Full wwPDB EM Validation Report

May 29, 2023 – 06:23 PM JST

PDB ID	:	7XZH
EMDB ID	:	EMD-33527
Title	:	Cryo-EM structure of human LRRC8A
Authors	:	Liu, H.; Liao, J.
Deposited on	:	2022-06-02
Resolution	:	2.78 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:

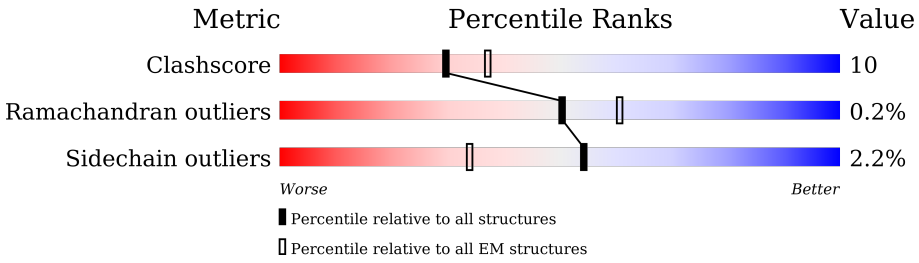
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	808	38% 73% 16% • 10%
1	B	808	38% 76% 14% 10%
1	C	808	38% 75% 15% • 10%
1	D	808	38% 73% 17% • 10%
1	E	808	38% 72% 18% • 10%
1	F	808	38% 74% 15% • 10%

2 Entry composition

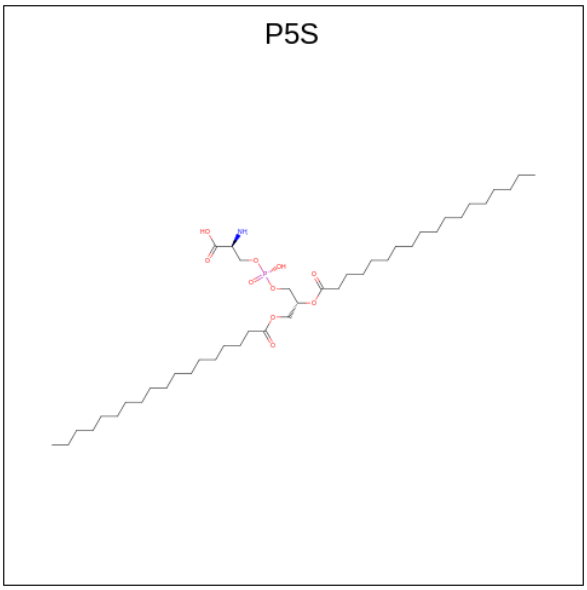
There are 4 unique types of molecules in this entry. The entry contains 37073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

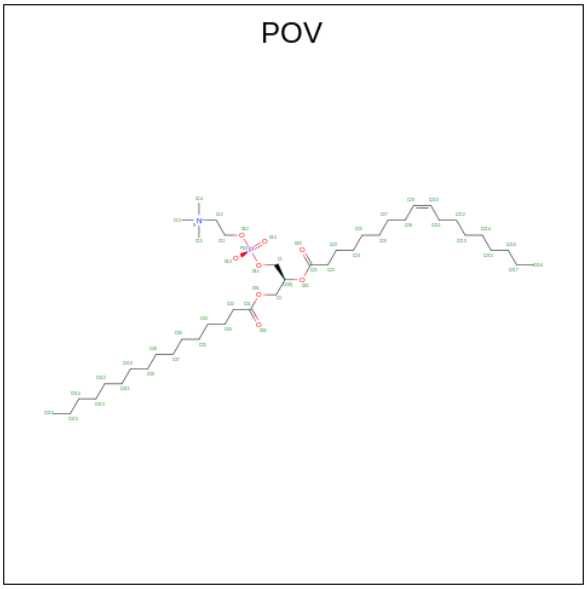
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	729	Total	C	N	O	S	0	0
			6025	3922	1013	1064	26		
1	B	730	Total	C	N	O	S	0	0
			6032	3926	1014	1066	26		
1	C	730	Total	C	N	O	S	0	0
			6032	3926	1014	1066	26		
1	D	730	Total	C	N	O	S	0	0
			6032	3926	1014	1066	26		
1	E	730	Total	C	N	O	S	0	0
			6032	3926	1014	1066	26		
1	F	730	Total	C	N	O	S	0	0
			6032	3926	1014	1066	26		

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



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			54	42	1	10	1	
2	B	1	Total	C	N	O	P	0
			54	42	1	10	1	
2	C	1	Total	C	N	O	P	0
			54	42	1	10	1	
2	D	1	Total	C	N	O	P	0
			54	42	1	10	1	
2	E	1	Total	C	N	O	P	0
			54	42	1	10	1	
2	F	1	Total	C	N	O	P	0
			54	42	1	10	1	

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
3	E	1	Total	C	N	O	P	0
			38	28	1	8	1	

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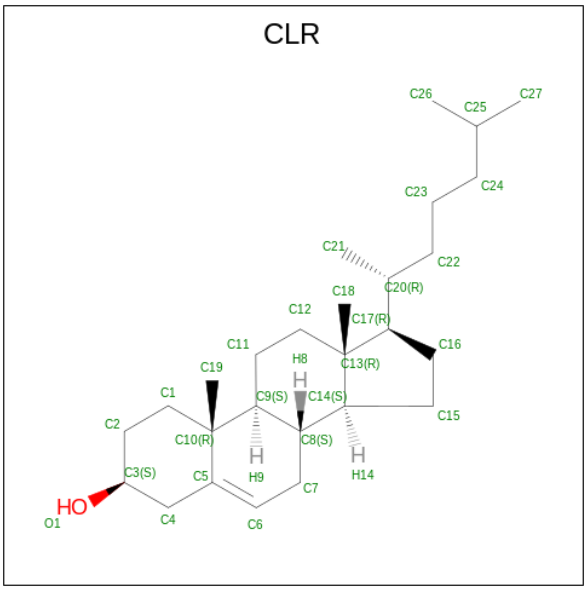
Mol	Chain	Residues	Atoms	AltConf
3	F	1	Total C N O P 38 28 1 8 1	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 28 27 1	0
4	A	1	Total C O 28 27 1	0
4	B	1	Total C O 28 27 1	0
4	B	1	Total C O 28 27 1	0
4	C	1	Total C O 28 27 1	0
4	C	1	Total C O 28 27 1	0
4	D	1	Total C O 28 27 1	0
4	D	1	Total C O 28 27 1	0
4	E	1	Total C O 28 27 1	0
4	E	1	Total C O 28 27 1	0

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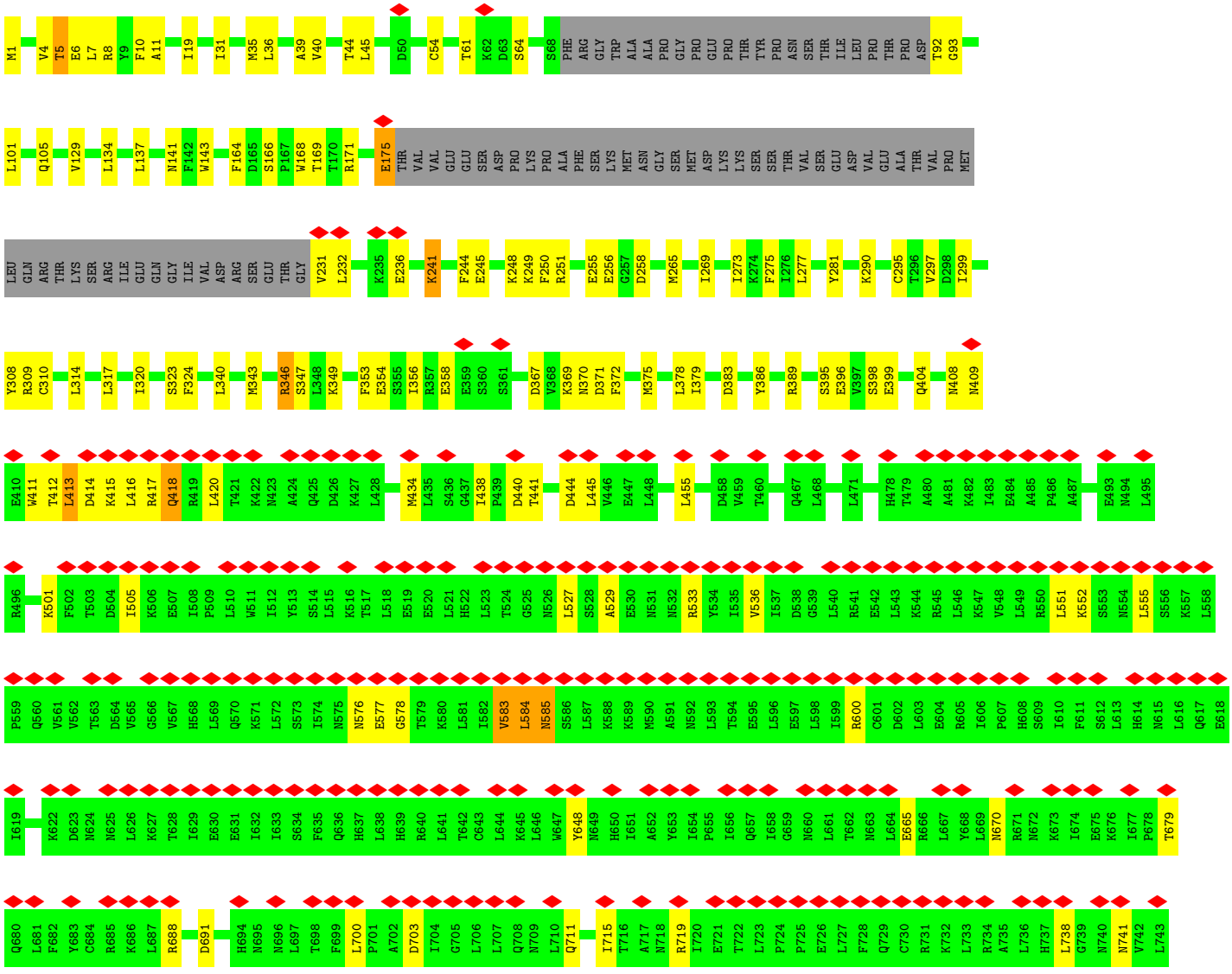
Mol	Chain	Residues	Atoms	AltConf
4	F	1	Total C O 28 27 1	0
4	F	1	Total C O 28 27 1	0

