31	1.24
1	D	569	SER	C-O	6.06	1.31	1.24
1	A	820	GLU	C-O	-5.34	1.17	1.24
1	B	820	GLU	C-O	-5.34	1.17	1.24
1	C	820	GLU	C-O	-5.34	1.17	1.24
1	D	820	GLU	C-O	-5.34	1.17	1.24
1	A	324	PRO	C-O	-5.25	1.17	1.24
1	B	324	PRO	C-O	-5.25	1.17	1.24
1	C	324	PRO	C-O	-5.25	1.17	1.24
1	D	324	PRO	C-O	-5.25	1.17	1.24

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	666	LEU	CA-C-O	-8.57	111.37	120.63
1	B	666	LEU	CA-C-O	-8.57	111.37	120.63
1	C	666	LEU	CA-C-O	-8.57	111.37	120.63
1	D	666	LEU	CA-C-O	-8.57	111.37	120.63
1	A	687	PHE	CA-C-O	-7.95	112.51	120.70
1	B	687	PHE	CA-C-O	-7.95	112.51	120.70
1	C	687	PHE	CA-C-O	-7.95	112.51	120.70
1	D	687	PHE	CA-C-O	-7.95	112.51	120.70
1	A	680	ASP	N-CA-C	-7.11	103.57	111.82
1	B	680	ASP	N-CA-C	-7.11	103.57	111.82
1	C	680	ASP	N-CA-C	-7.11	103.57	111.82
1	D	680	ASP	N-CA-C	-7.11	103.57	111.82
1	A	396	PHE	N-CA-CB	7.04	120.47	110.12
1	B	396	PHE	N-CA-CB	7.04	120.47	110.12
1	C	396	PHE	N-CA-CB	7.04	120.47	110.12
1	D	396	PHE	N-CA-CB	7.04	120.47	110.12
1	A	255	PHE	CA-CB-CG	6.92	120.72	113.80
1	B	255	PHE	CA-CB-CG	6.92	120.72	113.80
1	C	255	PHE	CA-CB-CG	6.92	120.72	113.80
1	D	255	PHE	CA-CB-CG	6.92	120.72	113.80
1	A	323	HIS	CA-C-O	-6.90	114.00	119.66
1	A	800	ASN	N-CA-CB	-6.90	100.03	111.20
1	B	323	HIS	CA-C-O	-6.90	114.00	119.66
1	B	800	ASN	N-CA-CB	-6.90	100.03	111.20
1	C	323	HIS	CA-C-O	-6.90	114.00	119.66
1	C	800	ASN	N-CA-CB	-6.90	100.03	111.20
1	D	323	HIS	CA-C-O	-6.90	114.00	119.66
1	D	800	ASN	N-CA-CB	-6.89	100.04	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	667	ILE	CA-C-O	-6.80	113.96	121.17
1	B	667	ILE	CA-C-O	-6.80	113.96	121.17
1	C	667	ILE	CA-C-O	-6.80	113.96	121.17
1	D	667	ILE	CA-C-O	-6.80	113.96	121.17
1	A	396	PHE	CB-CA-C	-6.46	100.08	110.79
1	B	396	PHE	CB-CA-C	-6.46	100.08	110.79
1	C	396	PHE	CB-CA-C	-6.46	100.08	110.79
1	D	396	PHE	CB-CA-C	-6.46	100.08	110.79
1	A	651	TYR	CA-C-O	-6.39	114.29	121.00
1	B	651	TYR	CA-C-O	-6.39	114.29	121.00
1	C	651	TYR	CA-C-O	-6.39	114.29	121.00
1	D	651	TYR	CA-C-O	-6.39	114.29	121.00
1	A	566	LEU	CB-CA-C	-6.35	100.30	110.84
1	B	566	LEU	CB-CA-C	-6.35	100.30	110.84
1	C	566	LEU	CB-CA-C	-6.35	100.30	110.84
1	D	566	LEU	CB-CA-C	-6.33	100.33	110.84
1	A	666	LEU	CA-C-N	6.23	128.41	120.56
1	A	666	LEU	C-N-CA	6.23	128.41	120.56
1	B	666	LEU	CA-C-N	6.23	128.41	120.56
1	B	666	LEU	C-N-CA	6.23	128.41	120.56
1	C	666	LEU	CA-C-N	6.23	128.41	120.56
1	C	666	LEU	C-N-CA	6.23	128.41	120.56
1	D	666	LEU	CA-C-N	6.23	128.41	120.56
1	D	666	LEU	C-N-CA	6.23	128.41	120.56
1	A	165	ILE	CA-C-O	-6.08	114.73	121.17
1	B	165	ILE	CA-C-O	-6.08	114.73	121.17
1	C	165	ILE	CA-C-O	-6.08	114.73	121.17
1	D	165	ILE	CA-C-O	-6.08	114.73	121.17
1	A	330	LEU	CA-C-O	-6.00	114.19	120.55
1	B	330	LEU	CA-C-O	-6.00	114.19	120.55
1	C	330	LEU	CA-C-O	-6.00	114.19	120.55
1	D	330	LEU	CA-C-O	-6.00	114.19	120.55
1	A	674	TYR	CA-C-O	5.95	129.03	120.51
1	B	674	TYR	CA-C-O	5.95	129.03	120.51
1	C	674	TYR	CA-C-O	5.95	129.03	120.51
1	D	674	TYR	CA-C-O	5.95	129.03	120.51
1	A	481	ILE	CA-C-O	-5.85	114.97	121.05
1	B	481	ILE	CA-C-O	-5.85	114.97	121.05
1	C	481	ILE	CA-C-O	-5.85	114.97	121.05
1	D	481	ILE	CA-C-O	-5.85	114.97	121.05
1	A	679	ASP	N-CA-C	-5.78	106.28	113.15
1	B	679	ASP	N-CA-C	-5.78	106.28	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	679	ASP	N-CA-C	-5.78	106.28	113.15
1	D	679	ASP	N-CA-C	-5.78	106.28	113.15
1	A	648	TYR	N-CA-CB	-5.76	101.36	110.28
1	B	648	TYR	N-CA-CB	-5.76	101.36	110.28
1	C	648	TYR	N-CA-CB	-5.76	101.36	110.28
1	D	648	TYR	N-CA-CB	-5.76	101.36	110.28
1	B	580	PHE	N-CA-C	-5.74	105.54	112.54
1	A	580	PHE	N-CA-C	-5.71	105.57	112.54
1	C	580	PHE	N-CA-C	-5.71	105.57	112.54
1	D	580	PHE	N-CA-C	-5.71	105.57	112.54
1	A	396	PHE	CA-C-O	-5.63	114.59	120.55
1	B	396	PHE	CA-C-O	-5.63	114.59	120.55
1	C	396	PHE	CA-C-O	-5.63	114.59	120.55
1	D	396	PHE	CA-C-O	-5.63	114.59	120.55
1	A	561	GLU	N-CA-C	-5.54	106.29	113.16
1	B	561	GLU	N-CA-C	-5.54	106.29	113.16
1	C	561	GLU	N-CA-C	-5.54	106.29	113.16
1	D	561	GLU	N-CA-C	-5.54	106.29	113.16
1	A	820	GLU	CA-C-O	-5.48	113.67	119.97
1	B	820	GLU	CA-C-O	-5.48	113.67	119.97
1	C	820	GLU	CA-C-O	-5.48	113.67	119.97
1	D	820	GLU	CA-C-O	-5.48	113.67	119.97
1	D	800	ASN	CB-CA-C	5.38	120.09	109.66
1	A	800	ASN	CB-CA-C	5.36	120.06	109.66
1	B	800	ASN	CB-CA-C	5.36	120.06	109.66
1	C	800	ASN	CB-CA-C	5.36	120.06	109.66
1	A	800	ASN	CA-C-O	-5.35	115.19	121.46
1	B	800	ASN	CA-C-O	-5.35	115.19	121.46
1	C	800	ASN	CA-C-O	-5.35	115.19	121.46
1	D	800	ASN	CA-C-O	-5.35	115.19	121.46
1	A	674	TYR	O-C-N	-5.15	115.74	122.59
1	B	674	TYR	O-C-N	-5.15	115.74	122.59
1	C	674	TYR	O-C-N	-5.15	115.74	122.59
1	D	674	TYR	O-C-N	-5.15	115.74	122.59
1	A	669	MET	CA-C-O	-5.07	114.14	119.97
1	B	669	MET	CA-C-O	-5.07	114.14	119.97
1	C	669	MET	CA-C-O	-5.07	114.14	119.97
1	D	669	MET	CA-C-O	-5.07	114.14	119.97
1	A	439	MET	CA-C-O	-5.04	115.71	121.00
1	B	439	MET	CA-C-O	-5.04	115.71	121.00
1	C	439	MET	CA-C-O	-5.04	115.71	121.00
1	D	439	MET	CA-C-O	-5.04	115.71	121.00

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain
1	A	188	ARG	Sidechain
1	A	248	LEU	Mainchain
1	A	278	ARG	Sidechain
1	A	308	ARG	Sidechain
1	A	56	ARG	Sidechain
1	B	185	ARG	Sidechain
1	B	188	ARG	Sidechain
1	B	248	LEU	Mainchain
1	B	278	ARG	Sidechain
1	B	308	ARG	Sidechain
1	B	56	ARG	Sidechain
1	C	185	ARG	Sidechain
1	C	188	ARG	Sidechain
1	C	248	LEU	Mainchain
1	C	278	ARG	Sidechain
1	C	308	ARG	Sidechain
1	C	56	ARG	Sidechain
1	D	185	ARG	Sidechain
1	D	188	ARG	Sidechain
1	D	248	LEU	Mainchain
1	D	278	ARG	Sidechain
1	D	308	ARG	Sidechain
1	D	56	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6001	0	6042	104	0
1	B	6001	0	6042	108	0
1	C	6001	0	6042	109	0
1	D	6001	0	6042	109	0
2	A	140	0	199	19	0
2	B	140	0	199	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	140	0	199	20	0
2	D	140	0	199	19	0
All	All	24564	0	24964	387	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 8.

