Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:16 AM UTC

PDB ID	:	8DRE / pdb_00008dre
EMDB ID	:	EMD-27676
Title	:	LRRC8A:C conformation 2 (oblong)
Authors	:	Kern, D.M.; Brohawn, S.G.
Deposited on	:	2022-07-20
Resolution	:	3.18 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:

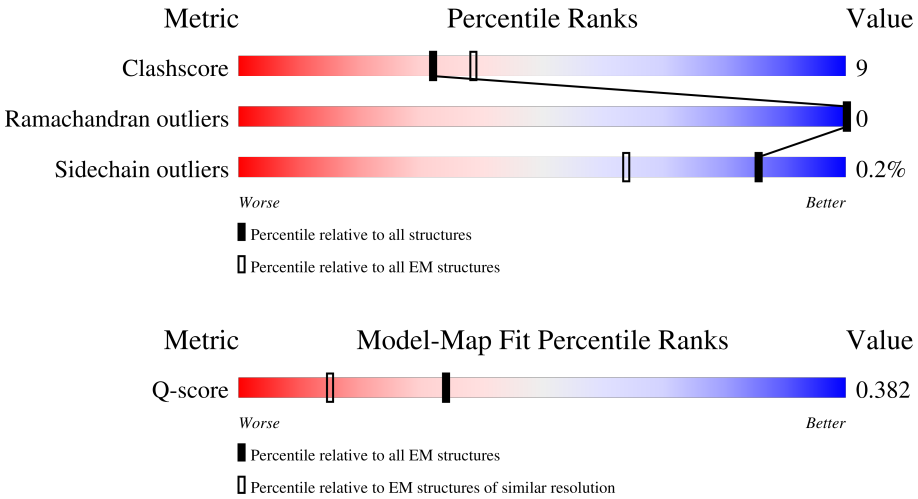
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

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

The reported resolution of this entry is 3.18 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	14470 (2.68 - 3.68)

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	911	6% 60% 19% 21%
1	B	911	29% 60% 18% 21%
1	C	911	6% 27% 5% 67%
1	D	911	28% 6% 65%

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Mol	Chain	Length	Quality of chain
1	E	911	6% 29% 5% 65%
2	F	813	23% 65% 21% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEE	F	903	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25940 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 Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	717	Total 5915	C 3849	N 996	O 1045	S 25	0	0
1	B	716	Total 5911	C 3847	N 995	O 1044	S 25	0	0
1	C	300	Total 2519	C 1670	N 400	O 432	S 17	0	0
1	D	316	Total 2653	C 1749	N 426	O 461	S 17	0	0
1	E	316	Total 2651	C 1749	N 426	O 459	S 17	0	0

There are 85 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68D	TRP	-	linker	UNP Q80WG5
A	68E	ALA	-	linker	UNP Q80WG5
A	68F	ALA	-	linker	UNP Q80WG5
A	68G	SER	-	linker	UNP Q80WG5
A	68H	SER	-	linker	UNP Q80WG5
A	68O	TRP	MET	conflict	UNP P0ABE7
A	72F	ILE	HIS	conflict	UNP P0ABE7
A	72J	LEU	-	linker	UNP P0ABE7
A	811	SER	-	expression tag	UNP Q80WG5
A	812	ASN	-	expression tag	UNP Q80WG5
A	813	SER	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	GLU	-	expression tag	UNP Q80WG5
A	816	VAL	-	expression tag	UNP Q80WG5
A	817	LEU	-	expression tag	UNP Q80WG5
A	818	PHE	-	expression tag	UNP Q80WG5
A	819	GLN	-	expression tag	UNP Q80WG5
B	68D	TRP	-	linker	UNP Q80WG5
B	68E	ALA	-	linker	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68F	ALA	-	linker	UNP Q80WG5
B	68G	SER	-	linker	UNP Q80WG5
B	68H	SER	-	linker	UNP Q80WG5
B	68O	TRP	MET	conflict	UNP P0ABE7
B	72F	ILE	HIS	conflict	UNP P0ABE7
B	72J	LEU	-	linker	UNP P0ABE7
B	811	SER	-	expression tag	UNP Q80WG5
B	812	ASN	-	expression tag	UNP Q80WG5
B	813	SER	-	expression tag	UNP Q80WG5
B	814	LEU	-	expression tag	UNP Q80WG5
B	815	GLU	-	expression tag	UNP Q80WG5
B	816	VAL	-	expression tag	UNP Q80WG5
B	817	LEU	-	expression tag	UNP Q80WG5
B	818	PHE	-	expression tag	UNP Q80WG5
B	819	GLN	-	expression tag	UNP Q80WG5
C	68D	TRP	-	linker	UNP Q80WG5
C	68E	ALA	-	linker	UNP Q80WG5
C	68F	ALA	-	linker	UNP Q80WG5
C	68G	SER	-	linker	UNP Q80WG5
C	68H	SER	-	linker	UNP Q80WG5
C	68O	TRP	MET	conflict	UNP P0ABE7
C	72F	ILE	HIS	conflict	UNP P0ABE7
C	72J	LEU	-	linker	UNP P0ABE7
C	811	SER	-	expression tag	UNP Q80WG5
C	812	ASN	-	expression tag	UNP Q80WG5
C	813	SER	-	expression tag	UNP Q80WG5
C	814	LEU	-	expression tag	UNP Q80WG5
C	815	GLU	-	expression tag	UNP Q80WG5
C	816	VAL	-	expression tag	UNP Q80WG5
C	817	LEU	-	expression tag	UNP Q80WG5
C	818	PHE	-	expression tag	UNP Q80WG5
C	819	GLN	-	expression tag	UNP Q80WG5
D	68D	TRP	-	linker	UNP Q80WG5
D	68E	ALA	-	linker	UNP Q80WG5
D	68F	ALA	-	linker	UNP Q80WG5
D	68G	SER	-	linker	UNP Q80WG5
D	68H	SER	-	linker	UNP Q80WG5
D	68O	TRP	MET	conflict	UNP P0ABE7
D	72F	ILE	HIS	conflict	UNP P0ABE7
D	72J	LEU	-	linker	UNP P0ABE7
D	811	SER	-	expression tag	UNP Q80WG5
D	812	ASN	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	813	SER	-	expression tag	UNP Q80WG5
D	814	LEU	-	expression tag	UNP Q80WG5
D	815	GLU	-	expression tag	UNP Q80WG5
D	816	VAL	-	expression tag	UNP Q80WG5
D	817	LEU	-	expression tag	UNP Q80WG5
D	818	PHE	-	expression tag	UNP Q80WG5
D	819	GLN	-	expression tag	UNP Q80WG5
E	68D	TRP	-	linker	UNP Q80WG5
E	68E	ALA	-	linker	UNP Q80WG5
E	68F	ALA	-	linker	UNP Q80WG5
E	68G	SER	-	linker	UNP Q80WG5
E	68H	SER	-	linker	UNP Q80WG5
E	68O	TRP	MET	conflict	UNP P0ABE7
E	72F	ILE	HIS	conflict	UNP P0ABE7
E	72J	LEU	-	linker	UNP P0ABE7
E	811	SER	-	expression tag	UNP Q80WG5
E	812	ASN	-	expression tag	UNP Q80WG5
E	813	SER	-	expression tag	UNP Q80WG5
E	814	LEU	-	expression tag	UNP Q80WG5
E	815	GLU	-	expression tag	UNP Q80WG5
E	816	VAL	-	expression tag	UNP Q80WG5
E	817	LEU	-	expression tag	UNP Q80WG5
E	818	PHE	-	expression tag	UNP Q80WG5
E	819	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	704	Total	C	N	O	S	0	0
			5751	3745	940	1029	37		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	804	SER	-	expression tag	UNP Q8R502
F	805	ASN	-	expression tag	UNP Q8R502
F	806	SER	-	expression tag	UNP Q8R502
F	807	GLU	-	expression tag	UNP Q8R502
F	808	ASN	-	expression tag	UNP Q8R502
F	809	LEU	-	expression tag	UNP Q8R502
F	810	TYR	-	expression tag	UNP Q8R502
F	811	PHE	-	expression tag	UNP Q8R502

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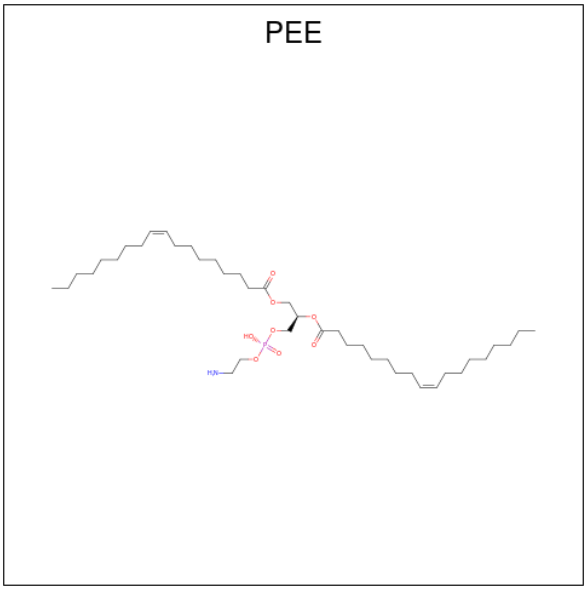
Chain	Residue	Modelled	Actual	Comment	Reference
F	812	GLN	-	expression tag	UNP Q8R502
F	813	GLY	-	expression tag	UNP Q8R502

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O P 44 34 1 8 1	0
3	A	1	Total C O 13 11 2	0
3	A	1	Total C O 13 11 2	0
3	B	1	Total C N O P 44 34 1 8 1	0
3	B	1	Total C O 11 9 2	0
3	B	1	Total C O 10 8 2	0
3	B	1	Total C N O P 51 41 1 8 1	0
3	C	1	Total C N O P 44 34 1 8 1	0
3	C	1	Total C O 11 9 2	0
3	D	1	Total C N O P 44 34 1 8 1	0

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Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total C O 9 7 2	0
3	D	1	Total C O 11 9 2	0
3	D	1	Total C N O P 51 41 1 8 1	0
3	E	1	Total C N O P 44 34 1 8 1	0
3	E	1	Total C O 10 8 2	0
3	E	1	Total C O 10 8 2	0
3	F	1	Total C N O P 44 34 1 8 1	0
3	F	1	Total C O 11 9 2	0
3	F	1	Total C O 8 6 2	0
3	F	1	Total C N O P 51 41 1 8 1	0

- Molecule 4 is water.

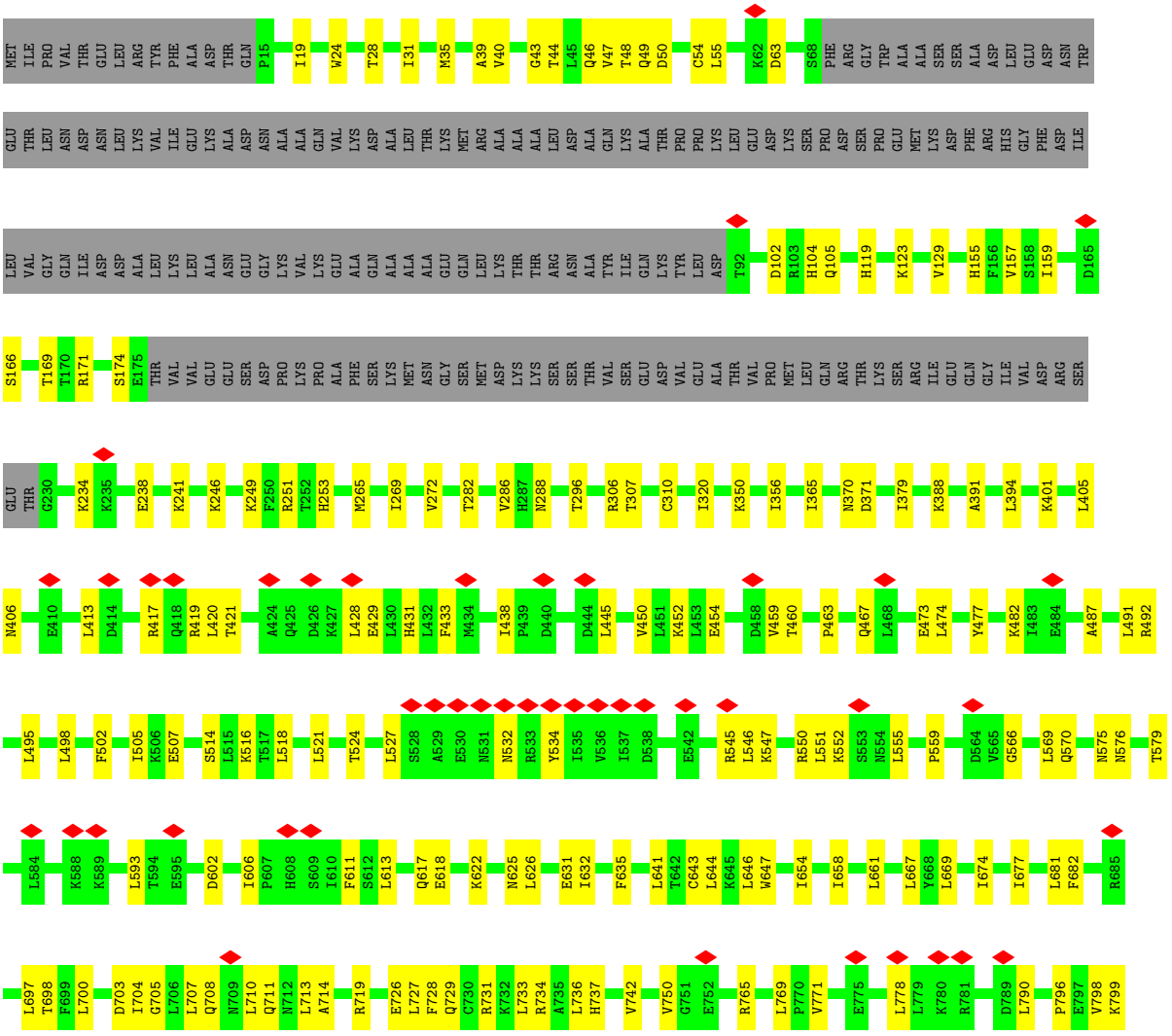
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total O 1 1	0
4	B	1	Total O 1 1	0
4	C	1	Total O 1 1	0
4	D	1	Total O 1 1	0
4	E	1	Total O 1 1	0
4	F	1	Total O 1 1	0

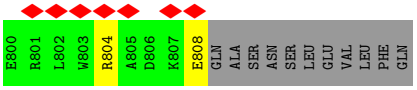
3 Residue-property plots (i)

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

• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

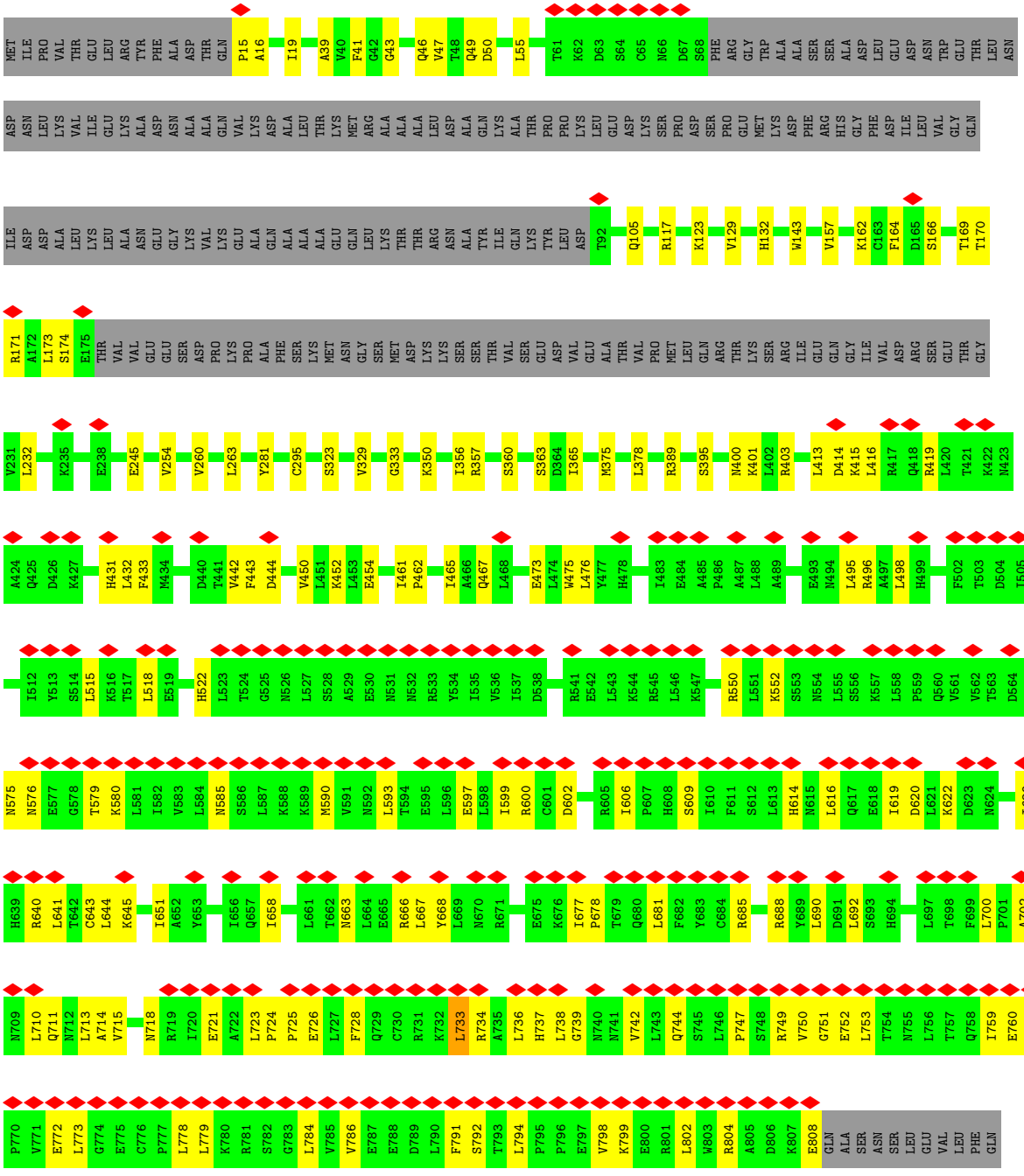
Chain A:





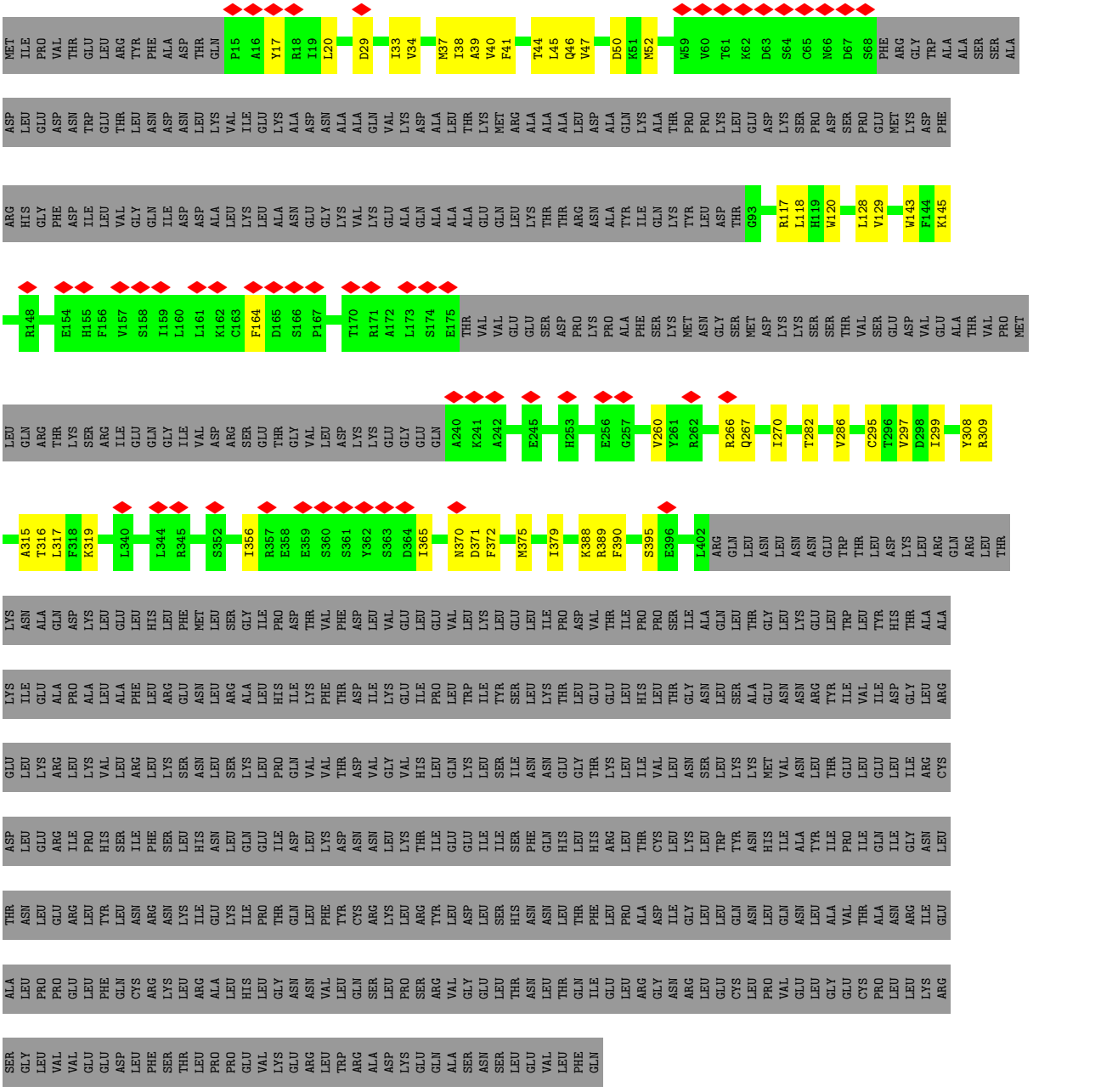
• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