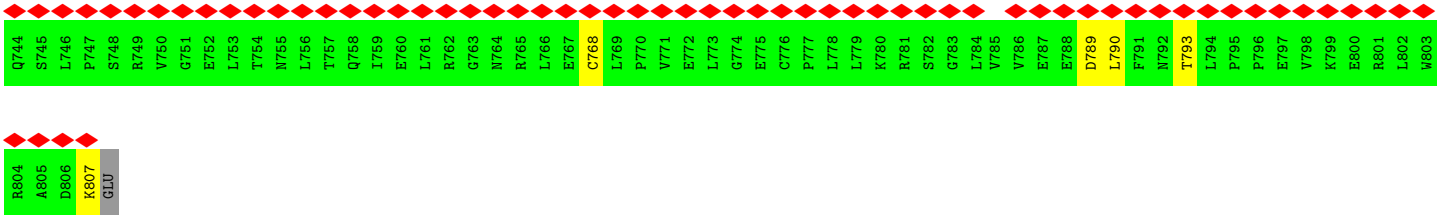
3 Residue-property plots (i)

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

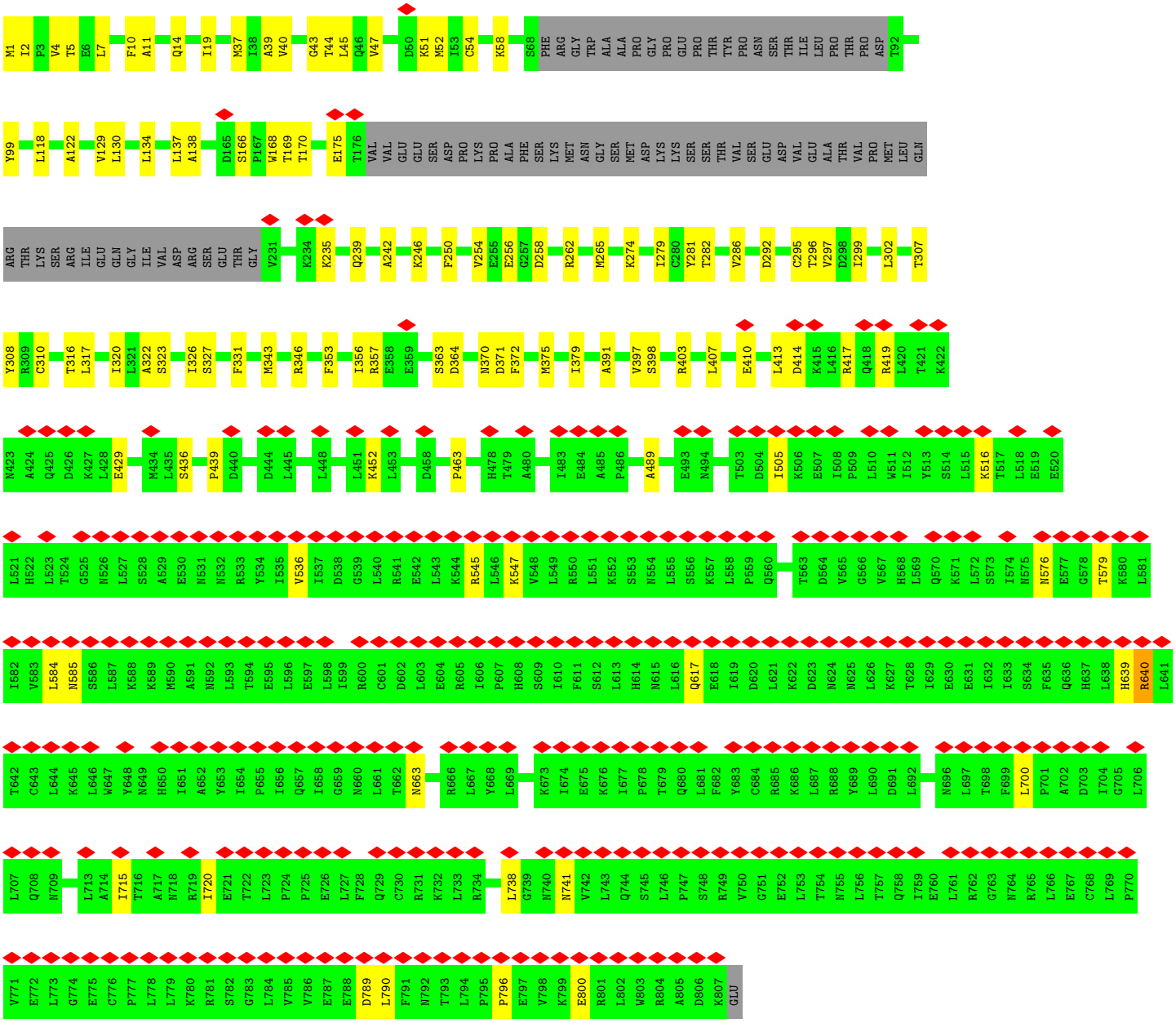
Chain A:



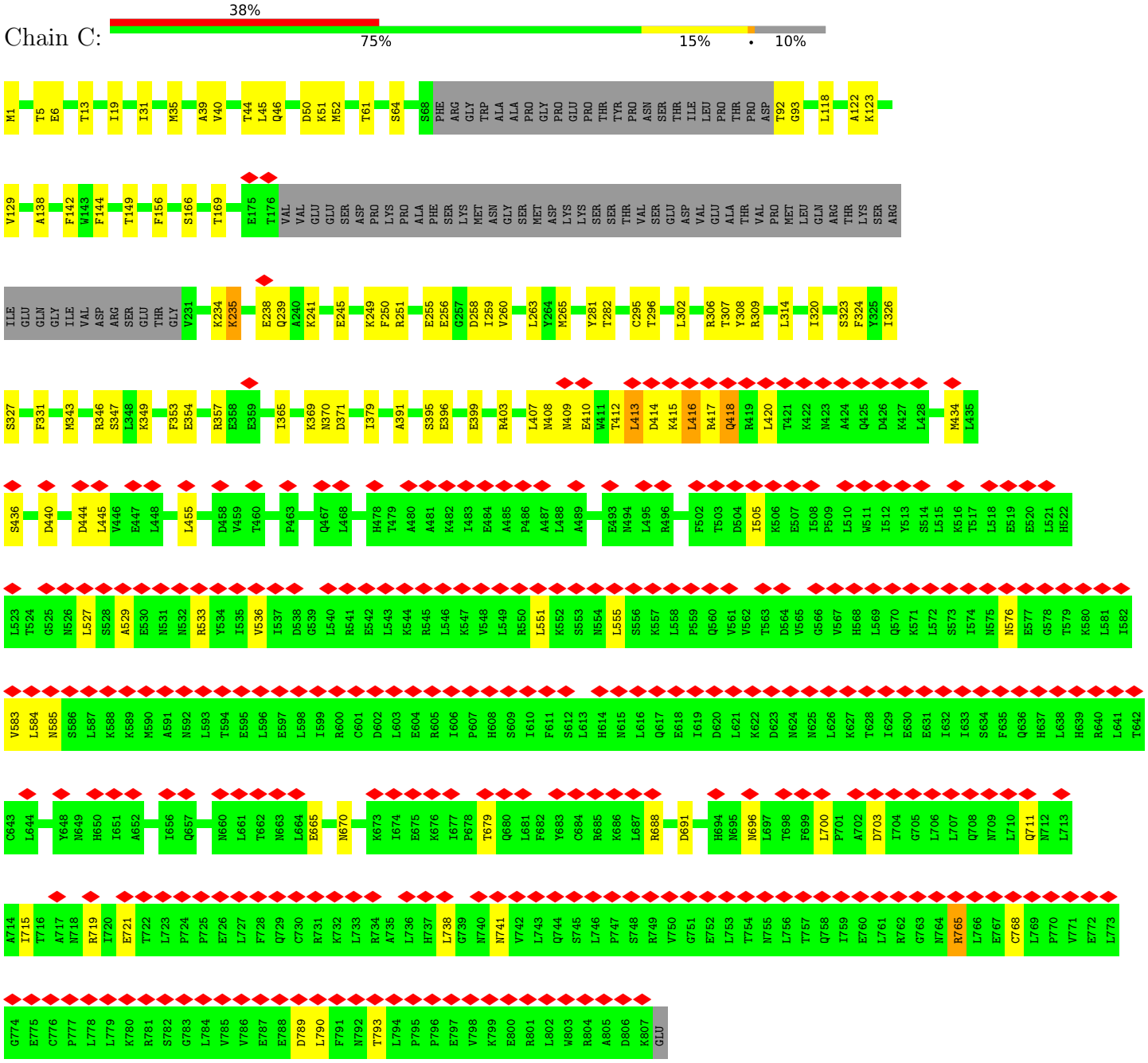


• Molecule 1: Volume-regulated anion channel subunit LRRC8A

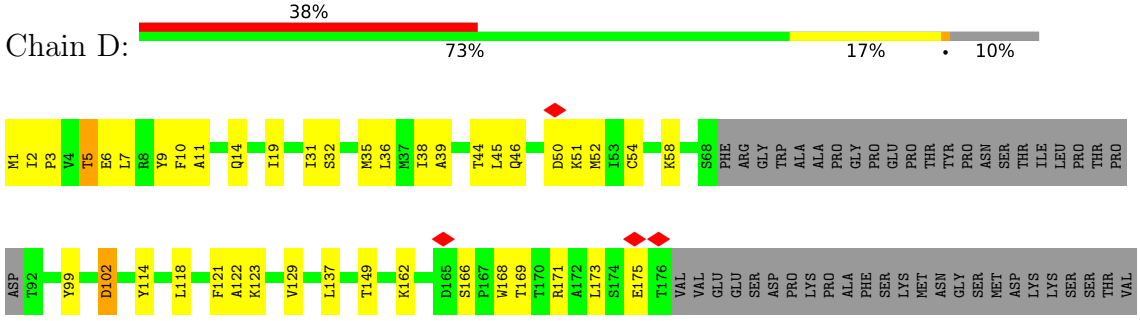
Chain B:

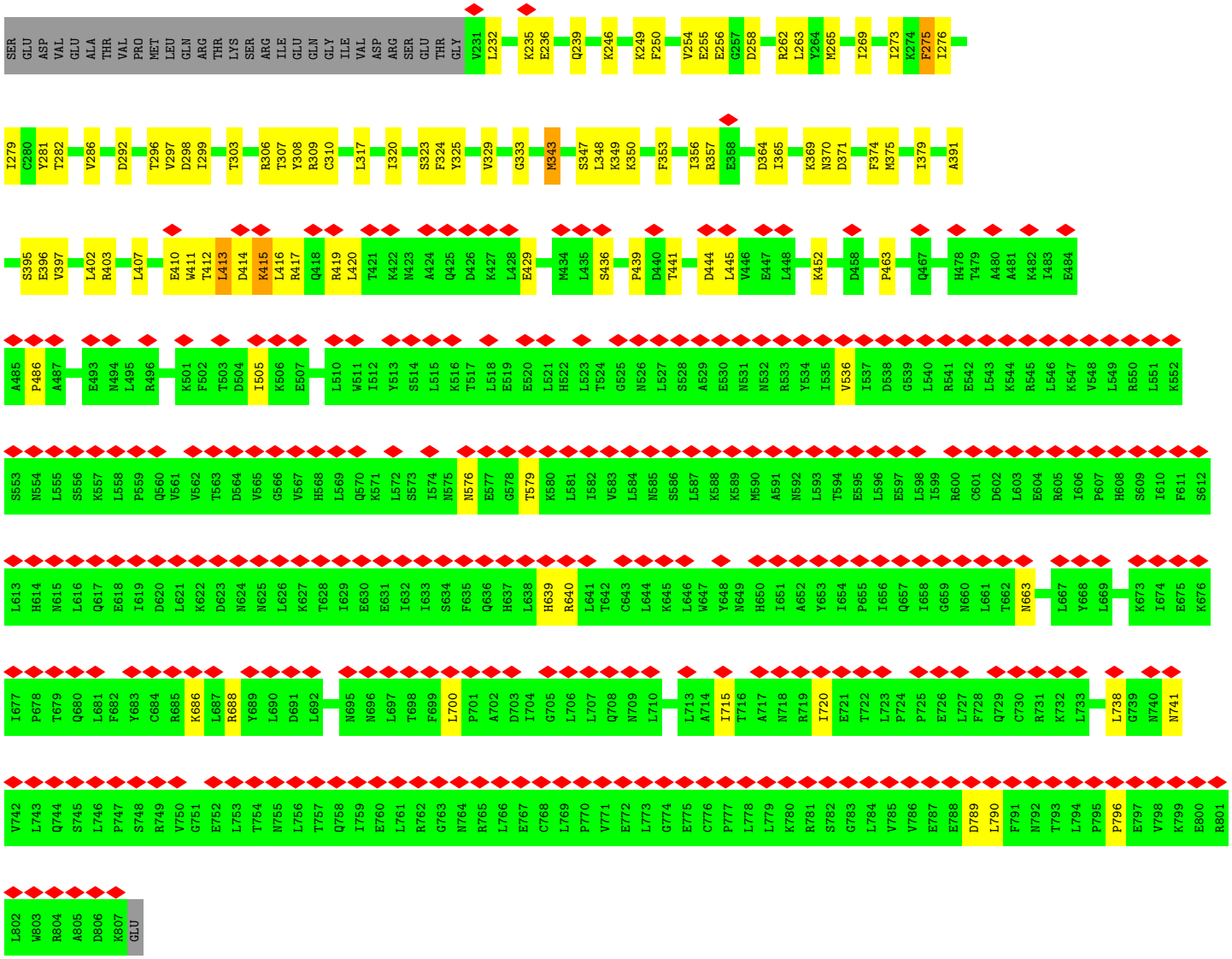


• Molecule 1: Volume-regulated anion channel subunit LRRC8A



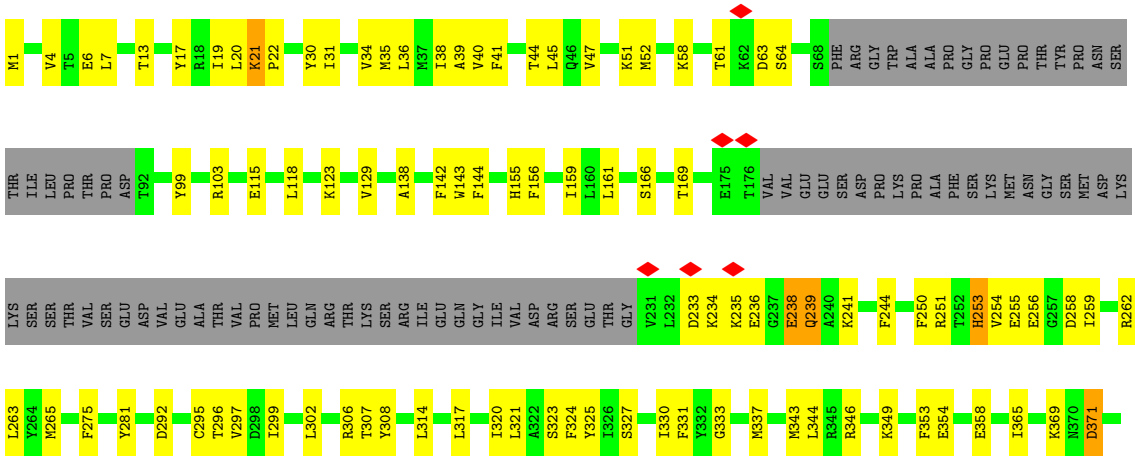
• Molecule 1: Volume-regulated anion channel subunit LRRC8A

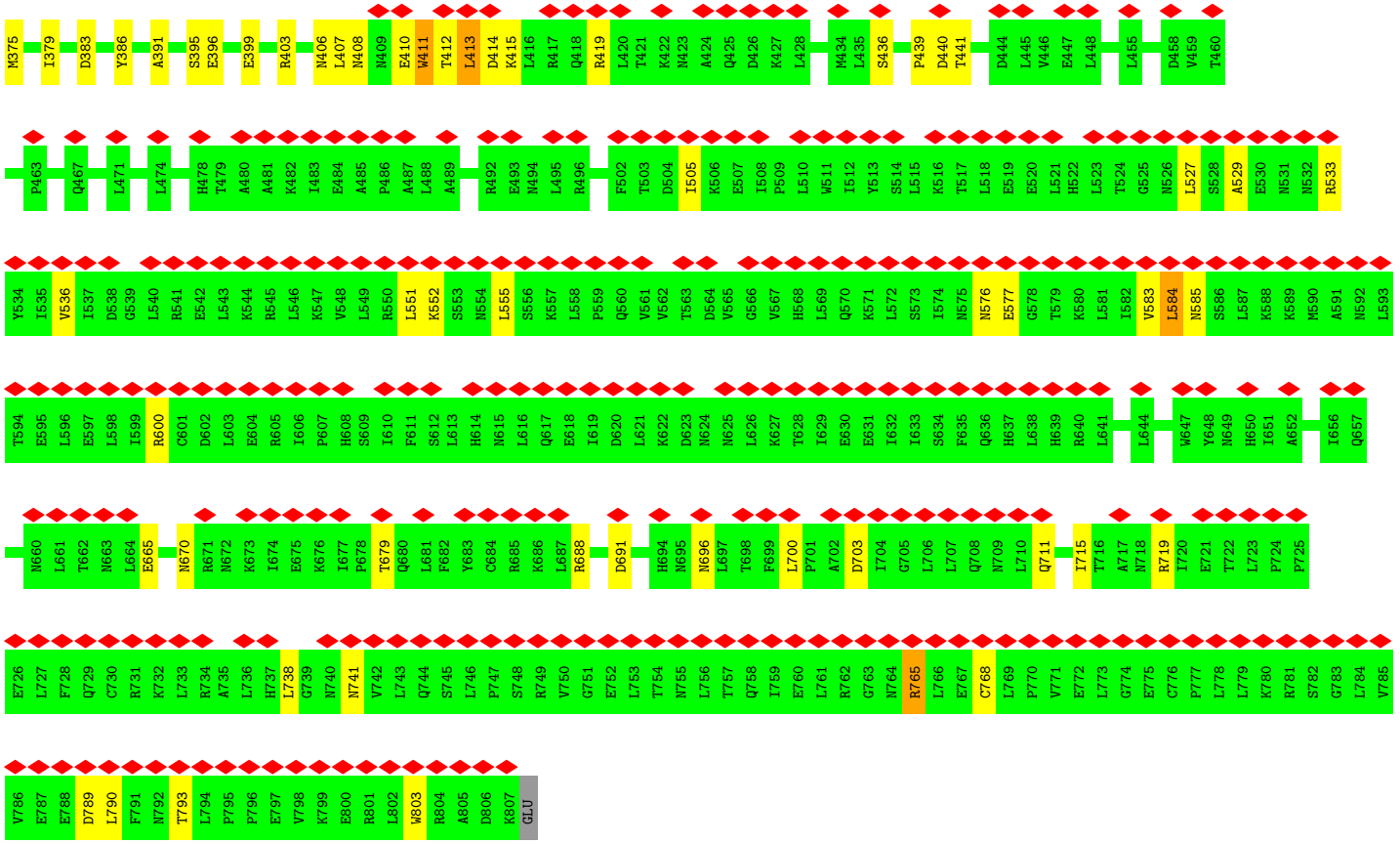




• Molecule 1: Volume-regulated anion channel subunit LRRC8A

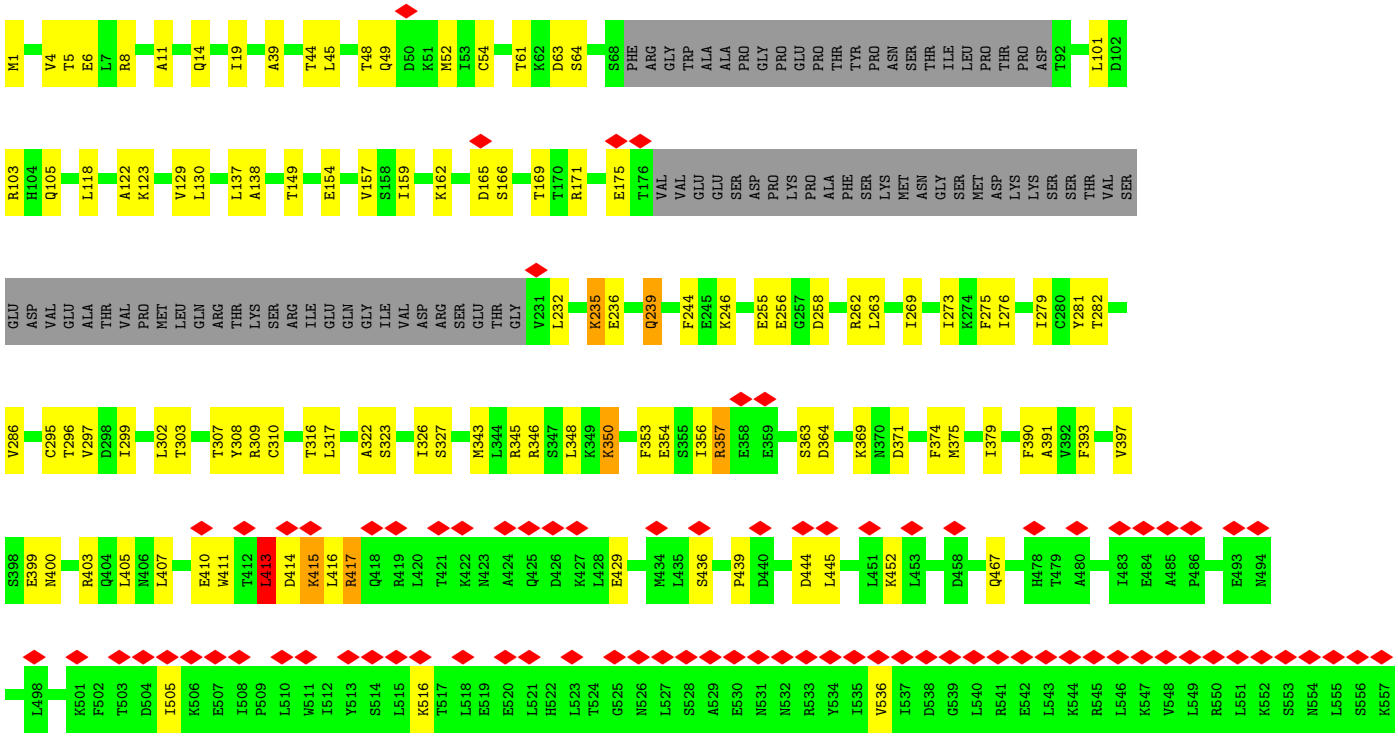
Chain E:

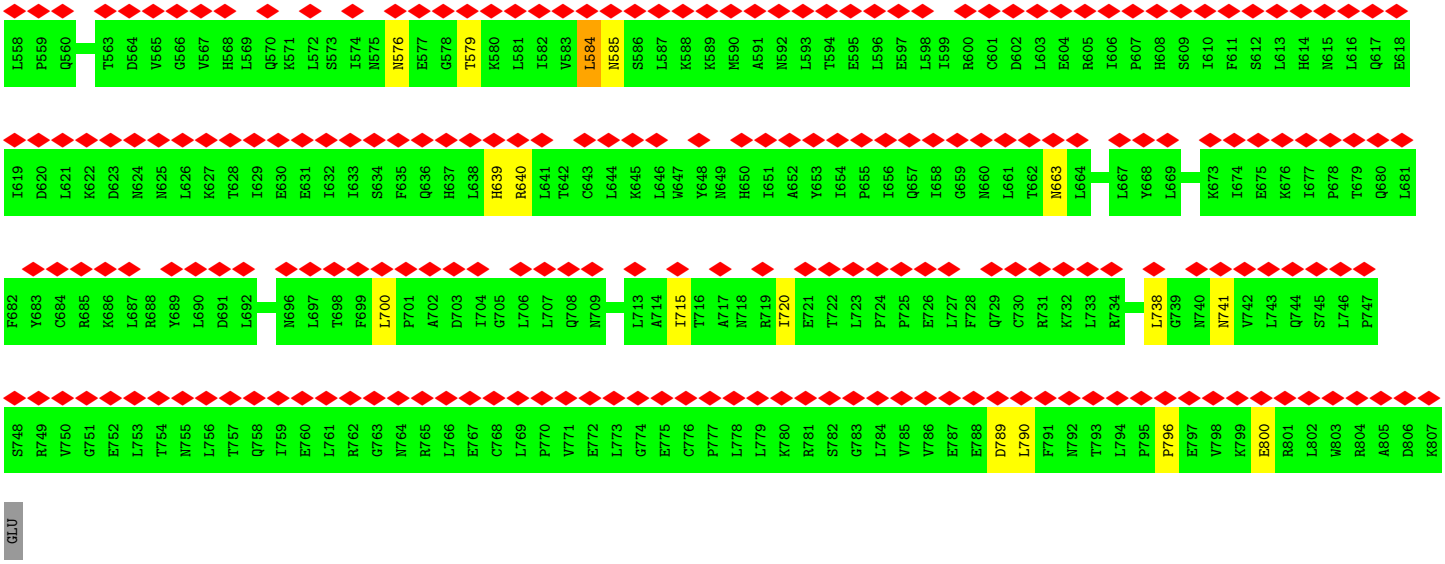




• Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain F:




L558 P559 Q560 T563 D564 V565 G566 V567 H568 L569 Q570 K571 L572 S573 I574 N575 N576 E577 G578 T579 K580 L581 I582 V583 L584 N585 S586 L587 K588 K589 M590 A591 N592 L593 T594 E595 L596 E597 L598 I599 R600 C601 D602 L603 E604 R605 I606 P607 H608 S609 I610 F611 S612 L613 H614 N615 L616 Q617 E618
I619 D620 L621 K622 D623 N624 N625 L626 K627 T628 I629 E630 E631 I632 I633 S634 F635 Q636 H637 L638 H639 R640 L641 T642 C643 L644 K645 L646 W647 Y648 N649 H650 I651 A652 Y653 I654 P655 I656 Q657 I658 G659 N660 L661 T662 N663 L664 L667 Y668 L669 K673 I674 E675 K676 I677 P678 T679 Q680 L681
F682 Y683 C684 R685 K686 L687 R688 Y689 L690 D691 L692 N696 L697 T698 F699 L700 P701 A702 D703 I704 G705 L706 L707 Q708 N709 L713 A714 I715 T716 A717 N718 R719 I720 E721 T722 L723 P724 P725 E726 L727 F728 Q729 C730 R731 K732 L733 R734 L738 G739 N740 N741 V742 L743 Q744 S745 L746 P747
S748 R749 V750 G751 E752 L753 T754 N755 L756 T757 Q758 I759 E760 L761 R762 G763 N764 R765 L766 E767 C768 L769 P770 V771 E772 L773 G774 E775 C776 P777 L778 L779 K780 R781 S782 G783 L784 V785 V786 E787 E788 D789 L790 F791 N792 T793 L794 P795 P796 E797 V798 K799 E800 R801 L802 W803 R804 A805 D806 K807
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.023	Depositor
Minimum map value	-0.735	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, P5S, CLR

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	0.39	0/6161	0.57	0/8353
1	B	0.38	0/6168	0.56	0/8363
1	C	0.39	0/6168	0.57	0/8363
1	D	0.38	0/6168	0.57	0/8363
1	E	0.38	0/6168	0.57	0/8363
1	F	0.38	0/6168	0.56	0/8363
All	All	0.38	0/37001	0.57	0/50168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6025	0	6189	148	0
1	B	6032	0	6196	128	0
1	C	6032	0	6196	120	0
1	D	6032	0	6196	144	0
1	E	6032	0	6196	138	0
1	F	6032	0	6196	134	0
2	A	54	0	80	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	54	0	80	2	0
2	C	54	0	80	4	0
2	D	54	0	80	3	0
2	E	54	0	80	2	0
2	F	54	0	80	6	0
3	A	38	0	48	5	0
3	B	38	0	48	2	0
3	C	38	0	48	1	0
3	D	38	0	48	0	0
3	E	38	0	48	0	0
3	F	38	0	48	1	0
4	A	56	0	92	17	0
4	B	56	0	92	14	0
4	C	56	0	92	13	0
4	D	56	0	92	20	0
4	E	56	0	92	26	0
4	F	56	0	92	17	0
All	All	37073	0	38489	761	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 10.