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:TRP:NE1	2:D:903:CPL:O11	1.91	1.04
1:C:469:TRP:NE1	2:C:901:CPL:O11	1.91	1.04
1:B:469:TRP:NE1	2:B:901:CPL:O11	1.91	1.03
1:A:469:TRP:NE1	2:A:901:CPL:O11	1.91	1.03
2:B:902:CPL:O1P	2:B:903:CPL:H342	1.74	0.88
2:A:902:CPL:O1P	2:A:903:CPL:H342	1.74	0.88
2:C:902:CPL:O1P	2:C:903:CPL:H342	1.74	0.88
2:D:901:CPL:O1P	2:D:902:CPL:H342	1.74	0.87
1:D:472:LEU:HD11	2:D:903:CPL:H371	1.60	0.84
1:C:472:LEU:HD11	2:C:901:CPL:H371	1.60	0.83
1:A:472:LEU:HD11	2:A:901:CPL:H371	1.60	0.82
1:C:664:ASN:HA	1:C:667:ILE:HD12	1.62	0.82
1:B:664:ASN:HA	1:B:667:ILE:HD12	1.62	0.81
1:B:472:LEU:HD11	2:B:901:CPL:H371	1.60	0.81
1:D:664:ASN:HA	1:D:667:ILE:HD12	1.62	0.80
1:A:664:ASN:HA	1:A:667:ILE:HD12	1.62	0.79
1:C:648:TYR:HB3	2:C:902:CPL:H322	1.72	0.72
1:D:648:TYR:HB3	2:D:901:CPL:H322	1.72	0.71
1:B:648:TYR:HB3	2:B:902:CPL:H322	1.72	0.71
1:A:648:TYR:HB3	2:A:902:CPL:H322	1.72	0.70
1:D:577:ILE:HD12	1:D:665:MET:HG2	1.80	0.63
1:B:577:ILE:HD12	1:B:665:MET:HG2	1.80	0.63
1:C:577:ILE:HD12	1:C:665:MET:HG2	1.80	0.63
1:A:577:ILE:HD12	1:A:665:MET:HG2	1.80	0.63
1:D:445:VAL:HG21	1:D:480:PHE:CD2	2.34	0.63
1:A:445:VAL:HG21	1:A:480:PHE:CD2	2.34	0.62
1:B:445:VAL:HG21	1:B:480:PHE:CD2	2.34	0.61
1:C:445:VAL:HG21	1:C:480:PHE:CD2	2.34	0.61
1:C:469:TRP:CD2	1:C:472:LEU:HD12	2.36	0.61
1:A:469:TRP:CD2	1:A:472:LEU:HD12	2.36	0.61
1:B:469:TRP:CD2	1:B:472:LEU:HD12	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:TRP:CD2	1:D:472:LEU:HD12	2.36	0.60
1:A:472:LEU:HD13	2:A:901:CPL:H141	1.85	0.59
1:B:472:LEU:HD13	2:B:901:CPL:H141	1.85	0.58
1:C:472:LEU:HD13	2:C:901:CPL:H141	1.85	0.58
1:D:472:LEU:HD13	2:D:903:CPL:H141	1.85	0.57
1:A:799:VAL:HG11	1:D:804:LEU:HD22	1.87	0.57
1:B:194:CYS:HG	1:B:196:CYS:HG	1.42	0.57
1:C:804:LEU:HD22	1:D:799:VAL:HG11	1.87	0.57
1:A:804:LEU:HD22	1:B:799:VAL:HG11	1.87	0.56
1:D:196:CYS:SG	1:D:199:CYS:SG	3.03	0.56
1:A:85:GLU:HA	1:A:117:ILE:CD1	2.36	0.56
1:B:85:GLU:HA	1:B:117:ILE:CD1	2.36	0.56
1:B:804:LEU:HD22	1:C:799:VAL:HG11	1.87	0.56
1:C:85:GLU:HA	1:C:117:ILE:CD1	2.36	0.56
1:D:85:GLU:HA	1:D:117:ILE:CD1	2.36	0.56
1:C:289:GLY:O	1:C:290:ASP:OD1	2.24	0.56
1:A:196:CYS:SG	1:A:199:CYS:SG	3.03	0.55
1:A:289:GLY:O	1:A:290:ASP:OD1	2.24	0.55
1:D:674:TYR:CE1	1:D:675:GLN:HB3	2.42	0.55
1:A:671:ASN:O	1:A:675:GLN:HG2	2.07	0.55
2:C:902:CPL:O1P	2:C:903:CPL:C34	2.53	0.55
1:D:289:GLY:O	1:D:290:ASP:OD1	2.24	0.55
1:D:671:ASN:O	1:D:675:GLN:HG2	2.07	0.55
1:A:588:PHE:CD2	1:A:592:MET:HE2	2.42	0.55
1:B:588:PHE:CD2	1:B:592:MET:HE2	2.42	0.55
1:B:671:ASN:O	1:B:675:GLN:HG2	2.07	0.55
1:C:588:PHE:CD2	1:C:592:MET:HE2	2.42	0.55
1:C:674:TYR:CE1	1:C:675:GLN:HB3	2.42	0.55
1:D:291:LEU:HD21	1:D:772:PRO:HD2	1.89	0.55
1:D:588:PHE:CD2	1:D:592:MET:HE2	2.42	0.55
1:A:674:TYR:CE1	1:A:675:GLN:HB3	2.42	0.55
1:B:291:LEU:HD21	1:B:772:PRO:HD2	1.89	0.55
1:B:804:LEU:HD22	1:C:799:VAL:CG1	2.37	0.54
1:C:291:LEU:HD21	1:C:772:PRO:HD2	1.89	0.54
1:C:671:ASN:O	1:C:675:GLN:HG2	2.07	0.54
1:B:670:ILE:HG21	1:C:670:ILE:HD11	1.89	0.54
2:D:901:CPL:O1P	2:D:902:CPL:C34	2.53	0.54
1:A:291:LEU:HD21	1:A:772:PRO:HD2	1.89	0.54
1:B:289:GLY:O	1:B:290:ASP:OD1	2.24	0.54
1:A:804:LEU:HD22	1:B:799:VAL:CG1	2.37	0.54
1:A:443:VAL:O	1:A:446:LEU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:VAL:CG1	1:D:804:LEU:HD22	2.37	0.54
1:C:804:LEU:HD22	1:D:799:VAL:CG1	2.37	0.54
1:A:670:ILE:HG21	1:B:670:ILE:HD11	1.90	0.54
1:B:443:VAL:O	1:B:446:LEU:HB3	2.08	0.54
1:B:670:ILE:HG21	1:C:670:ILE:CD1	2.38	0.54
1:B:469:TRP:CD1	2:B:901:CPL:H352	2.43	0.54
1:A:469:TRP:CD1	2:A:901:CPL:H352	2.43	0.54
1:A:670:ILE:HG21	1:B:670:ILE:CD1	2.38	0.54
1:B:674:TYR:CE1	1:B:675:GLN:HB3	2.42	0.54
1:B:261:LYS:HA	1:B:264:MET:HE2	1.90	0.53
1:C:261:LYS:HA	1:C:264:MET:HE2	1.90	0.53
1:A:261:LYS:HA	1:A:264:MET:HE2	1.90	0.53
1:C:196:CYS:SG	1:C:199:CYS:SG	3.03	0.53
1:C:670:ILE:HG21	1:D:670:ILE:CD1	2.38	0.53
1:D:443:VAL:O	1:D:446:LEU:HB3	2.08	0.53
1:C:443:VAL:O	1:C:446:LEU:HB3	2.08	0.53
1:C:670:ILE:HG21	1:D:670:ILE:HD11	1.89	0.53
1:D:261:LYS:HA	1:D:264:MET:HE2	1.90	0.53
1:D:469:TRP:CD1	2:D:903:CPL:H352	2.43	0.53
1:A:670:ILE:CD1	1:D:670:ILE:HG21	2.38	0.53
1:A:456:LEU:HD23	1:A:464:TYR:CD2	2.44	0.53
1:A:670:ILE:HD11	1:D:670:ILE:HG21	1.89	0.53
1:C:469:TRP:CD1	2:C:901:CPL:H352	2.43	0.53
1:C:456:LEU:HD23	1:C:464:TYR:CD2	2.44	0.53
1:B:469:TRP:NE1	2:B:901:CPL:O2P	2.43	0.52
1:C:469:TRP:NE1	2:C:901:CPL:O2P	2.43	0.52
1:D:469:TRP:NE1	2:D:903:CPL:O2P	2.43	0.52
1:A:622:PHE:CD2	2:D:901:CPL:H351	2.45	0.52
1:B:456:LEU:HD23	1:B:464:TYR:CD2	2.44	0.52
1:B:593:ILE:HD13	1:C:550:PHE:CZ	2.45	0.52
1:D:456:LEU:HD23	1:D:464:TYR:CD2	2.44	0.52
2:B:902:CPL:H351	1:C:622:PHE:CD2	2.45	0.52
1:C:291:LEU:HD11	1:C:772:PRO:HD3	1.92	0.52
1:C:593:ILE:HD13	1:D:550:PHE:CZ	2.45	0.52
2:A:902:CPL:H351	1:B:622:PHE:CD2	2.45	0.51
1:D:291:LEU:HD11	1:D:772:PRO:HD3	1.92	0.51
1:A:469:TRP:NE1	2:A:901:CPL:O2P	2.43	0.51
1:A:593:ILE:HD13	1:B:550:PHE:CZ	2.45	0.51
1:A:550:PHE:CZ	1:D:593:ILE:HD13	2.45	0.51
1:B:291:LEU:HD11	1:B:772:PRO:HD3	1.92	0.51
2:C:902:CPL:H351	1:D:622:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLY:HA2	1:D:598:LEU:HD13	1.93	0.51
1:B:444:TRP:CD1	1:B:448:MET:HE2	2.46	0.51
1:A:444:TRP:CD1	1:A:448:MET:HE2	2.46	0.51
1:C:598:LEU:HD13	1:D:540:GLY:HA2	1.93	0.50
1:A:598:LEU:HD13	1:B:540:GLY:HA2	1.93	0.50
1:C:469:TRP:CD1	2:C:901:CPL:O2P	2.65	0.50
1:A:543:ALA:O	1:A:547:VAL:HG23	2.12	0.50
1:B:469:TRP:CD1	2:B:901:CPL:O2P	2.65	0.50
1:C:444:TRP:CD1	1:C:448:MET:HE2	2.46	0.50
1:B:543:ALA:O	1:B:547:VAL:HG23	2.12	0.50
1:B:469:TRP:CZ2	2:B:901:CPL:H131	2.47	0.50
1:B:598:LEU:HD13	1:C:540:GLY:HA2	1.93	0.50
1:D:543:ALA:O	1:D:547:VAL:HG23	2.12	0.50
1:A:291:LEU:HD11	1:A:772:PRO:HD3	1.92	0.50
1:D:469:TRP:CD1	2:D:903:CPL:O2P	2.65	0.50
1:A:469:TRP:CZ2	2:A:901:CPL:H131	2.47	0.50
1:B:583:LEU:HB2	1:B:586:MET:HE2	1.93	0.50
1:D:444:TRP:CD1	1:D:448:MET:HE2	2.46	0.50
1:C:469:TRP:CZ2	2:C:901:CPL:H131	2.47	0.49
1:A:469:TRP:CD1	2:A:901:CPL:O2P	2.65	0.49
1:A:583:LEU:HB2	1:A:586:MET:HE2	1.93	0.49
1:C:445:VAL:HG11	1:C:480:PHE:HB3	1.94	0.49
1:C:583:LEU:HB2	1:C:586:MET:HE2	1.93	0.49
1:A:655:ASN:HB3	1:B:626:PHE:CZ	2.48	0.49
1:C:427:PHE:O	1:C:431:THR:HG23	2.12	0.49
1:D:445:VAL:HG11	1:D:480:PHE:HB3	1.94	0.49
1:B:655:ASN:HB3	1:C:626:PHE:CZ	2.47	0.49
1:A:626:PHE:CZ	1:D:655:ASN:HB3	2.47	0.49
1:B:820:GLU:O	1:B:824:GLN:HG3	2.12	0.49
1:C:593:ILE:CD1	1:D:550:PHE:CZ	2.96	0.49
1:C:655:ASN:HB3	1:D:626:PHE:CZ	2.47	0.49
1:C:820:GLU:O	1:C:824:GLN:HG3	2.12	0.49
1:B:799:VAL:HG12	1:C:799:VAL:HG21	1.94	0.49
1:D:469:TRP:CZ2	2:D:903:CPL:H131	2.47	0.49
1:D:583:LEU:HB2	1:D:586:MET:HE2	1.93	0.49
1:A:799:VAL:HG12	1:B:799:VAL:HG21	1.94	0.49
1:B:427:PHE:O	1:B:431:THR:HG23	2.12	0.49
1:D:427:PHE:O	1:D:431:THR:HG23	2.12	0.49
1:D:820:GLU:O	1:D:824:GLN:HG3	2.12	0.49
1:A:550:PHE:CZ	1:D:593:ILE:CD1	2.96	0.48
1:A:589:PHE:CD2	1:A:593:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:ILE:CD1	1:B:550:PHE:CZ	2.96	0.48
2:A:902:CPL:O1P	2:A:903:CPL:C34	2.53	0.48
1:A:427:PHE:O	1:A:431:THR:HG23	2.12	0.48
1:A:660:VAL:HA	1:B:669:MET:HE1	1.95	0.48
1:A:820:GLU:O	1:A:824:GLN:HG3	2.12	0.48
1:B:445:VAL:HG11	1:B:480:PHE:HB3	1.94	0.48
1:C:543:ALA:O	1:C:547:VAL:HG23	2.12	0.48
1:B:593:ILE:CD1	1:C:550:PHE:CZ	2.96	0.48
1:C:660:VAL:HA	1:D:669:MET:HE1	1.95	0.48
1:A:322:ALA:HA	1:A:327:GLN:HE21	1.79	0.48
1:A:445:VAL:HG11	1:A:480:PHE:HB3	1.94	0.48
1:B:589:PHE:CD2	1:B:593:ILE:HD11	2.48	0.48
1:A:669:MET:HE1	1:D:660:VAL:HA	1.95	0.48
1:D:322:ALA:HA	1:D:327:GLN:HE21	1.79	0.48
1:A:799:VAL:HG21	1:D:799:VAL:HG12	1.94	0.48
1:D:589:PHE:CD2	1:D:593:ILE:HD11	2.48	0.48
1:B:660:VAL:HA	1:C:669:MET:HE1	1.95	0.47
1:C:322:ALA:HA	1:C:327:GLN:HE21	1.79	0.47
1:C:799:VAL:HG12	1:D:799:VAL:HG21	1.94	0.47
1:A:641:LYS:HG2	2:A:903:CPL:HC71	1.96	0.47
1:B:322:ALA:HA	1:B:327:GLN:HE21	1.79	0.47
1:C:589:PHE:CD2	1:C:593:ILE:HD11	2.48	0.47
1:A:456:LEU:C	1:A:456:LEU:HD13	2.40	0.47
1:C:589:PHE:HA	1:C:592:MET:HE3	1.97	0.47
1:C:667:ILE:HD11	1:D:669:MET:HB3	1.97	0.47
1:A:128:ALA:C	1:A:130:SER:H	2.23	0.47
1:B:641:LYS:HG2	2:B:903:CPL:HC71	1.96	0.47
1:A:533:ASP:HB3	1:A:536:ILE:HD12	1.97	0.47
1:C:444:TRP:HD1	1:C:448:MET:HE2	1.80	0.47
1:C:641:LYS:HG2	2:C:903:CPL:HC71	1.96	0.47
1:D:128:ALA:C	1:D:130:SER:H	2.23	0.47
1:D:456:LEU:C	1:D:456:LEU:HD13	2.40	0.47
1:B:428:ARG:HD2	1:B:428:ARG:HA	1.71	0.47
1:B:456:LEU:C	1:B:456:LEU:HD13	2.40	0.47
1:C:456:LEU:HD13	1:C:456:LEU:C	2.40	0.47
1:D:589:PHE:HA	1:D:592:MET:HE3	1.97	0.47
1:D:641:LYS:HG2	2:D:902:CPL:HC71	1.96	0.47
1:A:669:MET:HB3	1:D:667:ILE:HD11	1.97	0.47
1:B:533:ASP:HB3	1:B:536:ILE:HD12	1.97	0.47
2:B:902:CPL:O1P	2:B:903:CPL:C34	2.53	0.47
1:A:444:TRP:HD1	1:A:448:MET:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:902:CPL:H361	2:B:902:CPL:H331	1.64	0.46
1:A:589:PHE:HA	1:A:592:MET:HE3	1.97	0.46
1:C:533:ASP:HB3	1:C:536:ILE:HD12	1.97	0.46
1:D:444:TRP:HD1	1:D:448:MET:HE2	1.80	0.46
1:A:428:ARG:HA	1:A:428:ARG:HD2	1.71	0.46
1:A:800:ASN:HB3	1:B:795:GLU:O	2.16	0.46
1:A:667:ILE:HD11	1:B:669:MET:HB3	1.97	0.46
1:B:667:ILE:HD11	1:C:669:MET:HB3	1.97	0.46
1:D:533:ASP:HB3	1:D:536:ILE:HD12	1.97	0.46
1:C:800:ASN:HB3	1:D:795:GLU:O	2.16	0.46
1:A:568:ILE:HD12	1:A:684:GLU:HG3	1.98	0.45
1:B:800:ASN:HB3	1:C:795:GLU:O	2.16	0.45
1:C:581:MET:HA	1:C:584:PHE:HB3	1.98	0.45
1:D:568:ILE:HD12	1:D:684:GLU:HG3	1.98	0.45
1:A:795:GLU:O	1:D:800:ASN:HB3	2.16	0.45
1:B:589:PHE:HA	1:B:592:MET:HE3	1.97	0.45
1:D:581:MET:HA	1:D:584:PHE:HB3	1.98	0.45
1:C:188:ARG:HA	1:C:221:LEU:HD11	1.99	0.45
2:C:903:CPL:HC73	2:C:903:CPL:HC41	1.75	0.45
1:B:128:ALA:C	1:B:130:SER:H	2.23	0.45
1:B:444:TRP:HD1	1:B:448:MET:HE2	1.80	0.45
1:C:476:MET:HE1	1:C:552:ARG:HD2	1.98	0.45
1:C:565:PRO:O	1:C:566:LEU:C	2.60	0.45
1:D:188:ARG:HA	1:D:221:LEU:HD11	1.99	0.45
1:B:188:ARG:HA	1:B:221:LEU:HD11	1.99	0.45
1:D:476:MET:HE1	1:D:552:ARG:HD2	1.98	0.45
1:A:565:PRO:O	1:A:566:LEU:C	2.60	0.45
1:A:667:ILE:CG2	1:B:673:SER:HB3	2.47	0.45
1:A:795:GLU:HB2	1:D:802:GLY:CA	2.47	0.45
2:D:902:CPL:HC73	2:D:902:CPL:HC41	1.75	0.45
1:B:469:TRP:CE2	2:B:901:CPL:O11	2.67	0.45
1:C:128:ALA:C	1:C:130:SER:H	2.23	0.45
1:C:568:ILE:HD12	1:C:684:GLU:HG3	1.98	0.45
1:B:568:ILE:HD12	1:B:684:GLU:HG3	1.98	0.45
1:B:581:MET:HA	1:B:584:PHE:HB3	1.98	0.45
1:B:667:ILE:CG2	1:C:673:SER:HB3	2.47	0.45
1:A:469:TRP:CE2	2:A:901:CPL:O11	2.67	0.45
1:A:581:MET:HA	1:A:584:PHE:HB3	1.98	0.45
1:A:188:ARG:HA	1:A:221:LEU:HD11	1.99	0.44
1:A:476:MET:HE1	1:A:552:ARG:HD2	1.98	0.44
1:A:673:SER:HB3	1:D:667:ILE:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:GLY:CA	1:C:795:GLU:HB2	2.47	0.44
1:C:667:ILE:CG2	1:D:673:SER:HB3	2.47	0.44
2:C:903:CPL:H332	2:C:903:CPL:H362	1.40	0.44
1:D:428:ARG:HA	1:D:428:ARG:HD2	1.71	0.44
2:B:903:CPL:H332	2:B:903:CPL:H362	1.40	0.44
1:D:565:PRO:O	1:D:566:LEU:C	2.60	0.44
1:A:802:GLY:CA	1:B:795:GLU:HB2	2.47	0.44
1:C:802:GLY:CA	1:D:795:GLU:HB2	2.47	0.44
2:A:903:CPL:H332	2:A:903:CPL:H362	1.40	0.44
1:B:476:MET:HE1	1:B:552:ARG:HD2	1.98	0.44
1:C:128:ALA:C	1:C:130:SER:N	2.76	0.44
1:C:449:MET:HE1	1:C:474:PHE:CE1	2.53	0.44
1:B:565:PRO:O	1:B:566:LEU:C	2.60	0.44
2:B:903:CPL:HC73	2:B:903:CPL:HC41	1.75	0.44
1:B:449:MET:HE1	1:B:474:PHE:CE1	2.53	0.43
2:B:903:CPL:HC2	2:B:903:CPL:H321	1.69	0.43
1:D:622:PHE:C	1:D:624:SER:H	2.27	0.43
1:C:622:PHE:C	1:C:624:SER:H	2.27	0.43
2:D:901:CPL:H331	2:D:901:CPL:H361	1.64	0.43
1:B:128:ALA:C	1:B:130:SER:N	2.76	0.43
1:C:469:TRP:HD1	2:C:901:CPL:H342	1.83	0.43
1:A:449:MET:HE1	1:A:474:PHE:CE1	2.53	0.43
1:D:469:TRP:HD1	2:D:903:CPL:H342	1.83	0.43
2:D:902:CPL:H152	2:D:902:CPL:H181	1.76	0.43
1:A:476:MET:O	1:A:477:LEU:C	2.61	0.43
1:B:476:MET:O	1:B:477:LEU:C	2.61	0.43
1:C:399:LEU:HD23	1:C:399:LEU:HA	1.87	0.43
1:C:674:TYR:CD1	1:C:675:GLN:N	2.87	0.43
2:D:903:CPL:H361	2:D:903:CPL:H331	1.71	0.43
1:D:783:ILE:HD13	1:D:783:ILE:HA	1.87	0.43
1:D:674:TYR:CD1	1:D:675:GLN:N	2.87	0.43
1:A:803:GLU:CB	1:D:804:LEU:HD23	2.49	0.42
2:A:902:CPL:H331	2:A:902:CPL:H361	1.64	0.42
2:A:903:CPL:HC73	2:A:903:CPL:HC41	1.75	0.42
1:B:674:TYR:CD1	1:B:675:GLN:N	2.87	0.42
1:C:804:LEU:HD23	1:D:803:GLU:CB	2.50	0.42
1:D:449:MET:HE1	1:D:474:PHE:CE1	2.53	0.42
1:B:469:TRP:HD1	2:B:901:CPL:H342	1.83	0.42
1:B:622:PHE:C	1:B:624:SER:H	2.27	0.42
1:C:276:LEU:HB3	1:C:785:ARG:HD2	2.01	0.42
1:D:476:MET:O	1:D:477:LEU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:VAL:HA	1:D:711:PRO:HD3	1.92	0.42
1:A:674:TYR:CD1	1:A:675:GLN:N	2.87	0.42
2:C:902:CPL:H331	2:C:902:CPL:H361	1.64	0.42
1:D:478:SER:HA	1:D:481:ILE:HG22	2.01	0.42
1:C:405:SER:HA	1:C:408:PHE:CE2	2.55	0.42
2:C:903:CPL:H321	2:C:903:CPL:HC2	1.69	0.42
1:B:219:LYS:HB2	1:B:219:LYS:HE3	1.72	0.42
1:C:457:TRP:C	1:C:459:GLU:N	2.78	0.42
2:C:901:CPL:H361	2:C:901:CPL:H331	1.71	0.42
1:A:405:SER:HA	1:A:408:PHE:CE2	2.55	0.42
1:A:469:TRP:HD1	2:A:901:CPL:H342	1.84	0.42
1:A:622:PHE:C	1:A:624:SER:H	2.27	0.42
1:A:670:ILE:HG13	1:D:667:ILE:HG23	2.02	0.42
1:D:585:ILE:HD13	1:D:585:ILE:HA	1.89	0.42
1:B:291:LEU:HD11	1:B:772:PRO:CD	2.50	0.42
1:B:804:LEU:HD23	1:C:803:GLU:CB	2.49	0.42
1:C:478:SER:HA	1:C:481:ILE:HG22	2.01	0.42
1:D:219:LYS:HG3	1:D:262:LEU:HD21	2.01	0.42
1:A:588:PHE:HD2	1:A:592:MET:HE2	1.85	0.42
1:B:219:LYS:HG3	1:B:262:LEU:HD21	2.01	0.42
1:D:405:SER:HA	1:D:408:PHE:CE2	2.55	0.42
1:A:478:SER:HA	1:A:481:ILE:HG22	2.01	0.42
1:A:804:LEU:HD23	1:B:803:GLU:CB	2.49	0.42
2:A:903:CPL:H321	2:A:903:CPL:HC2	1.69	0.42
1:B:667:ILE:HG23	1:C:670:ILE:HG13	2.02	0.42
1:C:435:THR:O	1:C:439:MET:HG2	2.20	0.42
1:A:360:LEU:HB3	1:A:361:PRO:HD3	2.02	0.41
1:B:552:ARG:NH1	1:B:552:ARG:HB3	2.35	0.41
1:B:663:LEU:HD23	1:C:666:LEU:HA	2.01	0.41
1:C:219:LYS:HG3	1:C:262:LEU:HD21	2.01	0.41
1:C:663:LEU:HD23	1:D:666:LEU:HA	2.01	0.41
1:D:128:ALA:C	1:D:130:SER:N	2.76	0.41
1:D:425:GLN:HE22	1:D:430:LYS:HB2	1.85	0.41
1:A:219:LYS:HG3	1:A:262:LEU:HD21	2.01	0.41
1:A:291:LEU:HD11	1:A:772:PRO:CD	2.50	0.41
1:A:552:ARG:HB3	1:A:552:ARG:NH1	2.35	0.41
1:B:276:LEU:HB3	1:B:785:ARG:HD2	2.01	0.41
1:B:478:SER:HA	1:B:481:ILE:HG22	2.01	0.41
1:C:291:LEU:HD11	1:C:772:PRO:CD	2.50	0.41
1:C:425:GLN:HE22	1:C:430:LYS:HB2	1.85	0.41
1:C:476:MET:O	1:C:477:LEU:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:TRP:C	1:D:459:GLU:N	2.77	0.41
1:A:667:ILE:HG23	1:B:670:ILE:HG13	2.02	0.41
1:D:674:TYR:O	1:D:677:ILE:HG22	2.21	0.41
1:A:663:LEU:HD23	1:B:666:LEU:HA	2.01	0.41
1:C:433:GLN:H	1:C:433:GLN:HG2	1.66	0.41
1:D:552:ARG:NH1	1:D:552:ARG:HB3	2.35	0.41
1:A:128:ALA:C	1:A:130:SER:N	2.76	0.41
1:A:534:PRO:HA	1:A:537:ILE:HG12	2.03	0.41
1:A:666:LEU:HA	1:D:663:LEU:HD23	2.01	0.41
1:A:674:TYR:O	1:A:677:ILE:HG22	2.21	0.41
1:B:414:LEU:HD12	1:B:414:LEU:HA	1.99	0.41
1:B:534:PRO:HA	1:B:537:ILE:HG12	2.03	0.41
1:C:674:TYR:O	1:C:677:ILE:HG22	2.21	0.41
1:D:276:LEU:HB3	1:D:785:ARG:HD2	2.01	0.41
1:D:286:ILE:HD13	1:D:286:ILE:HA	1.89	0.41
1:D:435:THR:O	1:D:439:MET:HG2	2.20	0.41
1:A:457:TRP:C	1:A:459:GLU:N	2.78	0.41
1:B:137:PRO:O	1:B:141:GLU:HG2	2.21	0.41
1:B:677:ILE:HG23	1:B:677:ILE:O	2.21	0.41
1:C:552:ARG:HB3	1:C:552:ARG:NH1	2.35	0.41
1:C:667:ILE:HG23	1:D:670:ILE:HG13	2.02	0.41
1:D:291:LEU:HD11	1:D:772:PRO:CD	2.50	0.41
1:B:405:SER:HA	1:B:408:PHE:CE2	2.55	0.41
1:B:435:THR:O	1:B:439:MET:HG2	2.20	0.41
1:B:783:ILE:HD13	1:B:783:ILE:HA	1.87	0.41
1:B:835:LYS:O	1:B:836:LEU:C	2.64	0.41
1:C:360:LEU:HB3	1:C:361:PRO:HD3	2.02	0.41
1:D:469:TRP:CE2	2:D:903:CPL:O11	2.67	0.41
1:C:469:TRP:CE2	2:C:901:CPL:O11	2.67	0.41
1:A:435:THR:O	1:A:439:MET:HG2	2.20	0.41
1:A:677:ILE:HG23	1:A:677:ILE:O	2.21	0.41
1:B:360:LEU:HB3	1:B:361:PRO:HD3	2.02	0.41
1:B:561:GLU:HB3	1:B:685:TRP:CH2	2.56	0.41
1:B:674:TYR:O	1:B:677:ILE:HG22	2.21	0.41
1:C:286:ILE:HD13	1:C:286:ILE:HA	1.89	0.41
1:C:588:PHE:HD2	1:C:592:MET:HE2	1.85	0.41
1:D:360:LEU:HB3	1:D:361:PRO:HD3	2.02	0.41
1:D:472:LEU:HD21	2:D:903:CPL:H382	2.03	0.41
1:A:137:PRO:O	1:A:141:GLU:HG2	2.21	0.41
1:A:389:HIS:CD2	1:A:705:PRO:HD3	2.56	0.41
1:B:804:LEU:HD23	1:C:803:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:HD13	1:A:286:ILE:HA	1.89	0.40
1:A:804:LEU:HD23	1:B:803:GLU:HB2	2.04	0.40
2:A:901:CPL:H361	2:A:901:CPL:H331	1.71	0.40
1:B:457:TRP:C	1:B:459:GLU:N	2.78	0.40
1:C:505:VAL:HG13	1:C:513:VAL:HG21	2.03	0.40
1:C:585:ILE:HD13	1:C:585:ILE:HA	1.89	0.40
1:C:677:ILE:HG23	1:C:677:ILE:O	2.21	0.40
1:C:835:LYS:O	1:C:836:LEU:C	2.64	0.40
2:C:903:CPL:H152	2:C:903:CPL:H181	1.75	0.40
1:B:585:ILE:HD13	1:B:585:ILE:HA	1.89	0.40
1:C:389:HIS:CD2	1:C:705:PRO:HD3	2.56	0.40
1:D:677:ILE:HG23	1:D:677:ILE:O	2.21	0.40
1:A:276:LEU:HB3	1:A:785:ARG:HD2	2.01	0.40
1:B:348:ILE:O	1:B:351:LEU:HG	2.22	0.40
1:C:137:PRO:O	1:C:141:GLU:HG2	2.21	0.40
1:D:468:LEU:O	1:D:469:TRP:C	2.65	0.40
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.87	0.40
1:D:389:HIS:CD2	1:D:705:PRO:HD3	2.56	0.40
1:D:399:LEU:HD23	1:D:399:LEU:HA	1.87	0.40
1:D:835:LYS:O	1:D:836:LEU:C	2.64	0.40
1:A:425:GLN:HE22	1:A:430:LYS:HB2	1.85	0.40
1:B:236:LEU:O	1:B:240:GLU:HG3	2.22	0.40
1:C:348:ILE:O	1:C:351:LEU:HG	2.22	0.40
1:C:428:ARG:HA	1:C:428:ARG:HD2	1.71	0.40
1:C:561:GLU:HB3	1:C:685:TRP:CH2	2.56	0.40
1:D:137:PRO:O	1:D:141:GLU:HG2	2.21	0.40
1:D:251:ILE:H	1:D:251:ILE:HG13	1.73	0.40
1:D:534:PRO:HA	1:D:537:ILE:HG12	2.03	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	739/848 (87%)	690 (93%)	46 (6%)	3 (0%)	30	61
1	B	739/848 (87%)	690 (93%)	46 (6%)	3 (0%)	30	61
1	C	739/848 (87%)	690 (93%)	46 (6%)	3 (0%)	30	61
1	D	739/848 (87%)	691 (94%)	45 (6%)	3 (0%)	30	61
All	All	2956/3392 (87%)	2761 (93%)	183 (6%)	12 (0%)	31	61