Chain B:



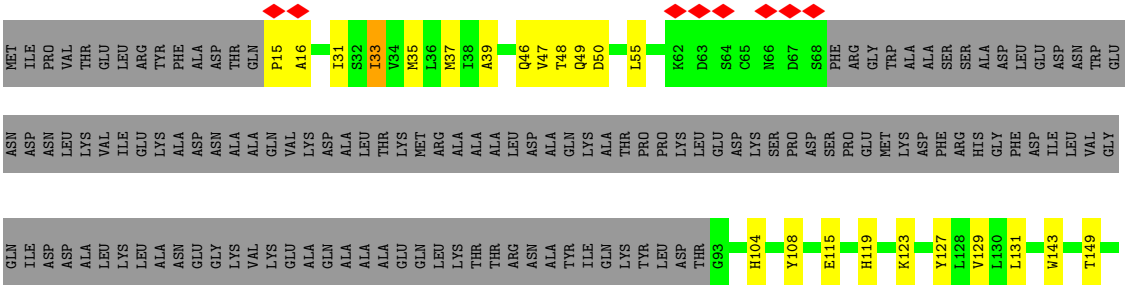
• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

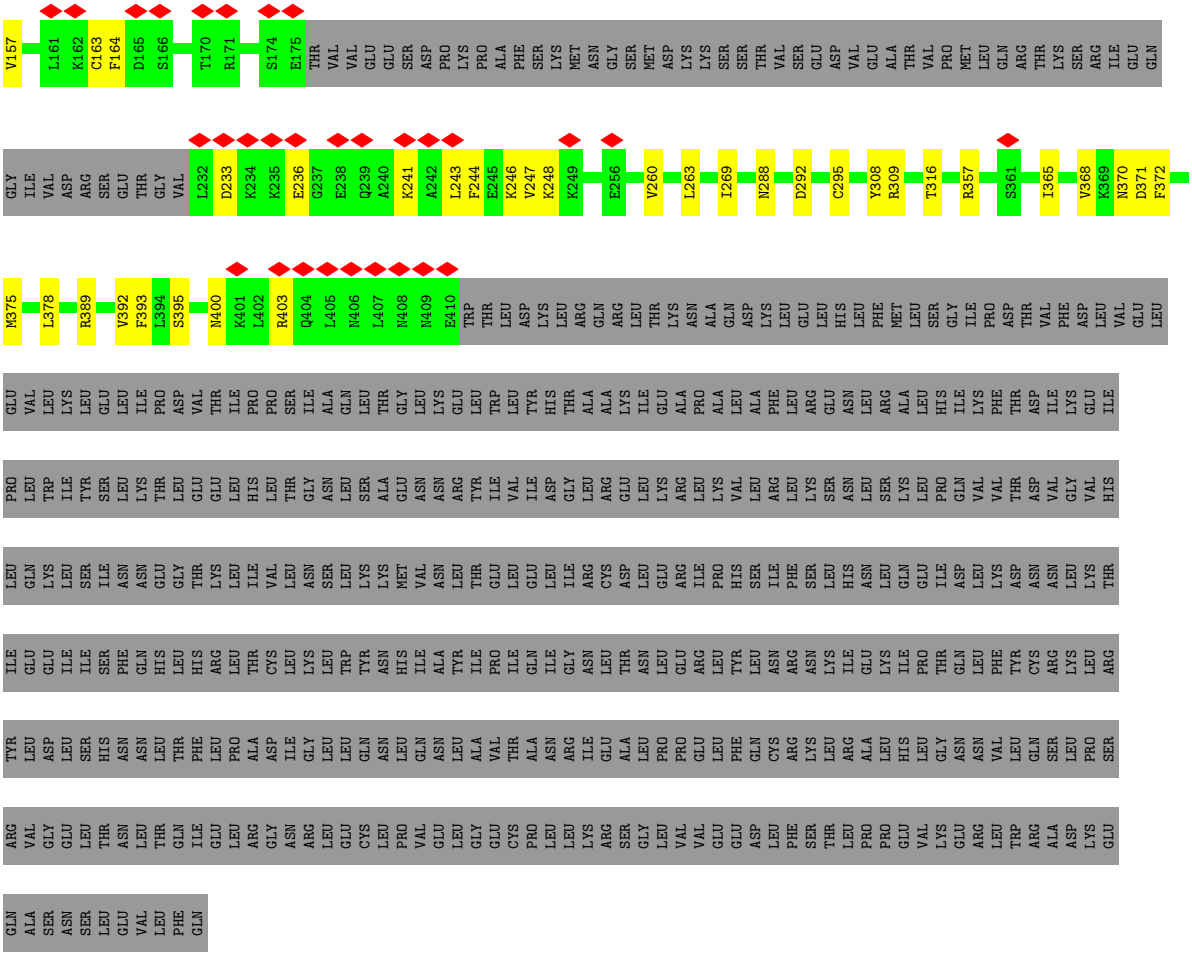
Chain C:



• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

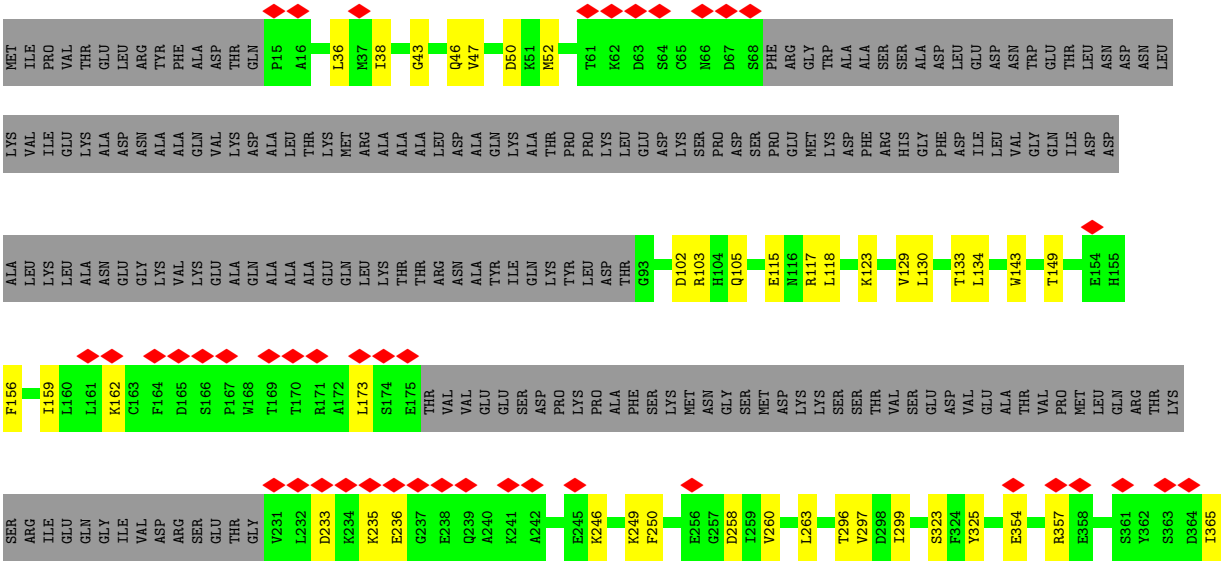
Chain D:

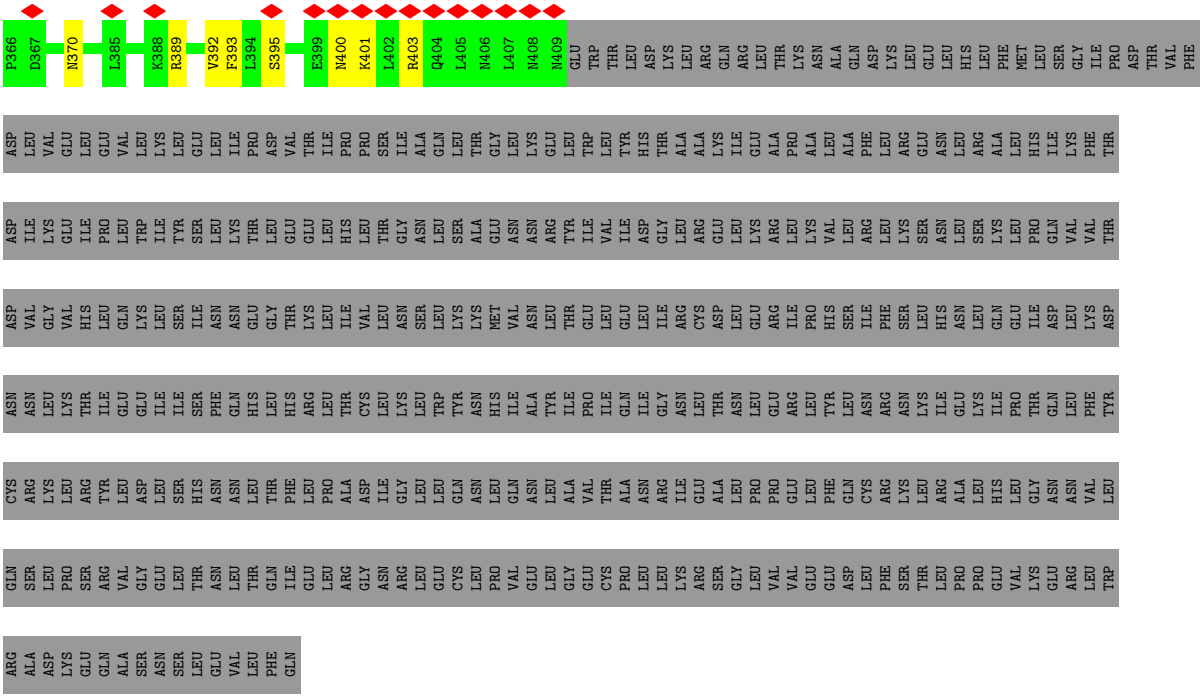




• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

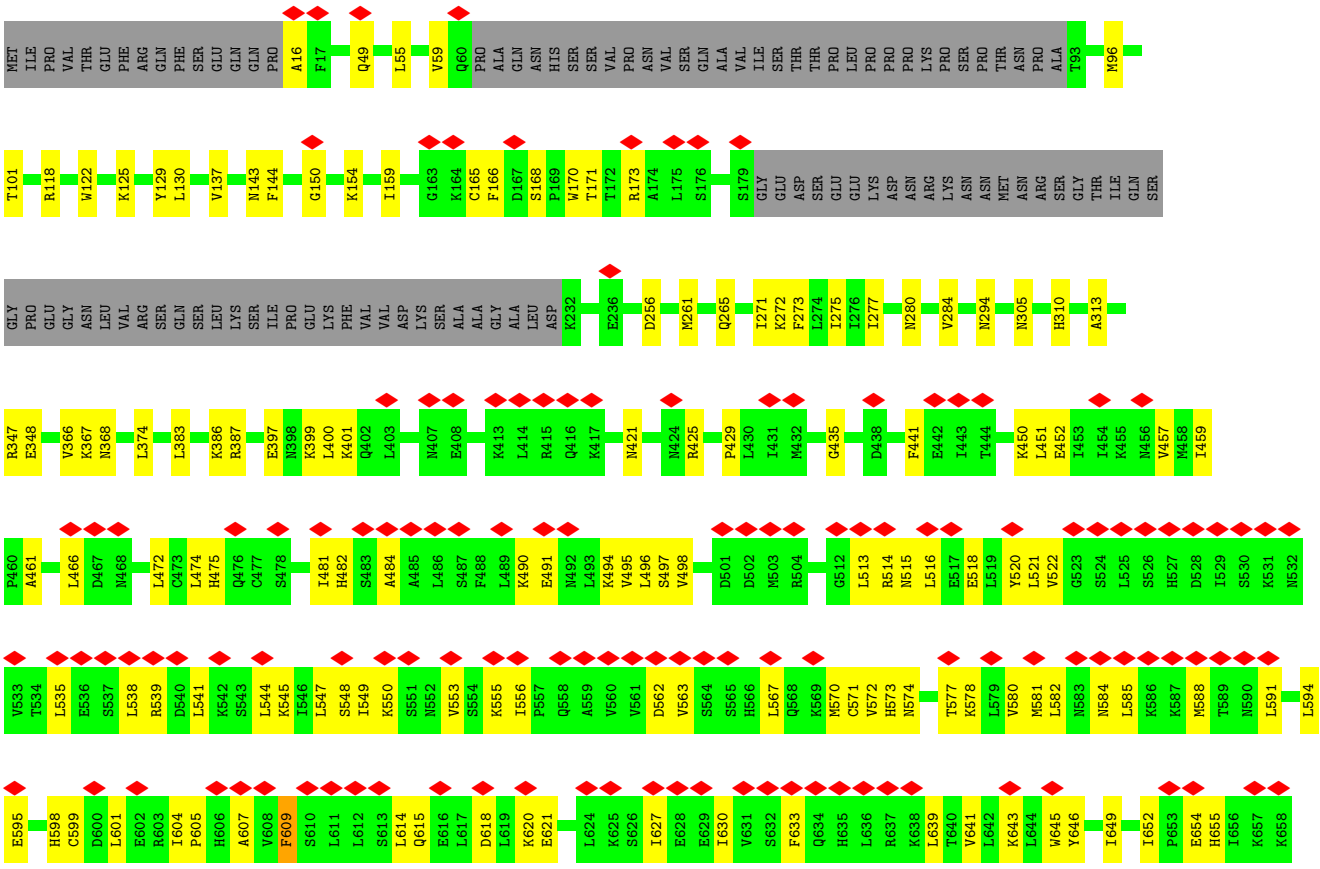
Chain E:

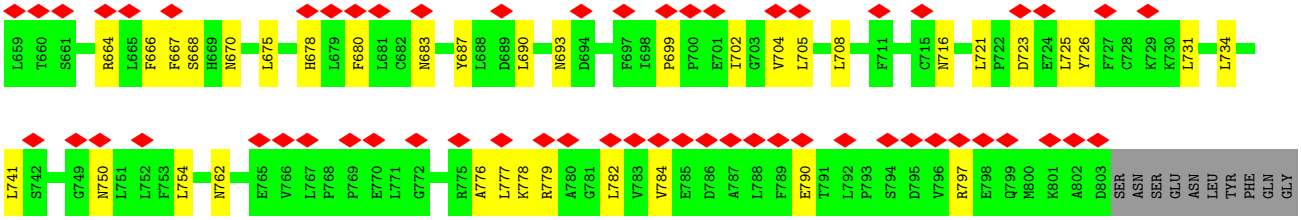




• Molecule 2: Volume-regulated anion channel subunit LRRC8C

Chain F:




L659 T660 S661 R664 L665 F666 F667 S668 H669 N670 L675 H678 L679 F680 L681 C682 N683 Y687 L688 D689 L690 N693 D694 F697 I698 P699 P700 E701 I702 G703 V704 L705 L708 F711 C715 N716 L721 P722 D723 E724 L725 Y726 F727 C728 K729 K730 L731 L734
L741 S742 G749 N750 L751 L752 F753 L754 N762 E765 V766 L767 P768 P769 E770 L771 G772 R775 A776 L777 K778 R779 A780 G781 L782 V783 V784 E785 D786 A787 L788 F789 E790 T791 L792 P793 S794 D795 V796 R797 E798 Q799 M800 K801 A802 D803 SER ASN SER GLU ASN LEU TYR PHE GLN GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126955	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)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.746	Depositor
Minimum map value	-1.867	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.475	Depositor
Map size (Å)	435.968, 435.968, 435.968	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	1/6048 (0.0%)	0.39	0/8197
1	B	0.19	1/6044 (0.0%)	0.42	0/8192
1	C	0.17	0/2594	0.38	0/3515
1	D	0.17	0/2728	0.37	0/3693
1	E	0.16	0/2726	0.35	1/3691 (0.0%)
2	F	0.20	1/5877 (0.0%)	0.43	4/7943 (0.1%)
All	All	0.18	3/26017 (0.0%)	0.40	5/35231 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	399	LYS	C-N	8.38	1.45	1.33
1	B	401	LYS	C-N	-6.09	1.25	1.33
1	A	401	LYS	C-N	-5.76	1.26	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	399	LYS	CA-C-N	-7.57	110.14	120.28
2	F	399	LYS	C-N-CA	-7.57	110.14	120.28
2	F	399	LYS	O-C-N	6.21	128.79	122.09
2	F	368	ASN	CB-CA-C	-5.76	109.95	116.63
1	E	370	ASN	CB-CA-C	-5.57	110.17	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5915	0	6074	117	0
1	B	5911	0	6071	119	0
1	C	2519	0	2510	34	0
1	D	2653	0	2641	45	0
1	E	2651	0	2644	33	0
2	F	5751	0	5887	114	0
3	A	70	0	101	1	0
3	B	116	0	173	7	0
3	C	55	0	79	1	0
3	D	115	0	171	7	0
3	E	64	0	89	3	0
3	F	114	0	169	8	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
4	E	1	0	0	1	0
4	F	1	0	0	0	0
All	All	25940	0	26609	450	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (450) 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:B:476:LEU:HD12	1:B:476:LEU:O	1.70	0.89
3:F:901:PEE:H38	3:F:904:PEE:H45	1.65	0.79
2:F:582:LEU:HB3	2:F:607:ALA:HB2	1.67	0.77
1:E:38:ILE:HG22	3:F:901:PEE:H40	1.67	0.77
1:B:620:ASP:HA	1:B:645:LYS:HB2	1.69	0.74
1:A:241:LYS:NZ	1:A:406:ASN:ND2	2.36	0.73
3:F:901:PEE:H38	3:F:904:PEE:C27	2.20	0.71
2:F:585:LEU:HB3	2:F:607:ALA:HB1	1.71	0.71
1:B:725:PRO:HA	1:B:728:PHE:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLY:HA2	1:A:569:LEU:HB2	1.74	0.70
1:C:365:ILE:HG13	1:C:395:SER:HB3	1.74	0.69
2:F:556:ILE:O	2:F:584:ASN:ND2	2.26	0.69
1:A:241:LYS:HZ2	1:A:406:ASN:HD21	1.40	0.69
2:F:630:ILE:HG23	2:F:633:PHE:HD2	1.58	0.68
1:D:143:TRP:HD1	1:D:263:LEU:HD23	1.59	0.67
1:B:49:GLN:NE2	1:C:47:VAL:O	2.28	0.67
1:D:48:THR:HG22	1:D:49:GLN:HG3	1.77	0.66
1:D:164:PHE:HA	1:D:389:ARG:HH12	1.61	0.66
1:B:432:LEU:HD11	1:B:442:VAL:HG21	1.79	0.65
1:D:47:VAL:HG11	3:D:904:PEE:H30	1.77	0.65
2:F:165:CYS:HB3	2:F:387:ARG:HH12	1.60	0.65
1:D:46:GLN:HA	1:D:50:ASP:HB2	1.78	0.65
1:B:495:LEU:HD21	1:B:498:LEU:HD12	1.77	0.65
1:B:751:GLY:HA3	1:B:772:GLU:HB3	1.79	0.65
1:D:104:HIS:ND1	4:D:1001:HOH:O	2.29	0.64
2:F:790:GLU:O	2:F:797:ARG:NH2	2.31	0.64
2:F:495:VAL:HG13	2:F:518:GLU:HB2	1.79	0.64
1:B:143:TRP:HE1	1:B:260:VAL:HG13	1.64	0.63
1:A:710:LEU:HD21	1:A:713:LEU:HB2	1.80	0.63
1:B:164:PHE:HA	1:B:389:ARG:HD2	1.80	0.63
1:A:429:GLU:HG2	1:A:452:LYS:HD2	1.79	0.63
2:F:675:LEU:HD11	2:F:690:LEU:HD13	1.80	0.63
1:B:749:ARG:NH1	1:B:752:GLU:OE1	2.31	0.63
2:F:615:GLN:HA	2:F:639:LEU:HA	1.81	0.62
1:B:452:LYS:HE3	1:B:454:GLU:HB2	1.79	0.62
1:B:585:ASN:HA	1:B:609:SER:HB3	1.81	0.62
1:B:46:GLN:HA	1:B:50:ASP:HB2	1.81	0.62
2:F:627:ILE:HB	2:F:630:ILE:HD11	1.80	0.62
1:D:46:GLN:NE2	1:D:123:LYS:O	2.33	0.61
2:F:421:ASN:HD21	2:F:425:ARG:HB2	1.64	0.61
1:A:241:LYS:NZ	1:A:406:ASN:HD21	1.98	0.61
2:F:550:LYS:HG2	2:F:573:HIS:HB2	1.84	0.60
1:A:804:ARG:O	1:A:808:GLU:N	2.33	0.60
1:D:365:ILE:HG12	1:D:395:SER:HB3	1.83	0.60
2:F:643:LYS:HB3	2:F:645:TRP:HZ3	1.66	0.60
1:B:764:ASN:HD21	1:B:766:LEU:HB2	1.66	0.60
2:F:16:ALA:HB3	2:F:159:ILE:HG12	1.83	0.60
1:B:645:LYS:HD3	1:B:668:TYR:HB2	1.83	0.60
1:E:46:GLN:HA	1:E:50:ASP:HB2	1.81	0.60
2:F:630:ILE:HB	2:F:655:HIS:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:GLN:HA	1:A:641:LEU:HA	1.83	0.59
1:D:127:TYR:HB3	3:D:901:PEE:H30	1.83	0.59
1:B:715:VAL:HG13	1:B:718:ASN:HD21	1.66	0.59
1:A:241:LYS:HZ2	1:A:406:ASN:ND2	1.98	0.59
1:B:400:ASN:OD1	1:B:403:ARG:NH2	2.35	0.59
2:F:310:HIS:HB3	2:F:313:ALA:HB2	1.85	0.58
1:A:492:ARG:HH21	1:A:514:SER:HB2	1.69	0.58
1:B:723:LEU:HB2	1:B:747:PRO:HD2	1.83	0.58
2:F:574:ASN:ND2	2:F:577:THR:O	2.36	0.58
2:F:168:SER:O	2:F:171:THR:OG1	2.22	0.58
2:F:435:GLY:HA2	2:F:457:VAL:HG22	1.86	0.58
1:B:580:LYS:NZ	1:B:602:ASP:O	2.35	0.58
1:B:678:PRO:HD2	1:B:681:LEU:HD22	1.85	0.58
1:D:37:MET:HE1	1:E:134:LEU:HD21	1.86	0.58
1:E:400:ASN:OD1	1:E:403:ARG:NH2	2.35	0.58
1:D:49:GLN:NE2	1:E:47:VAL:O	2.36	0.57
1:D:400:ASN:OD1	1:D:403:ARG:NH2	2.36	0.57
1:B:690:LEU:HD22	1:B:713:LEU:HG	1.86	0.57
2:F:779:ARG:NH1	2:F:782:LEU:O	2.36	0.57
1:A:474:LEU:HD23	1:A:498:LEU:HD13	1.86	0.57
1:B:759:ILE:HG12	1:B:784:LEU:HB2	1.86	0.57
1:E:143:TRP:HE1	1:E:260:VAL:HG13	1.69	0.57
2:F:588:MET:HG3	2:F:591:LEU:HD12	1.87	0.56
1:B:643:CYS:HB3	1:B:666:ARG:HB3	1.86	0.56
1:A:769:LEU:HD13	1:A:790:LEU:HB3	1.87	0.56
2:F:383:LEU:HA	2:F:386:LYS:HG2	1.87	0.56
2:F:496:LEU:HD12	2:F:516:LEU:HD11	1.88	0.56
1:A:521:LEU:HB2	1:A:546:LEU:HD11	1.88	0.56
1:B:692:LEU:H	1:B:714:ALA:HB3	1.70	0.56
2:F:144:PHE:HD2	2:F:265:GLN:HB2	1.70	0.56
1:B:769:LEU:HB3	1:B:773:LEU:HD12	1.87	0.56
2:F:731:LEU:HD21	2:F:734:LEU:HD13	1.87	0.56
1:A:282:THR:O	1:A:286:VAL:HB	2.05	0.56
1:B:643:CYS:HB2	1:B:645:LYS:HZ1	1.71	0.56
2:F:754:LEU:H	2:F:776:ALA:HB3	1.71	0.56
1:B:365:ILE:HG12	1:B:395:SER:HB3	1.88	0.56
2:F:491:GLU:HA	2:F:514:ARG:HH12	1.69	0.56
1:A:516:LYS:HB3	1:B:600:ARG:HH12	1.71	0.55
2:F:59:VAL:HG21	2:F:101:THR:HG22	1.87	0.55
2:F:609:PHE:HZ	2:F:630:ILE:HA	1.71	0.55
2:F:643:LYS:HA	2:F:666:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:GLU:OE2	1:A:452:LYS:NZ	2.39	0.55
1:B:597:GLU:HA	1:B:620:ASP:HB3	1.89	0.55
1:A:241:LYS:HZ1	1:A:406:ASN:CG	2.14	0.55
1:A:431:HIS:HA	1:A:452:LYS:HB2	1.88	0.55
1:B:616:LEU:HD13	1:B:619:ILE:HD11	1.89	0.55
1:B:356:ILE:O	1:B:360:SER:OG	2.24	0.55
2:F:170:TRP:CZ2	2:F:400:LEU:HB2	2.42	0.55
1:B:357:ARG:NH2	1:B:365:ILE:O	2.41	0.54
1:B:632:ILE:HD12	1:B:658:ILE:HB	1.89	0.54
1:B:733:LEU:HD11	1:B:753:LEU:HD13	1.88	0.54
1:A:46:GLN:NE2	1:A:123:LYS:O	2.40	0.54
1:A:593:LEU:HB2	1:A:613:LEU:HD21	1.89	0.54
1:D:39:ALA:HB2	1:D:129:VAL:HG12	1.89	0.54
2:F:280:ASN:O	2:F:284:VAL:HB	2.07	0.54
2:F:664:ARG:HA	2:F:687:TYR:HB3	1.88	0.54
1:C:164:PHE:HA	1:C:389:ARG:HD3	1.89	0.54
1:E:102:ASP:OD2	1:E:105:GLN:NE2	2.36	0.54
1:C:316:THR:HA	1:C:319:LYS:HE3	1.88	0.53
2:F:541:LEU:HD12	2:F:544:LEU:HD22	1.89	0.53
2:F:726:TYR:O	2:F:750:ASN:ND2	2.36	0.53
1:B:375:MET:HA	1:B:378:LEU:HD12	1.91	0.53
3:B:901:PEE:H42	3:B:904:PEE:H44	1.90	0.53
1:A:102:ASP:HB2	1:A:105:GLN:HG3	1.89	0.53
1:A:555:LEU:O	1:A:576:ASN:ND2	2.41	0.53
1:A:241:LYS:HZ1	1:A:406:ASN:ND2	2.07	0.53
1:A:728:PHE:O	1:A:731:ARG:NH1	2.41	0.53
1:B:728:PHE:HE2	1:B:747:PRO:HB2	1.72	0.53
1:D:31:ILE:O	1:D:35:MET:HG3	2.08	0.53
1:C:45:LEU:HD21	1:C:317:LEU:HD23	1.91	0.53
2:F:459:ILE:HB	2:F:481:ILE:HG13	1.89	0.53
2:F:544:LEU:HD23	2:F:563:VAL:HG11	1.89	0.53
1:A:104:HIS:ND1	4:A:1001:HOH:O	2.33	0.53
1:A:704:ILE:HD12	1:A:707:LEU:HD12	1.90	0.53
1:D:368:VAL:HG21	1:D:372:PHE:HD2	1.72	0.53
2:F:521:LEU:N	2:F:548:SER:O	2.42	0.53
1:B:714:ALA:HA	1:B:737:HIS:HB2	1.90	0.53
1:C:34:VAL:HG23	1:C:37:MET:HE2	1.90	0.53
2:F:705:LEU:HD13	2:F:708:LEU:HD22	1.89	0.52
1:E:118:LEU:HD23	1:E:123:LYS:HG3	1.91	0.52
1:B:641:LEU:O	1:B:663:ASN:ND2	2.42	0.52
1:B:726:GLU:N	1:B:726:GLU:OE1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:HD21	1:A:661:LEU:HD22	1.91	0.52
1:B:779:LEU:HD13	1:B:784:LEU:HD13	1.92	0.52
2:F:594:LEU:HB2	2:F:614:LEU:HD11	1.91	0.52
1:B:431:HIS:HD2	1:B:452:LYS:HG2	1.75	0.52
1:D:292:ASP:HB3	1:D:309:ARG:HH12	1.74	0.52
1:D:295:CYS:SG	1:D:308:TYR:HB2	2.49	0.52
2:F:143:ASN:OD1	2:F:143:ASN:N	2.43	0.52
1:A:463:PRO:HA	1:A:487:ALA:HB2	1.92	0.52
1:A:698:THR:HA	1:A:719:ARG:HB3	1.92	0.51
1:B:606:ILE:HD12	1:B:631:GLU:HB2	1.92	0.51
1:A:39:ALA:HB2	1:A:129:VAL:HG12	1.92	0.51
1:A:43:GLY:O	1:A:47:VAL:HG23	2.10	0.51
1:E:258:ASP:OD1	1:E:258:ASP:N	2.42	0.51
2:F:539:ARG:HB3	2:F:562:ASP:HB3	1.92	0.51
3:D:904:PEE:H18	3:F:904:PEE:H54	1.92	0.51
1:C:120:TRP:HZ3	1:C:128:LEU:HD11	1.74	0.51
1:A:505:ILE:HD13	1:A:532:ASN:HB3	1.93	0.50
1:B:452:LYS:NZ	1:B:475:TRP:O	2.40	0.50
1:D:149:THR:HG21	1:D:263:LEU:HD22	1.91	0.50
1:C:356:ILE:HG23	1:C:388:LYS:HG3	1.92	0.50
1:A:635:PHE:HB3	1:A:661:LEU:HD21	1.94	0.50
1:A:498:LEU:HB3	1:A:518:LEU:HD21	1.94	0.50
1:A:460:THR:HG22	1:A:482:LYS:HB2	1.93	0.50
1:B:688:ARG:HA	1:B:710:LEU:HA	1.93	0.49
2:F:547:LEU:HG	2:F:549:ILE:HD11	1.94	0.49
1:B:644:LEU:O	1:B:645:LYS:NZ	2.39	0.49
1:E:149:THR:HG21	1:E:263:LEU:HD22	1.92	0.49
1:B:721:GLU:O	1:B:744:GLN:N	2.35	0.49
1:C:46:GLN:HA	1:C:50:ASP:HB2	1.93	0.49
1:D:357:ARG:NH1	1:D:365:ILE:O	2.42	0.49
1:E:103:ARG:NH1	4:E:1001:HOH:O	2.45	0.49
1:B:329:VAL:O	1:B:333:GLY:N	2.44	0.49
2:F:548:SER:HA	2:F:571:CYS:HB3	1.95	0.49
2:F:778:LYS:O	2:F:782:LEU:N	2.45	0.49
1:A:31:ILE:HG22	1:A:35:MET:HE2	1.95	0.49
1:A:576:ASN:HB3	1:A:579:THR:HB	1.94	0.49
1:B:552:LYS:HG3	1:B:575:ASN:HB2	1.94	0.49
1:B:123:LYS:NZ	3:B:901:PEE:O2P	2.44	0.48
2:F:741:LEU:HB2	2:F:762:ASN:HD21	1.78	0.48
1:E:365:ILE:HG12	1:E:395:SER:HB3	1.95	0.48
1:B:700:LEU:HD21	1:B:704:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:522:VAL:HG23	2:F:550:LYS:HB3	1.95	0.48
2:F:570:MET:HE1	2:F:572:VAL:HG23	1.95	0.48
1:B:522:HIS:CE1	1:B:550:ARG:HG3	2.48	0.48
2:F:474:LEU:HB2	2:F:498:VAL:HG22	1.95	0.48
1:A:48:THR:HG22	1:A:49:GLN:HG3	1.96	0.48
1:B:736:LEU:HB3	1:B:738:LEU:HG	1.95	0.48
2:F:441:PHE:HA	2:F:466:LEU:HD21	1.95	0.48
1:A:602:ASP:OD1	1:A:625:ASN:ND2	2.46	0.48
2:F:137:VAL:HB	2:F:272:LYS:HE2	1.96	0.48
2:F:166:PHE:HD1	2:F:387:ARG:HE	1.61	0.48
1:C:389:ARG:HH22	1:D:246:LYS:NZ	2.12	0.48
1:D:143:TRP:HE1	1:D:260:VAL:HG13	1.79	0.48
1:E:130:LEU:HD21	3:E:901:PEE:H39	1.96	0.48
1:B:597:GLU:OE1	1:B:597:GLU:N	2.47	0.48
1:B:629:ILE:HD13	1:B:651:ILE:HD13	1.96	0.48
1:E:156:PHE:HD1	1:E:250:PHE:HZ	1.60	0.48
2:F:122:TRP:HA	2:F:125:LYS:HE2	1.95	0.48
2:F:604:ILE:HD11	2:F:627:ILE:HG22	1.95	0.48
1:A:19:ILE:HD11	1:A:157:VAL:HG22	1.95	0.47
1:A:265:MET:HG3	1:A:269:ILE:HD11	1.95	0.47
1:D:247:VAL:HG11	1:D:393:PHE:HB3	1.96	0.47
1:A:63:ASP:OD1	1:A:306:ARG:NH1	2.46	0.47
1:B:171:ARG:HG3	1:B:232:LEU:HD11	1.96	0.47
1:D:131:LEU:HD11	3:D:901:PEE:H27	1.96	0.47
1:A:438:ILE:HG12	1:A:459:VAL:HG21	1.95	0.47
1:B:599:ILE:HG23	1:B:622:LYS:HD3	1.96	0.47
1:A:618:GLU:HG3	1:A:643:CYS:HB3	1.97	0.47
2:F:578:LYS:HG3	2:F:580:VAL:HG13	1.97	0.47
1:A:420:LEU:HD11	1:A:445:LEU:HD21	1.95	0.47
1:A:796:PRO:HA	1:A:799:LYS:HB2	1.96	0.47
1:A:320:ILE:HG22	3:A:903:PEE:H15	1.96	0.47
1:B:323:SER:HB3	3:B:902:PEE:H15	1.95	0.47
1:C:39:ALA:HB2	1:C:129:VAL:HG12	1.97	0.47
2:F:680:PHE:HB3	2:F:702:ILE:HA	1.96	0.47
1:B:443:PHE:HE2	1:B:462:PRO:HD2	1.80	0.47
2:F:348:GLU:OE2	2:F:367:LYS:NZ	2.41	0.47
1:B:685:ARG:HA	1:B:707:LEU:HD22	1.96	0.47
2:F:723:ASP:HA	2:F:726:TYR:HD2	1.80	0.47
1:A:370:ASN:HB3	1:A:371:ASP:H	1.54	0.47
1:A:545:ARG:HG2	1:A:547:LYS:HE3	1.97	0.46
1:B:791:PHE:HE1	1:B:802:LEU:HD13	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:SER:OG	3:E:902:PEE:O2	2.33	0.46
1:A:527:LEU:HD11	1:A:551:LEU:HD22	1.97	0.46
1:D:244:PHE:O	1:D:248:LYS:HG2	2.14	0.46
1:E:173:LEU:HD11	1:E:389:ARG:HG2	1.98	0.46
1:A:550:ARG:HH12	1:A:575:ASN:HB2	1.80	0.46
1:B:702:ALA:HA	1:B:726:GLU:HG2	1.98	0.46
1:C:372:PHE:HZ	1:C:390:PHE:HE2	1.64	0.46
2:F:150:GLY:O	2:F:154:LYS:HG3	2.16	0.46
1:A:55:LEU:HD11	1:B:105:GLN:HA	1.97	0.46
1:A:611:PHE:HE1	1:A:631:GLU:HB3	1.81	0.46
1:C:370:ASN:HB3	1:C:371:ASP:H	1.55	0.46
2:F:490:LYS:HG3	2:F:513:LEU:HA	1.98	0.46
2:F:683:ASN:HB3	2:F:704:VAL:HG12	1.98	0.46
1:B:431:HIS:HA	1:B:452:LYS:HG2	1.98	0.46
1:B:804:ARG:O	1:B:808:GLU:N	2.35	0.45
1:D:392:VAL:HG23	1:D:393:PHE:HD1	1.81	0.45
2:F:620:LYS:HG2	2:F:621:GLU:HG3	1.97	0.45
1:A:714:ALA:HA	1:A:737:HIS:HB2	1.98	0.45
1:D:164:PHE:HA	1:D:389:ARG:NH1	2.30	0.45
1:B:50:ASP:O	3:B:904:PEE:N	2.38	0.45
2:F:170:TRP:HA	2:F:173:ARG:HB2	1.99	0.45
2:F:452:GLU:HG3	2:F:475:HIS:HB3	1.98	0.45
2:F:545:LYS:HA	2:F:567:LEU:HA	1.97	0.45
2:F:680:PHE:HE2	2:F:699:PRO:HD2	1.82	0.45
2:F:571:CYS:HA	2:F:595:GLU:HB3	1.99	0.45
1:B:515:LEU:HB3	1:B:518:LEU:HD23	1.98	0.45
1:B:739:GLY:HA3	1:B:760:GLU:HG2	1.98	0.45
1:D:375:MET:HA	1:D:378:LEU:HD12	1.99	0.45
2:F:654:GLU:HG2	2:F:678:HIS:CG	2.51	0.45
1:E:297:VAL:HG23	1:E:299:ILE:HG12	1.99	0.45
1:B:39:ALA:HB2	1:B:129:VAL:HG12	1.99	0.45
1:B:442:VAL:HG13	1:B:443:PHE:CD1	2.52	0.45
1:D:55:LEU:HD11	1:E:105:GLN:HA	1.99	0.45
3:F:901:PEE:H46	3:F:904:PEE:H46	1.98	0.45
1:B:43:GLY:HA3	3:B:904:PEE:H47	1.98	0.45
2:F:649:ILE:HG21	2:F:667:PHE:HE2	1.82	0.45
1:B:632:ILE:HA	1:B:635:PHE:HD2	1.82	0.45
1:A:726:GLU:O	1:A:729:GLN:HB2	2.16	0.44
2:F:397:GLU:O	2:F:401:LYS:HG2	2.16	0.44
2:F:601:LEU:HD22	2:F:605:PRO:HG3	2.00	0.44
2:F:618:ASP:HA	2:F:643:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:782:LEU:HG	2:F:784:VAL:HG23	1.99	0.44
1:A:49:GLN:NE2	1:B:47:VAL:O	2.50	0.44
1:A:431:HIS:CE1	1:A:433:PHE:HB2	2.51	0.44
1:B:166:SER:O	1:B:169:THR:OG1	2.29	0.44
1:C:40:VAL:O	1:C:44:THR:HG23	2.17	0.44
2:F:129:TYR:HD2	3:F:901:PEE:H35	1.83	0.44
1:A:454:GLU:HA	1:A:477:TYR:HB2	1.98	0.44
1:A:622:LYS:HB2	1:A:647:TRP:NE1	2.32	0.44
1:B:461:ILE:HG21	1:B:465:ILE:HD12	1.99	0.44
1:A:171:ARG:HH21	1:A:405:LEU:HD21	1.82	0.44
1:A:677:ILE:HG13	1:A:697:LEU:HD11	1.99	0.44
1:B:169:THR:O	1:B:173:LEU:N	2.49	0.44
2:F:49:GLN:HB2	3:F:904:PEE:H3	2.00	0.44
1:B:450:VAL:HG13	1:B:473:GLU:HB3	1.99	0.44
2:F:170:TRP:NE1	2:F:400:LEU:HD13	2.32	0.44
2:F:535:LEU:O	2:F:538:LEU:HG	2.16	0.44
1:A:24:TRP:O	1:A:28:THR:HG23	2.17	0.44
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.78	0.44
1:A:431:HIS:HB2	1:A:452:LYS:HD3	1.99	0.44
1:E:246:LYS:HA	1:E:249:LYS:HG2	1.99	0.44
2:F:652:ILE:O	2:F:678:HIS:NE2	2.40	0.44
1:A:606:ILE:HG13	1:A:626:LEU:HD21	1.98	0.44
1:A:658:ILE:HD12	1:A:661:LEU:HD12	1.99	0.44
1:B:614:HIS:O	1:B:640:ARG:NH1	2.51	0.44
1:B:792:SER:HA	1:B:799:LYS:HD3	2.00	0.44
1:B:162:LYS:HE3	1:B:162:LYS:HB2	1.88	0.43
1:C:52:MET:HE3	1:C:118:LEU:HD22	1.99	0.43
1:E:392:VAL:HG23	1:E:393:PHE:HD1	1.83	0.43
2:F:494:LYS:HZ2	2:F:515:ASN:HD22	1.65	0.43
1:A:296:THR:HG23	1:A:307:THR:HG22	2.00	0.43
1:A:674:ILE:H	1:A:674:ILE:HG13	1.65	0.43
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.88	0.43
1:A:467:GLN:HE22	1:B:433:PHE:HB3	1.83	0.43
1:A:711:GLN:O	1:A:734:ARG:N	2.43	0.43
2:F:461:ALA:HB2	2:F:482:HIS:CE1	2.54	0.43
2:F:497:SER:HB2	2:F:520:TYR:HD1	1.83	0.43
1:A:356:ILE:HG12	1:A:388:LYS:HA	2.00	0.43
1:A:420:LEU:HD22	1:A:428:LEU:HG	1.99	0.43
1:C:389:ARG:HH12	1:D:246:LYS:NZ	2.16	0.43
1:E:233:ASP:HB3	1:E:236:GLU:HB3	1.99	0.43
2:F:271:ILE:O	2:F:275:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HD12	1:A:379:ILE:HD11	2.00	0.43
2:F:294:ASN:OD1	2:F:305:ASN:ND2	2.52	0.43
2:F:643:LYS:HB3	2:F:645:TRP:CZ3	2.51	0.43
2:F:668:SER:O	2:F:670:ASN:ND2	2.51	0.43
1:B:761:LEU:HB3	1:B:764:ASN:OD1	2.18	0.43
1:C:266:ARG:O	1:C:270:ILE:HG13	2.19	0.43
1:C:297:VAL:HG23	1:C:299:ILE:HG12	2.01	0.43
1:E:159:ILE:HA	1:E:162:LYS:HG2	2.00	0.43
2:F:122:TRP:HZ3	2:F:130:LEU:HD11	1.83	0.43
2:F:429:PRO:HA	2:F:450:LYS:HB3	1.99	0.43
1:A:54:CYS:HA	1:A:310:CYS:HA	2.01	0.43
1:B:769:LEU:HD11	1:B:786:VAL:HG21	2.00	0.43
1:E:36:LEU:HB2	1:E:133:THR:HG21	2.00	0.43
1:A:251:ARG:HD2	1:A:394:LEU:HD22	2.01	0.43
1:C:309:ARG:NH2	1:D:108:TYR:OH	2.51	0.43
1:D:233:ASP:OD2	1:E:235:LYS:NZ	2.52	0.43
2:F:721:LEU:HD13	2:F:725:LEU:HD21	2.00	0.43
1:A:166:SER:O	1:A:169:THR:OG1	2.37	0.43
1:A:171:ARG:O	1:A:174:SER:OG	2.36	0.43
1:A:365:ILE:HD13	1:A:391:ALA:HB1	2.01	0.43
1:A:632:ILE:O	1:A:635:PHE:HB2	2.19	0.43
1:A:700:LEU:HD13	1:A:727:LEU:HD22	2.01	0.43
1:B:750:VAL:HG13	1:B:773:LEU:HD21	2.00	0.43
1:C:17:TYR:HB3	1:C:20:LEU:HD12	2.00	0.43
1:A:234:LYS:NZ	1:A:238:GLU:OE2	2.52	0.43
1:A:428:LEU:HD12	1:A:428:LEU:HA	1.90	0.43
1:B:323:SER:OG	3:B:902:PEE:O2	2.37	0.43
1:B:496:ARG:HD3	1:B:496:ARG:HA	1.86	0.43
1:A:771:VAL:HG13	1:A:798:VAL:HG21	2.00	0.42
1:B:254:VAL:HG11	1:B:375:MET:HE1	2.01	0.42
2:F:96:MET:HE3	2:F:96:MET:HB2	1.88	0.42
2:F:451:LEU:HB2	2:F:474:LEU:HD13	2.01	0.42
1:C:34:VAL:HA	1:C:37:MET:HG2	2.01	0.42
1:D:123:LYS:NZ	3:D:901:PEE:O2P	2.52	0.42
1:B:41:PHE:HB2	3:C:901:PEE:H41	2.00	0.42
1:B:15:PRO:HB2	1:B:16:ALA:H	1.65	0.42
1:B:619:ILE:HD13	1:B:619:ILE:HA	1.96	0.42
2:F:256:ASP:HB2	2:F:347:ARG:HH21	1.83	0.42
2:F:366:VAL:HG21	2:F:374:LEU:HD12	2.01	0.42
1:A:682:PHE:HB3	1:A:703:ASP:OD2	2.19	0.42
1:B:263:LEU:HA	1:B:263:LEU:HD12	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:LEU:HD21	1:B:667:LEU:HD12	2.01	0.42
1:B:677:ILE:HA	1:B:678:PRO:HD3	1.92	0.42
1:D:33:ILE:HD12	1:D:33:ILE:HA	1.81	0.42
2:F:118:ARG:HG2	2:F:118:ARG:HH11	1.84	0.42
2:F:555:LYS:HE2	2:F:581:MET:HG2	2.00	0.42
1:C:282:THR:O	1:C:286:VAL:HB	2.19	0.42
2:F:273:PHE:CE1	2:F:277:ILE:HG13	2.54	0.42
2:F:516:LEU:HD23	2:F:516:LEU:HA	1.94	0.42
1:A:647:TRP:H	1:A:647:TRP:CD1	2.38	0.42
1:A:713:LEU:HD22	1:A:727:LEU:HD11	2.00	0.42
1:B:170:THR:O	1:B:174:SER:N	2.52	0.42
1:C:315:ALA:O	1:C:319:LYS:N	2.51	0.42
2:F:693:ASN:N	2:F:716:ASN:OD1	2.46	0.42
1:A:644:LEU:HG	1:A:646:LEU:HG	2.02	0.42
1:A:733:LEU:HD13	1:A:736:LEU:HD11	2.01	0.42
1:A:682:PHE:HD1	1:A:703:ASP:HB3	1.85	0.42
1:B:19:ILE:HD11	1:B:157:VAL:HG22	2.01	0.42
1:B:444:ASP:OD1	1:B:467:GLN:NE2	2.52	0.42
1:A:450:VAL:HG22	1:A:473:GLU:HB2	2.02	0.42
1:A:534:TYR:CE1	1:A:559:PRO:HG3	2.55	0.42
2:F:472:LEU:HB2	2:F:496:LEU:HD23	2.02	0.42
1:A:534:TYR:HE1	1:A:555:LEU:HD22	1.85	0.41
1:A:545:ARG:NH2	1:B:600:ARG:HD2	2.36	0.41
1:D:233:ASP:HB3	1:D:236:GLU:HB3	2.02	0.41
1:D:370:ASN:HB3	1:D:371:ASP:H	1.52	0.41
2:F:649:ILE:HD13	2:F:649:ILE:HA	1.95	0.41
2:F:777:LEU:HD21	2:F:782:LEU:HD13	2.00	0.41
1:A:246:LYS:HA	1:A:249:LYS:HG2	2.03	0.41
1:A:570:GLN:HA	1:A:593:LEU:HA	2.01	0.41
1:D:269:ILE:HD13	1:D:269:ILE:HA	1.94	0.41
3:E:901:PEE:H63	3:E:901:PEE:H56	1.86	0.41
1:A:46:GLN:HA	1:A:50:ASP:HB2	2.01	0.41
1:B:350:LYS:HE2	1:B:350:LYS:HB2	1.78	0.41
1:B:715:VAL:HB	1:B:738:LEU:HD22	2.02	0.41
2:F:144:PHE:CZ	2:F:261:MET:HE2	2.55	0.41
2:F:482:HIS:CE1	2:F:484:ALA:H	2.38	0.41
2:F:482:HIS:HE1	2:F:484:ALA:HB3	1.85	0.41
2:F:553:VAL:N	2:F:574:ASN:OD1	2.54	0.41
2:F:721:LEU:HG	2:F:741:LEU:HD21	2.01	0.41
1:B:576:ASN:HB3	1:B:579:THR:HB	2.01	0.41
1:C:117:ARG:HG3	1:C:295:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:ARG:NH2	1:E:296:THR:O	2.53	0.41
1:A:40:VAL:O	1:A:44:THR:HG22	2.20	0.41
1:A:419:ARG:HA	1:A:419:ARG:HD2	1.82	0.41
1:A:491:LEU:HD22	1:A:495:LEU:HB2	2.02	0.41
1:A:654:ILE:HG21	1:A:681:LEU:HD12	2.02	0.41
1:B:43:GLY:HA3	3:B:904:PEE:H41	2.02	0.41
1:C:143:TRP:HE1	1:C:260:VAL:HG13	1.86	0.41
2:F:598:HIS:HB2	2:F:621:GLU:HB2	2.03	0.41
1:A:265:MET:O	1:A:269:ILE:HD12	2.20	0.41
1:A:502:PHE:HB2	1:A:507:GLU:HB2	2.03	0.41
1:A:705:GLY:O	1:A:708:GLN:NE2	2.52	0.41
1:A:778:LEU:HD23	1:A:778:LEU:HA	1.86	0.41
1:C:267:GLN:HE21	1:C:267:GLN:HB2	1.66	0.41
1:C:316:THR:OG1	1:D:115:GLU:OE2	2.36	0.41
1:A:379:ILE:HD13	1:A:379:ILE:HA	1.92	0.41
1:A:413:LEU:O	1:A:417:ARG:HG2	2.21	0.41
1:A:421:THR:O	1:A:429:GLU:N	2.51	0.41
1:A:524:THR:HB	1:A:552:LYS:HE3	2.02	0.41
1:A:667:LEU:HG	1:A:669:LEU:HG	2.03	0.41
1:B:414:ASP:OD1	1:B:414:ASP:N	2.54	0.41
1:B:580:LYS:HD3	1:B:580:LYS:HA	1.85	0.41
1:B:707:LEU:HB3	1:B:710:LEU:HD23	2.02	0.41
1:B:711:GLN:OE1	1:B:734:ARG:NE	2.45	0.41
2:F:574:ASN:HB3	2:F:599:CYS:HA	2.02	0.41
2:F:620:LYS:HD2	2:F:646:TYR:HD2	1.85	0.41
2:F:641:VAL:HA	2:F:664:ARG:HB2	2.02	0.41
1:A:174:SER:HB3	1:B:245:GLU:HG2	2.03	0.41
1:B:117:ARG:HA	1:B:117:ARG:HD3	1.96	0.41
1:B:724:PRO:HG2	1:B:726:GLU:HB2	2.03	0.41
1:B:742:VAL:HA	1:B:765:ARG:HD3	2.02	0.41
1:C:317:LEU:HD12	1:C:317:LEU:HA	1.94	0.41
1:E:235:LYS:HD3	1:E:235:LYS:HA	1.87	0.41
2:F:778:LYS:HD3	2:F:778:LYS:HA	1.88	0.41
1:B:55:LEU:HD23	1:B:55:LEU:HA	1.89	0.41
1:C:29:ASP:O	1:C:33:ILE:HG12	2.21	0.41
1:D:49:GLN:HE22	1:E:47:VAL:HG13	1.86	0.41
1:D:316:THR:OG1	1:E:115:GLU:OE2	2.29	0.41
1:E:401:LYS:HB3	1:E:401:LYS:HE3	1.87	0.41
2:F:387:ARG:HG2	2:F:387:ARG:HH11	1.86	0.41
2:F:490:LYS:O	2:F:514:ARG:NH1	2.54	0.41
1:A:419:ARG:O	1:A:419:ARG:NH1	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:HIS:CD2	1:A:288:ASN:HD22	2.39	0.40
1:B:415:LYS:C	1:B:419:ARG:HH21	2.30	0.40
1:B:794:LEU:HD22	1:B:798:VAL:HG11	2.02	0.40
1:C:145:LYS:HA	1:C:145:LYS:HD3	1.80	0.40
1:C:375:MET:O	1:C:379:ILE:HG12	2.21	0.40
1:D:15:PRO:HB2	1:D:16:ALA:H	1.68	0.40
1:D:16:ALA:HB1	1:D:157:VAL:HG11	2.02	0.40
1:D:163:CYS:HA	1:D:243:LEU:HD21	2.03	0.40
1:D:241:LYS:HE2	1:D:241:LYS:HB3	1.89	0.40
1:E:129:VAL:HG23	1:E:325:TYR:CE1	2.56	0.40
1:A:105:GLN:HA	2:F:55:LEU:HD11	2.03	0.40
1:A:742:VAL:HA	1:A:765:ARG:HG2	2.02	0.40
1:B:590:MET:HG3	1:B:593:LEU:HB2	2.02	0.40
1:C:38:ILE:HG22	3:D:901:PEE:H36	2.03	0.40
1:C:295:CYS:SG	1:C:308:TYR:HB2	2.62	0.40
2:F:171:THR:HG21	2:F:387:ARG:HH11	1.86	0.40
1:A:155:HIS:O	1:A:159:ILE:HG23	2.21	0.40
1:A:269:ILE:HA	1:A:272:VAL:HG12	2.02	0.40
1:B:117:ARG:HG3	1:B:295:CYS:HB2	2.04	0.40
1:B:132:HIS:NE2	1:B:281:TYR:OH	2.53	0.40
1:B:413:LEU:HA	1:B:416:LEU:HD12	2.04	0.40
1:B:759:ILE:HD11	1:B:784:LEU:HD12	2.04	0.40
1:D:243:LEU:HG	1:D:393:PHE:CE2	2.56	0.40
1:E:246:LYS:HE3	1:E:246:LYS:HB2	1.78	0.40
1:B:363:SER:O	1:B:363:SER:OG	2.37	0.40
1:B:721:GLU:HB3	1:B:744:GLN:HG2	2.03	0.40
1:B:778:LEU:HD23	1:B:778:LEU:HA	1.90	0.40
1:C:41:PHE:HB2	3:D:901:PEE:H42	2.03	0.40
1:D:119:HIS:CE1	1:D:288:ASN:HD22	2.40	0.40
1:E:43:GLY:HA3	3:F:904:PEE:H78	2.04	0.40
1:E:354:GLU:HA	1:E:357:ARG:HG2	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	711/911 (78%)	686 (96%)	25 (4%)	0	100	100
1	B	710/911 (78%)	676 (95%)	34 (5%)	0	100	100
1	C	294/911 (32%)	283 (96%)	11 (4%)	0	100	100
1	D	310/911 (34%)	305 (98%)	5 (2%)	0	100	100
1	E	310/911 (34%)	304 (98%)	6 (2%)	0	100	100
2	F	698/813 (86%)	673 (96%)	25 (4%)	0	100	100
All	All	3033/5368 (56%)	2927 (96%)	106 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	665/830 (80%)	663 (100%)	2 (0%)	86	86
1	B	665/830 (80%)	664 (100%)	1 (0%)	87	88
1	C	279/830 (34%)	279 (100%)	0	100	100
1	D	294/830 (35%)	293 (100%)	1 (0%)	86	86
1	E	294/830 (35%)	293 (100%)	1 (0%)	86	86
2	F	659/756 (87%)	658 (100%)	1 (0%)	87	88
All	All	2856/4906 (58%)	2850 (100%)	6 (0%)	85	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	HIS
1	A	750	VAL
1	B	733	LEU
1	D	33	ILE