All (761) 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:E:331:PHE:CE1	4:E:904:CLR:H261	1.43	1.52
1:E:407:LEU:CD2	1:E:439:PRO:HG3	1.63	1.27
1:C:790:LEU:O	1:C:793:THR:HG22	1.38	1.22
1:E:790:LEU:O	1:E:793:THR:HG22	1.38	1.20
1:E:331:PHE:CE1	4:E:904:CLR:C26	2.25	1.18
1:A:700:LEU:HD21	1:A:715:ILE:HD13	1.24	1.16
1:A:790:LEU:O	1:A:793:THR:HG22	1.38	1.16
1:B:403:ARG:HD2	1:B:436:SER:HB2	1.18	1.15
1:D:407:LEU:HD11	1:D:439:PRO:HG3	1.26	1.15
1:B:403:ARG:HD2	1:B:436:SER:CB	1.77	1.15
1:E:700:LEU:HD21	1:E:715:ILE:HD13	1.23	1.14
1:B:4:VAL:CG2	1:B:40:VAL:HG21	1.78	1.13
1:E:407:LEU:HD21	1:E:439:PRO:HG3	1.19	1.12
1:C:700:LEU:HD21	1:C:715:ILE:HD13	1.23	1.09
1:F:403:ARG:HD2	1:F:436:SER:HB2	1.17	1.09
1:E:331:PHE:CZ	4:E:904:CLR:C26	2.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:MET:CE	1:D:463:PRO:HG2	1.82	1.07
1:D:403:ARG:HD2	1:D:436:SER:HB2	1.15	1.07
1:F:403:ARG:HD2	1:F:436:SER:CB	1.86	1.04
1:B:4:VAL:HG22	1:B:40:VAL:HG21	1.39	1.04
1:C:434:MET:HE1	1:D:463:PRO:HG2	1.40	1.03
1:B:796:PRO:HB2	1:C:665:GLU:OE2	1.59	1.02
1:D:403:ARG:CD	1:D:436:SER:HB2	1.89	1.00
1:A:807:LYS:O	1:E:803:TRP:HZ2	1.43	0.99
1:E:331:PHE:HE1	4:E:904:CLR:H261	1.19	0.98
1:C:434:MET:CE	1:D:463:PRO:CG	2.40	0.98
1:A:665:GLU:OE2	1:F:796:PRO:HB2	1.64	0.97
1:A:600:ARG:HG2	1:B:545:ARG:NH2	1.79	0.97
1:A:600:ARG:CD	1:B:545:ARG:NH2	2.28	0.96
1:F:403:ARG:CD	1:F:436:SER:CB	2.44	0.96
1:C:434:MET:SD	1:D:463:PRO:HG2	2.07	0.94
1:E:331:PHE:CZ	4:E:904:CLR:H263	2.03	0.93
1:D:323:SER:OG	4:D:904:CLR:H71	1.68	0.93
1:E:323:SER:OG	4:E:904:CLR:H71	1.69	0.91
1:D:279:ILE:HD11	1:D:329:VAL:HG12	1.53	0.91
1:B:4:VAL:HG23	1:B:40:VAL:HG21	1.53	0.90
1:D:324:PHE:CE1	4:D:903:CLR:H241	2.06	0.90
1:A:584:LEU:O	1:A:585:ASN:CB	2.18	0.90
1:B:4:VAL:HG22	1:B:40:VAL:CG2	2.02	0.89
1:D:700:LEU:HD21	1:D:715:ILE:HD13	1.55	0.89
1:F:403:ARG:CD	1:F:436:SER:HB2	2.03	0.89
1:D:403:ARG:HD2	1:D:436:SER:CB	2.02	0.89
1:B:700:LEU:HD21	1:B:715:ILE:HD13	1.55	0.89
1:B:403:ARG:CD	1:B:436:SER:CB	2.51	0.88
1:A:323:SER:HB3	4:A:903:CLR:H183	1.55	0.88
1:F:700:LEU:HD21	1:F:715:ILE:HD13	1.54	0.87
1:B:4:VAL:CG2	1:B:40:VAL:CG2	2.53	0.86
1:E:323:SER:HB3	4:E:903:CLR:H121	1.58	0.86
1:A:600:ARG:CG	1:B:545:ARG:NH2	2.37	0.86
1:D:403:ARG:CD	1:D:436:SER:CB	2.53	0.86
1:A:600:ARG:HG2	1:B:545:ARG:HH21	1.38	0.86
1:B:796:PRO:HB2	1:C:665:GLU:CD	1.96	0.86
1:E:700:LEU:HD21	1:E:715:ILE:CD1	2.05	0.86
1:C:700:LEU:HD21	1:C:715:ILE:CD1	2.05	0.85
1:A:665:GLU:CD	1:F:796:PRO:HB2	1.96	0.85
1:D:324:PHE:CD1	4:D:903:CLR:H241	2.11	0.84
1:A:700:LEU:HD21	1:A:715:ILE:CD1	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ARG:CD	1:B:545:ARG:HH22	1.88	0.84
1:E:19:ILE:HG22	1:E:379:ILE:HD12	1.59	0.83
1:A:807:LYS:O	1:E:803:TRP:CZ2	2.31	0.83
1:A:600:ARG:HD2	1:B:545:ARG:HH22	1.43	0.82
1:E:45:LEU:CD2	1:E:317:LEU:HD22	2.10	0.82
1:B:796:PRO:CB	1:C:665:GLU:OE2	2.27	0.82
1:D:407:LEU:CD1	1:D:439:PRO:HG3	2.10	0.81
1:E:331:PHE:CZ	4:E:904:CLR:H261	2.03	0.81
1:C:434:MET:HE1	1:D:463:PRO:CG	2.04	0.81
1:C:719:ARG:HH22	1:D:639:HIS:CB	1.94	0.80
1:B:796:PRO:CB	1:C:665:GLU:OE1	2.30	0.80
1:E:323:SER:OG	4:E:904:CLR:C7	2.29	0.79
1:A:688:ARG:CZ	1:F:800:GLU:HG3	2.13	0.78
1:E:715:ILE:HG22	1:E:715:ILE:O	1.84	0.77
1:E:403:ARG:HD3	1:E:436:SER:HB2	1.64	0.77
1:F:715:ILE:HG22	1:F:715:ILE:O	1.84	0.77
1:D:715:ILE:O	1:D:715:ILE:HG22	1.84	0.77
1:A:584:LEU:O	1:A:585:ASN:HB3	1.83	0.77
1:A:715:ILE:HG22	1:A:715:ILE:O	1.84	0.77
1:A:414:ASP:HA	1:A:417:ARG:HD2	1.64	0.77
1:D:1:MET:HG3	1:D:44:THR:HG22	1.67	0.77
1:E:407:LEU:HD21	1:E:439:PRO:CG	2.10	0.77
1:B:715:ILE:O	1:B:715:ILE:HG22	1.84	0.76
1:E:45:LEU:CD2	1:E:317:LEU:CD2	2.64	0.76
1:C:715:ILE:HG22	1:C:715:ILE:O	1.84	0.76
1:A:323:SER:HB3	4:A:903:CLR:C18	2.15	0.76
1:F:413:LEU:HG	1:F:417:ARG:HH21	1.51	0.76
1:C:434:MET:SD	1:D:463:PRO:CG	2.73	0.76
1:C:434:MET:CE	1:D:463:PRO:HG3	2.15	0.75
1:E:323:SER:HB2	4:E:903:CLR:H122	1.68	0.75
1:D:407:LEU:HD11	1:D:439:PRO:CG	2.14	0.75
1:E:323:SER:CB	4:E:903:CLR:C12	2.65	0.74
1:A:413:LEU:HD13	1:A:444:ASP:HB2	1.70	0.74
1:E:1:MET:HG3	1:E:44:THR:HG22	1.70	0.74
1:A:265:MET:HA	1:A:343:MET:HE1	1.68	0.73
1:F:232:LEU:HB2	1:F:405:LEU:HD21	1.69	0.73
1:B:796:PRO:CB	1:C:665:GLU:CD	2.57	0.73
1:E:323:SER:HB3	4:E:904:CLR:H151	1.71	0.73
1:E:323:SER:HB3	4:E:903:CLR:C12	2.18	0.73
1:F:1:MET:HG3	1:F:44:THR:HG22	1.71	0.73
1:E:577:GLU:OE2	1:F:516:LYS:NZ	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG22	1:A:379:ILE:HD12	1.72	0.72
1:F:403:ARG:HD3	1:F:436:SER:CB	2.20	0.72
1:A:583:VAL:O	1:A:584:LEU:HB3	1.89	0.72
1:F:244:PHE:HE1	1:F:393:PHE:HA	1.53	0.72
1:E:258:ASP:H	1:E:371:ASP:HB2	1.53	0.71
1:A:434:MET:CE	1:B:463:PRO:HG2	2.21	0.71
1:F:416:LEU:HB3	1:F:445:LEU:HD11	1.71	0.71
1:C:265:MET:HA	1:C:343:MET:HE1	1.72	0.71
1:D:403:ARG:HD3	1:D:436:SER:CB	2.19	0.70
1:C:258:ASP:H	1:C:371:ASP:HB2	1.54	0.70
1:E:403:ARG:HD3	1:E:436:SER:CB	2.21	0.70
1:A:600:ARG:NE	1:B:545:ARG:NH2	2.39	0.70
1:D:258:ASP:H	1:D:371:ASP:HB2	1.57	0.69
1:B:796:PRO:HB3	1:C:665:GLU:OE1	1.92	0.69
1:A:665:GLU:OE1	1:F:796:PRO:HB2	1.91	0.69
1:C:765:ARG:HB3	1:D:688:ARG:HD2	1.76	0.68
1:E:45:LEU:HD23	1:E:317:LEU:HD22	1.74	0.68
1:C:434:MET:HE3	1:D:463:PRO:HG3	1.72	0.68
1:E:45:LEU:HD21	1:E:317:LEU:HD22	1.75	0.68
1:E:258:ASP:OD1	1:E:349:LYS:NZ	2.24	0.68
1:D:416:LEU:HB3	1:D:445:LEU:HD11	1.74	0.68
1:A:265:MET:O	1:A:269:ILE:HG12	1.94	0.68
1:B:796:PRO:CG	1:C:665:GLU:OE2	2.42	0.68
1:C:700:LEU:CD2	1:C:715:ILE:HD13	2.13	0.68
1:A:700:LEU:CD2	1:A:715:ILE:HD13	2.14	0.67
1:A:501:LYS:HZ1	1:B:489:ALA:HB3	1.59	0.67
1:C:52:MET:SD	1:C:118:LEU:HD12	2.33	0.67
1:C:719:ARG:HD3	1:D:640:ARG:HG2	1.77	0.67
1:E:700:LEU:CD2	1:E:715:ILE:HD13	2.13	0.67
1:A:408:ASN:HD21	1:A:440:ASP:HB2	1.59	0.66
1:A:583:VAL:O	1:A:584:LEU:CB	2.44	0.66
1:C:413:LEU:HD22	1:C:417:ARG:HE	1.60	0.66
1:F:413:LEU:HD21	1:F:444:ASP:HB2	1.76	0.66
1:B:796:PRO:HG2	1:C:665:GLU:OE2	1.95	0.66
1:C:239:GLN:OE1	1:C:239:GLN:N	2.24	0.66
1:D:324:PHE:CE1	4:D:903:CLR:C24	2.78	0.66