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	PRO
1	A	772	PRO
1	B	371	PRO
1	B	772	PRO
1	C	371	PRO
1	C	772	PRO
1	D	371	PRO
1	D	772	PRO
1	A	582	VAL
1	B	582	VAL
1	C	582	VAL
1	D	582	VAL

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	657/754 (87%)	646 (98%)	11 (2%)	53	74
1	B	657/754 (87%)	646 (98%)	11 (2%)	53	74
1	C	657/754 (87%)	646 (98%)	11 (2%)	53	74
1	D	657/754 (87%)	646 (98%)	11 (2%)	53	74
All	All	2628/3016 (87%)	2584 (98%)	44 (2%)	52	74

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PHE
1	A	477	LEU
1	A	526	ARG
1	A	586	MET
1	A	619	LYS
1	A	641	LYS
1	A	665	MET
1	A	666	LEU
1	A	669	MET
1	A	674	TYR
1	A	709	LEU
1	B	27	PHE
1	B	477	LEU
1	B	526	ARG
1	B	586	MET
1	B	619	LYS
1	B	641	LYS
1	B	665	MET
1	B	666	LEU
1	B	669	MET
1	B	674	TYR
1	B	709	LEU
1	C	27	PHE
1	C	477	LEU
1	C	526	ARG
1	C	586	MET
1	C	619	LYS
1	C	641	LYS
1	C	665	MET
1	C	666	LEU
1	C	669	MET
1	C	674	TYR
1	C	709	LEU
1	D	27	PHE
1	D	477	LEU
1	D	526	ARG
1	D	586	MET
1	D	619	LYS
1	D	641	LYS
1	D	665	MET
1	D	666	LEU
1	D	669	MET
1	D	674	TYR

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Mol	Chain	Res	Type
1	D	709	LEU

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

Mol	Chain	Res	Type
1	D	84	ASN
1	D	327	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)

12 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	$\#\|Z\| > 2$
2	CPL	B	901	-	49,49,51	0.31	0	55,57,59	0.33	0
2	CPL	D	901	-	40,40,51	0.35	0	46,48,59	0.34	0
2	CPL	A	903	-	48,48,51	0.30	0	54,56,59	0.35	0
2	CPL	A	902	-	40,40,51	0.35	0	46,48,59	0.34	0
2	CPL	D	902	-	48,48,51	0.30	0	54,56,59	0.35	0
2	CPL	B	903	-	48,48,51	0.30	0	54,56,59	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CPL	C	903	-	48,48,51	0.30	0	54,56,59	0.35	0
2	CPL	A	901	-	49,49,51	0.30	0	55,57,59	0.33	0
2	CPL	C	901	-	49,49,51	0.30	0	55,57,59	0.33	0
2	CPL	D	903	-	49,49,51	0.31	0	55,57,59	0.33	0
2	CPL	C	902	-	40,40,51	0.35	0	46,48,59	0.34	0
2	CPL	B	902	-	40,40,51	0.35	0	46,48,59	0.34	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
2	CPL	B	901	-	-	33/53/53/55	-
2	CPL	D	901	-	-	28/44/44/55	-
2	CPL	A	903	-	-	34/52/52/55	-
2	CPL	A	902	-	-	28/44/44/55	-
2	CPL	D	902	-	-	34/52/52/55	-
2	CPL	B	903	-	-	34/52/52/55	-
2	CPL	C	903	-	-	34/52/52/55	-
2	CPL	A	901	-	-	33/53/53/55	-
2	CPL	C	901	-	-	33/53/53/55	-
2	CPL	D	903	-	-	33/53/53/55	-
2	CPL	C	902	-	-	28/44/44/55	-
2	CPL	B	902	-	-	28/44/44/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (380) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	CPL	C1-O3P-P-O1P
2	A	901	CPL	C1-O3P-P-O2P
2	A	901	CPL	C1-O3P-P-O4P
2	A	901	CPL	C4-O4P-P-O1P
2	A	901	CPL	C4-O4P-P-O2P
2	A	901	CPL	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	A	902	CPL	C1-O3P-P-O1P
2	A	902	CPL	C1-O3P-P-O2P
2	A	902	CPL	C1-O3P-P-O4P
2	A	902	CPL	C4-O4P-P-O1P
2	A	902	CPL	C4-O4P-P-O3P
2	A	903	CPL	C2-C1-O3P-P
2	A	903	CPL	O4P-C4-C5-N
2	A	903	CPL	C32-C31-O2-C2
2	A	903	CPL	O31-C31-O2-C2
2	A	903	CPL	C1-O3P-P-O4P
2	A	903	CPL	C4-O4P-P-O3P
2	B	901	CPL	C1-O3P-P-O1P
2	B	901	CPL	C1-O3P-P-O2P
2	B	901	CPL	C1-O3P-P-O4P
2	B	901	CPL	C4-O4P-P-O1P
2	B	901	CPL	C4-O4P-P-O2P
2	B	901	CPL	C4-O4P-P-O3P
2	B	902	CPL	C1-O3P-P-O1P
2	B	902	CPL	C1-O3P-P-O2P
2	B	902	CPL	C1-O3P-P-O4P
2	B	902	CPL	C4-O4P-P-O1P
2	B	902	CPL	C4-O4P-P-O3P
2	B	903	CPL	C2-C1-O3P-P
2	B	903	CPL	O4P-C4-C5-N
2	B	903	CPL	C32-C31-O2-C2
2	B	903	CPL	O31-C31-O2-C2
2	B	903	CPL	C1-O3P-P-O4P
2	B	903	CPL	C4-O4P-P-O3P
2	C	901	CPL	C1-O3P-P-O1P
2	C	901	CPL	C1-O3P-P-O2P
2	C	901	CPL	C1-O3P-P-O4P
2	C	901	CPL	C4-O4P-P-O1P
2	C	901	CPL	C4-O4P-P-O2P
2	C	901	CPL	C4-O4P-P-O3P
2	C	902	CPL	C1-O3P-P-O1P
2	C	902	CPL	C1-O3P-P-O2P
2	C	902	CPL	C1-O3P-P-O4P
2	C	902	CPL	C4-O4P-P-O1P
2	C	902	CPL	C4-O4P-P-O3P
2	C	903	CPL	C2-C1-O3P-P
2	C	903	CPL	O4P-C4-C5-N
2	C	903	CPL	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
2	C	903	CPL	O31-C31-O2-C2
2	C	903	CPL	C1-O3P-P-O4P
2	C	903	CPL	C4-O4P-P-O3P
2	D	901	CPL	C1-O3P-P-O1P
2	D	901	CPL	C1-O3P-P-O2P
2	D	901	CPL	C1-O3P-P-O4P
2	D	901	CPL	C4-O4P-P-O1P
2	D	901	CPL	C4-O4P-P-O3P
2	D	902	CPL	C2-C1-O3P-P
2	D	902	CPL	O4P-C4-C5-N
2	D	902	CPL	C32-C31-O2-C2
2	D	902	CPL	O31-C31-O2-C2
2	D	902	CPL	C1-O3P-P-O4P
2	D	902	CPL	C4-O4P-P-O3P
2	D	903	CPL	C1-O3P-P-O1P
2	D	903	CPL	C1-O3P-P-O2P
2	D	903	CPL	C1-O3P-P-O4P
2	D	903	CPL	C4-O4P-P-O1P
2	D	903	CPL	C4-O4P-P-O2P
2	D	903	CPL	C4-O4P-P-O3P
2	A	901	CPL	O11-C11-O3-C3
2	A	902	CPL	O11-C11-O3-C3
2	B	901	CPL	O11-C11-O3-C3
2	B	902	CPL	O11-C11-O3-C3
2	C	901	CPL	O11-C11-O3-C3
2	C	902	CPL	O11-C11-O3-C3
2	D	901	CPL	O11-C11-O3-C3
2	D	903	CPL	O11-C11-O3-C3
2	A	901	CPL	C12-C11-O3-C3
2	B	901	CPL	C12-C11-O3-C3
2	C	901	CPL	C12-C11-O3-C3
2	D	903	CPL	C12-C11-O3-C3
2	A	902	CPL	C12-C11-O3-C3
2	A	903	CPL	C12-C11-O3-C3
2	B	902	CPL	C12-C11-O3-C3
2	B	903	CPL	C12-C11-O3-C3
2	C	902	CPL	C12-C11-O3-C3
2	C	903	CPL	C12-C11-O3-C3
2	D	901	CPL	C12-C11-O3-C3
2	D	902	CPL	C12-C11-O3-C3
2	A	903	CPL	O11-C11-O3-C3
2	B	903	CPL	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	C	903	CPL	O11-C11-O3-C3
2	D	902	CPL	O11-C11-O3-C3
2	A	902	CPL	C33-C34-C35-C36
2	B	902	CPL	C33-C34-C35-C36
2	C	902	CPL	C33-C34-C35-C36
2	D	901	CPL	C33-C34-C35-C36
2	A	903	CPL	C38-C39-C40-C41
2	A	903	CPL	C41-C42-C43-C44
2	B	903	CPL	C38-C39-C40-C41
2	B	903	CPL	C41-C42-C43-C44
2	C	903	CPL	C38-C39-C40-C41
2	C	903	CPL	C41-C42-C43-C44
2	D	902	CPL	C38-C39-C40-C41
2	D	902	CPL	C41-C42-C43-C44
2	A	903	CPL	C15-C16-C17-C18
2	B	903	CPL	C15-C16-C17-C18
2	C	903	CPL	C15-C16-C17-C18
2	D	902	CPL	C15-C16-C17-C18
2	A	901	CPL	C33-C34-C35-C36
2	B	901	CPL	C33-C34-C35-C36
2	C	901	CPL	C33-C34-C35-C36
2	A	903	CPL	C21-C22-C23-C24
2	B	903	CPL	C21-C22-C23-C24
2	C	903	CPL	C21-C22-C23-C24
2	D	902	CPL	C21-C22-C23-C24
2	D	903	CPL	C33-C34-C35-C36
2	A	901	CPL	C16-C17-C18-C19
2	A	901	CPL	C18-C19-C20-C21
2	A	903	CPL	C33-C34-C35-C36
2	B	901	CPL	C16-C17-C18-C19
2	B	901	CPL	C18-C19-C20-C21
2	B	903	CPL	C33-C34-C35-C36
2	C	901	CPL	C16-C17-C18-C19
2	C	901	CPL	C18-C19-C20-C21
2	C	903	CPL	C33-C34-C35-C36
2	D	902	CPL	C33-C34-C35-C36
2	D	903	CPL	C16-C17-C18-C19
2	D	903	CPL	C18-C19-C20-C21
2	A	903	CPL	C4-C5-N-C7
2	B	903	CPL	C4-C5-N-C7
2	C	903	CPL	C4-C5-N-C7
2	D	902	CPL	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
2	A	902	CPL	C35-C36-C37-C38
2	D	901	CPL	C35-C36-C37-C38
2	B	902	CPL	C35-C36-C37-C38
2	C	902	CPL	C35-C36-C37-C38
2	A	902	CPL	C4-C5-N-C6
2	A	902	CPL	C4-C5-N-C7
2	A	902	CPL	C4-C5-N-C8
2	A	903	CPL	C4-C5-N-C6
2	B	902	CPL	C4-C5-N-C6
2	B	902	CPL	C4-C5-N-C7
2	B	902	CPL	C4-C5-N-C8
2	B	903	CPL	C4-C5-N-C6
2	C	902	CPL	C4-C5-N-C6
2	C	902	CPL	C4-C5-N-C7
2	C	902	CPL	C4-C5-N-C8
2	C	903	CPL	C4-C5-N-C6
2	D	901	CPL	C4-C5-N-C6
2	D	901	CPL	C4-C5-N-C7
2	D	901	CPL	C4-C5-N-C8
2	D	902	CPL	C4-C5-N-C6
2	B	901	CPL	C20-C21-C22-C23
2	D	903	CPL	C20-C21-C22-C23
2	A	901	CPL	C20-C21-C22-C23
2	C	901	CPL	C20-C21-C22-C23
2	A	901	CPL	C31-C32-C33-C34
2	B	901	CPL	C31-C32-C33-C34
2	A	901	CPL	C32-C31-O2-C2
2	B	901	CPL	C32-C31-O2-C2
2	C	901	CPL	C32-C31-O2-C2
2	D	903	CPL	C32-C31-O2-C2
2	A	901	CPL	O31-C31-O2-C2
2	B	901	CPL	O31-C31-O2-C2
2	C	901	CPL	O31-C31-O2-C2
2	D	903	CPL	O31-C31-O2-C2
2	C	901	CPL	C31-C32-C33-C34
2	D	903	CPL	C31-C32-C33-C34
2	A	901	CPL	C43-C44-C45-C46
2	B	901	CPL	C43-C44-C45-C46
2	C	901	CPL	C43-C44-C45-C46
2	D	903	CPL	C43-C44-C45-C46
2	A	903	CPL	C4-C5-N-C8
2	B	903	CPL	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
2	C	903	CPL	C4-C5-N-C8
2	D	902	CPL	C4-C5-N-C8
2	A	903	CPL	C32-C33-C34-C35
2	B	903	CPL	C32-C33-C34-C35
2	C	903	CPL	C32-C33-C34-C35
2	D	902	CPL	C32-C33-C34-C35
2	A	903	CPL	C11-C12-C13-C14
2	B	903	CPL	C11-C12-C13-C14
2	C	903	CPL	C11-C12-C13-C14
2	D	902	CPL	C11-C12-C13-C14
2	A	901	CPL	C38-C39-C40-C41
2	B	901	CPL	C38-C39-C40-C41
2	C	901	CPL	C38-C39-C40-C41
2	D	903	CPL	C38-C39-C40-C41
2	A	901	CPL	C15-C16-C17-C18
2	B	901	CPL	C15-C16-C17-C18
2	C	901	CPL	C15-C16-C17-C18
2	D	903	CPL	C15-C16-C17-C18
2	A	901	CPL	C35-C36-C37-C38
2	B	901	CPL	C35-C36-C37-C38
2	C	901	CPL	C35-C36-C37-C38
2	D	903	CPL	C35-C36-C37-C38
2	A	901	CPL	C11-C12-C13-C14
2	B	901	CPL	C11-C12-C13-C14
2	C	901	CPL	C11-C12-C13-C14
2	D	903	CPL	C11-C12-C13-C14
2	A	903	CPL	C34-C35-C36-C37
2	C	903	CPL	C34-C35-C36-C37
2	D	902	CPL	C34-C35-C36-C37
2	B	903	CPL	C34-C35-C36-C37
2	A	903	CPL	C13-C14-C15-C16
2	B	903	CPL	C13-C14-C15-C16
2	C	903	CPL	C13-C14-C15-C16
2	D	902	CPL	C13-C14-C15-C16
2	B	902	CPL	C32-C31-O2-C2
2	D	901	CPL	C32-C31-O2-C2
2	A	901	CPL	C36-C37-C38-C39
2	B	901	CPL	C36-C37-C38-C39
2	C	901	CPL	C36-C37-C38-C39
2	D	903	CPL	C36-C37-C38-C39
2	A	902	CPL	O3P-C1-C2-C3
2	B	902	CPL	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	902	CPL	O3P-C1-C2-C3
2	D	901	CPL	O3P-C1-C2-C3
2	A	901	CPL	C13-C14-C15-C16
2	D	903	CPL	C13-C14-C15-C16
2	B	901	CPL	C13-C14-C15-C16
2	C	901	CPL	C13-C14-C15-C16
2	A	902	CPL	C32-C31-O2-C2
2	C	902	CPL	C32-C31-O2-C2
2	A	903	CPL	C19-C20-C21-C22
2	B	903	CPL	C19-C20-C21-C22
2	C	903	CPL	C19-C20-C21-C22
2	D	902	CPL	C19-C20-C21-C22
2	A	903	CPL	C16-C17-C18-C19
2	C	903	CPL	C16-C17-C18-C19
2	D	902	CPL	C16-C17-C18-C19
2	B	903	CPL	C16-C17-C18-C19
2	B	903	CPL	C12-C13-C14-C15
2	A	903	CPL	C12-C13-C14-C15
2	C	903	CPL	C12-C13-C14-C15
2	D	902	CPL	C12-C13-C14-C15
2	A	902	CPL	C32-C33-C34-C35
2	B	902	CPL	C32-C33-C34-C35
2	C	902	CPL	C32-C33-C34-C35
2	D	901	CPL	C32-C33-C34-C35
2	A	902	CPL	C37-C38-C39-C40
2	B	902	CPL	C37-C38-C39-C40
2	C	902	CPL	C37-C38-C39-C40
2	D	901	CPL	C37-C38-C39-C40
2	A	901	CPL	O2-C2-C3-O3
2	B	901	CPL	O2-C2-C3-O3
2	C	901	CPL	O2-C2-C3-O3
2	D	903	CPL	O2-C2-C3-O3
2	A	902	CPL	C40-C41-C42-C43
2	B	902	CPL	C40-C41-C42-C43
2	C	902	CPL	C40-C41-C42-C43
2	D	901	CPL	C40-C41-C42-C43
2	A	902	CPL	O31-C31-O2-C2
2	B	902	CPL	O31-C31-O2-C2
2	C	902	CPL	O31-C31-O2-C2
2	D	901	CPL	O31-C31-O2-C2
2	A	902	CPL	O3P-C1-C2-O2
2	A	903	CPL	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	902	CPL	O3P-C1-C2-O2
2	B	903	CPL	O3P-C1-C2-O2
2	C	902	CPL	O3P-C1-C2-O2
2	C	903	CPL	O3P-C1-C2-O2
2	D	901	CPL	O3P-C1-C2-O2
2	D	902	CPL	O3P-C1-C2-O2
2	A	903	CPL	C5-C4-O4P-P
2	B	903	CPL	C5-C4-O4P-P
2	C	903	CPL	C5-C4-O4P-P
2	D	902	CPL	C5-C4-O4P-P
2	A	901	CPL	C41-C42-C43-C44
2	B	901	CPL	C41-C42-C43-C44
2	C	901	CPL	C41-C42-C43-C44
2	D	903	CPL	C41-C42-C43-C44
2	A	901	CPL	O4P-C4-C5-N
2	A	902	CPL	O4P-C4-C5-N
2	B	901	CPL	O4P-C4-C5-N
2	B	902	CPL	O4P-C4-C5-N
2	C	901	CPL	O4P-C4-C5-N
2	C	902	CPL	O4P-C4-C5-N
2	D	901	CPL	O4P-C4-C5-N
2	D	903	CPL	O4P-C4-C5-N
2	A	903	CPL	O3P-C1-C2-C3
2	B	903	CPL	O3P-C1-C2-C3
2	C	903	CPL	O3P-C1-C2-C3
2	D	902	CPL	O3P-C1-C2-C3
2	A	903	CPL	O2-C2-C3-O3
2	B	903	CPL	O2-C2-C3-O3
2	C	903	CPL	O2-C2-C3-O3
2	D	902	CPL	O2-C2-C3-O3
2	A	903	CPL	C1-C2-C3-O3
2	B	903	CPL	C1-C2-C3-O3
2	C	903	CPL	C1-C2-C3-O3
2	D	902	CPL	C1-C2-C3-O3
2	A	902	CPL	C4-O4P-P-O2P
2	A	903	CPL	C1-O3P-P-O1P
2	A	903	CPL	C4-O4P-P-O1P
2	B	902	CPL	C4-O4P-P-O2P
2	B	903	CPL	C1-O3P-P-O1P
2	B	903	CPL	C4-O4P-P-O1P
2	C	902	CPL	C4-O4P-P-O2P
2	C	903	CPL	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
2	C	903	CPL	C4-O4P-P-O1P
2	D	901	CPL	C4-O4P-P-O2P
2	D	902	CPL	C1-O3P-P-O1P
2	D	902	CPL	C4-O4P-P-O1P
2	A	901	CPL	C3-C2-O2-C31
2	B	901	CPL	C3-C2-O2-C31
2	C	901	CPL	C3-C2-O2-C31
2	D	903	CPL	C3-C2-O2-C31
2	B	901	CPL	C14-C15-C16-C17
2	D	903	CPL	C14-C15-C16-C17
2	A	901	CPL	C14-C15-C16-C17
2	C	901	CPL	C14-C15-C16-C17
2	A	901	CPL	C32-C33-C34-C35
2	C	901	CPL	C32-C33-C34-C35
2	D	903	CPL	C32-C33-C34-C35
2	B	901	CPL	C32-C33-C34-C35
2	A	901	CPL	C1-C2-O2-C31
2	B	901	CPL	C1-C2-O2-C31
2	C	901	CPL	C1-C2-O2-C31
2	D	903	CPL	C1-C2-O2-C31
2	A	903	CPL	C40-C41-C42-C43
2	B	903	CPL	C40-C41-C42-C43
2	C	903	CPL	C40-C41-C42-C43
2	D	902	CPL	C40-C41-C42-C43
2	A	902	CPL	C2-C1-O3P-P
2	B	902	CPL	C2-C1-O3P-P
2	C	902	CPL	C2-C1-O3P-P
2	D	901	CPL	C2-C1-O3P-P
2	A	902	CPL	C12-C13-C14-C15
2	C	902	CPL	C12-C13-C14-C15
2	B	902	CPL	C12-C13-C14-C15
2	D	901	CPL	C12-C13-C14-C15
2	A	903	CPL	C22-C23-C24-C25
2	B	903	CPL	C22-C23-C24-C25
2	D	902	CPL	C22-C23-C24-C25
2	C	903	CPL	C22-C23-C24-C25
2	A	902	CPL	C42-C43-C44-C45
2	B	902	CPL	C42-C43-C44-C45
2	C	902	CPL	C42-C43-C44-C45
2	D	901	CPL	C42-C43-C44-C45
2	A	901	CPL	C1-C2-C3-O3
2	B	901	CPL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	901	CPL	C1-C2-C3-O3
2	D	903	CPL	C1-C2-C3-O3
2	D	901	CPL	O2-C31-C32-C33
2	C	902	CPL	O2-C31-C32-C33
2	A	902	CPL	O2-C31-C32-C33
2	B	902	CPL	O2-C31-C32-C33
2	A	901	CPL	O3P-C1-C2-O2
2	B	901	CPL	O3P-C1-C2-O2
2	C	901	CPL	O3P-C1-C2-O2
2	D	903	CPL	O3P-C1-C2-O2
2	A	903	CPL	C42-C43-C44-C45
2	B	903	CPL	C42-C43-C44-C45
2	C	903	CPL	C42-C43-C44-C45
2	D	902	CPL	C42-C43-C44-C45
2	C	902	CPL	O31-C31-C32-C33
2	B	903	CPL	C18-C19-C20-C21
2	C	903	CPL	C18-C19-C20-C21
2	A	903	CPL	C18-C19-C20-C21
2	D	902	CPL	C18-C19-C20-C21
2	C	901	CPL	C23-C24-C25-C26
2	D	903	CPL	C23-C24-C25-C26
2	A	902	CPL	O31-C31-C32-C33
2	B	902	CPL	O31-C31-C32-C33
2	D	901	CPL	O31-C31-C32-C33
2	A	901	CPL	C23-C24-C25-C26
2	B	901	CPL	C23-C24-C25-C26
2	B	902	CPL	C45-C46-C47-C48
2	A	902	CPL	C45-C46-C47-C48
2	C	902	CPL	C45-C46-C47-C48
2	D	901	CPL	C45-C46-C47-C48
2	A	901	CPL	O2-C31-C32-C33
2	B	901	CPL	O2-C31-C32-C33
2	C	901	CPL	O2-C31-C32-C33
2	D	903	CPL	O2-C31-C32-C33
2	A	902	CPL	C38-C39-C40-C41
2	B	902	CPL	C38-C39-C40-C41
2	C	902	CPL	C38-C39-C40-C41
2	D	901	CPL	C38-C39-C40-C41