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Mol	Chain	Res	Type
1	E	52	MET
2	F	609	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	239	GLN
1	A	406	ASN
1	A	554	ASN
1	A	663	ASN
1	A	740	ASN
1	B	46	GLN
1	B	253	HIS
1	B	377	HIS
1	B	526	ASN
1	B	624	ASN
1	B	660	ASN
1	B	744	GLN
1	B	764	ASN
1	D	253	HIS
1	E	381	GLN
1	E	409	ASN
2	F	112	ASN
2	F	113	GLN
2	F	402	GLN
2	F	423	HIS
2	F	447	GLN
2	F	482	HIS
2	F	492	ASN
2	F	515	ASN
2	F	558	GLN
2	F	606	HIS
2	F	762	ASN
2	F	799	GLN

5.3.3 RNA

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)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEE	A	903	-	12,12,50	1.09	1 (8%)	12,12,55	1.14	1 (8%)
3	PEE	A	902	-	12,12,50	1.74	3 (25%)	12,12,55	1.69	3 (25%)
3	PEE	E	902	-	9,9,50	1.72	2 (22%)	9,9,55	1.62	2 (22%)
3	PEE	D	901	-	43,43,50	1.36	4 (9%)	46,48,55	1.05	2 (4%)
3	PEE	E	903	-	9,9,50	1.71	2 (22%)	9,9,55	1.61	2 (22%)
3	PEE	B	901	-	43,43,50	1.35	5 (11%)	46,48,55	1.05	2 (4%)
3	PEE	B	904	-	50,50,50	1.29	4 (8%)	53,55,55	0.96	1 (1%)
3	PEE	C	901	-	43,43,50	1.35	4 (9%)	46,48,55	1.05	2 (4%)
3	PEE	F	901	-	43,43,50	0.76	2 (4%)	46,48,55	0.64	1 (2%)
3	PEE	A	901	-	43,43,50	1.35	4 (9%)	46,48,55	1.06	2 (4%)
3	PEE	E	901	-	43,43,50	1.35	5 (11%)	46,48,55	1.04	2 (4%)
3	PEE	F	902	-	10,10,50	1.64	2 (20%)	10,10,55	1.56	2 (20%)
3	PEE	D	903	-	10,10,50	0.56	0	10,10,55	0.80	0
3	PEE	F	903	-	7,7,50	1.94	2 (28%)	7,7,55	1.82	2 (28%)
3	PEE	D	904	-	50,50,50	1.29	4 (8%)	53,55,55	0.96	1 (1%)
3	PEE	D	902	-	8,8,50	1.81	2 (25%)	8,8,55	1.70	2 (25%)
3	PEE	C	902	-	10,10,50	1.62	2 (20%)	10,10,55	1.57	2 (20%)
3	PEE	B	902	-	10,10,50	0.58	0	10,10,55	0.80	0
3	PEE	B	903	-	9,9,50	0.61	0	9,9,55	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PEE	F	904	-	50,50,50	1.29	4 (8%)	53,55,55	0.98	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEE	A	903	-	-	6/10/10/54	-
3	PEE	A	902	-	-	5/10/10/54	-
3	PEE	E	902	-	-	5/7/7/54	-
3	PEE	D	901	-	-	20/47/47/54	-
3	PEE	E	903	-	-	1/7/7/54	-
3	PEE	B	901	-	-	19/47/47/54	-
3	PEE	B	904	-	-	28/54/54/54	-
3	PEE	C	901	-	-	16/47/47/54	-
3	PEE	F	901	-	-	15/47/47/54	-
3	PEE	A	901	-	-	18/47/47/54	-
3	PEE	E	901	-	-	18/47/47/54	-
3	PEE	F	902	-	-	4/8/8/54	-
3	PEE	D	903	-	-	5/8/8/54	-
3	PEE	F	903	-	-	4/5/5/54	-
3	PEE	D	904	-	-	29/54/54/54	-
3	PEE	D	902	-	-	4/6/6/54	-
3	PEE	C	902	-	-	4/8/8/54	-
3	PEE	B	902	-	-	4/8/8/54	-
3	PEE	B	903	-	-	4/7/7/54	-
3	PEE	F	904	-	-	27/54/54/54	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	PEE	P-O4P	4.79	1.78	1.59
3	D	901	PEE	P-O4P	4.77	1.78	1.59
3	C	901	PEE	P-O4P	4.76	1.78	1.59
3	D	904	PEE	P-O4P	4.75	1.78	1.59
3	F	904	PEE	P-O4P	4.74	1.77	1.59
3	E	901	PEE	P-O4P	4.71	1.77	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	904	PEE	P-O4P	4.70	1.77	1.59
3	B	901	PEE	P-O4P	4.69	1.77	1.59
3	F	902	PEE	O4-C10	4.34	1.36	1.22
3	E	902	PEE	O4-C10	4.32	1.36	1.22
3	F	903	PEE	O4-C10	4.31	1.36	1.22
3	C	902	PEE	O4-C10	4.29	1.36	1.22
3	D	902	PEE	O4-C10	4.29	1.36	1.22
3	E	903	PEE	O4-C10	4.29	1.36	1.22
3	A	902	PEE	O4-C10	4.25	1.36	1.22
3	F	904	PEE	C39-C38	3.97	1.54	1.31
3	D	904	PEE	C39-C38	3.94	1.54	1.31
3	B	904	PEE	C39-C38	3.94	1.54	1.31
3	F	904	PEE	C18-C19	3.78	1.53	1.31
3	D	901	PEE	C18-C19	3.78	1.53	1.31
3	B	904	PEE	C18-C19	3.74	1.53	1.31
3	C	901	PEE	C18-C19	3.73	1.52	1.31
3	A	901	PEE	C18-C19	3.73	1.52	1.31
3	B	901	PEE	C18-C19	3.72	1.52	1.31
3	D	904	PEE	C18-C19	3.68	1.52	1.31
3	E	901	PEE	C18-C19	3.66	1.52	1.31
3	F	901	PEE	C18-C19	3.43	1.51	1.31
3	D	901	PEE	C38-C39	3.39	1.54	1.29
3	C	901	PEE	C38-C39	3.38	1.54	1.29
3	A	901	PEE	C38-C39	3.37	1.54	1.29
3	E	901	PEE	C38-C39	3.35	1.53	1.29
3	B	901	PEE	C38-C39	3.34	1.53	1.29
3	A	903	PEE	C18-C19	3.20	1.52	1.29
3	A	902	PEE	C18-C19	3.16	1.52	1.29
3	F	901	PEE	C38-C39	2.99	1.51	1.29
3	D	902	PEE	O2-C10	-2.68	1.21	1.30
3	E	902	PEE	O2-C10	-2.68	1.22	1.30
3	E	903	PEE	O2-C10	-2.67	1.22	1.30
3	F	903	PEE	O2-C10	-2.67	1.22	1.30
3	A	902	PEE	O2-C10	-2.66	1.22	1.30
3	C	902	PEE	O2-C10	-2.65	1.22	1.30
3	F	902	PEE	O2-C10	-2.65	1.22	1.30
3	B	901	PEE	O4P-C4	-2.08	1.36	1.44
3	B	904	PEE	O4P-C4	-2.07	1.36	1.44
3	E	901	PEE	O2-C2	-2.06	1.41	1.46
3	A	901	PEE	O4P-C4	-2.04	1.36	1.44
3	E	901	PEE	O4P-C4	-2.04	1.36	1.44
3	F	904	PEE	O4P-C4	-2.03	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	904	PEE	O4P-C4	-2.02	1.36	1.44
3	C	901	PEE	O4P-C4	-2.01	1.36	1.44
3	B	901	PEE	O2-C2	-2.01	1.41	1.46
3	D	901	PEE	O4P-C4	-2.00	1.36	1.44