1:C:40:VAL:O	1:C:44:THR:HG23	1.96	0.66
1:D:796:PRO:HB2	1:E:665:GLU:OE2	1.96	0.66
1:A:413:LEU:HD11	1:A:417:ARG:HH21	1.61	0.65
1:C:719:ARG:HH22	1:D:639:HIS:C	2.00	0.65
1:A:600:ARG:HD2	1:B:545:ARG:NH2	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:SER:HB3	4:C:901:CLR:H122	1.79	0.65
1:D:265:MET:HA	1:D:343:MET:HE1	1.79	0.65
1:D:39:ALA:HB2	1:D:129:VAL:HG12	1.78	0.65
1:F:258:ASP:H	1:F:371:ASP:HB2	1.60	0.65
1:A:600:ARG:CG	1:B:545:ARG:HH22	2.05	0.65
1:C:719:ARG:HH22	1:D:639:HIS:HB3	1.61	0.65
1:A:501:LYS:NZ	1:B:489:ALA:HB3	2.12	0.64
1:D:306:ARG:HH11	1:D:306:ARG:HA	1.62	0.64
1:B:796:PRO:HB2	1:C:665:GLU:OE1	1.93	0.64
1:F:171:ARG:HD2	1:F:232:LEU:HD21	1.80	0.64
1:A:584:LEU:O	1:A:585:ASN:HB2	1.98	0.64
1:C:92:THR:OG1	1:C:93:GLY:N	2.27	0.64
1:C:258:ASP:OD1	1:C:349:LYS:NZ	2.31	0.63
1:C:19:ILE:HG22	1:C:379:ILE:HD12	1.79	0.63
1:A:455:LEU:CD1	1:B:463:PRO:HB2	2.28	0.63
1:D:286:VAL:CG1	4:D:904:CLR:H12	2.28	0.63
1:E:45:LEU:HD21	1:E:317:LEU:CD2	2.29	0.63
1:A:320:ILE:HG12	4:A:903:CLR:H112	1.80	0.63
1:D:256:GLU:OE1	1:D:256:GLU:N	2.25	0.62
1:E:406:ASN:OD1	1:E:407:LEU:N	2.32	0.62
1:F:255:GLU:HG2	1:F:369:LYS:HB2	1.79	0.62
1:E:40:VAL:O	1:E:44:THR:HG23	2.00	0.62
1:E:259:ILE:N	1:E:371:ASP:OD2	2.32	0.62
1:F:364:ASP:OD2	1:F:397:VAL:N	2.30	0.62
1:F:48:THR:OG1	1:F:49:GLN:OE1	2.06	0.62
1:A:323:SER:CB	4:A:903:CLR:H183	2.27	0.62
1:C:696:ASN:HA	1:D:640:ARG:NH2	2.14	0.62
1:D:6:GLU:HG3	1:E:4:VAL:HG13	1.82	0.62
3:A:902:POV:O32	4:B:901:CLR:H41	2.00	0.62
1:B:407:LEU:HG	1:B:439:PRO:HG3	1.81	0.62
1:A:6:GLU:OE2	1:B:4:VAL:HB	2.00	0.61
1:B:800:GLU:HG3	1:C:688:ARG:CZ	2.30	0.61
1:D:416:LEU:CB	1:D:445:LEU:HD11	2.30	0.61
1:E:696:ASN:HB3	1:F:640:ARG:HH22	1.64	0.61
1:C:6:GLU:HG2	1:D:5:THR:HG23	1.82	0.61
1:B:2:ILE:HD12	1:B:2:ILE:H	1.65	0.61
1:B:364:ASP:OD2	1:B:397:VAL:N	2.33	0.61
1:A:665:GLU:OE1	1:F:796:PRO:CB	2.47	0.61
1:A:40:VAL:O	1:A:44:THR:HG23	2.00	0.61
1:B:265:MET:HA	1:B:343:MET:HE1	1.83	0.61
1:B:256:GLU:OE2	1:B:256:GLU:N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASP:O	1:B:262:ARG:NH1	2.33	0.61
1:D:276:ILE:HG22	1:D:276:ILE:O	2.00	0.61
1:F:258:ASP:O	1:F:262:ARG:NH1	2.34	0.60
1:A:324:PHE:CD1	4:A:903:CLR:H262	2.36	0.60
1:A:324:PHE:HE1	4:A:903:CLR:H261	1.67	0.60
1:B:130:LEU:HD23	3:B:904:POV:H21B	1.83	0.60
1:D:411:TRP:O	1:D:441:THR:HG21	2.02	0.60
1:F:118:LEU:HD22	1:F:123:LYS:HG3	1.83	0.60
1:F:39:ALA:HB2	1:F:129:VAL:HG12	1.84	0.60
1:F:403:ARG:HD3	1:F:436:SER:HB3	1.84	0.60
1:A:249:LYS:NZ	1:B:170:THR:O	2.34	0.60
1:E:256:GLU:OE2	1:E:256:GLU:N	2.29	0.59
1:D:324:PHE:HE1	4:D:903:CLR:H241	1.58	0.59
1:B:39:ALA:HB2	1:B:129:VAL:HG12	1.85	0.59
1:F:286:VAL:CG1	4:F:904:CLR:H12	2.32	0.59
1:B:258:ASP:H	1:B:371:ASP:HB2	1.68	0.59
1:D:258:ASP:O	1:D:262:ARG:NH1	2.36	0.59
1:B:4:VAL:HG23	1:B:40:VAL:CG2	2.27	0.59
1:D:415:LYS:HE2	1:E:414:ASP:HB2	1.84	0.59
1:A:552:LYS:HE2	1:B:516:LYS:NZ	2.18	0.59
1:D:364:ASP:OD2	1:D:397:VAL:HG13	2.03	0.59
1:F:429:GLU:OE1	1:F:452:LYS:NZ	2.28	0.59
1:F:14:GLN:OE1	1:F:14:GLN:N	2.34	0.58
1:E:323:SER:HB2	4:E:903:CLR:C12	2.29	0.58
1:F:403:ARG:CD	1:F:436:SER:HB3	2.33	0.58
1:D:413:LEU:HD11	1:D:444:ASP:HB2	1.85	0.58
1:A:404:GLN:NE2	1:A:438:ILE:O	2.36	0.58
1:C:408:ASN:HD21	1:C:440:ASP:HB2	1.68	0.58
1:F:276:ILE:O	1:F:276:ILE:HG22	2.02	0.58
1:F:323:SER:OG	4:F:904:CLR:H71	2.03	0.58
1:E:330:ILE:HG21	4:E:904:CLR:C27	2.34	0.58
1:D:324:PHE:HE1	4:D:903:CLR:C24	2.17	0.58
1:C:719:ARG:NH2	1:D:639:HIS:C	2.58	0.57
1:D:323:SER:HG	4:D:904:CLR:H71	1.69	0.57
1:B:43:GLY:O	1:B:47:VAL:HG23	2.04	0.57
1:E:407:LEU:CD2	1:E:439:PRO:CG	2.59	0.57
1:E:320:ILE:HG22	4:E:903:CLR:H12	1.87	0.57
1:F:323:SER:HB3	4:F:904:CLR:H151	1.86	0.57
1:A:375:MET:O	1:A:379:ILE:HG12	2.05	0.57
1:C:46:GLN:HG3	1:C:50:ASP:HB2	1.87	0.57
1:A:7:LEU:HB3	1:A:36:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLU:OE1	1:C:256:GLU:N	2.25	0.56
1:D:357:ARG:HD3	1:D:365:ILE:H	1.68	0.56
1:E:118:LEU:HD22	1:E:123:LYS:HG2	1.88	0.56
1:B:14:GLN:OE1	1:B:14:GLN:N	2.38	0.56
1:D:11:ALA:HB2	1:D:137:LEU:HD22	1.88	0.56
1:F:327:SER:OG	4:F:903:CLR:H211	2.05	0.56
1:F:576:ASN:ND2	1:F:579:THR:O	2.38	0.56
1:E:375:MET:O	1:E:379:ILE:HG12	2.05	0.56
1:A:323:SER:CB	4:A:903:CLR:C18	2.85	0.56
1:A:738:LEU:O	1:A:741:ASN:ND2	2.39	0.56
1:D:576:ASN:ND2	1:D:579:THR:O	2.38	0.56
1:C:738:LEU:O	1:C:741:ASN:ND2	2.39	0.55
1:A:166:SER:O	1:A:169:THR:OG1	2.24	0.55
1:E:233:ASP:HB3	1:E:236:GLU:HB3	1.88	0.55
1:F:303:THR:OG1	1:F:308:TYR:OH	2.23	0.55
1:B:576:ASN:ND2	1:B:579:THR:O	2.38	0.55
1:C:39:ALA:HB2	1:C:129:VAL:HG12	1.88	0.55
1:A:241:LYS:HE3	1:A:241:LYS:HA	1.87	0.55
1:D:2:ILE:HD12	1:D:2:ILE:H	1.70	0.55
1:D:413:LEU:HD11	1:D:444:ASP:CB	2.37	0.55
1:A:11:ALA:HB2	1:A:137:LEU:HD13	1.88	0.55
1:A:31:ILE:O	1:A:35:MET:HG3	2.06	0.55
1:E:738:LEU:O	1:E:741:ASN:ND2	2.39	0.55
1:A:371:ASP:O	1:A:375:MET:HE2	2.07	0.55
1:F:346:ARG:HH11	1:F:346:ARG:HB3	1.72	0.55
1:D:275:PHE:O	1:D:279:ILE:HG12	2.06	0.55
1:F:11:ALA:HB2	1:F:137:LEU:HD22	1.88	0.55
1:F:357:ARG:HD3	1:F:363:SER:HA	1.88	0.55
1:A:7:LEU:HD23	1:A:36:LEU:HD11	1.89	0.55
1:B:346:ARG:HH11	1:B:346:ARG:HB3	1.72	0.55
1:D:292:ASP:OD1	1:D:292:ASP:N	2.33	0.54
1:E:407:LEU:HD23	1:E:439:PRO:HG3	1.78	0.54
1:E:45:LEU:CD2	1:E:317:LEU:HD21	2.36	0.54
1:F:235:LYS:NZ	1:F:239:GLN:HG2	2.22	0.54
1:A:688:ARG:NH2	1:A:711:GLN:OE1	2.41	0.54
1:C:413:LEU:HD11	1:C:444:ASP:CB	2.38	0.54
1:F:715:ILE:O	1:F:715:ILE:CG2	2.56	0.54
1:D:715:ILE:O	1:D:715:ILE:CG2	2.56	0.54
1:F:130:LEU:HD23	3:F:902:POV:H21B	1.90	0.54
1:C:1:MET:HG3	1:C:44:THR:HG22	1.90	0.54
1:F:407:LEU:CG	1:F:439:PRO:HG3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:LEU:HB3	1:C:445:LEU:HD11	1.90	0.54
1:D:306:ARG:HA	1:D:306:ARG:NH1	2.23	0.54
1:A:231:VAL:N	1:A:409:ASN:OD1	2.41	0.53
1:F:45:LEU:HD21	1:F:317:LEU:HD23	1.90	0.53
1:D:2:ILE:HB	1:D:7:LEU:HD21	1.90	0.53
1:A:39:ALA:HB2	1:A:129:VAL:HG12	1.90	0.53
1:B:715:ILE:O	1:B:715:ILE:CG2	2.56	0.53
1:C:166:SER:O	1:C:169:THR:HG22	2.08	0.53
1:F:415:LYS:HG3	1:F:416:LEU:HD12	1.90	0.53