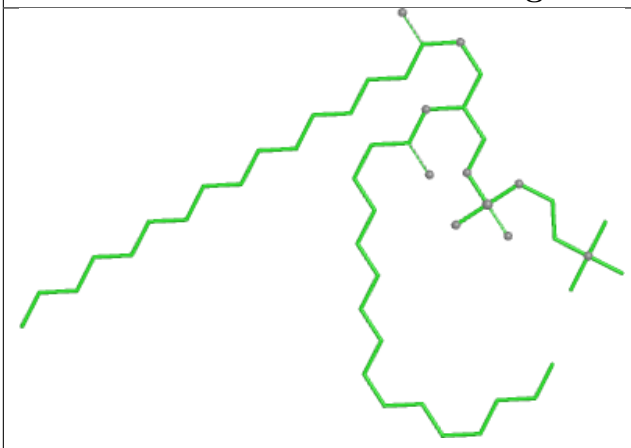
There are no ring outliers.

12 monomers are involved in 76 short contacts:

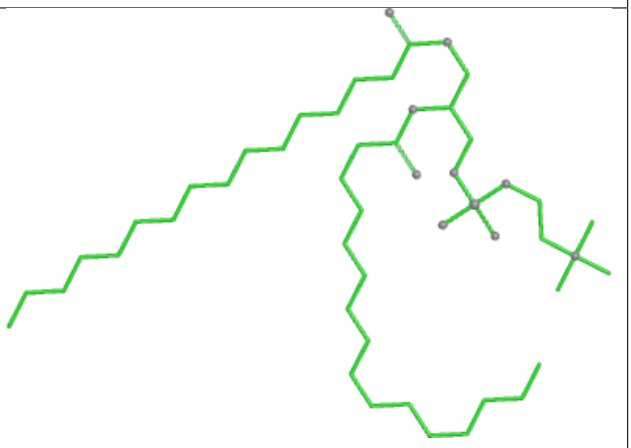
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	CPL	9	0
2	D	901	CPL	5	0
2	A	903	CPL	6	0
2	A	902	CPL	5	0
2	D	902	CPL	5	0
2	B	903	CPL	6	0
2	C	903	CPL	7	0
2	A	901	CPL	10	0
2	C	901	CPL	10	0
2	D	903	CPL	11	0
2	C	902	CPL	5	0
2	B	902	CPL	5	0