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	901	PEE	O2P-P-O1P	4.49	133.34	112.44
3	D	904	PEE	O2P-P-O1P	4.48	133.29	112.44
3	C	901	PEE	O2P-P-O1P	4.48	133.29	112.44
3	B	901	PEE	O2P-P-O1P	4.47	133.25	112.44
3	F	904	PEE	O2P-P-O1P	4.46	133.18	112.44
3	A	901	PEE	O2P-P-O1P	4.46	133.18	112.44
3	E	901	PEE	O2P-P-O1P	4.44	133.10	112.44
3	B	904	PEE	O2P-P-O1P	4.43	133.06	112.44
3	C	902	PEE	O2-C10-C11	3.39	124.72	114.00
3	E	902	PEE	O2-C10-C11	3.38	124.67	114.00
3	F	902	PEE	O2-C10-C11	3.37	124.66	114.00
3	A	902	PEE	O2-C10-C11	3.37	124.66	114.00
3	F	903	PEE	O2-C10-C11	3.37	124.64	114.00
3	E	903	PEE	O2-C10-C11	3.34	124.55	114.00
3	D	902	PEE	O2-C10-C11	3.33	124.53	114.00
3	C	902	PEE	O4-C10-C11	-2.68	114.58	123.09
3	F	903	PEE	O4-C10-C11	-2.68	114.59	123.09
3	E	902	PEE	O4-C10-C11	-2.68	114.60	123.09
3	A	902	PEE	O4-C10-C11	-2.68	114.60	123.09
3	E	903	PEE	O4-C10-C11	-2.65	114.68	123.09
3	F	902	PEE	O4-C10-C11	-2.65	114.69	123.09
3	D	902	PEE	O4-C10-C11	-2.65	114.69	123.09
3	A	903	PEE	C17-C18-C19	-2.43	112.07	130.48
3	A	902	PEE	C17-C18-C19	-2.39	112.40	130.48
3	A	901	PEE	C37-C38-C39	-2.22	113.68	130.48
3	D	901	PEE	C37-C38-C39	-2.21	113.71	130.48
3	B	901	PEE	C37-C38-C39	-2.21	113.71	130.48
3	C	901	PEE	C37-C38-C39	-2.21	113.71	130.48
3	E	901	PEE	C37-C38-C39	-2.20	113.83	130.48
3	F	901	PEE	C37-C38-C39	-2.14	114.30	130.48

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	PEE	C4-O4P-P-O3P
3	A	901	PEE	C4-O4P-P-O2P
3	A	901	PEE	C4-O4P-P-O1P
3	A	901	PEE	O4P-C4-C5-N
3	A	903	PEE	C17-C18-C19-C20
3	B	901	PEE	C1-O3P-P-O1P
3	B	901	PEE	C1-O3P-P-O4P
3	B	901	PEE	O4P-C4-C5-N
3	B	904	PEE	C1-O3P-P-O2P
3	B	904	PEE	C1-O3P-P-O4P
3	B	904	PEE	C4-O4P-P-O3P
3	B	904	PEE	C4-O4P-P-O2P
3	B	904	PEE	C4-O4P-P-O1P
3	B	904	PEE	O4P-C4-C5-N
3	C	901	PEE	C1-O3P-P-O2P
3	C	901	PEE	O4P-C4-C5-N
3	D	901	PEE	C1-O3P-P-O2P
3	D	901	PEE	C4-O4P-P-O3P
3	D	901	PEE	C4-O4P-P-O1P
3	D	901	PEE	O4P-C4-C5-N
3	D	904	PEE	O2-C2-C3-O3
3	D	904	PEE	C2-C1-O3P-P
3	D	904	PEE	C1-O3P-P-O1P
3	D	904	PEE	C1-O3P-P-O4P
3	D	904	PEE	C4-O4P-P-O3P
3	D	904	PEE	C4-O4P-P-O2P
3	D	904	PEE	O4P-C4-C5-N
3	E	901	PEE	C1-O3P-P-O2P
3	E	901	PEE	C1-O3P-P-O4P
3	E	901	PEE	C4-O4P-P-O2P
3	E	901	PEE	O4P-C4-C5-N
3	F	901	PEE	C1-O3P-P-O2P
3	F	901	PEE	C1-O3P-P-O4P
3	F	904	PEE	C11-C10-O2-C2
3	F	904	PEE	C1-O3P-P-O1P
3	F	904	PEE	C1-O3P-P-O4P
3	F	904	PEE	C4-O4P-P-O3P
3	F	904	PEE	C4-O4P-P-O2P
3	F	904	PEE	C5-C4-O4P-P
3	F	904	PEE	O4-C10-O2-C2
3	D	904	PEE	C37-C38-C39-C40
3	F	904	PEE	C37-C38-C39-C40
3	A	901	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
3	D	904	PEE	C21-C22-C23-C24
3	A	901	PEE	C10-C11-C12-C13
3	D	902	PEE	C10-C11-C12-C13
3	D	904	PEE	C30-C31-C32-C33
3	A	901	PEE	O5-C30-O3-C3
3	F	904	PEE	C10-C11-C12-C13
3	B	904	PEE	C35-C36-C37-C38
3	B	904	PEE	C17-C18-C19-C20
3	B	904	PEE	C37-C38-C39-C40
3	E	901	PEE	C17-C18-C19-C20
3	E	901	PEE	C10-C11-C12-C13
3	D	904	PEE	C17-C18-C19-C20
3	B	904	PEE	C22-C23-C24-C25
3	B	904	PEE	C34-C35-C36-C37
3	A	901	PEE	C17-C18-C19-C20
3	F	901	PEE	C17-C18-C19-C20
3	A	902	PEE	C13-C14-C15-C16
3	B	903	PEE	C13-C14-C15-C16
3	D	901	PEE	C11-C12-C13-C14
3	A	901	PEE	C19-C20-C21-C22
3	F	901	PEE	C11-C10-O2-C2
3	F	904	PEE	C11-C12-C13-C14
3	A	901	PEE	C37-C38-C39-C40
3	B	901	PEE	C13-C14-C15-C16
3	B	904	PEE	C10-C11-C12-C13
3	E	901	PEE	C31-C32-C33-C34
3	B	901	PEE	C22-C23-C24-C25
3	B	901	PEE	C11-C12-C13-C14
3	E	901	PEE	C13-C14-C15-C16
3	E	901	PEE	C31-C30-O3-C3
3	E	901	PEE	C34-C35-C36-C37
3	F	901	PEE	O4-C10-O2-C2
3	A	902	PEE	C15-C16-C17-C18
3	C	902	PEE	C13-C14-C15-C16
3	E	902	PEE	C13-C14-C15-C16
3	C	901	PEE	C14-C15-C16-C17
3	A	901	PEE	C35-C36-C37-C38
3	D	904	PEE	C35-C36-C37-C38
3	D	904	PEE	C40-C41-C42-C43
3	C	901	PEE	C11-C12-C13-C14
3	F	904	PEE	C12-C13-C14-C15
3	D	904	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	901	PEE	C22-C23-C24-C25
3	E	901	PEE	O5-C30-O3-C3
3	B	904	PEE	C40-C41-C42-C43
3	E	903	PEE	C13-C14-C15-C16
3	F	901	PEE	C23-C24-C25-C26
3	E	901	PEE	C14-C15-C16-C17
3	D	904	PEE	C1-C2-C3-O3
3	D	904	PEE	C15-C16-C17-C18
3	D	903	PEE	C13-C14-C15-C16
3	E	902	PEE	C10-C11-C12-C13
3	F	904	PEE	C31-C30-O3-C3
3	C	901	PEE	C32-C33-C34-C35
3	D	904	PEE	C34-C35-C36-C37
3	B	901	PEE	C34-C35-C36-C37
3	D	904	PEE	C13-C14-C15-C16
3	A	903	PEE	C11-C12-C13-C14
3	B	901	PEE	C15-C16-C17-C18
3	D	901	PEE	C35-C36-C37-C38
3	B	904	PEE	C11-C12-C13-C14
3	C	901	PEE	C12-C13-C14-C15
3	F	904	PEE	C2-C1-O3P-P
3	F	902	PEE	C13-C14-C15-C16
3	B	901	PEE	C24-C25-C26-C27
3	A	901	PEE	C31-C32-C33-C34
3	D	904	PEE	C22-C23-C24-C25
3	F	904	PEE	O5-C30-O3-C3
3	B	901	PEE	C37-C38-C39-C40
3	C	901	PEE	C37-C38-C39-C40
3	D	901	PEE	C37-C38-C39-C40
3	D	903	PEE	C15-C16-C17-C18
3	B	904	PEE	C1-C2-C3-O3
3	A	901	PEE	C14-C15-C16-C17
3	F	904	PEE	C22-C23-C24-C25
3	D	902	PEE	C11-C12-C13-C14
3	D	904	PEE	O3P-C1-C2-O2
3	C	901	PEE	C35-C36-C37-C38
3	F	904	PEE	C42-C43-C44-C45
3	B	904	PEE	O2-C2-C3-O3
3	B	904	PEE	C19-C20-C21-C22
3	D	901	PEE	C14-C15-C16-C17
3	F	901	PEE	C31-C32-C33-C34
3	D	904	PEE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	E	901	PEE	O3P-C1-C2-C3
3	B	904	PEE	C43-C44-C45-C46
3	B	904	PEE	C30-C31-C32-C33
3	E	901	PEE	C23-C24-C25-C26
3	F	903	PEE	C11-C12-C13-C14
3	F	904	PEE	C3-C2-O2-C10
3	D	901	PEE	C15-C16-C17-C18
3	B	904	PEE	C33-C34-C35-C36
3	B	903	PEE	C11-C12-C13-C14
3	F	904	PEE	C30-C31-C32-C33
3	A	901	PEE	C23-C24-C25-C26
3	C	902	PEE	C15-C16-C17-C18
3	F	904	PEE	C23-C24-C25-C26
3	D	904	PEE	C24-C25-C26-C27
3	D	904	PEE	C10-C11-C12-C13
3	D	901	PEE	C19-C20-C21-C22
3	D	904	PEE	C23-C24-C25-C26
3	A	901	PEE	C13-C14-C15-C16
3	F	901	PEE	C2-C1-O3P-P
3	E	901	PEE	O3P-C1-C2-O2
3	D	901	PEE	C31-C32-C33-C34
3	B	901	PEE	C1-O3P-P-O2P
3	D	901	PEE	C4-O4P-P-O2P
3	F	901	PEE	C1-O3P-P-O1P
3	F	904	PEE	C1-O3P-P-O2P
3	E	901	PEE	C2-C1-O3P-P
3	F	902	PEE	C15-C16-C17-C18
3	F	901	PEE	O3P-C1-C2-O2
3	D	903	PEE	C11-C12-C13-C14
3	D	904	PEE	C42-C43-C44-C45
3	B	904	PEE	C41-C42-C43-C44
3	B	902	PEE	C11-C12-C13-C14
3	D	901	PEE	C20-C21-C22-C23
3	C	901	PEE	C19-C20-C21-C22
3	C	901	PEE	C15-C16-C17-C18
3	D	901	PEE	C16-C17-C18-C19
3	F	904	PEE	C16-C17-C18-C19
3	A	901	PEE	C36-C37-C38-C39
3	C	901	PEE	C22-C23-C24-C25
3	F	904	PEE	C40-C41-C42-C43
3	B	904	PEE	C23-C24-C25-C26
3	D	901	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	D	901	PEE	C31-C30-O3-C3
3	D	904	PEE	C43-C44-C45-C46
3	B	904	PEE	O2-C10-C11-C12
3	F	904	PEE	C15-C16-C17-C18
3	D	903	PEE	O2-C10-C11-C12
3	B	901	PEE	C16-C17-C18-C19
3	B	901	PEE	C20-C21-C22-C23
3	D	901	PEE	O5-C30-O3-C3
3	E	902	PEE	O4-C10-C11-C12
3	B	904	PEE	O3P-C1-C2-O2
3	B	901	PEE	C14-C15-C16-C17
3	F	903	PEE	O4-C10-C11-C12
3	B	904	PEE	O3P-C1-C2-C3
3	D	902	PEE	O4-C10-C11-C12
3	A	903	PEE	C16-C17-C18-C19
3	F	901	PEE	C16-C17-C18-C19
3	D	903	PEE	O4-C10-C11-C12
3	C	902	PEE	O4-C10-C11-C12
3	F	904	PEE	C20-C21-C22-C23
3	F	902	PEE	O4-C10-C11-C12
3	F	902	PEE	O2-C10-C11-C12
3	F	904	PEE	C34-C35-C36-C37
3	A	903	PEE	C10-C11-C12-C13
3	F	901	PEE	C36-C37-C38-C39
3	F	903	PEE	O2-C10-C11-C12
3	C	901	PEE	C20-C21-C22-C23
3	E	902	PEE	O2-C10-C11-C12
3	B	903	PEE	O2-C10-C11-C12
3	C	901	PEE	C16-C17-C18-C19
3	E	901	PEE	C16-C17-C18-C19
3	F	904	PEE	O2-C10-C11-C12
3	D	902	PEE	O2-C10-C11-C12
3	C	901	PEE	C17-C18-C19-C20
3	A	903	PEE	O2-C10-C11-C12
3	A	901	PEE	C34-C35-C36-C37
3	F	901	PEE	O3P-C1-C2-C3
3	B	904	PEE	C16-C17-C18-C19
3	C	902	PEE	O2-C10-C11-C12
3	C	901	PEE	O3-C30-C31-C32
3	B	902	PEE	O2-C10-C11-C12
3	D	901	PEE	C36-C37-C38-C39
3	A	902	PEE	C16-C17-C18-C19

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	B	903	PEE	O4-C10-C11-C12
3	B	902	PEE	C13-C14-C15-C16
3	B	902	PEE	O4-C10-C11-C12
3	D	901	PEE	C22-C23-C24-C25
3	B	901	PEE	C12-C13-C14-C15
3	B	901	PEE	C36-C37-C38-C39
3	B	901	PEE	O3-C30-C31-C32
3	A	902	PEE	O4-C10-C11-C12
3	B	904	PEE	C20-C21-C22-C23
3	B	904	PEE	C12-C13-C14-C15
3	E	901	PEE	C36-C37-C38-C39
3	F	901	PEE	C18-C19-C20-C21
3	F	904	PEE	C36-C37-C38-C39
3	A	903	PEE	O4-C10-C11-C12
3	D	901	PEE	C34-C35-C36-C37
3	B	901	PEE	C35-C36-C37-C38
3	B	901	PEE	C33-C34-C35-C36
3	C	901	PEE	O2-C2-C3-O3
3	F	903	PEE	C10-C11-C12-C13
3	E	902	PEE	C11-C12-C13-C14
3	A	902	PEE	O2-C10-C11-C12
3	D	904	PEE	O3-C30-C31-C32
3	F	901	PEE	C13-C14-C15-C16
3	D	904	PEE	O2-C10-C11-C12
3	D	904	PEE	O5-C30-C31-C32

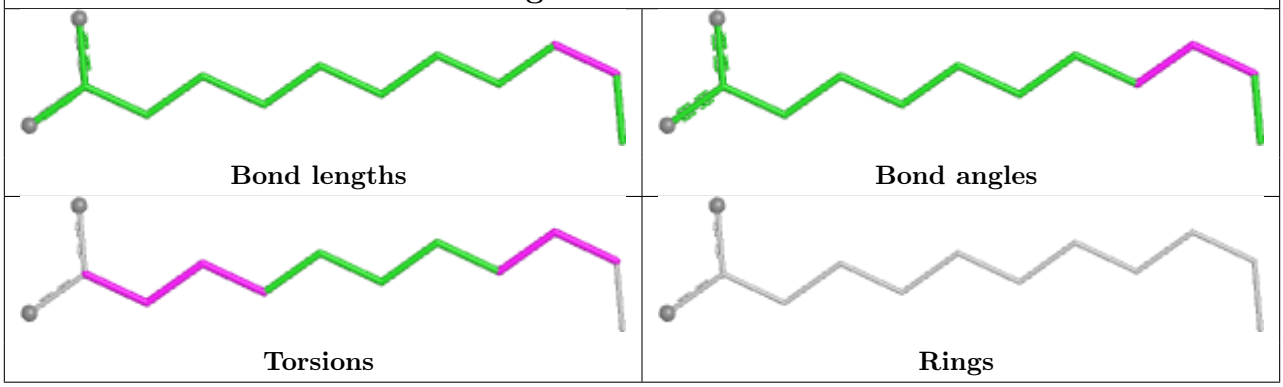
There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	PEE	1	0
3	E	902	PEE	1	0
3	D	901	PEE	5	0
3	B	901	PEE	2	0
3	B	904	PEE	4	0
3	C	901	PEE	1	0
3	F	901	PEE	5	0
3	E	901	PEE	2	0
3	D	904	PEE	2	0
3	B	902	PEE	2	0
3	F	904	PEE	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 PEE A 903



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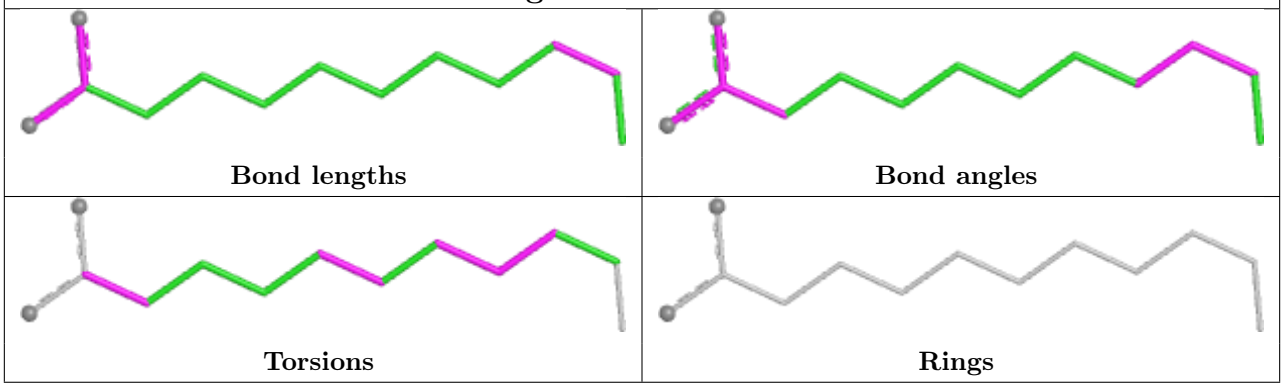

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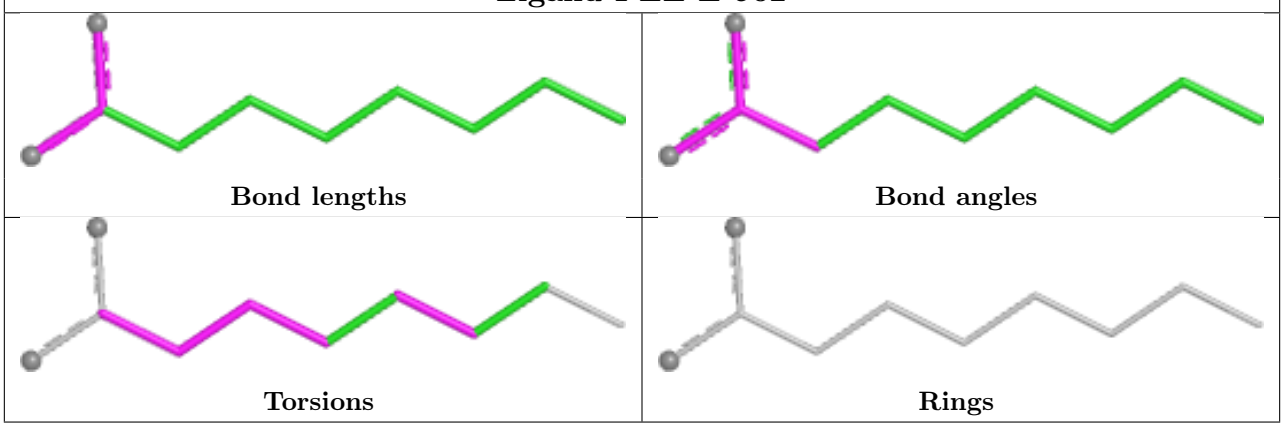

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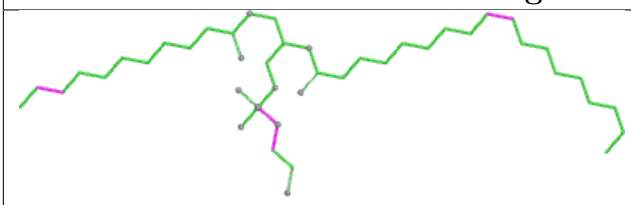
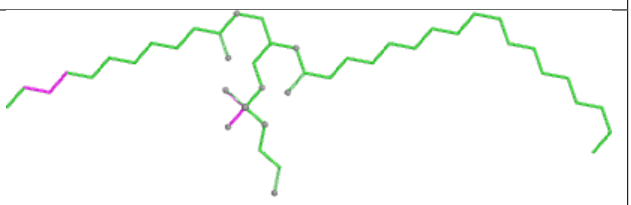
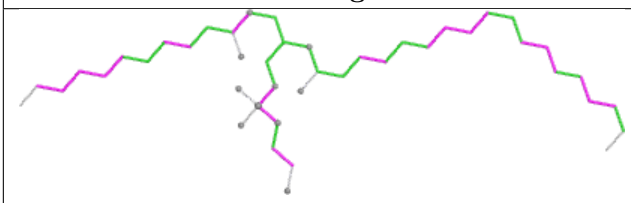