1:C:320:ILE:HG22	4:C:901:CLR:H6	1.90	0.53
1:F:11:ALA:HB2	1:F:137:LEU:HD13	1.91	0.53
1:C:259:ILE:N	1:C:371:ASP:OD2	2.41	0.53
1:B:323:SER:HB3	4:B:901:CLR:H121	1.90	0.53
1:A:258:ASP:OD1	1:A:349:LYS:NZ	2.37	0.53
3:C:904:POV:O22	4:D:903:CLR:H6	2.08	0.53
1:C:455:LEU:HD11	1:D:486:PRO:CB	2.39	0.53
1:C:700:LEU:CD2	1:C:715:ILE:CD1	2.83	0.53
1:F:411:TRP:HA	1:F:415:LYS:HE2	1.91	0.53
1:A:577:GLU:OE2	1:B:516:LYS:NZ	2.30	0.53
1:C:238:GLU:OE1	1:C:238:GLU:N	2.25	0.53
1:C:455:LEU:HD21	1:D:486:PRO:HG3	1.91	0.53
1:C:455:LEU:HD21	1:D:486:PRO:CG	2.39	0.53
1:D:429:GLU:OE1	1:D:452:LYS:NZ	2.28	0.53
1:F:413:LEU:HG	1:F:417:ARG:NH2	2.22	0.53
1:D:54:CYS:HA	1:D:310:CYS:HA	1.91	0.52
1:E:7:LEU:HB3	1:E:36:LEU:HD21	1.90	0.52
1:F:286:VAL:HG13	4:F:904:CLR:H12	1.91	0.52
1:A:251:ARG:O	1:A:255:GLU:HB2	2.08	0.52
1:B:51:LYS:HB2	1:B:51:LYS:NZ	2.25	0.52
1:F:232:LEU:HD13	1:F:405:LEU:HD11	1.91	0.52
1:A:552:LYS:HE2	1:B:516:LYS:HZ1	1.74	0.52
1:C:413:LEU:HD21	1:C:444:ASP:HB2	1.92	0.52
1:E:413:LEU:HG	1:E:441:THR:HG22	1.91	0.52
1:A:134:LEU:HD11	1:B:37:MET:HE1	1.90	0.52
1:A:413:LEU:CB	1:A:441:THR:HB	2.40	0.52
1:A:413:LEU:HD12	1:A:445:LEU:CD2	2.40	0.52
1:D:324:PHE:HD1	4:D:903:CLR:H241	1.69	0.52
1:E:688:ARG:NH2	1:E:711:GLN:OE1	2.41	0.52
1:A:324:PHE:CE1	4:A:903:CLR:H261	2.45	0.51
1:E:235:LYS:O	1:E:239:GLN:HG3	2.10	0.51
1:F:350:LYS:HD2	1:F:350:LYS:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:715:ILE:O	1:E:715:ILE:CG2	2.56	0.51
1:F:52:MET:SD	1:F:118:LEU:HD12	2.50	0.51
1:A:324:PHE:HD1	4:A:903:CLR:H262	1.75	0.51
1:C:715:ILE:O	1:C:715:ILE:CG2	2.56	0.51
1:D:276:ILE:O	1:D:276:ILE:CG2	2.58	0.51
1:E:31:ILE:O	1:E:35:MET:HG3	2.10	0.51
1:E:700:LEU:CD2	1:E:715:ILE:CD1	2.83	0.51
1:D:38:ILE:HD11	1:D:325:TYR:HD1	1.75	0.51
1:D:324:PHE:CD1	4:D:903:CLR:C24	2.90	0.51
1:B:505:ILE:HD13	1:B:536:VAL:HG22	1.93	0.51
1:C:118:LEU:HD21	1:C:122:ALA:HB3	1.93	0.51
1:F:282:THR:CG2	1:F:326:ILE:HD11	2.40	0.51
1:B:45:LEU:HD21	1:B:317:LEU:HD23	1.93	0.51
1:C:407:LEU:HD23	1:C:410:GLU:OE1	2.11	0.51
1:F:505:ILE:HD13	1:F:536:VAL:HG22	1.93	0.51
1:D:129:VAL:HG13	1:D:325:TYR:CE1	2.46	0.51
1:E:17:TYR:O	1:E:21:LYS:HG2	2.10	0.51
1:A:256:GLU:OE2	1:A:256:GLU:N	2.31	0.50
1:D:411:TRP:CZ3	1:D:415:LYS:HD3	2.45	0.50
1:E:13:THR:HG21	1:E:144:PHE:CD2	2.46	0.50
1:F:323:SER:HB2	4:F:903:CLR:H112	1.92	0.50
1:F:407:LEU:HD21	1:F:439:PRO:HG3	1.94	0.50
1:F:149:THR:HG21	1:F:263:LEU:HD22	1.93	0.50
1:D:3:PRO:O	1:D:7:LEU:HD23	2.12	0.50
1:D:286:VAL:HG13	4:D:904:CLR:H12	1.93	0.50
1:E:19:ILE:HD12	1:E:19:ILE:H	1.77	0.50
1:A:258:ASP:H	1:A:371:ASP:HB2	1.77	0.50
1:E:47:VAL:O	1:F:49:GLN:NE2	2.45	0.50
1:F:166:SER:O	1:F:169:THR:HG22	2.12	0.50
1:B:242:ALA:O	1:B:246:LYS:HG3	2.11	0.50
1:C:251:ARG:O	1:C:255:GLU:HB2	2.11	0.50
1:A:700:LEU:CD2	1:A:715:ILE:CD1	2.83	0.50
1:B:297:VAL:HG23	1:B:299:ILE:HG12	1.94	0.50
1:C:688:ARG:NH2	1:C:711:GLN:OE1	2.41	0.50
1:B:346:ARG:HB3	1:B:346:ARG:NH1	2.26	0.50
1:A:555:LEU:N	1:A:576:ASN:OD1	2.45	0.49
1:E:39:ALA:HB2	1:E:129:VAL:HG12	1.93	0.49
1:F:345:ARG:HH12	1:F:346:ARG:NH2	2.10	0.49
1:A:248:LYS:HZ3	1:A:248:LYS:HB2	1.77	0.49
1:B:322:ALA:O	1:B:326:ILE:HG13	2.12	0.49
1:D:7:LEU:HB3	1:D:36:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:ILE:HD13	1:D:536:VAL:HG22	1.93	0.49
1:E:61:THR:O	1:E:64:SER:OG	2.24	0.49
1:A:241:LYS:HD3	1:A:245:GLU:OE1	2.12	0.49
1:C:790:LEU:O	1:C:793:THR:CG2	2.33	0.49
1:E:555:LEU:N	1:E:576:ASN:OD1	2.45	0.49
1:F:357:ARG:HB2	1:F:363:SER:HA	1.94	0.49
1:C:255:GLU:HG2	1:C:369:LYS:HB2	1.94	0.49
1:E:45:LEU:HG	1:E:314:LEU:HD11	1.94	0.49
1:B:11:ALA:HB2	1:B:137:LEU:HD22	1.95	0.49
1:B:800:GLU:HG3	1:C:688:ARG:NH2	2.27	0.49
1:F:411:TRP:CZ3	1:F:439:PRO:HG2	2.48	0.49
1:B:357:ARG:HD2	1:B:363:SER:HA	1.93	0.49
1:C:555:LEU:N	1:C:576:ASN:OD1	2.45	0.49
1:D:175:GLU:OE1	1:D:175:GLU:N	2.40	0.49
1:D:353:PHE:HD1	1:D:356:ILE:HD13	1.77	0.49
1:C:416:LEU:O	1:C:420:LEU:HG	2.12	0.49
1:E:20:LEU:O	1:E:22:PRO:HD3	2.13	0.49
1:E:251:ARG:O	1:E:255:GLU:HB2	2.12	0.49
1:A:245:GLU:HA	1:A:248:LYS:NZ	2.28	0.49
1:E:142:PHE:HD2	1:E:263:LEU:HD21	1.78	0.49
1:F:276:ILE:O	1:F:276:ILE:CG2	2.60	0.49
1:A:1:MET:HG3	1:A:44:THR:HG22	1.95	0.49
1:A:45:LEU:HD21	1:A:317:LEU:HD23	1.93	0.49
1:A:790:LEU:O	1:A:793:THR:CG2	2.33	0.49
1:D:166:SER:O	1:D:169:THR:HG22	2.13	0.49
1:E:115:GLU:OE1	1:F:316:THR:OG1	2.28	0.49
1:A:501:LYS:NZ	1:B:489:ALA:CB	2.76	0.48
1:B:1:MET:HB2	1:B:44:THR:HG22	1.94	0.48
1:E:768:CYS:HA	1:E:793:THR:HG21	1.94	0.48
1:D:255:GLU:HG2	1:D:369:LYS:HB2	1.95	0.48
1:E:292:ASP:OD1	1:E:292:ASP:O	2.30	0.48
1:A:324:PHE:CE1	4:A:903:CLR:C26	2.96	0.48
1:B:302:LEU:HD11	1:C:309:ARG:HG2	1.95	0.48
4:C:902:CLR:H193	4:C:902:CLR:H111	1.60	0.48
1:C:327:SER:OG	4:C:901:CLR:H213	2.14	0.48
1:C:768:CYS:HA	1:C:793:THR:HG21	1.95	0.48
1:D:232:LEU:HB3	1:D:236:GLU:OE2	2.13	0.48
1:C:407:LEU:HD11	1:C:436:SER:OG	2.14	0.48
1:C:670:ASN:ND2	1:C:691:ASP:OD2	2.47	0.48
1:D:168:TRP:CE2	1:D:402:LEU:HD23	2.49	0.48
1:B:235:LYS:O	1:B:239:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:696:ASN:CB	1:F:640:ARG:HH22	2.25	0.48
1:B:4:VAL:HG23	1:B:40:VAL:HG11	1.96	0.48
1:E:6:GLU:OE1	1:E:6:GLU:N	2.41	0.48
1:E:6:GLU:HG2	1:F:4:VAL:HB	1.94	0.48
1:F:353:PHE:CE1	1:F:391:ALA:HB2	2.49	0.48
1:F:400:ASN:HA	1:F:403:ARG:HG2	1.96	0.48
1:A:768:CYS:HA	1:A:793:THR:HG21	1.95	0.48
1:E:408:ASN:HD21	1:E:440:ASP:H	1.61	0.48
1:A:715:ILE:O	1:A:715:ILE:CG2	2.56	0.48
1:B:54:CYS:HA	1:B:310:CYS:HA	1.96	0.48
1:F:323:SER:CB	4:F:904:CLR:H151	2.44	0.48
1:F:413:LEU:HA	1:F:416:LEU:HD13	1.95	0.48
1:A:789:ASP:OD1	1:A:790:LEU:N	2.47	0.48
1:B:286:VAL:CG1	4:B:902:CLR:H12	2.44	0.48
1:B:323:SER:CB	4:B:901:CLR:H112	2.43	0.48
1:E:234:LYS:O	1:E:238:GLU:HG3	2.13	0.48
1:E:403:ARG:HD3	1:E:436:SER:OG	2.13	0.48
1:E:670:ASN:ND2	1:E:691:ASP:OD2	2.47	0.48
1:F:700:LEU:CD2	1:F:715:ILE:HD13	2.35	0.48
1:B:2:ILE:HB	1:B:7:LEU:HD21	1.96	0.47
1:E:155:HIS:O	1:E:159:ILE:HD13	2.14	0.47
1:E:258:ASP:OD2	1:E:262:ARG:NH1	2.45	0.47
1:F:175:GLU:OE1	1:F:175:GLU:N	2.46	0.47