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

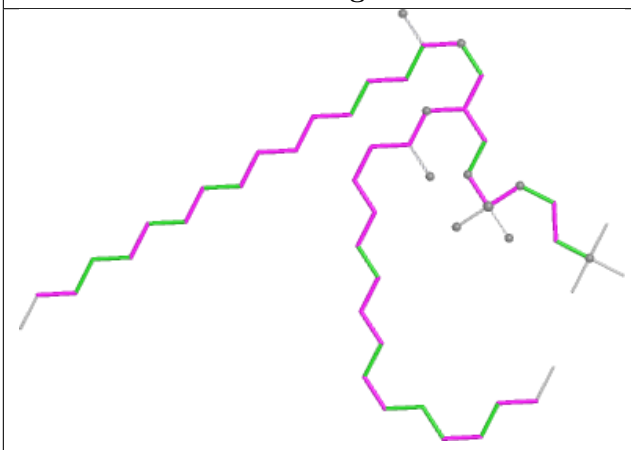
Ligand CPL B 901



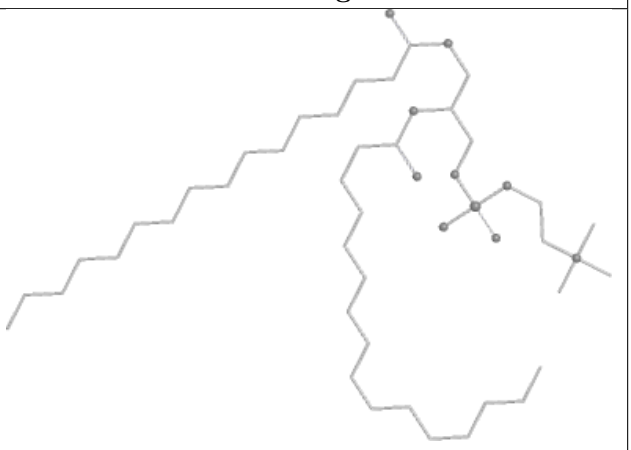
Bond lengths



Bond angles

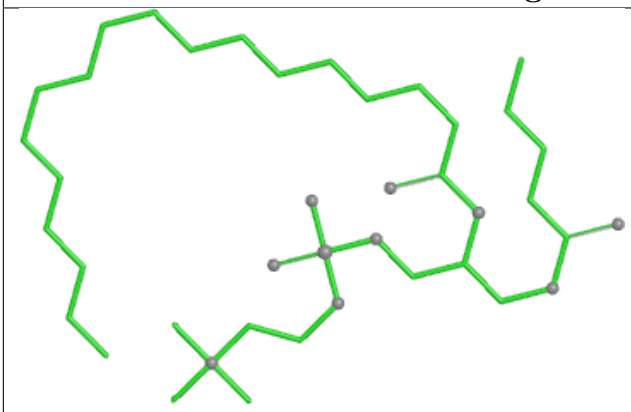


Torsions

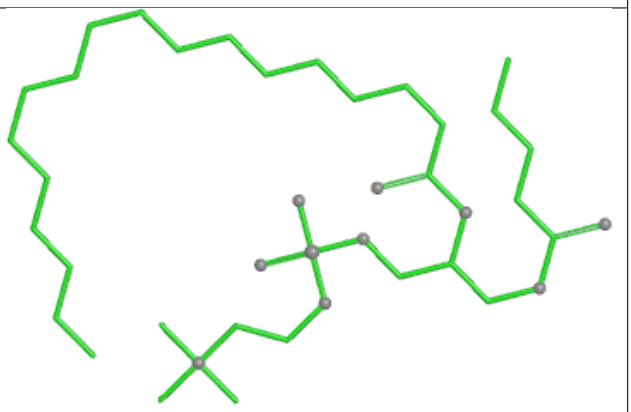


Rings

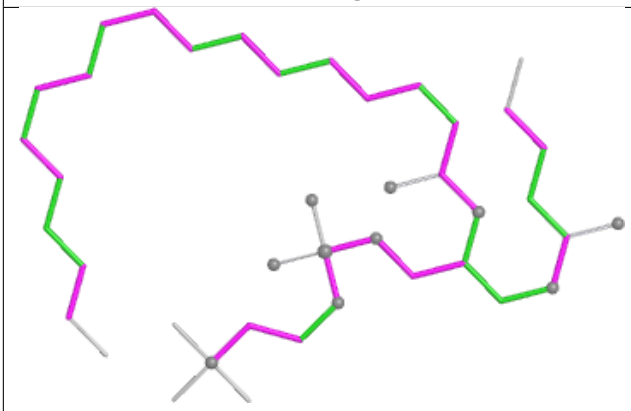
Ligand CPL D 901



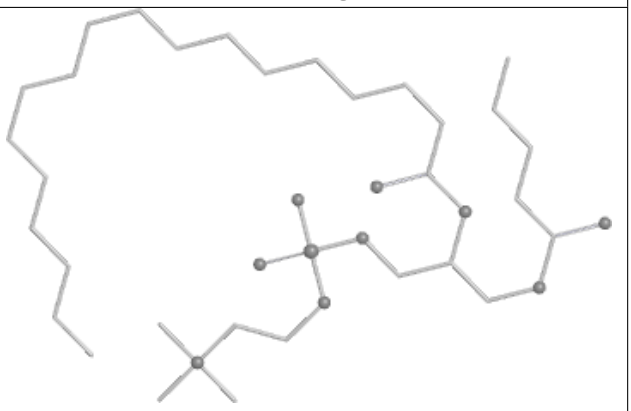
Bond lengths



Bond angles

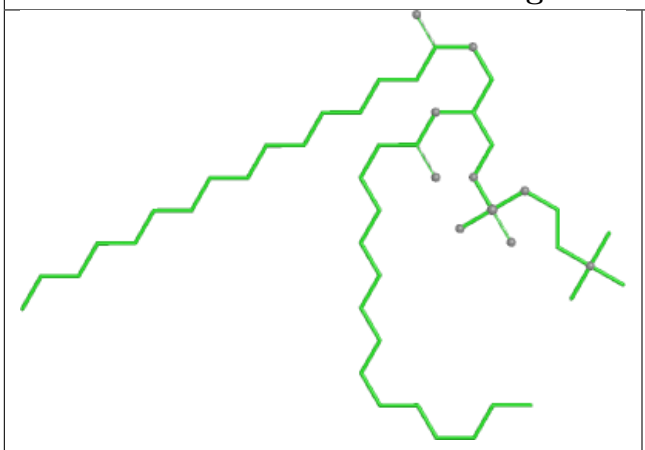


Torsions

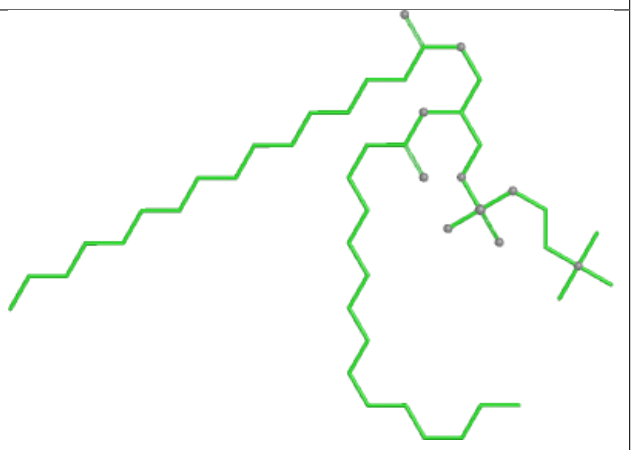


Rings

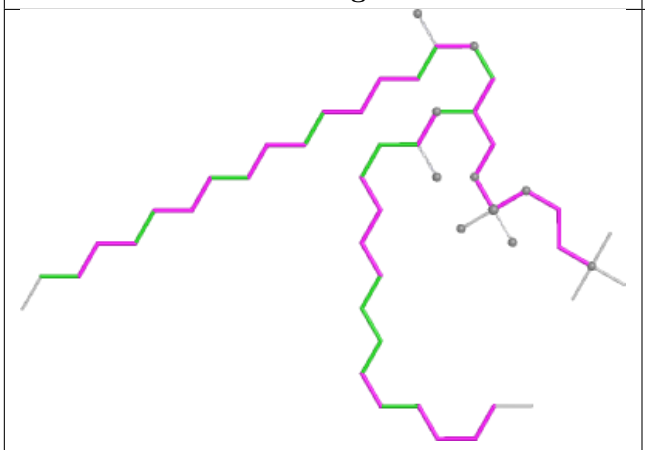
Ligand CPL A 903



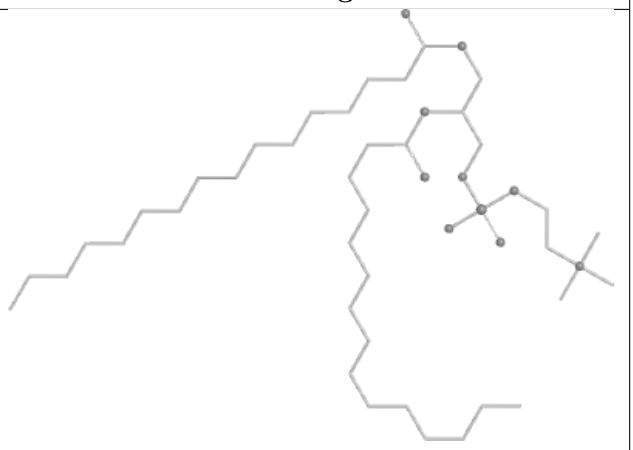
Bond lengths



Bond angles

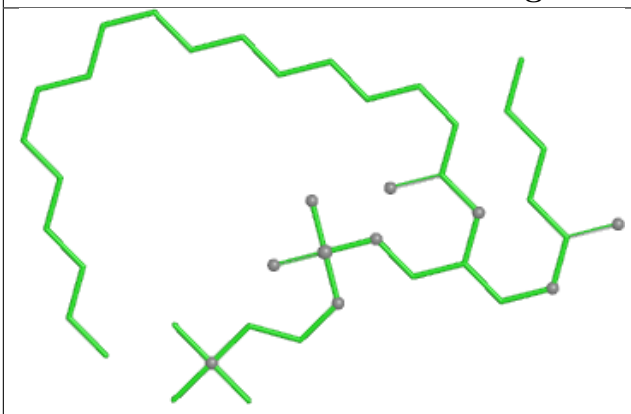


Torsions

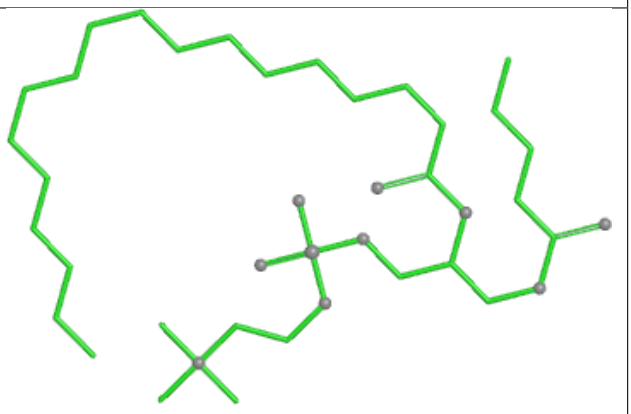


Rings

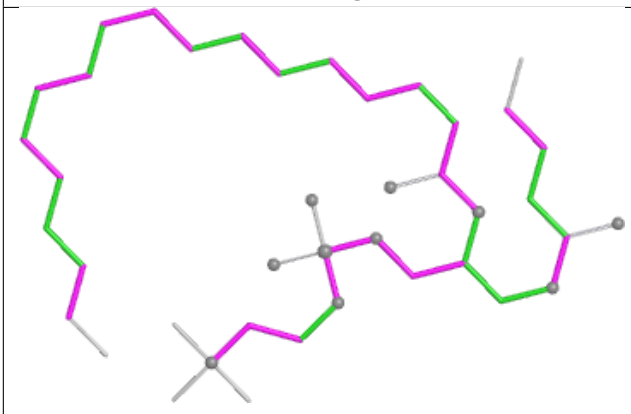
Ligand CPL A 902



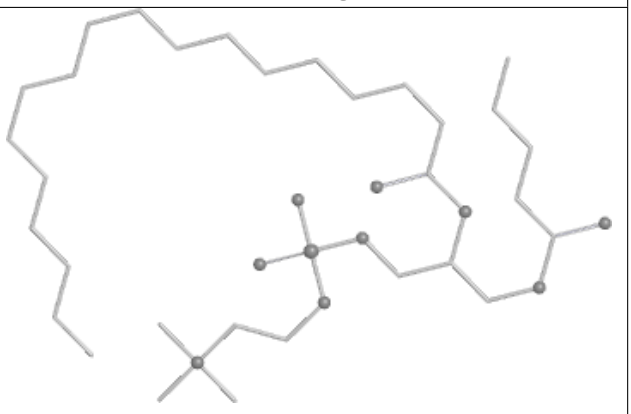
Bond lengths



Bond angles

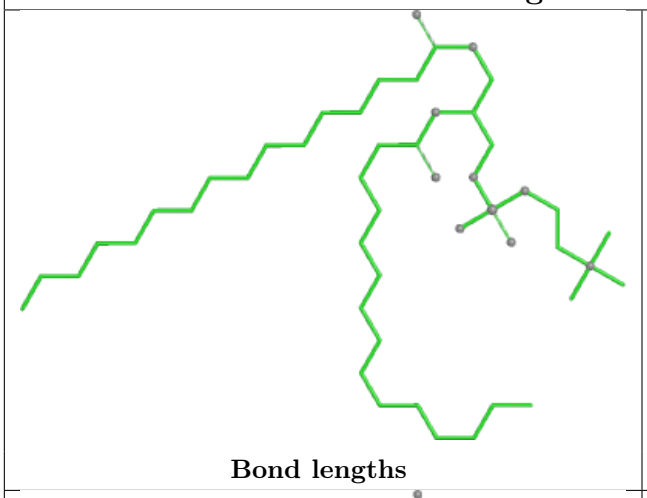


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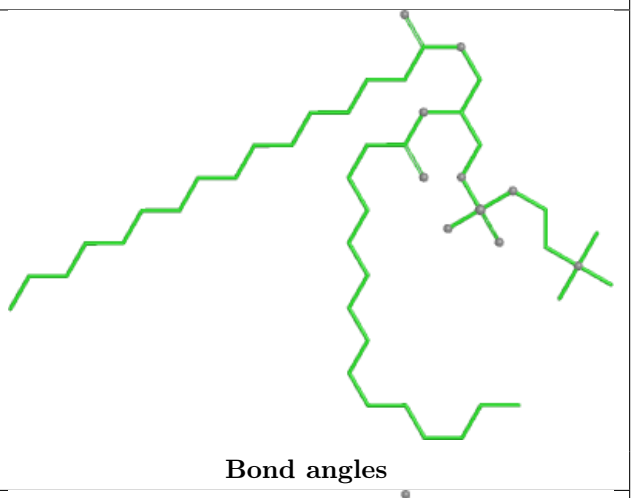


Rings

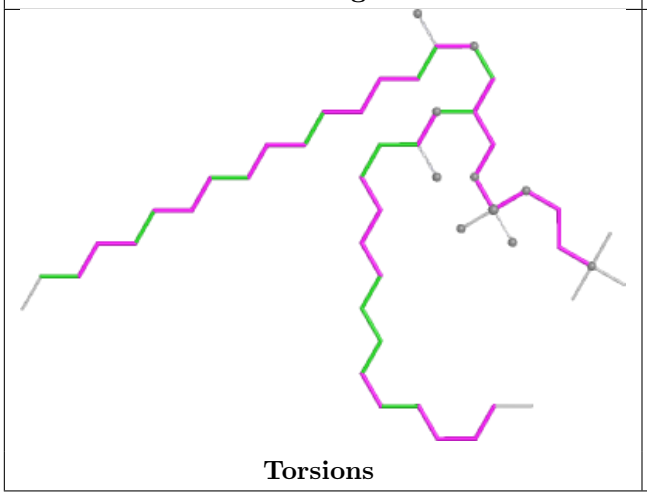
Ligand CPL D 902



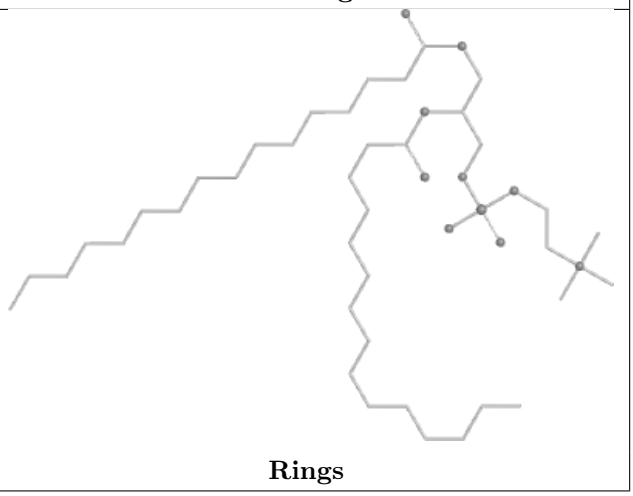
Bond lengths



Bond angles

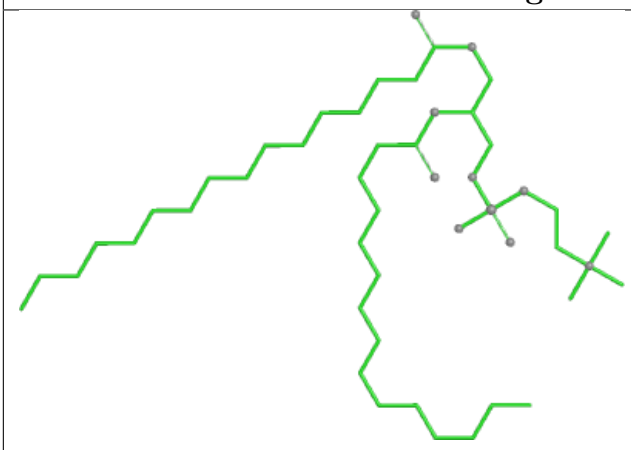


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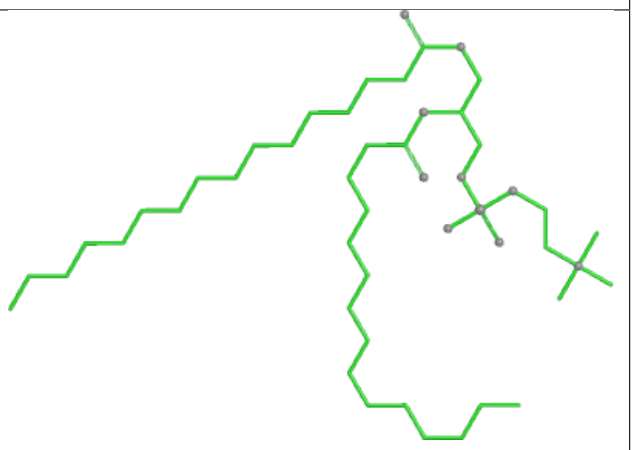


Rings

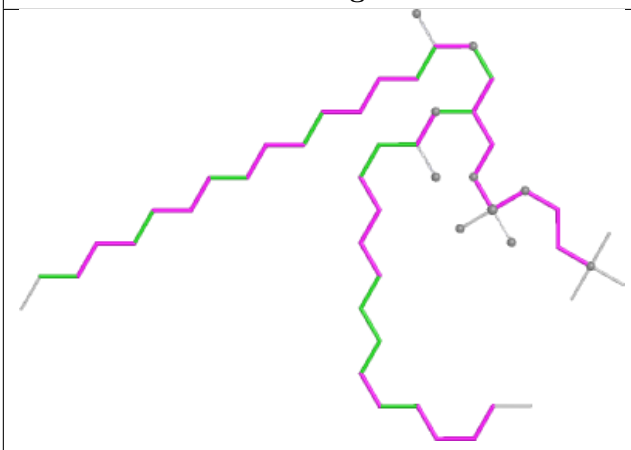
Ligand CPL B 903



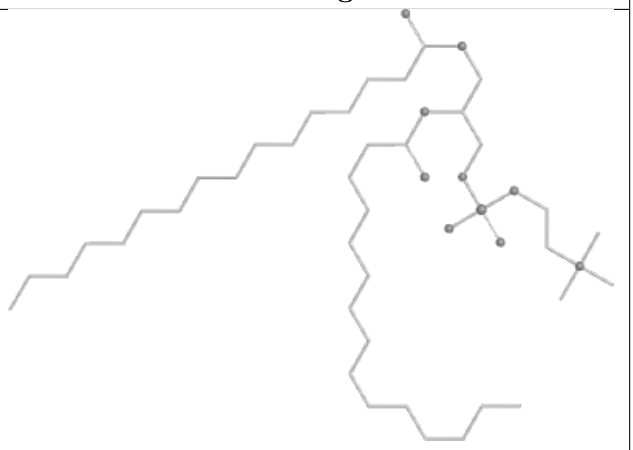
Bond lengths



Bond angles

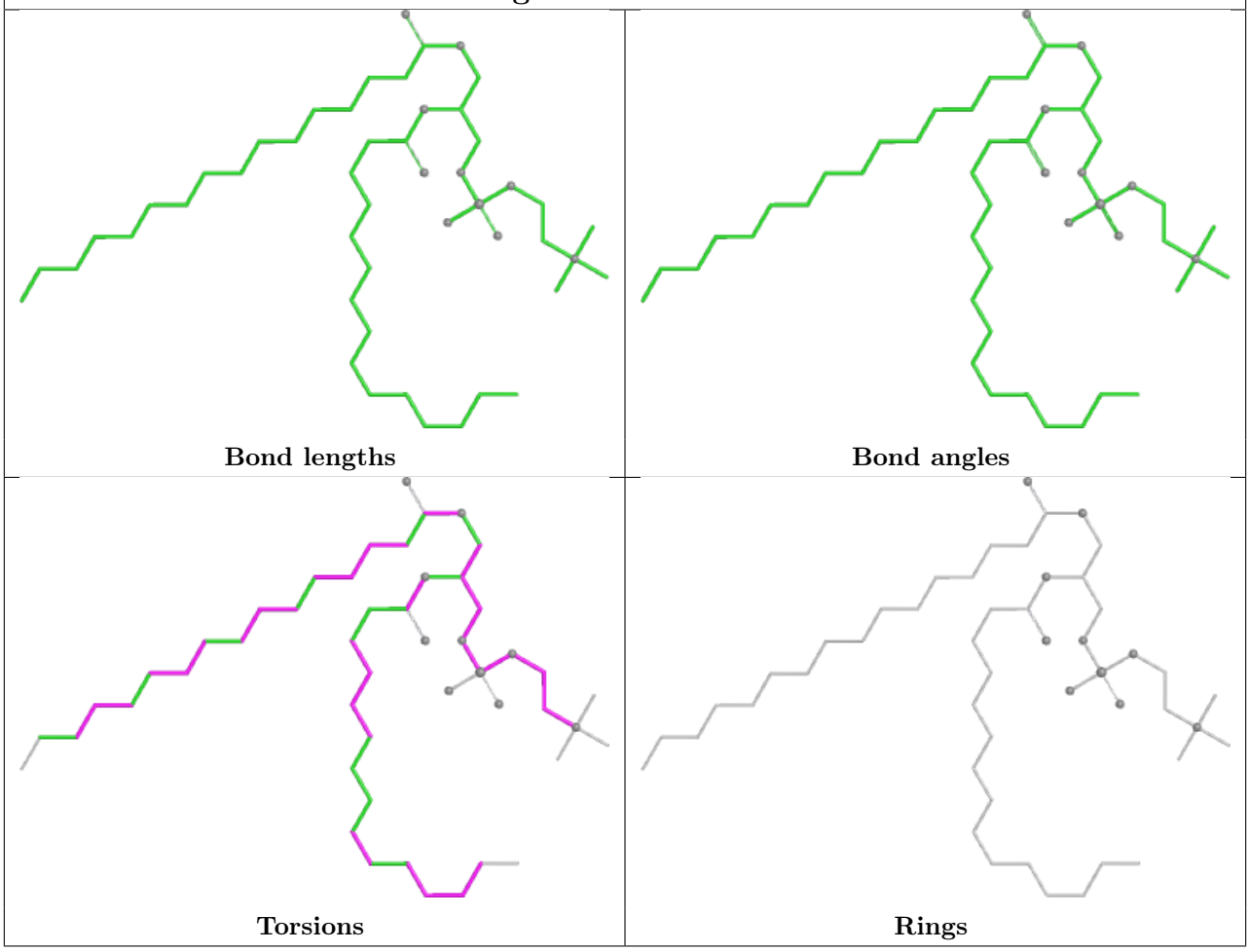


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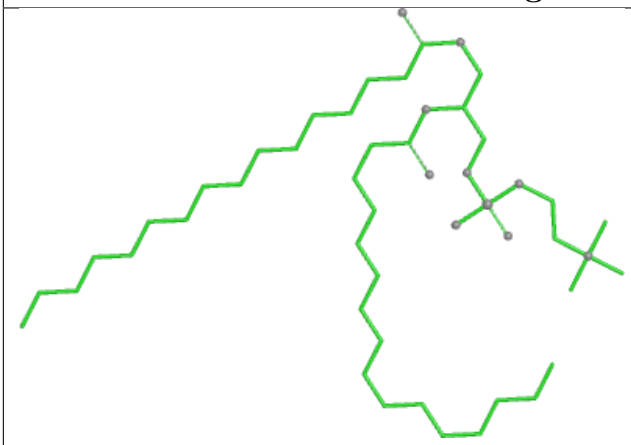