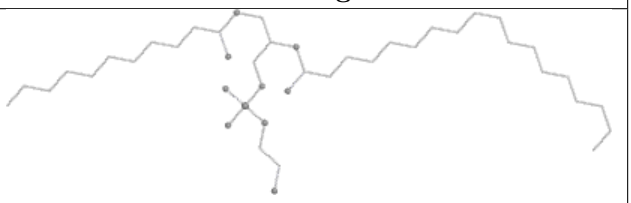
Bond lengths



Bond angles

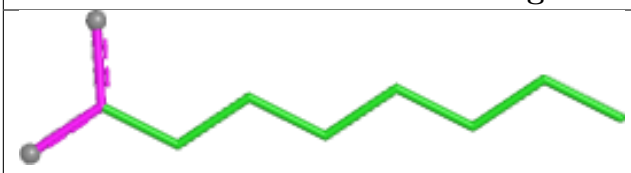


Torsions

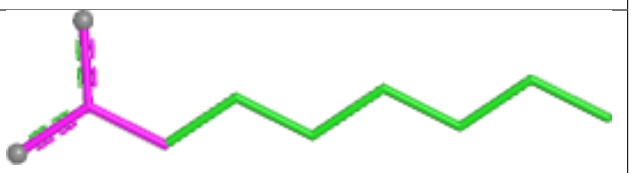


Rings

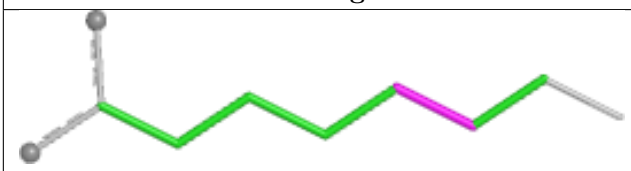
Ligand PEE E 903



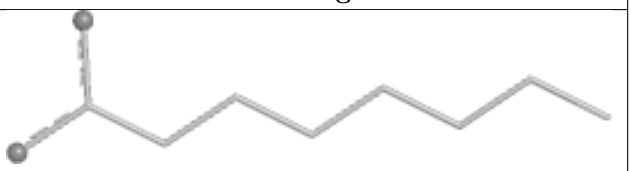
Bond lengths



Bond angles

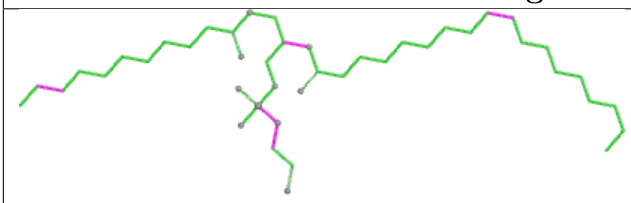


Torsions



Rings

Ligand PEE B 901



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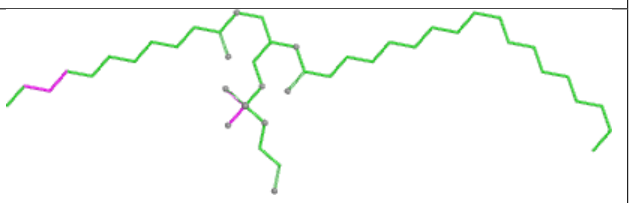
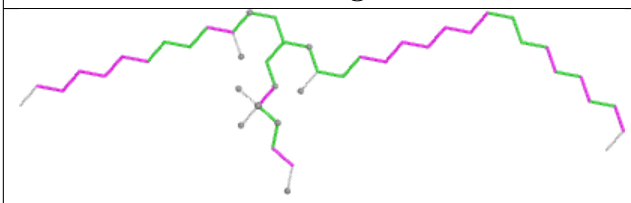


Bond angles



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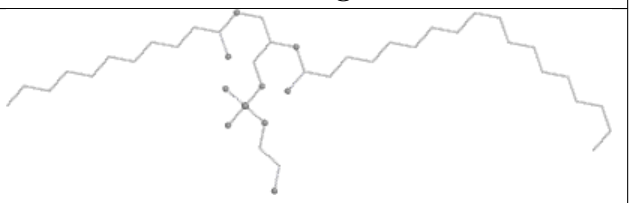

Rings

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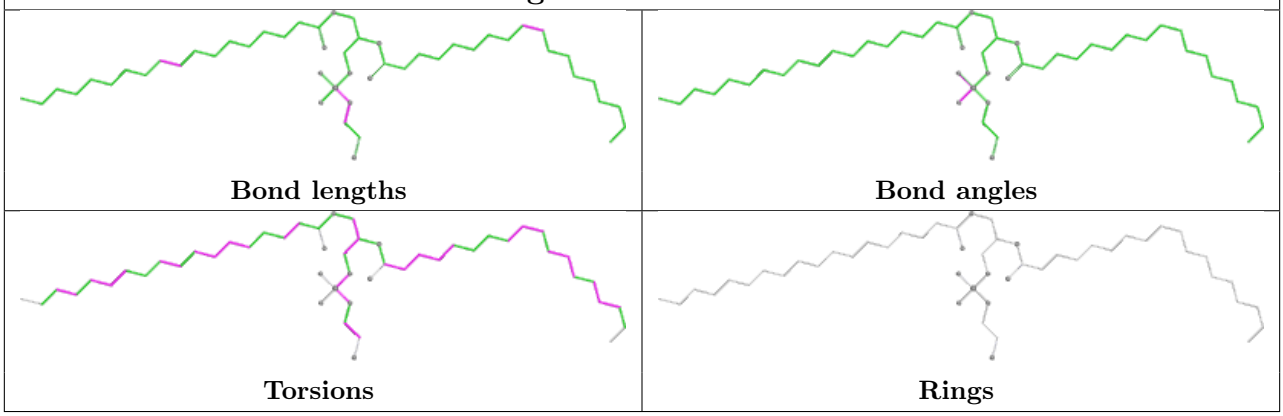

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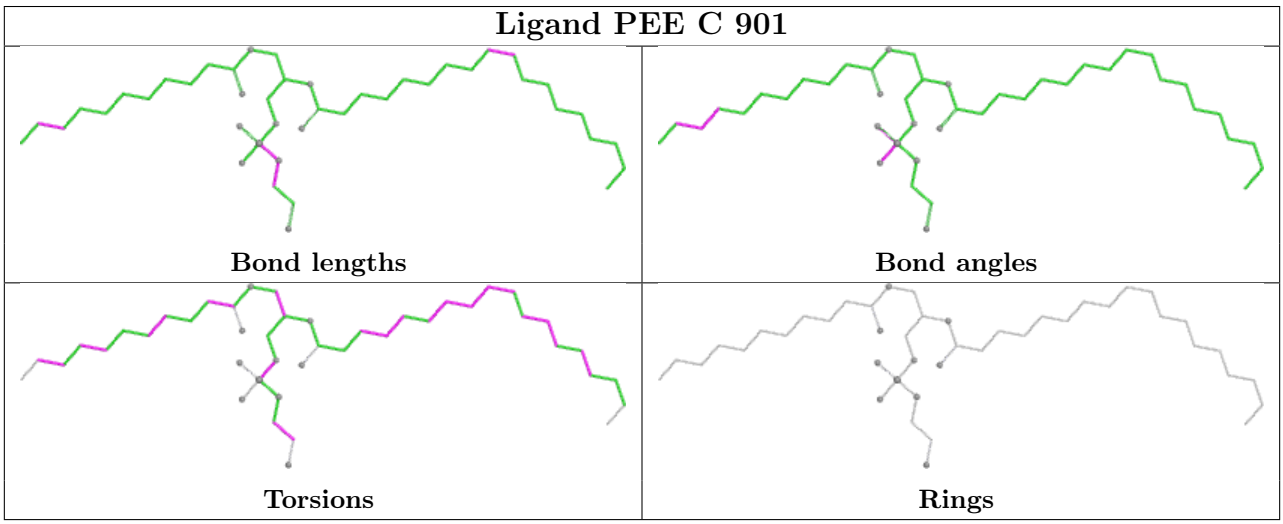

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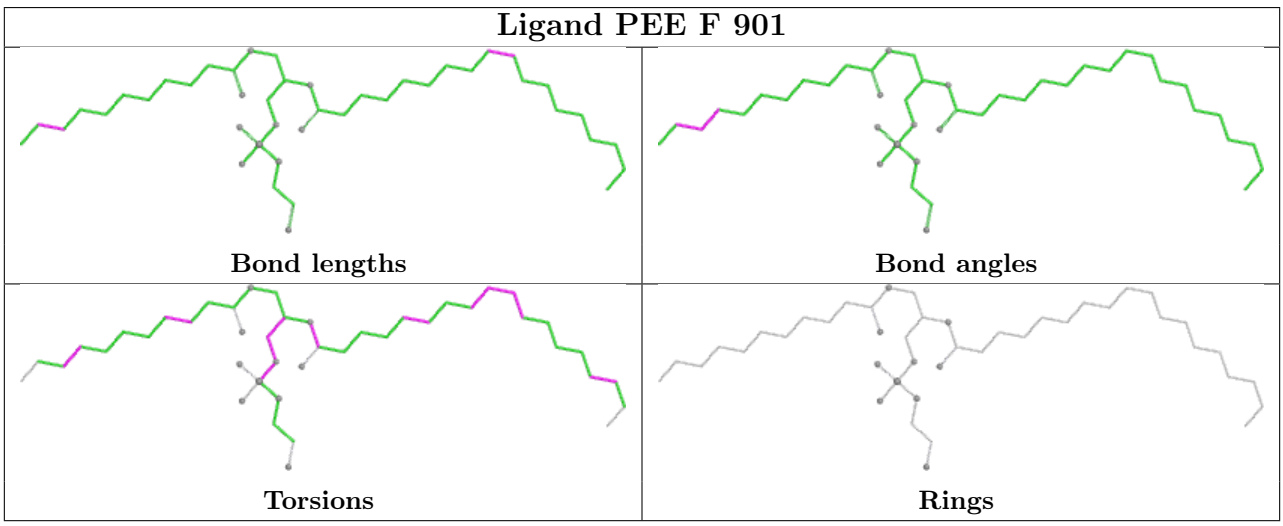

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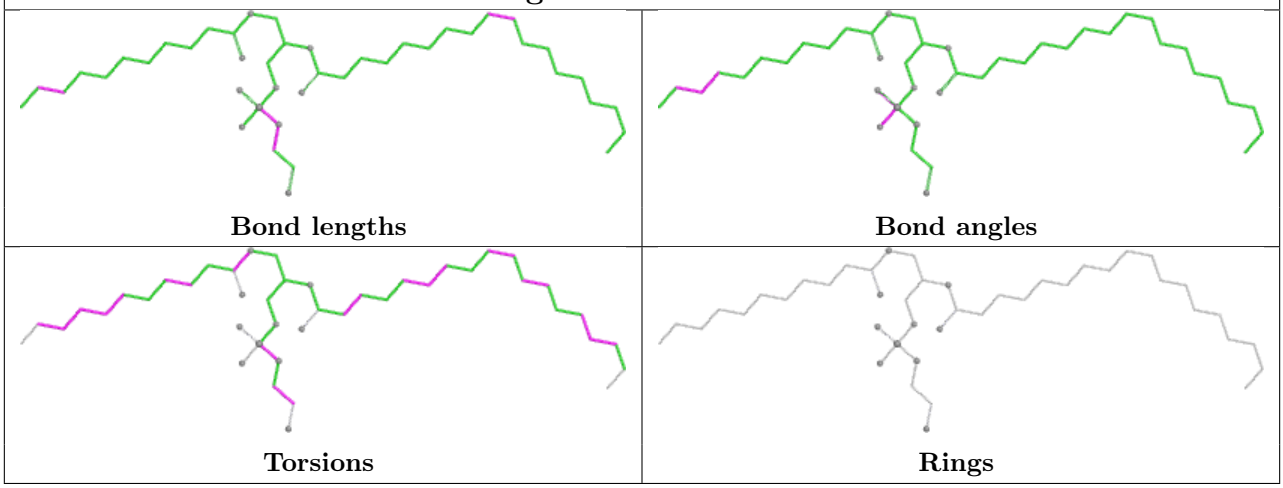

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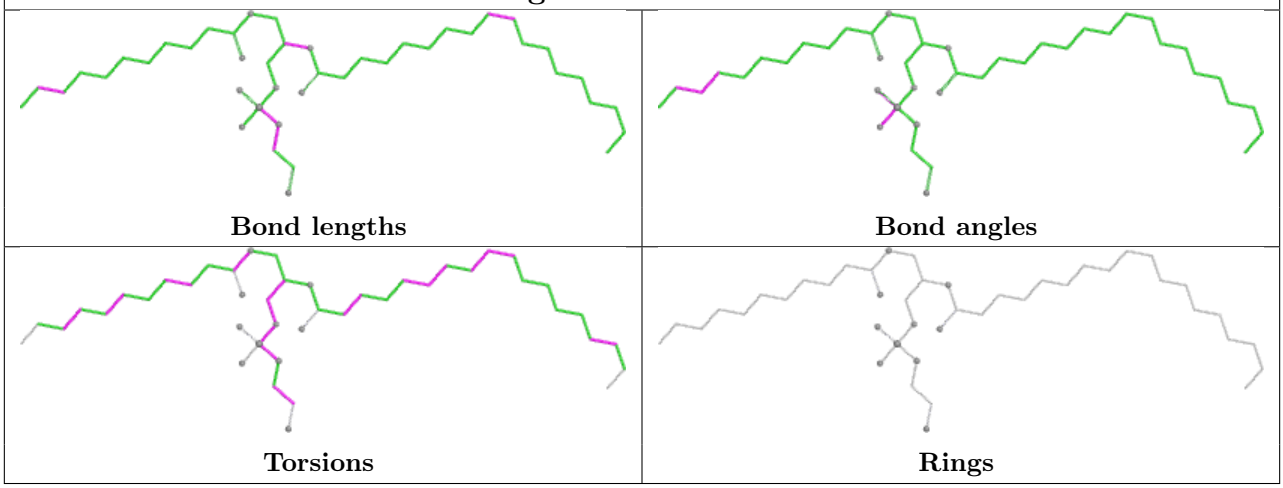

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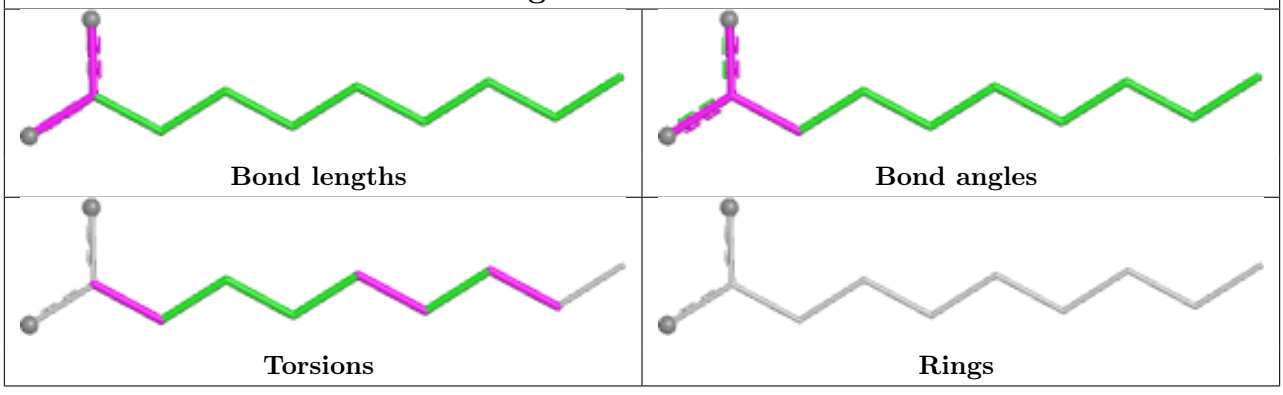

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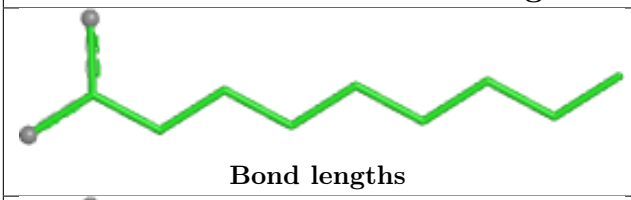
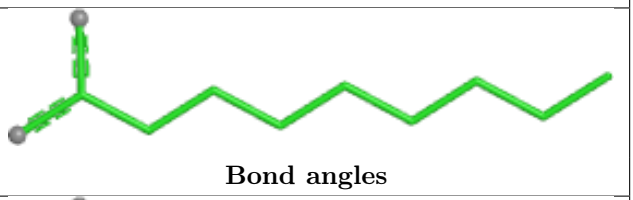
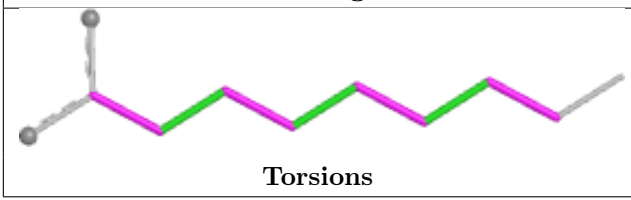
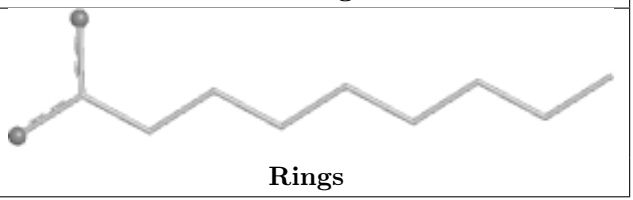

Bond lengths

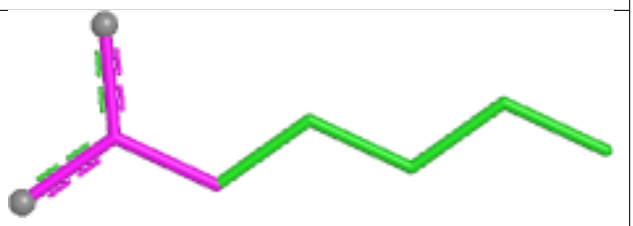

Bond angles


Torsions


Rings

Ligand PEE F 903

Bond lengths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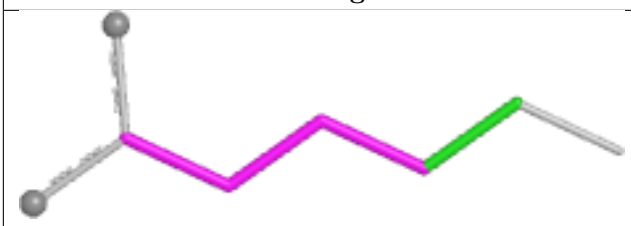
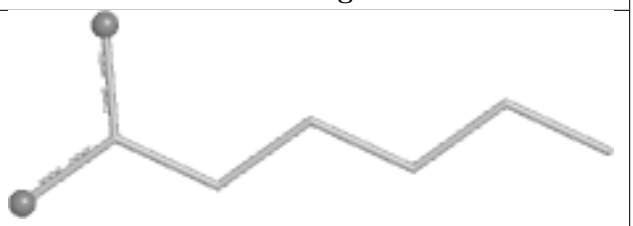
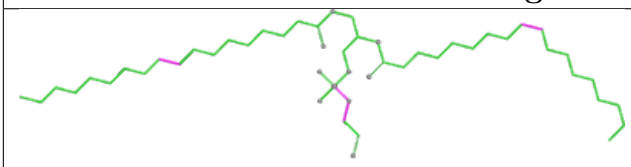

Torsions


Rings

Ligand PEE D 904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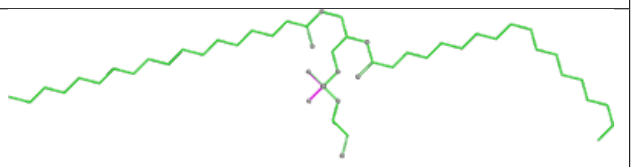
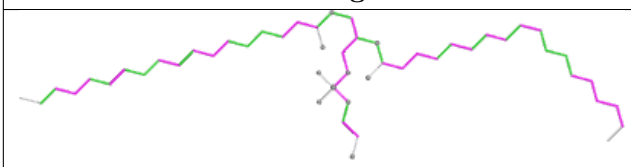