Rings

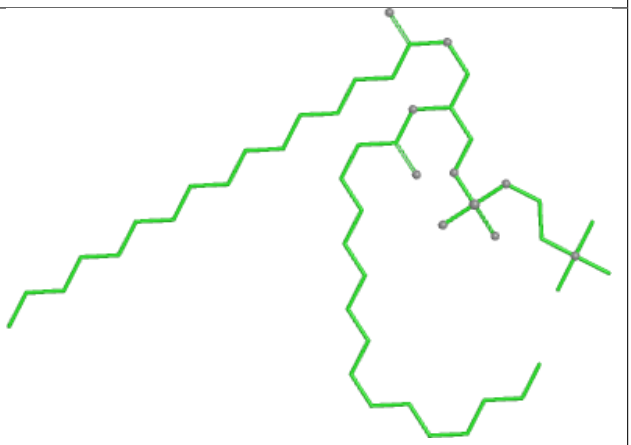
Ligand CPL C 903



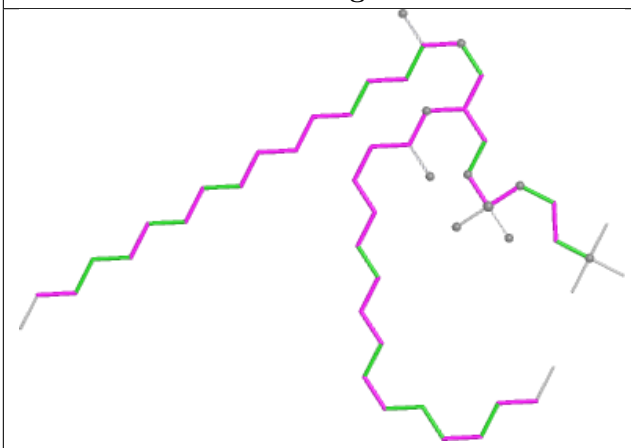
Ligand CPL A 901



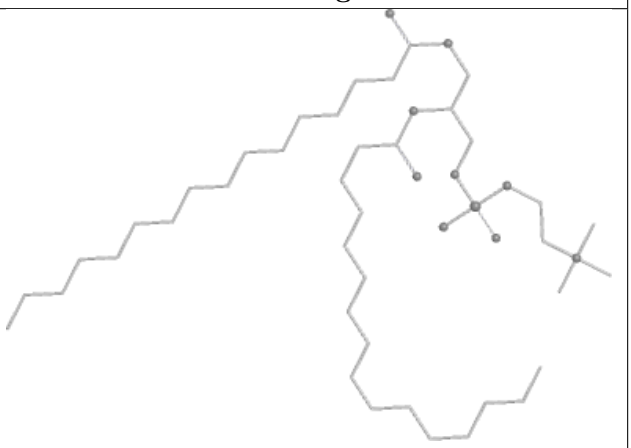
Bond lengths



Bond angles

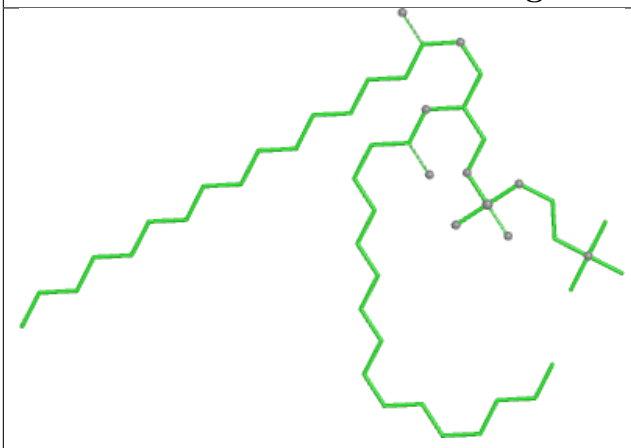


Torsions

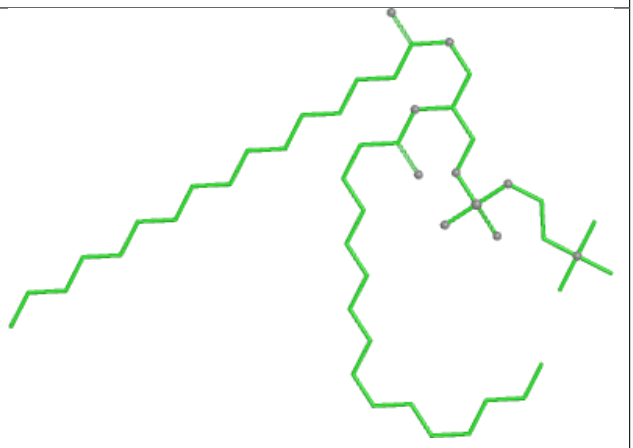


Rings

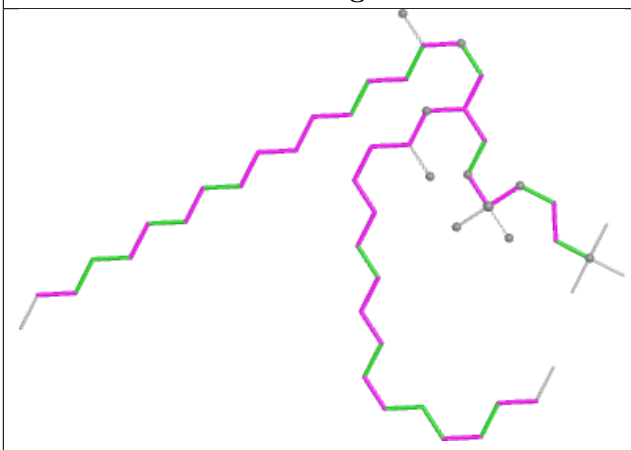
Ligand CPL C 901



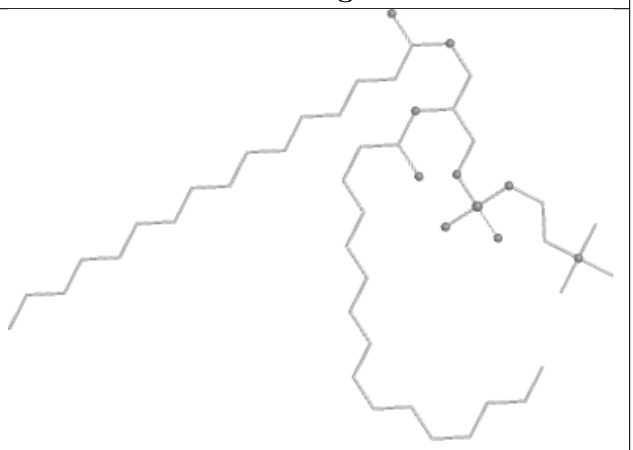
Bond lengths



Bond angles

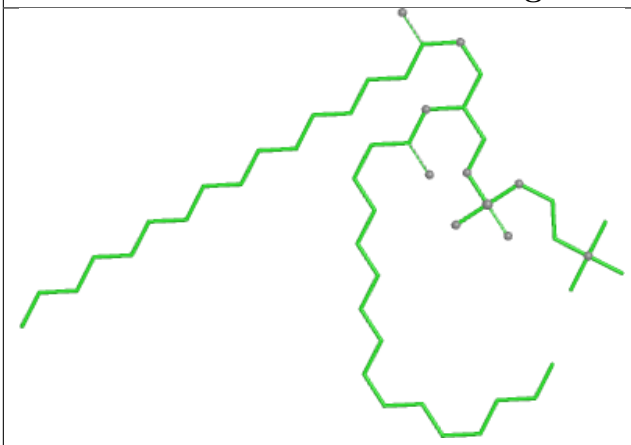


Torsions

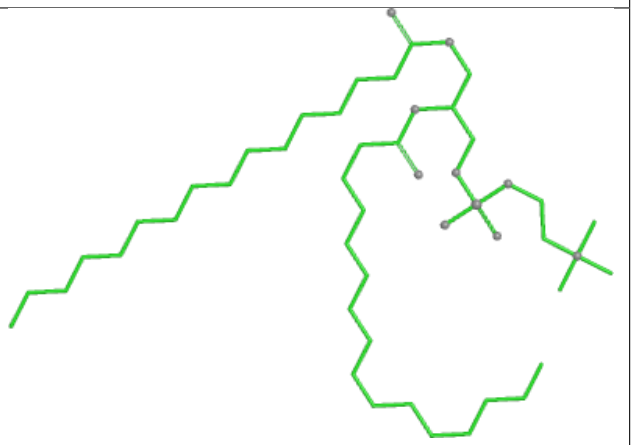


Rings

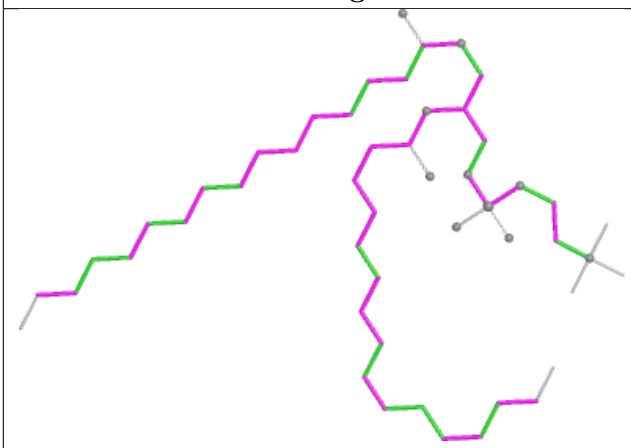
Ligand CPL D 903



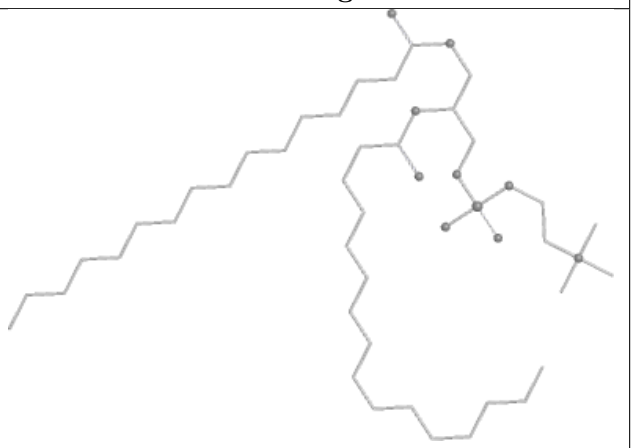
Bond lengths



Bond angles

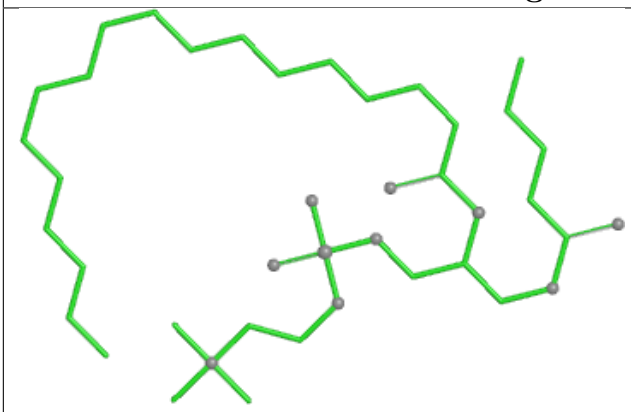


Torsions

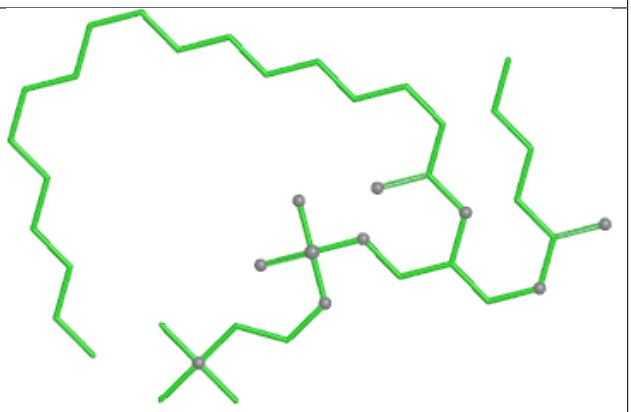


Rings

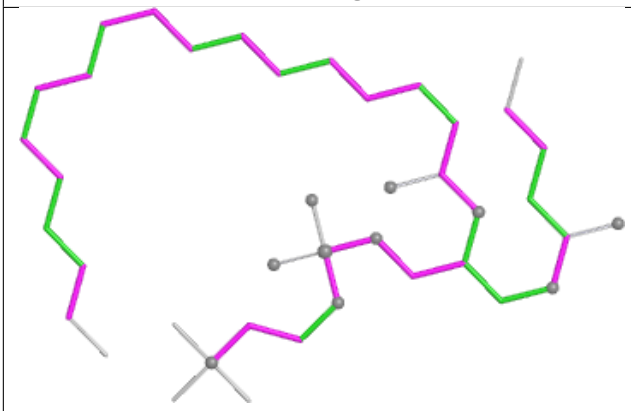
Ligand CPL C 902



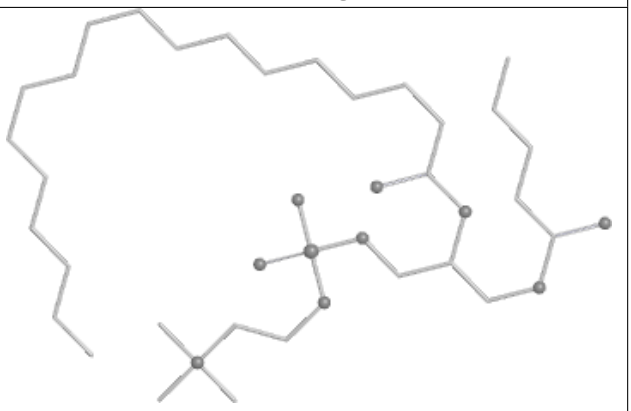
Bond lengths



Bond angles

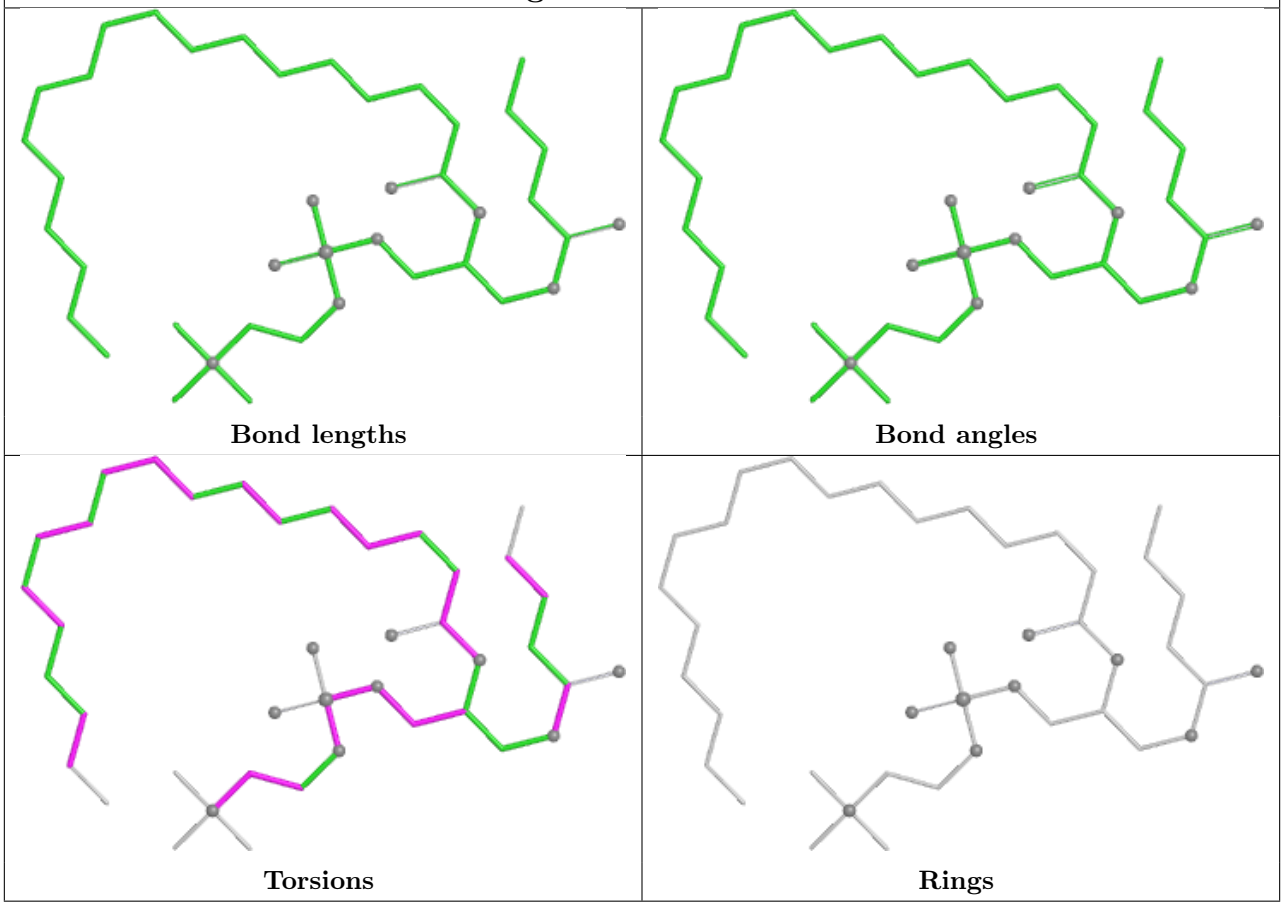


Torsions



Rings

Ligand CPL B 902



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.

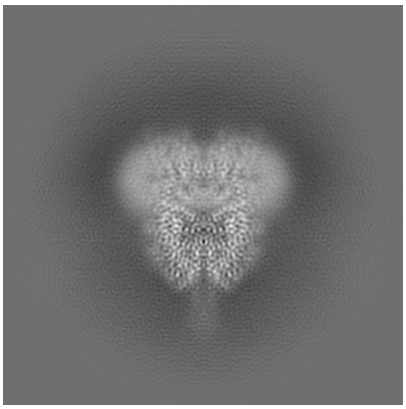
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70596. These allow visual inspection of the internal detail of the map and identification of artifacts.

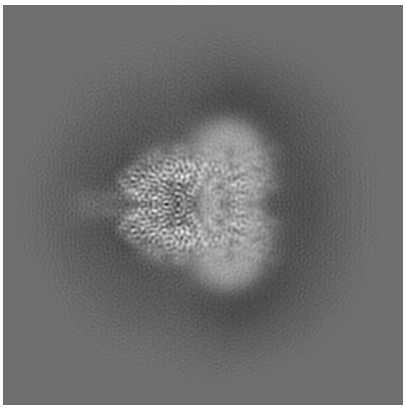
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

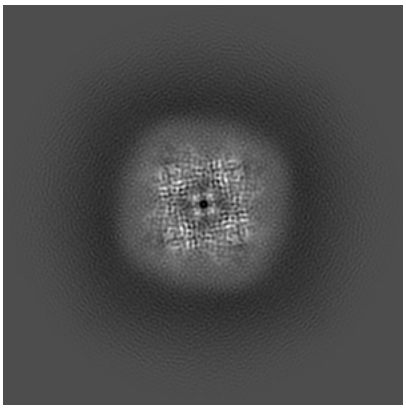
6.1.1 Primary map



X

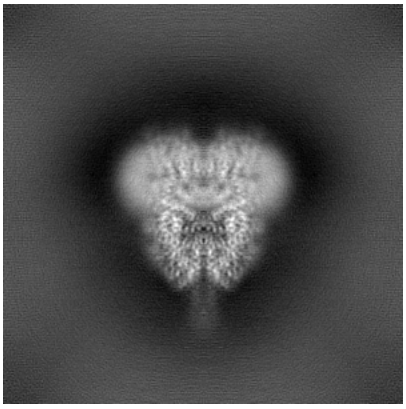


Y

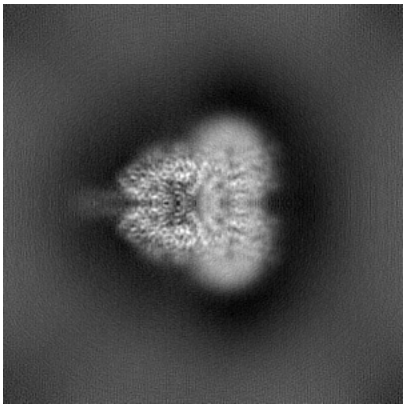


Z

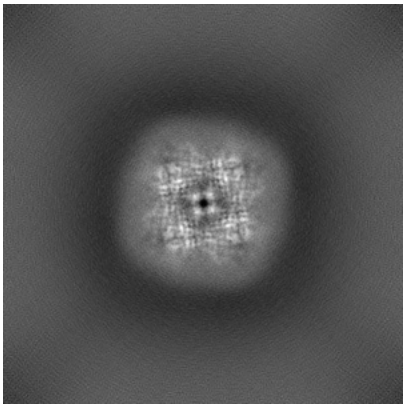
6.1.2 Raw map



X



Y

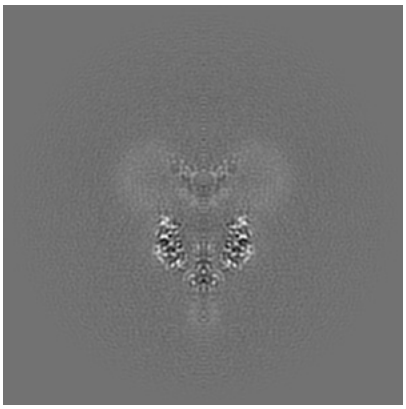


Z

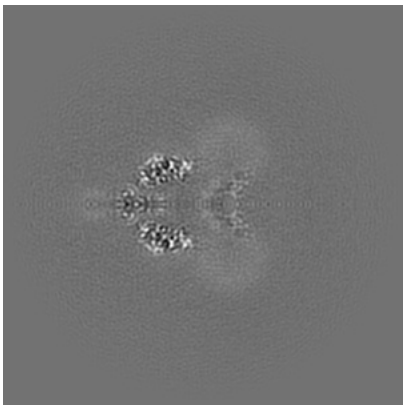
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

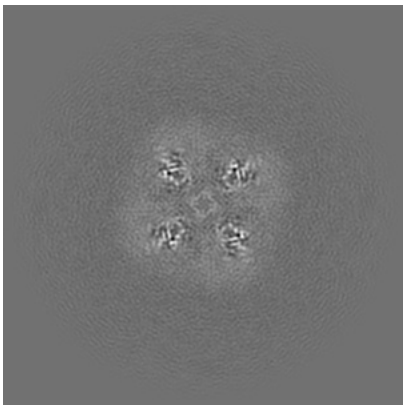
6.2.1 Primary map



X Index: 150

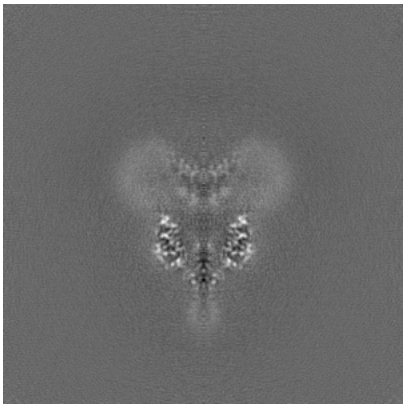


Y Index: 150

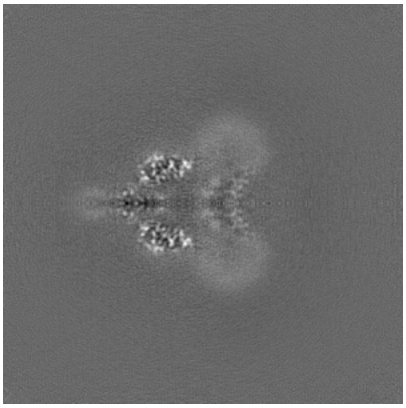


Z Index: 150

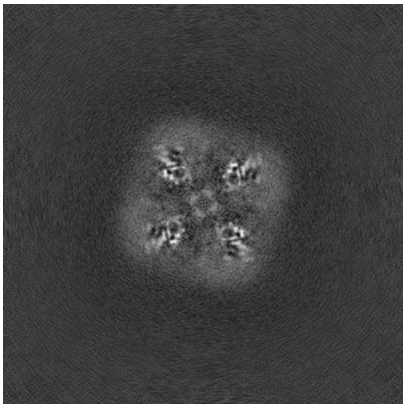
6.2.2 Raw map



X Index: 150



Y Index: 150

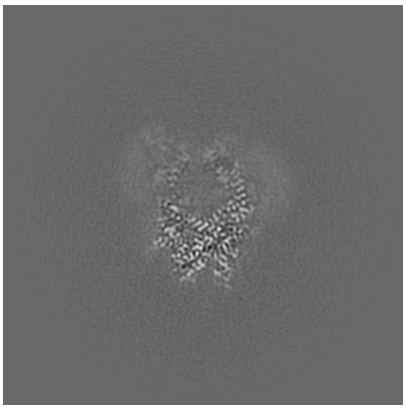


Z Index: 150

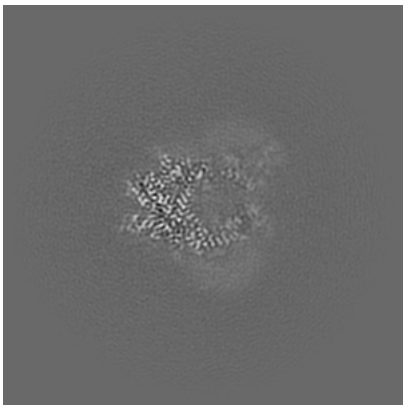
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

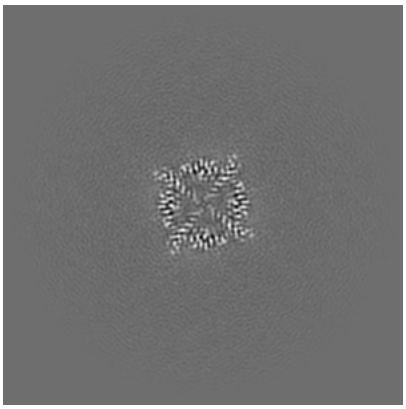
6.3.1 Primary map



X Index: 127

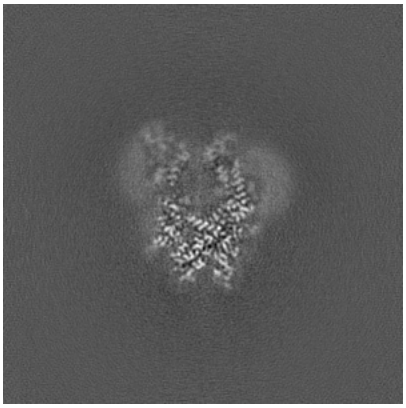


Y Index: 127

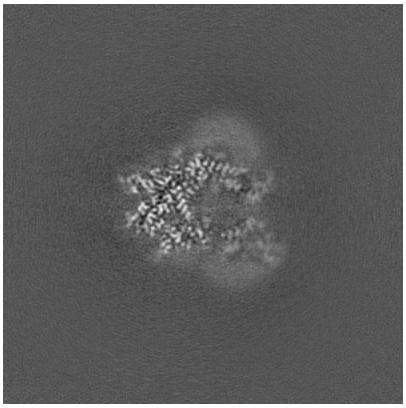


Z Index: 121

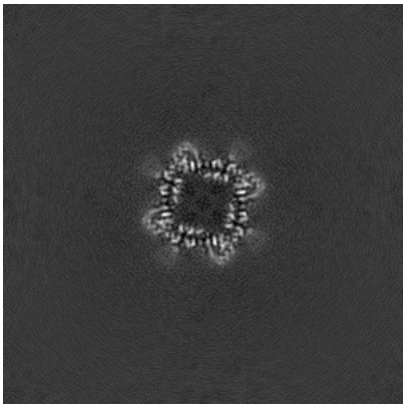
6.3.2 Raw map



X Index: 127



Y Index: 173

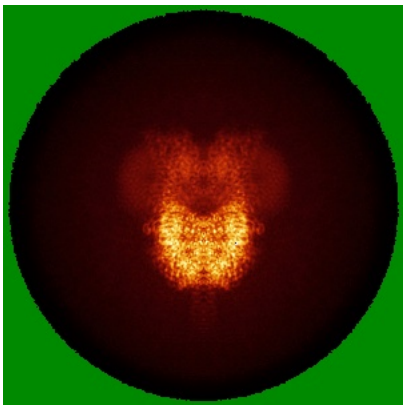


Z Index: 130

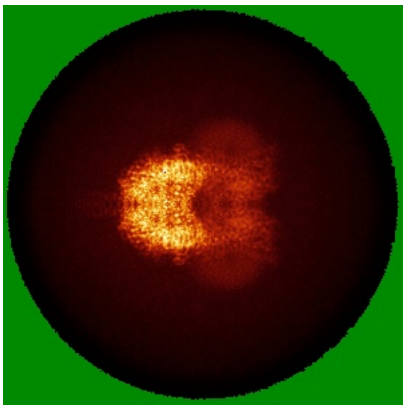
The images above show the largest variance slices of the map in three orthogonal directions.

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

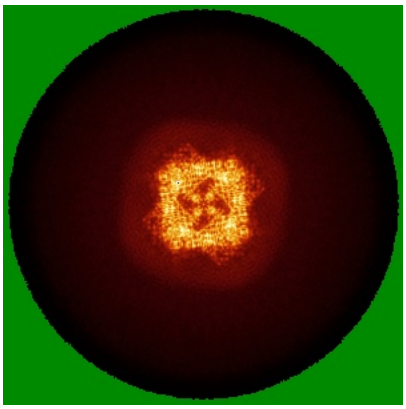
6.4.1 Primary map



X

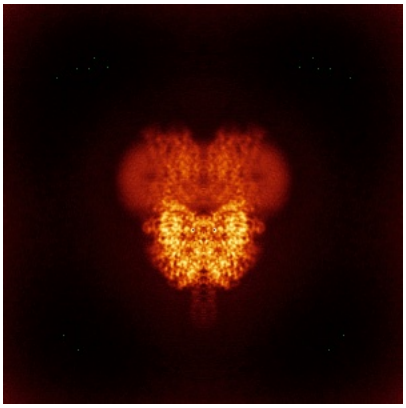


Y

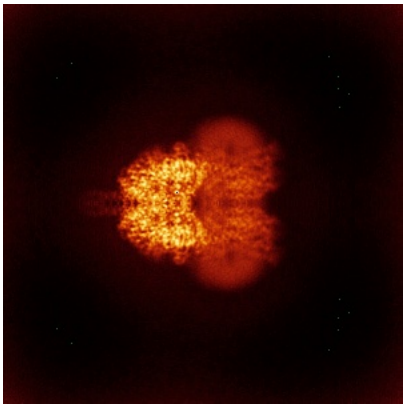


Z

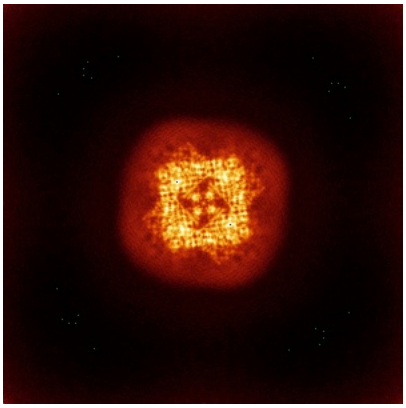
6.4.2 Raw map



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 0.06. 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.

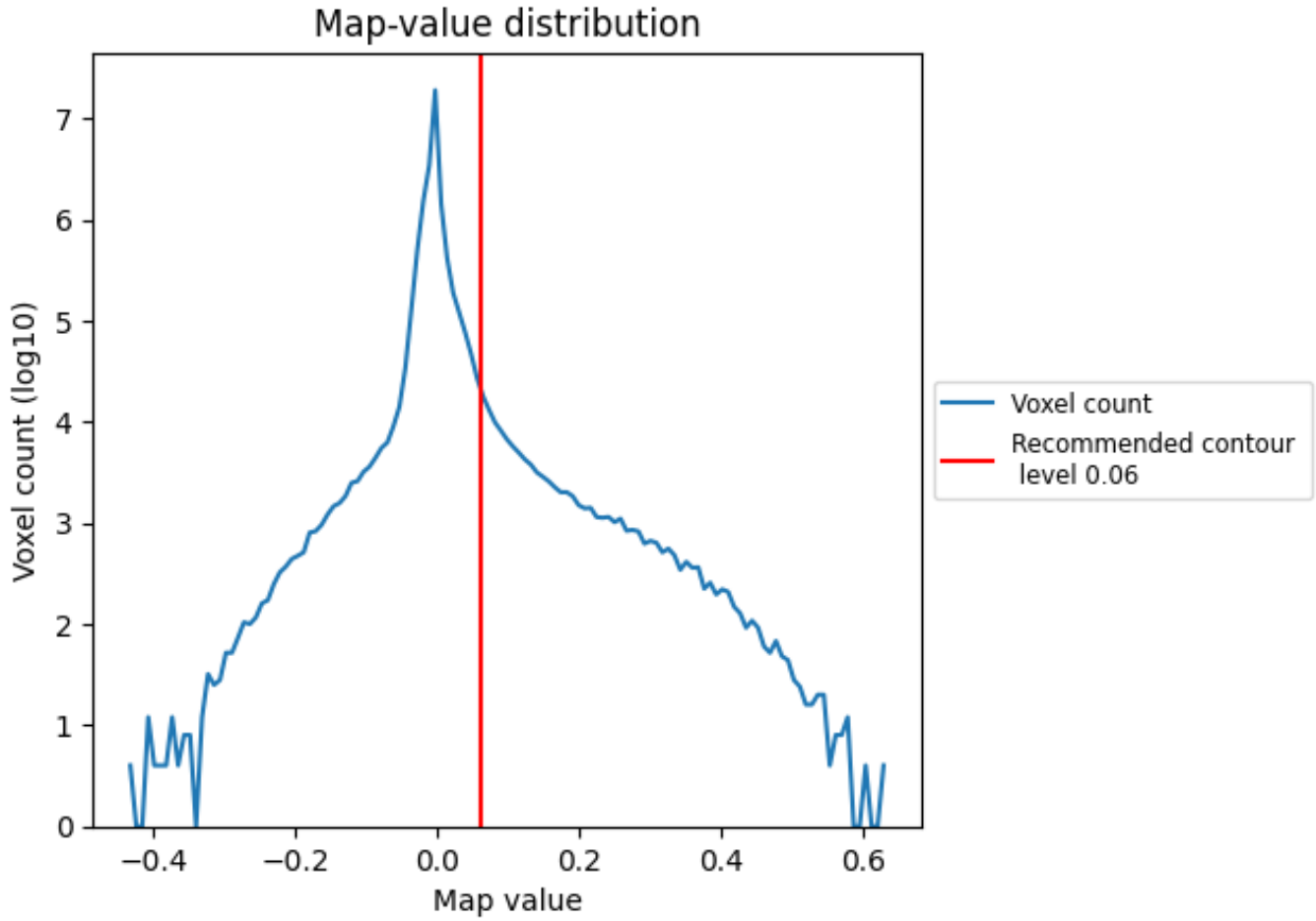
6.6 Mask visualisation (i)