Bond angles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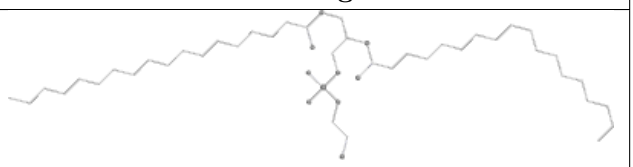
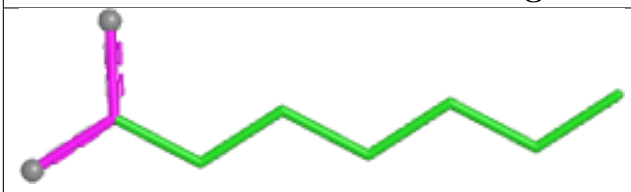
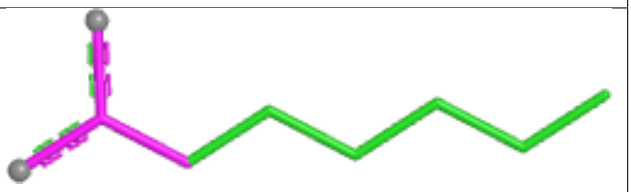
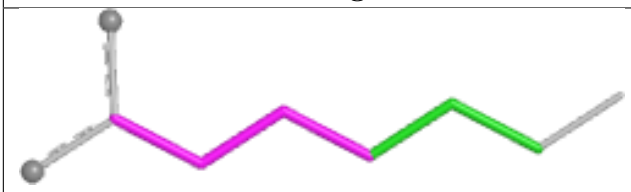
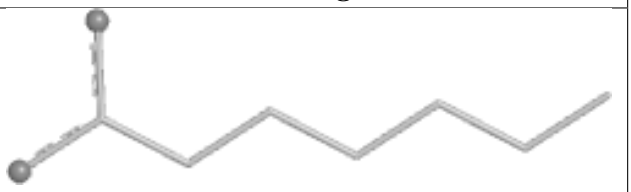
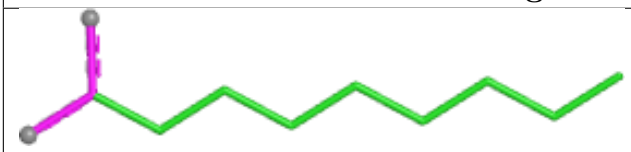
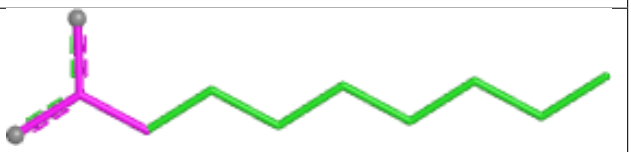
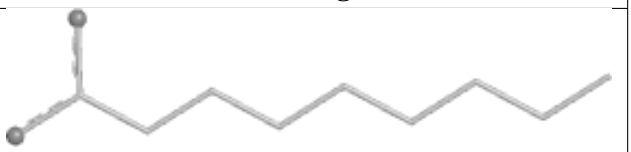

Rings

Ligand PEE D 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE C 902	
 Bond lengths	 Bond angles
Torsions	 Rings

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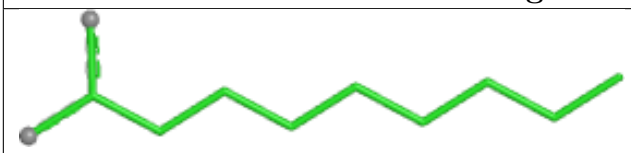
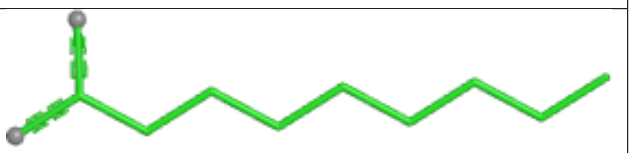
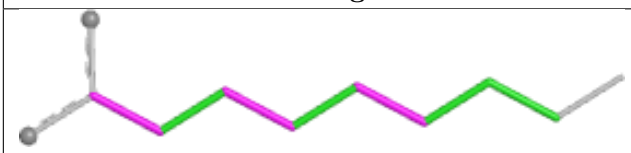
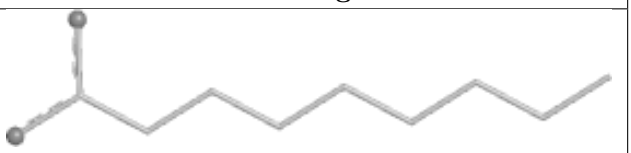
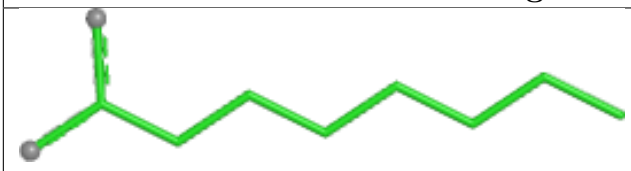
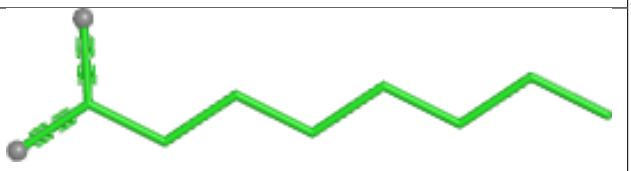
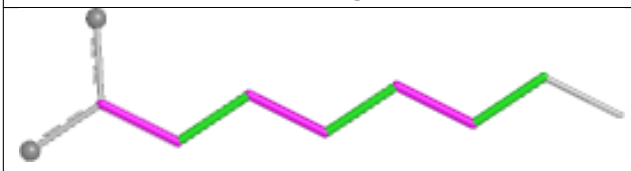
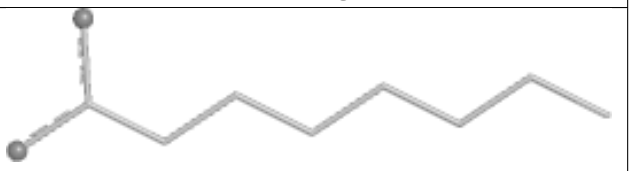
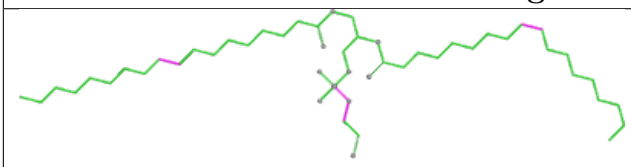
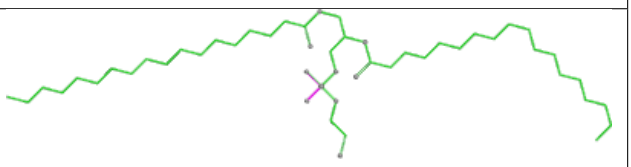
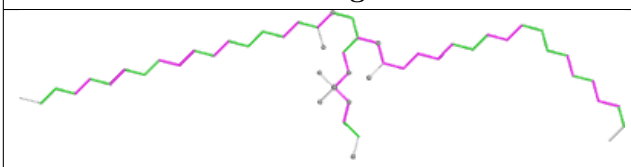
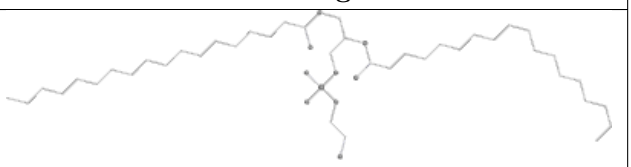
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE B 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE F 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

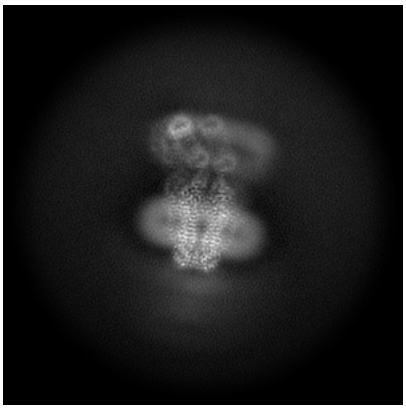
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27676. These allow visual inspection of the internal detail of the map and identification of artifacts.

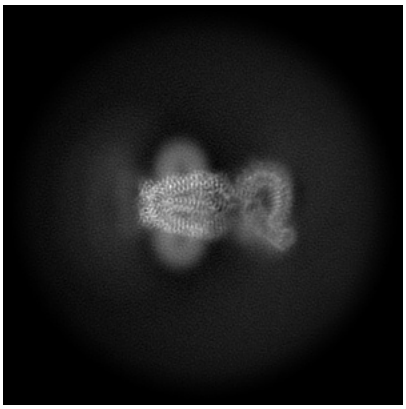
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

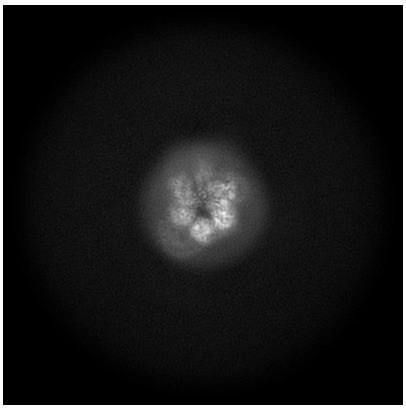
6.1.1 Primary map



X

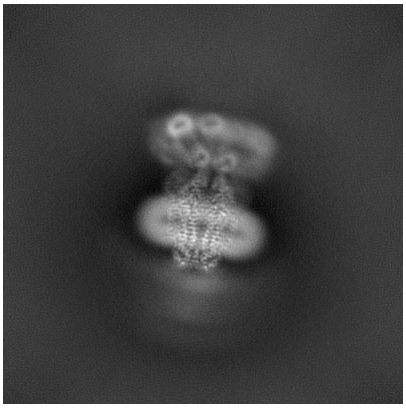


Y

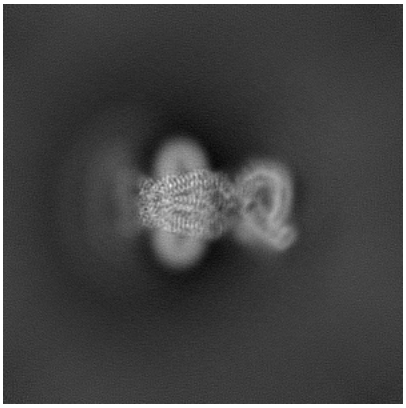


Z

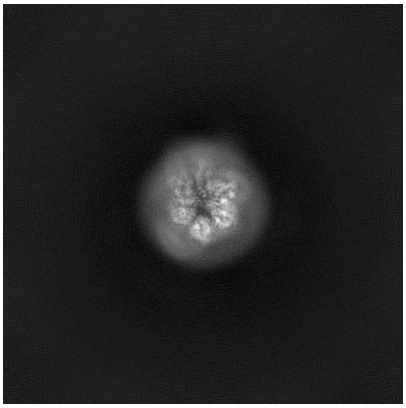
6.1.2 Raw map



X



Y



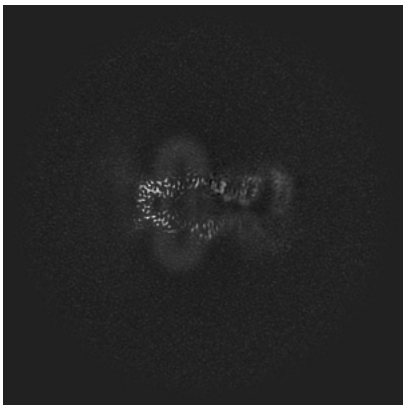
Z

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

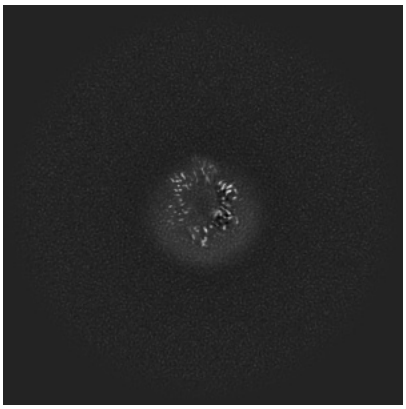
6.2 Central slices (i)

6.2.1 Primary map

X Index: 208

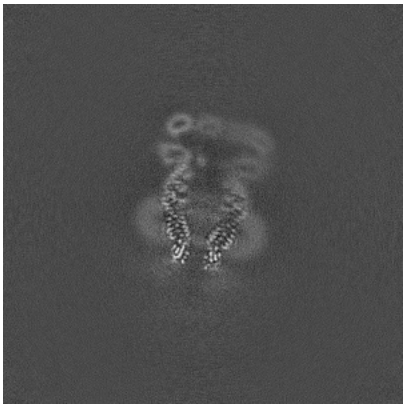


Y Index: 208



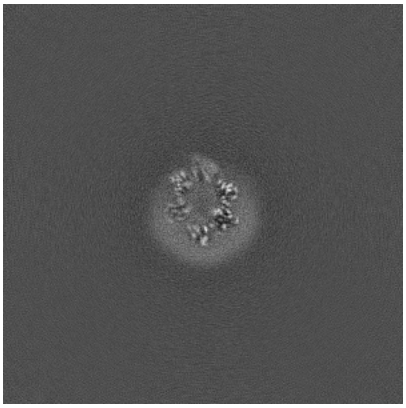
Z Index: 208

6.2.2 Raw map



X Index: 208

Y Index: 208

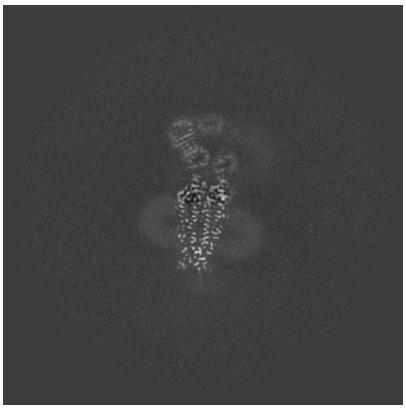


Z Index: 208

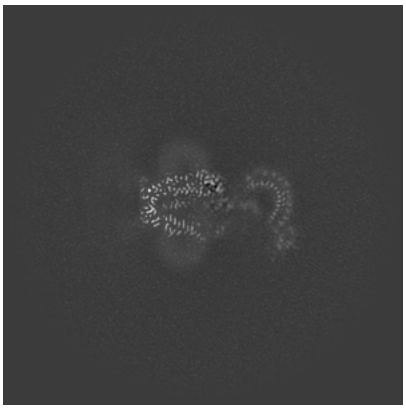
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

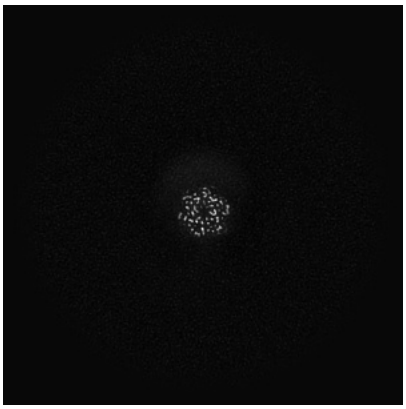
6.3.1 Primary map



X Index: 228

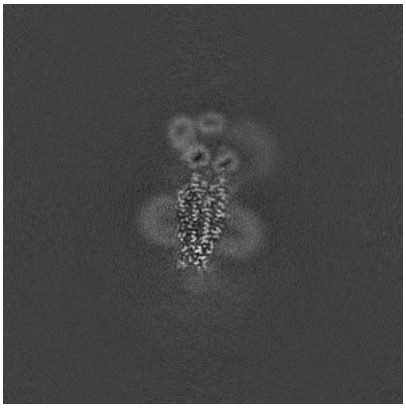


Y Index: 190

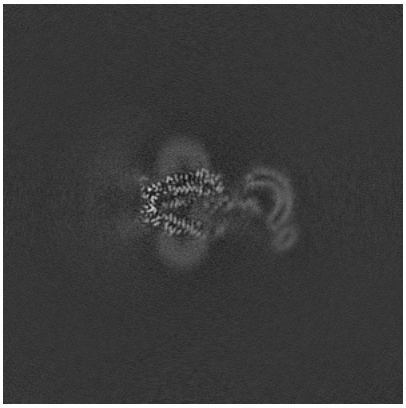


Z Index: 153

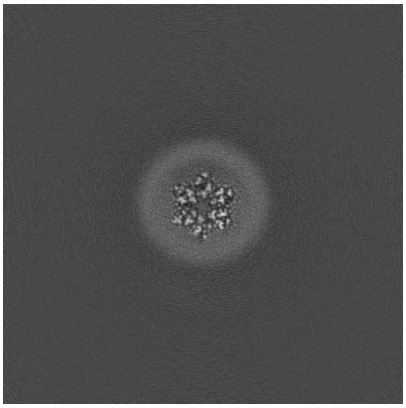
6.3.2 Raw map



X Index: 228



Y Index: 190

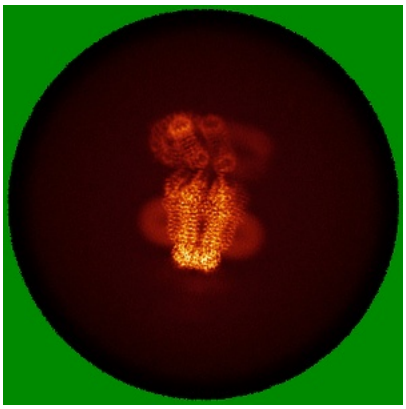


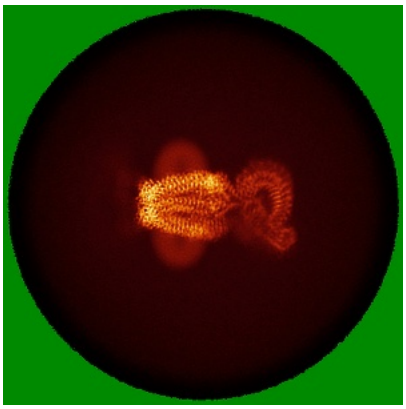
Z Index: 174

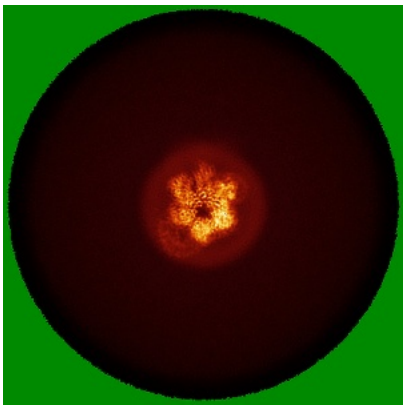
The images above show the largest variance slices of the map in three orthogonal directions.

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

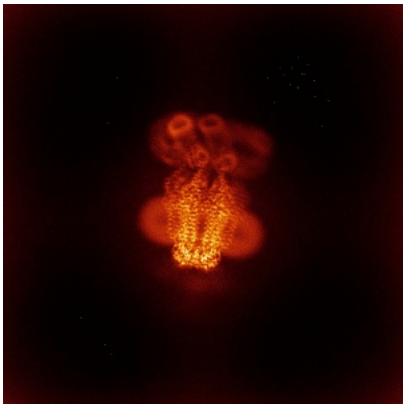
6.4.1 Primary map

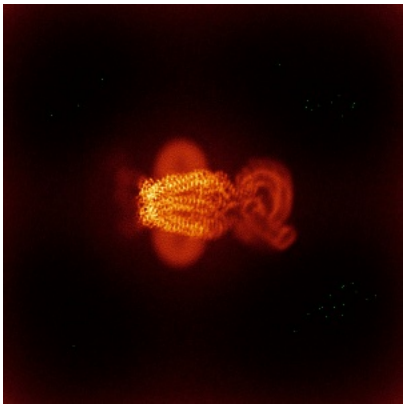

X

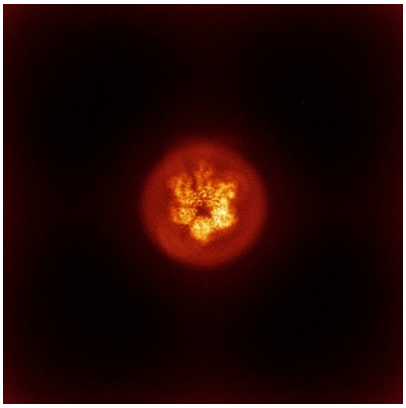

Y


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 0.475. 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.