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

7 Map analysis

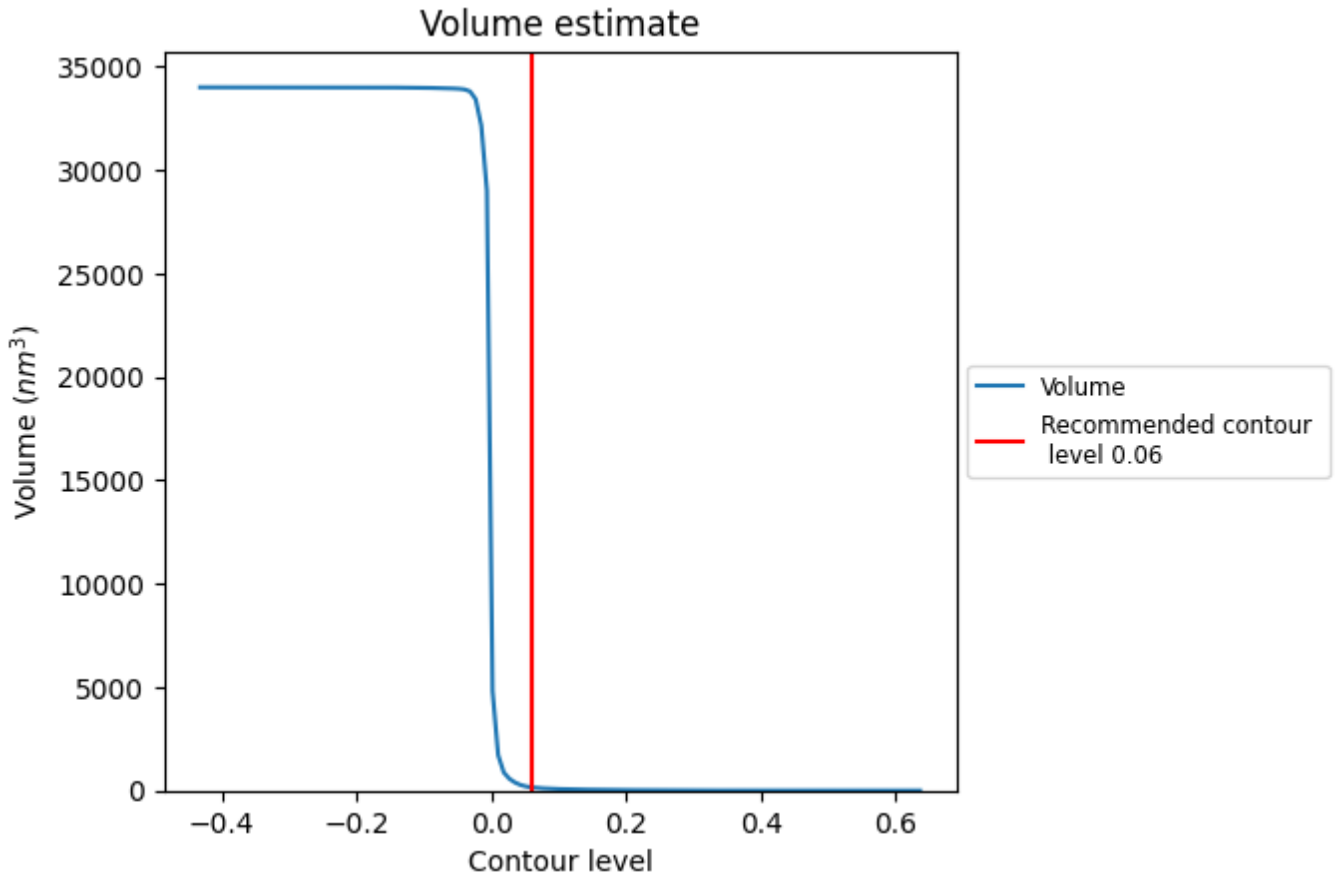
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

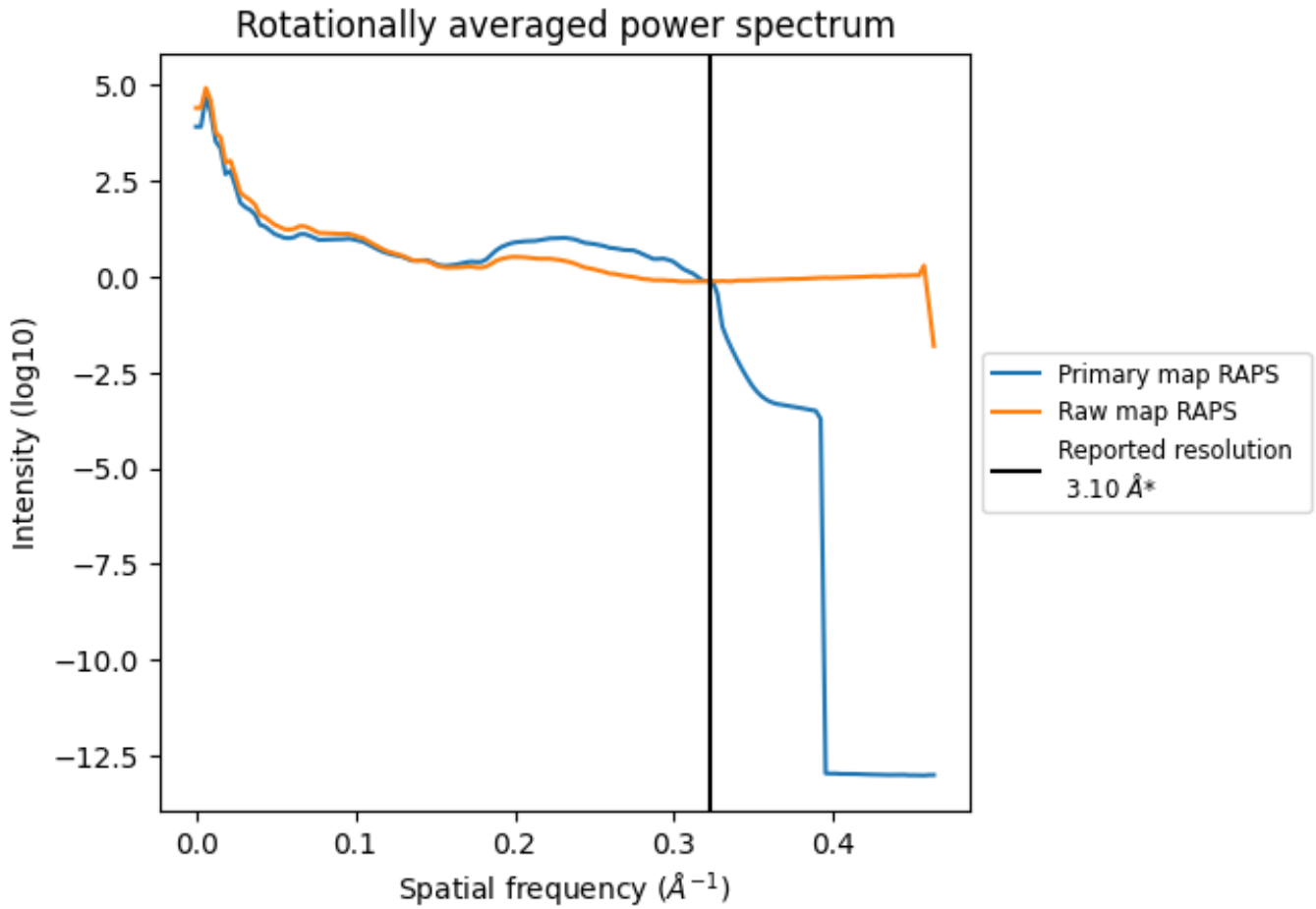
7.2 Volume estimate (i)



The volume at the recommended contour level is 156 nm^3; this corresponds to an approximate mass of 141 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)

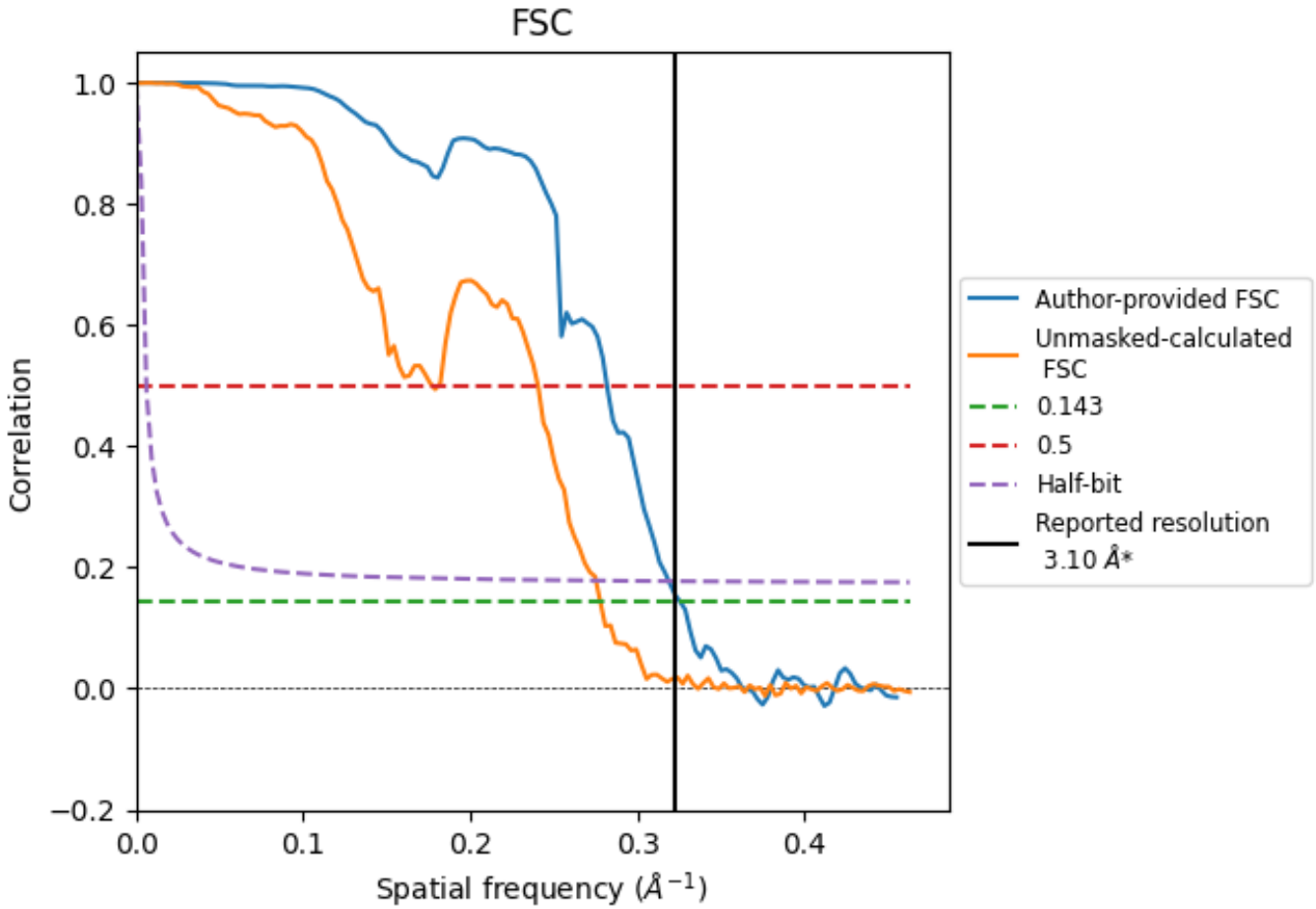


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

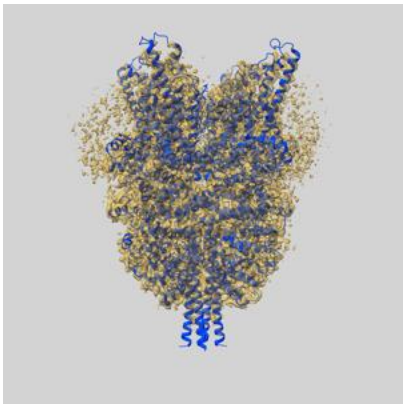
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.55	3.14
Unmasked-calculated*	3.60	5.64	3.63

*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 3.60 differs from the reported value 3.1 by more than 10 %

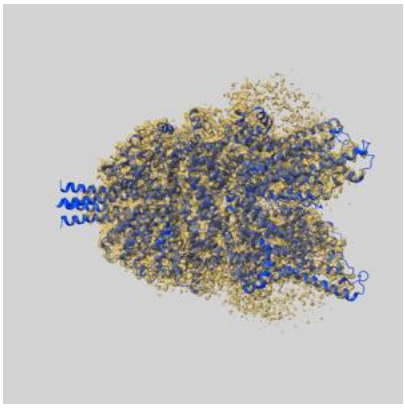
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70596 and PDB model 9OLL. Per-residue inclusion information can be found in section 3 on page 5.

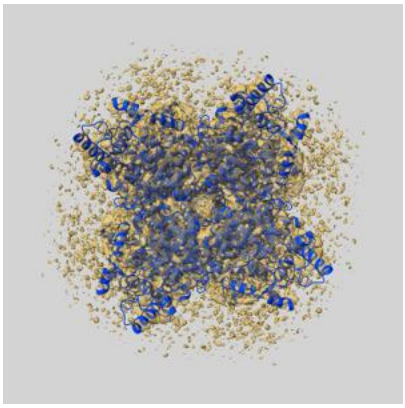
9.1 Map-model overlay



X



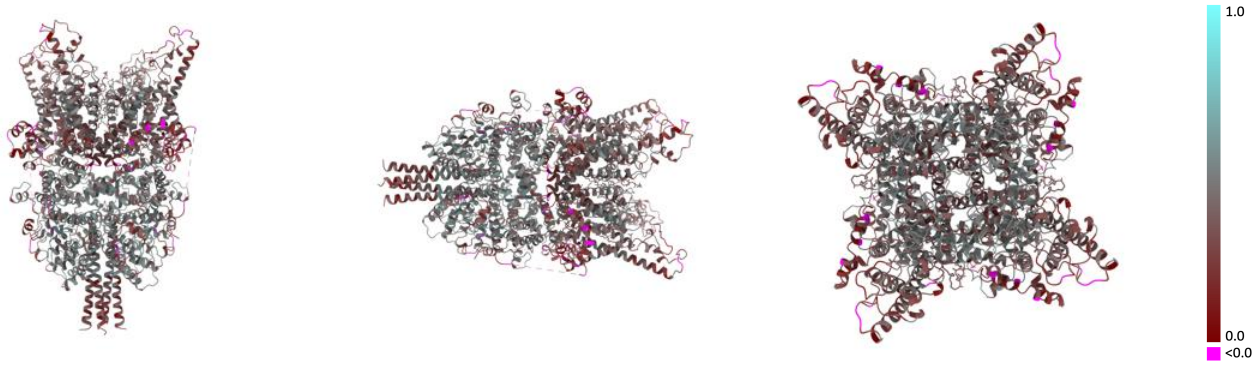
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

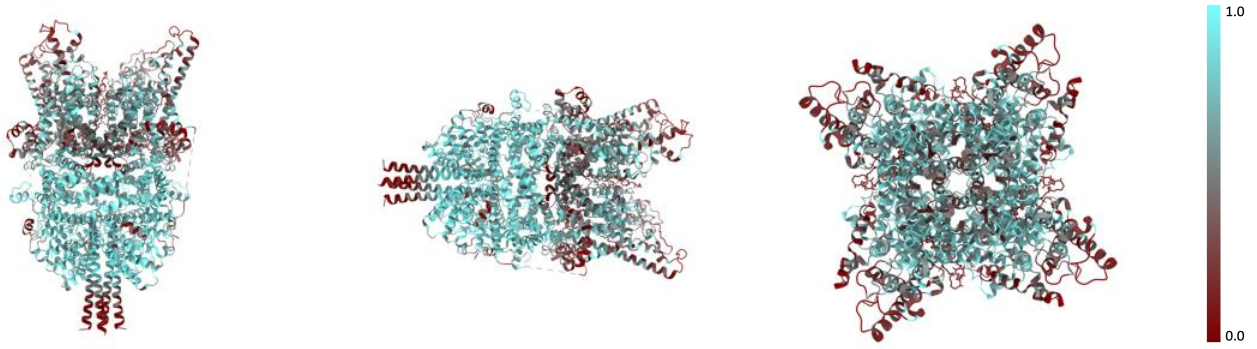
9.2 Q-score mapped to coordinate model (i)



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.

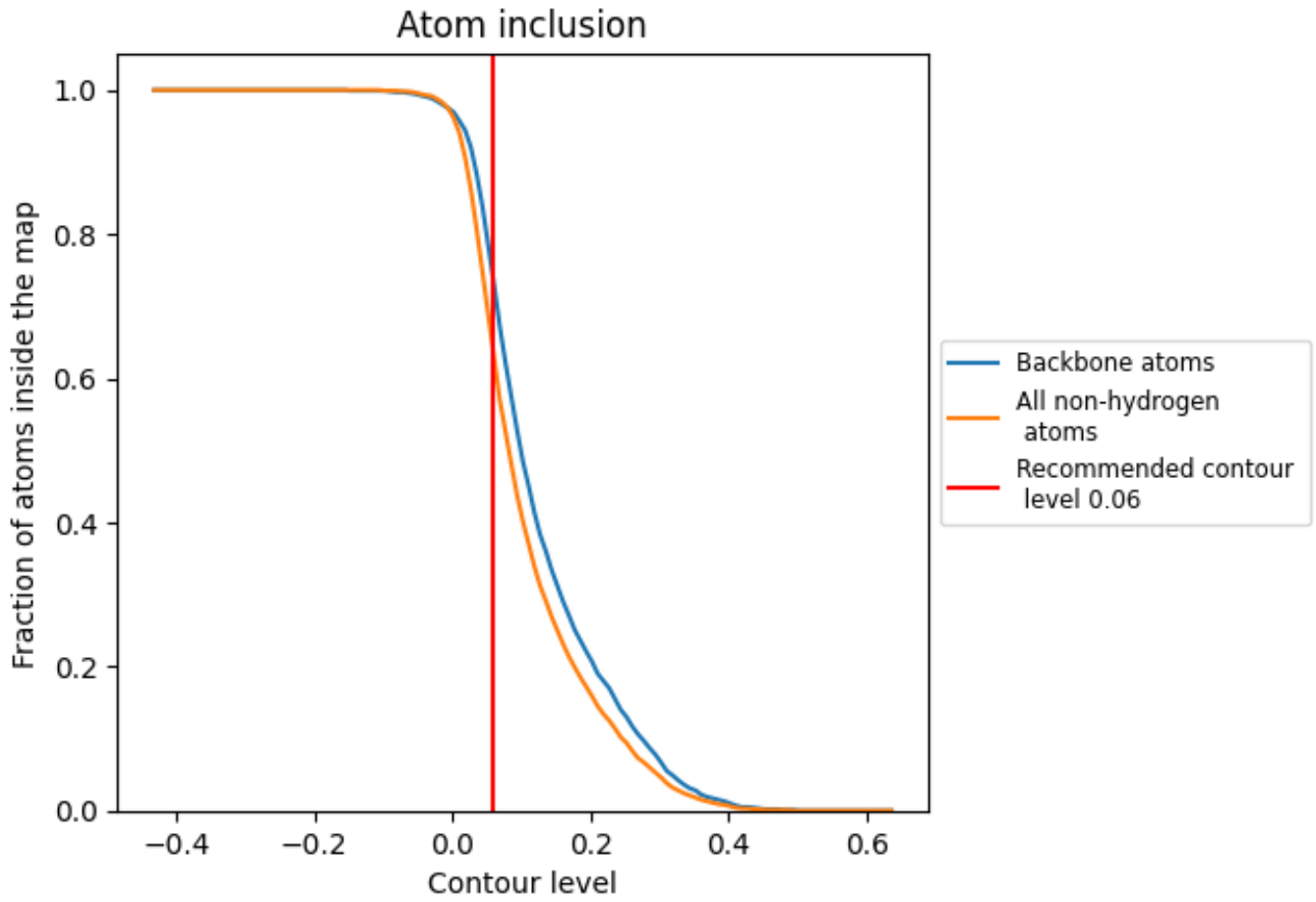
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 63% 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 (0.06) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6320	0.3920
A	0.6330	0.3920
B	0.6310	0.3930
C	0.6310	0.3920
D	0.6320	0.3920