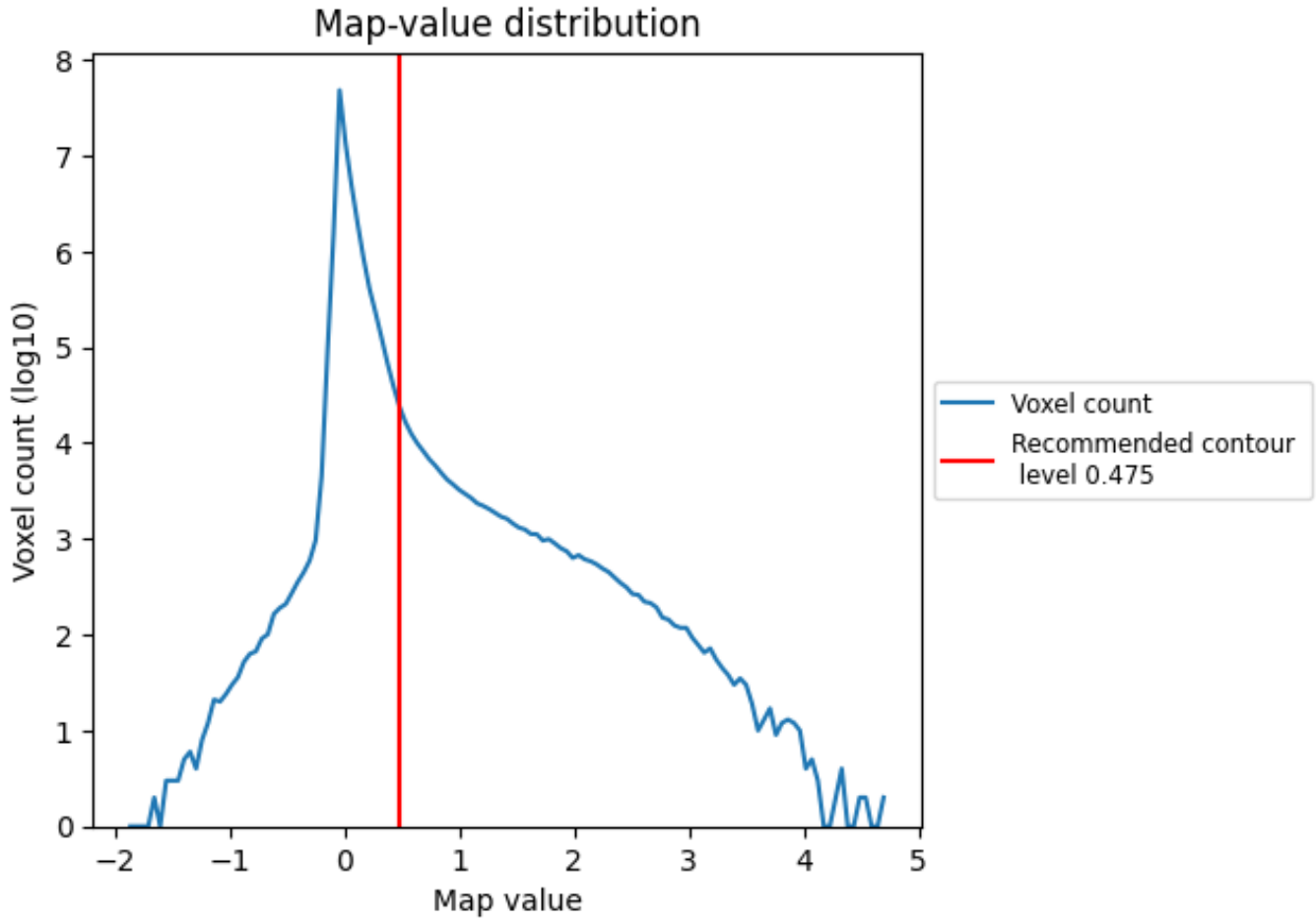
6.6 Mask visualisation (i)

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

7 Map analysis

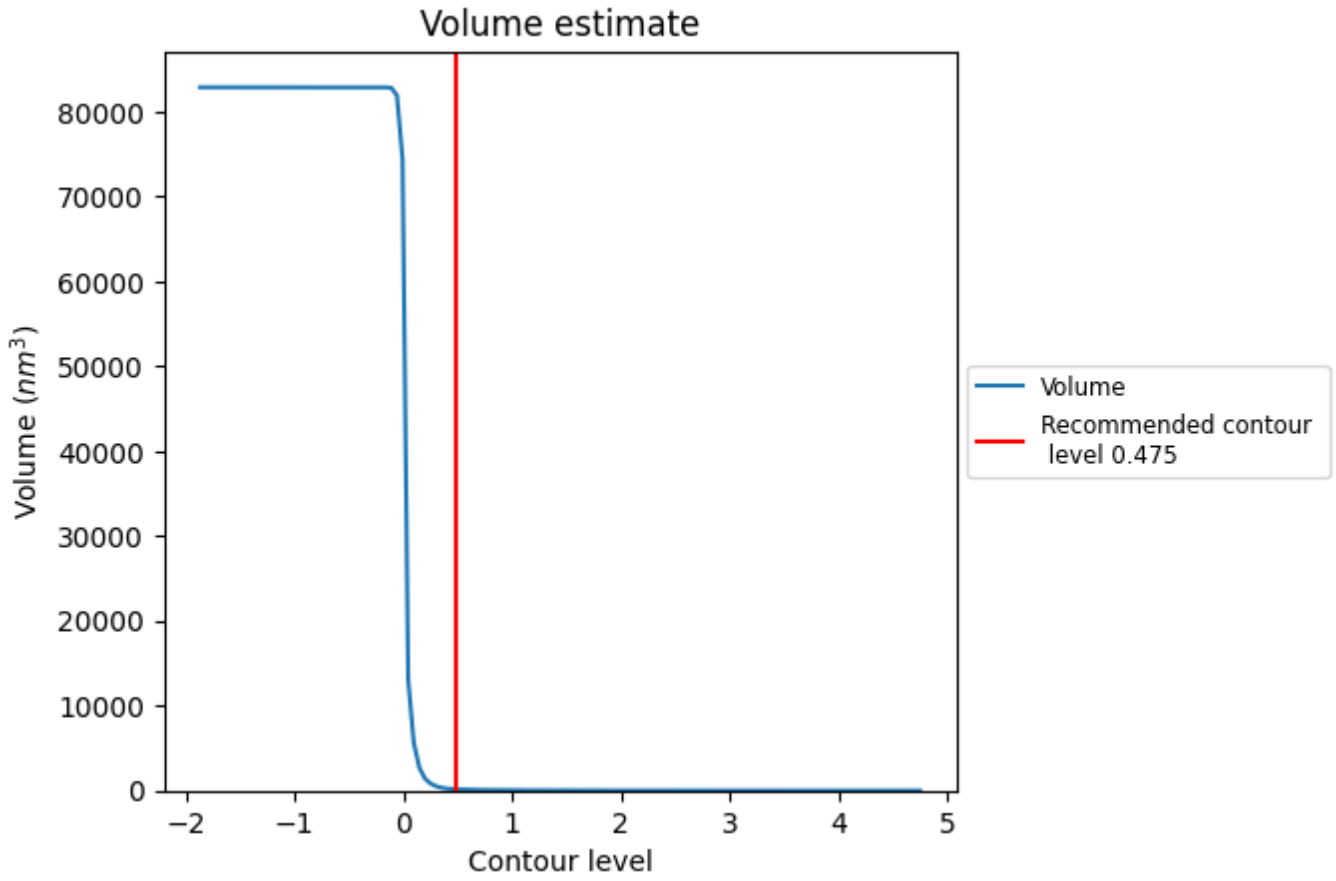
This section contains the results of statistical analysis of the map.

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.

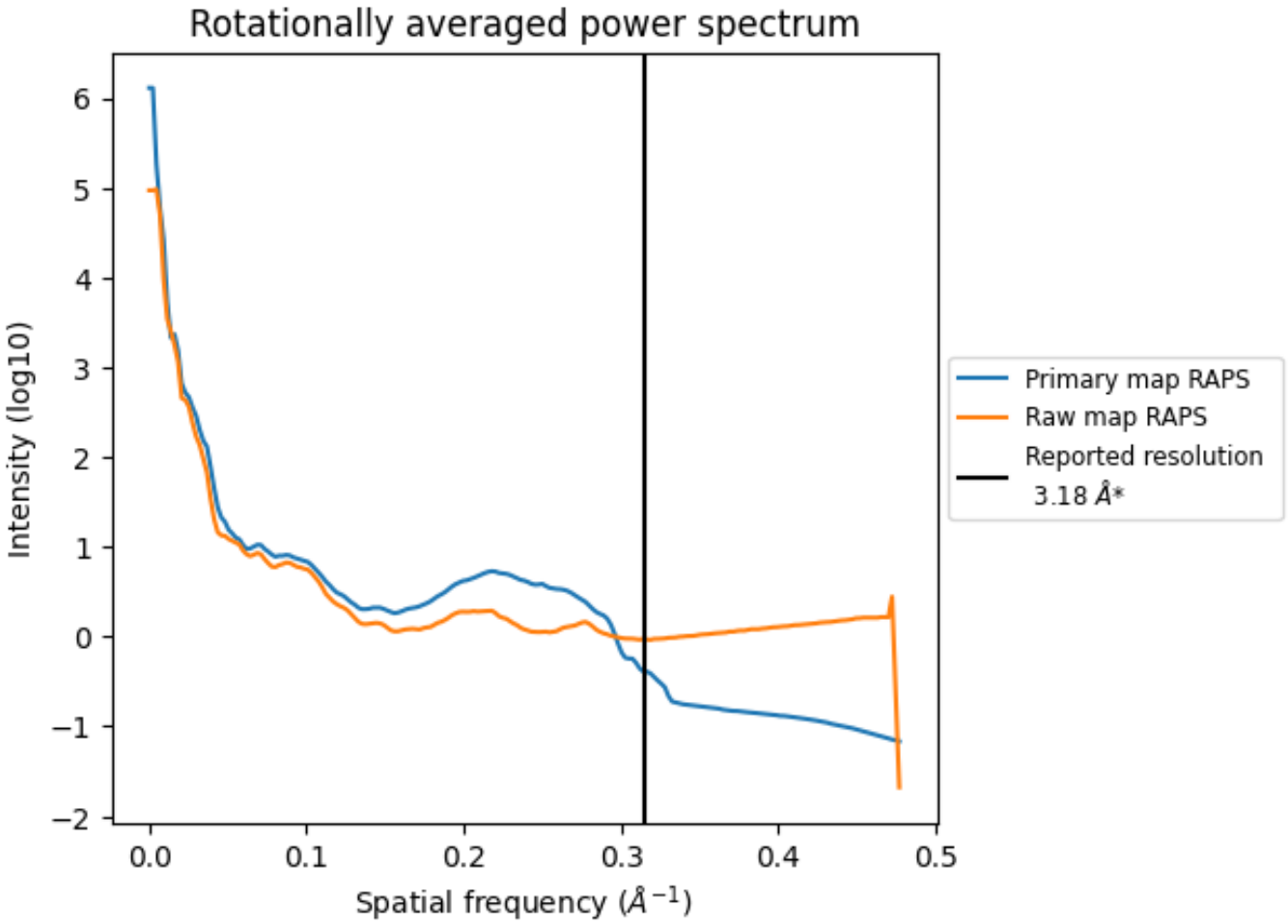
7.2 Volume estimate



The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 143 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)

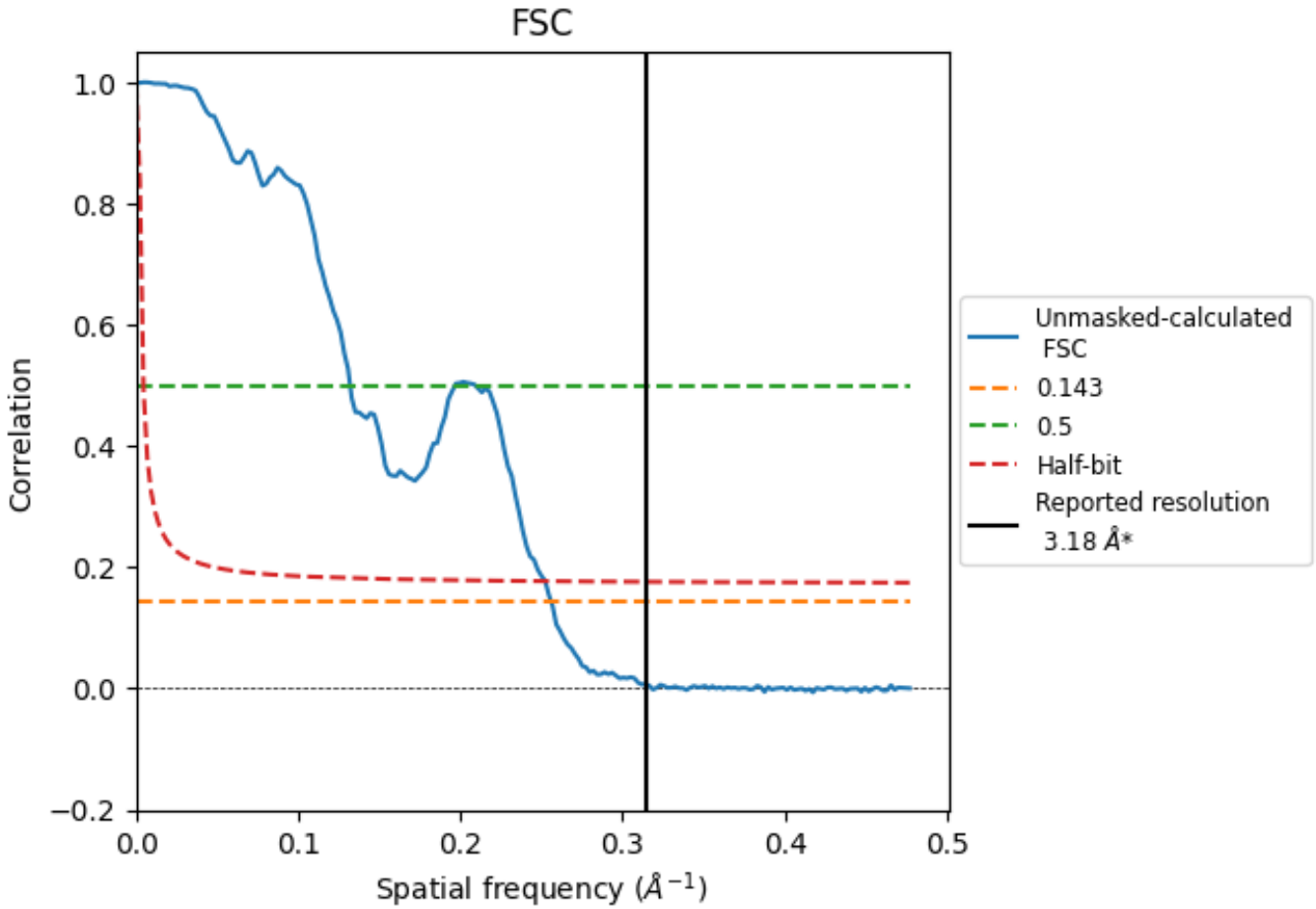


*Reported resolution corresponds to spatial frequency of 0.314 $Å^{-1}$

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 0.314 Å^{-1}

8.2 Resolution estimates (i)

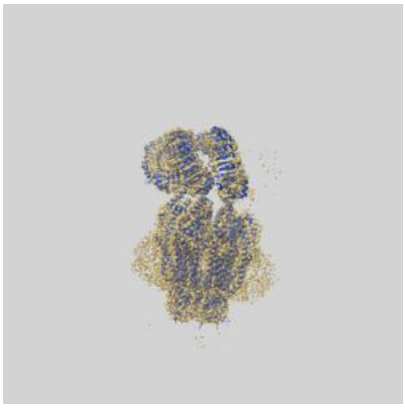
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	7.58	3.96

*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 3.91 differs from the reported value 3.18 by more than 10 %

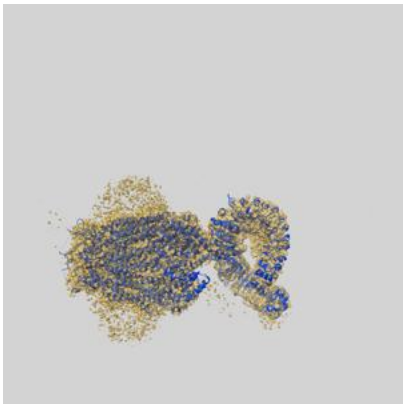
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27676 and PDB model 8DRE. Per-residue inclusion information can be found in section 3 on page 9.

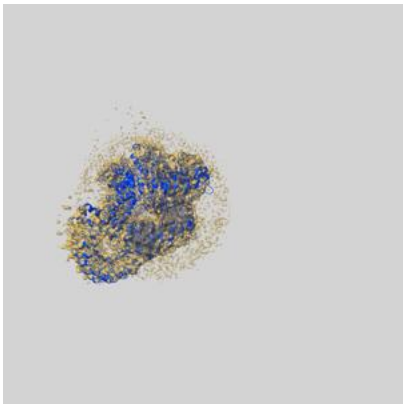
9.1 Map-model overlay



X



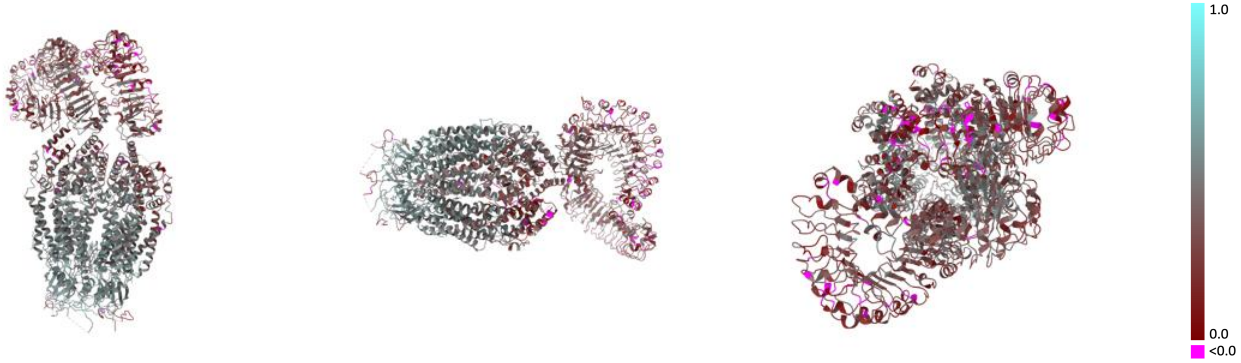
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.475 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.

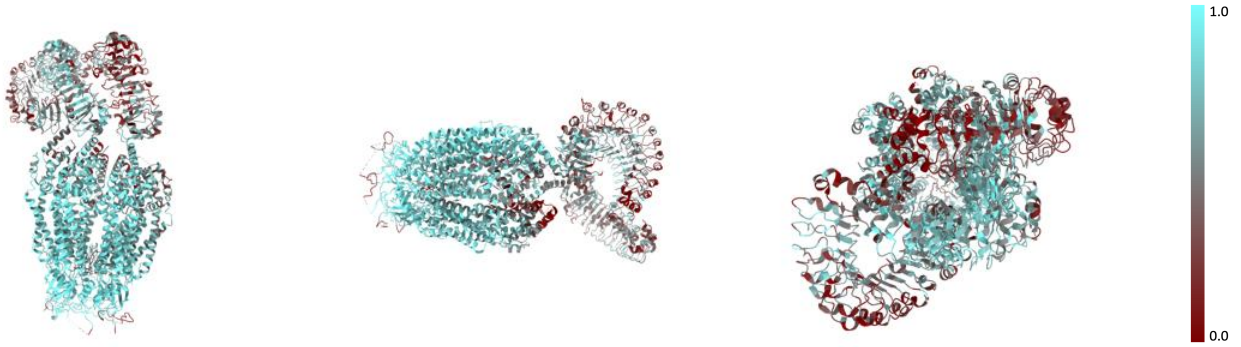
9.2 Q-score mapped to coordinate model (i)



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.

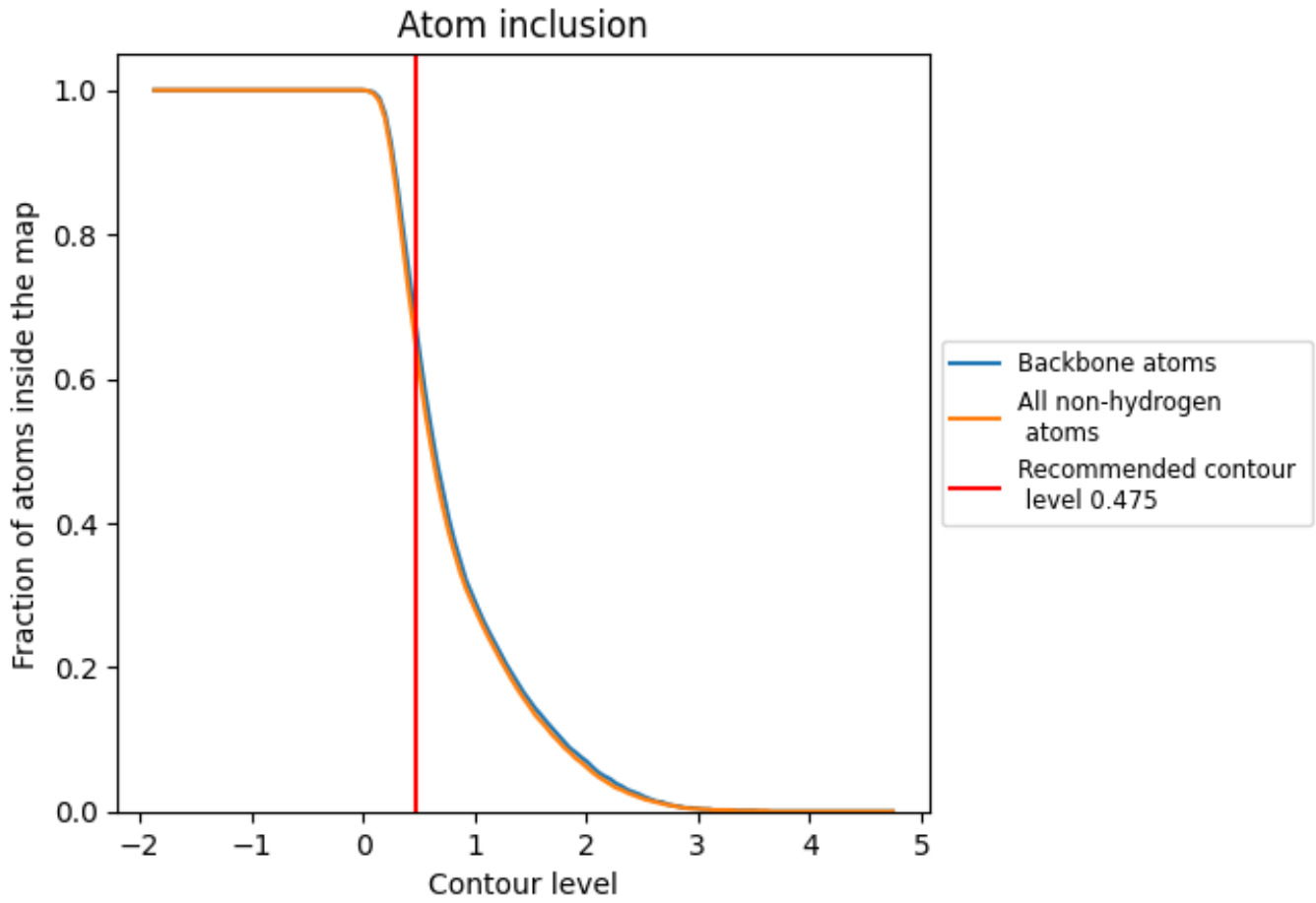
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.475).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.475) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.3820
A	0.7340	0.4110
B	0.5530	0.3460
C	0.6910	0.4040
D	0.7380	0.4370
E	0.7020	0.4220
F	0.5870	0.3350