1:F:346:ARG:HB3	1:F:346:ARG:NH1	2.29	0.47
1:D:171:ARG:HD3	1:D:232:LEU:HD21	1.96	0.47
1:D:700:LEU:CD2	1:D:715:ILE:HD13	2.35	0.47
1:E:396:GLU:HA	1:E:399:GLU:OE1	2.14	0.47
1:A:670:ASN:ND2	1:A:691:ASP:OD2	2.47	0.47
1:C:234:LYS:HE2	1:C:409:ASN:HB2	1.97	0.47
1:D:14:GLN:OE1	1:D:14:GLN:N	2.39	0.47
1:D:396:GLU:OE1	1:D:396:GLU:HA	2.14	0.47
1:F:54:CYS:HA	1:F:310:CYS:HA	1.97	0.47
1:A:258:ASP:H	1:A:371:ASP:CB	2.28	0.47
1:A:346:ARG:O	1:A:346:ARG:NH1	2.43	0.47
1:B:617:GLN:HG2	1:B:640:ARG:HB3	1.97	0.47
1:C:320:ILE:HG22	4:C:901:CLR:C6	2.44	0.47
1:C:529:ALA:O	1:C:533:ARG:NH1	2.48	0.47
1:E:789:ASP:OD1	1:E:790:LEU:N	2.47	0.47
1:C:138:ALA:HA	2:C:903:P5S:H36B	1.96	0.47
1:C:789:ASP:OD1	1:C:790:LEU:N	2.47	0.47
4:C:901:CLR:H221	4:C:901:CLR:H162	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:ILE:HG21	4:E:904:CLR:H273	1.96	0.47
1:A:245:GLU:HA	1:A:248:LYS:HZ3	1.80	0.47
1:A:529:ALA:O	1:A:533:ARG:NH1	2.48	0.47
1:C:235:LYS:O	1:C:235:LYS:HD3	2.14	0.47
1:C:296:THR:HG23	1:C:307:THR:HG22	1.97	0.47
1:A:665:GLU:CD	1:F:796:PRO:CB	2.75	0.47
3:A:902:POV:H2	4:B:901:CLR:H6	1.95	0.47
1:D:10:PHE:HD2	1:E:30:TYR:CE2	2.33	0.47
1:E:45:LEU:HD23	1:E:317:LEU:CD2	2.38	0.47
1:A:5:THR:N	1:F:6:GLU:OE2	2.36	0.46
1:B:166:SER:O	1:B:169:THR:HG22	2.15	0.46
1:B:353:PHE:HD1	1:B:356:ILE:HD13	1.79	0.46
1:E:295:CYS:SG	1:E:308:TYR:HB2	2.55	0.46
1:A:232:LEU:HB2	1:A:409:ASN:HD21	1.80	0.46
1:A:309:ARG:HG2	1:F:302:LEU:HD11	1.96	0.46
1:B:52:MET:SD	1:B:118:LEU:HD12	2.56	0.46
1:B:296:THR:HG23	1:B:307:THR:HG22	1.96	0.46
1:B:403:ARG:CD	1:B:436:SER:OG	2.63	0.46
1:D:296:THR:HG23	1:D:307:THR:HG22	1.98	0.46
1:E:297:VAL:HG23	1:E:299:ILE:HG12	1.98	0.46
4:F:903:CLR:H182	4:F:903:CLR:H8	1.59	0.46
1:A:648:TYR:HE1	1:B:547:LYS:HZ1	1.62	0.46
1:D:323:SER:HB3	4:D:904:CLR:H151	1.97	0.46
1:D:149:THR:HG21	1:D:263:LEU:HD22	1.97	0.46
1:F:244:PHE:CE2	1:F:399:GLU:HA	2.50	0.46
1:A:347:SER:O	1:A:347:SER:OG	2.34	0.46
1:A:455:LEU:CD1	1:B:463:PRO:CB	2.94	0.46
1:A:665:GLU:OE2	1:F:796:PRO:CB	2.49	0.46
4:D:903:CLR:H182	4:D:903:CLR:H8	1.55	0.46
1:E:19:ILE:CG2	1:E:379:ILE:HD12	2.36	0.46
1:F:346:ARG:O	1:F:346:ARG:HG2	2.16	0.46
1:A:5:THR:HG23	1:F:6:GLU:HG2	1.98	0.46
1:C:245:GLU:OE1	1:C:249:LYS:HE3	2.15	0.46
1:C:396:GLU:HA	1:C:399:GLU:OE1	2.15	0.46
1:D:416:LEU:O	1:D:420:LEU:HG	2.16	0.46
1:A:4:VAL:O	1:A:8:ARG:N	2.48	0.46
1:A:54:CYS:HA	1:A:310:CYS:HA	1.98	0.46
1:A:396:GLU:HA	1:A:399:GLU:OE1	2.16	0.46
1:B:4:VAL:CG2	1:B:40:VAL:CB	2.92	0.46
1:D:58:LYS:HG3	1:D:99:TYR:HE1	1.80	0.46
1:D:269:ILE:O	1:D:273:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:PHE:CE1	1:D:279:ILE:HG13	2.51	0.46
2:D:901:P5S:H44	2:D:901:P5S:H48	1.72	0.46
4:D:904:CLR:H183	4:D:904:CLR:H20	1.75	0.46
1:E:34:VAL:O	1:E:38:ILE:HG23	2.15	0.46
1:E:365:ILE:HG12	1:E:395:SER:HB3	1.98	0.46
1:A:354:GLU:O	1:A:358:GLU:HG2	2.15	0.46
4:A:903:CLR:H222	4:A:904:CLR:H161	1.97	0.46
1:B:403:ARG:HD3	1:B:436:SER:CB	2.44	0.46
1:B:700:LEU:CD2	1:B:715:ILE:HD13	2.35	0.46
1:E:529:ALA:O	1:E:533:ARG:NH1	2.48	0.46
1:A:244:PHE:CD1	1:A:399:GLU:HG3	2.50	0.46
1:C:347:SER:O	1:C:347:SER:OG	2.34	0.46
1:C:365:ILE:HG12	1:C:395:SER:HB3	1.98	0.46
1:C:719:ARG:NH2	1:D:639:HIS:HB3	2.29	0.46
1:D:31:ILE:O	1:D:35:MET:HG3	2.16	0.46
1:D:303:THR:OG1	1:D:308:TYR:OH	2.22	0.46
1:F:407:LEU:HG	1:F:439:PRO:HG3	1.97	0.46
2:F:901:P5S:H40A	2:F:901:P5S:HA	1.98	0.46
1:A:61:THR:N	1:A:64:SER:O	2.38	0.45
1:B:413:LEU:O	1:B:417:ARG:HG3	2.15	0.45
1:B:429:GLU:OE1	1:B:452:LYS:NZ	2.28	0.45
1:D:258:ASP:H	1:D:371:ASP:CB	2.27	0.45
1:E:52:MET:SD	1:E:118:LEU:HD12	2.57	0.45
1:E:61:THR:N	1:E:64:SER:O	2.40	0.45
1:A:175:GLU:H	1:A:175:GLU:HG2	1.39	0.45
1:C:434:MET:SD	1:D:463:PRO:HB2	2.56	0.45
1:B:175:GLU:OE2	1:B:175:GLU:N	2.42	0.45
1:C:418:GLN:HE21	1:C:418:GLN:HB2	1.52	0.45
1:D:279:ILE:HD11	1:D:329:VAL:CG1	2.33	0.45
1:A:584:LEU:O	1:A:584:LEU:HG	2.17	0.45
4:B:902:CLR:H221	4:B:902:CLR:H162	1.50	0.45
1:D:411:TRP:CE3	1:D:416:LEU:HG	2.51	0.45
1:E:331:PHE:HZ	4:E:904:CLR:H263	1.69	0.45
1:B:375:MET:O	1:B:379:ILE:HG12	2.17	0.45
1:C:142:PHE:HA	2:C:903:P5S:H35	1.98	0.45
4:F:904:CLR:H183	4:F:904:CLR:H20	1.74	0.45
1:C:403:ARG:HD3	1:C:436:SER:OG	2.16	0.45
1:A:370:ASN:C	1:A:372:PHE:H	2.20	0.45
1:D:297:VAL:HG23	1:D:299:ILE:HG12	1.99	0.45
1:D:353:PHE:CE1	1:D:391:ALA:HB2	2.52	0.45
1:D:413:LEU:HD12	1:D:445:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:SER:O	1:E:169:THR:HG22	2.16	0.45
1:E:324:PHE:CE1	4:E:903:CLR:H241	2.52	0.45
4:F:903:CLR:H111	4:F:903:CLR:H193	1.72	0.45
1:A:418:GLN:HE21	1:A:418:GLN:HB2	1.58	0.45
1:B:327:SER:OG	4:B:901:CLR:H211	2.16	0.45
1:B:331:PHE:HE2	4:B:901:CLR:H271	1.80	0.45
1:D:118:LEU:HD21	1:D:122:ALA:HB3	1.98	0.45
1:D:162:LYS:HD3	1:D:246:LYS:HZ1	1.82	0.45
1:F:118:LEU:HD21	1:F:122:ALA:HB3	1.99	0.45
1:A:320:ILE:HG13	4:A:903:CLR:C1	2.47	0.45
1:A:320:ILE:CG1	4:A:903:CLR:H112	2.47	0.45
1:A:412:THR:O	1:A:416:LEU:HG	2.16	0.45
1:C:407:LEU:CD1	1:C:436:SER:OG	2.65	0.45
1:E:6:GLU:CG	1:F:4:VAL:HB	2.46	0.45
1:E:253:HIS:CD2	1:E:254:VAL:HG23	2.52	0.45
1:E:327:SER:OG	4:E:903:CLR:C21	2.64	0.45
1:F:327:SER:OG	4:F:903:CLR:C21	2.65	0.45
1:A:101:LEU:HD22	1:A:105:GLN:OE1	2.17	0.45
4:B:902:CLR:H111	4:B:902:CLR:H193	1.75	0.45
1:D:169:THR:O	1:D:173:LEU:HD12	2.16	0.45
1:D:323:SER:HB2	4:D:903:CLR:H112	1.98	0.45
4:F:903:CLR:H211	4:F:903:CLR:H232	1.48	0.45
1:A:273:ILE:O	1:A:277:LEU:HG	2.16	0.44
1:A:418:GLN:H	1:A:418:GLN:HG3	1.52	0.44
1:B:4:VAL:HG23	1:B:40:VAL:CB	2.46	0.44
1:B:7:LEU:O	1:B:10:PHE:HD1	2.00	0.44
1:C:156:PHE:HD1	1:C:250:PHE:HZ	1.65	0.44
1:E:244:PHE:CD1	1:E:399:GLU:HG3	2.52	0.44
1:F:789:ASP:OD1	1:F:790:LEU:N	2.50	0.44
2:F:901:P5S:H32	2:F:901:P5S:H29A	1.79	0.44
1:C:149:THR:HG21	1:C:263:LEU:HD22	1.98	0.44
1:D:789:ASP:OD1	1:D:790:LEU:N	2.50	0.44
4:D:903:CLR:H212	4:D:903:CLR:H183	1.98	0.44
1:F:232:LEU:HB3	1:F:236:GLU:OE2	2.17	0.44
1:B:282:THR:HG22	1:B:326:ILE:HD11	1.99	0.44
4:B:902:CLR:H183	4:B:902:CLR:H20	1.75	0.44
1:C:282:THR:HG22	1:C:326:ILE:HD11	2.00	0.44
1:B:265:MET:SD	1:B:343:MET:HE3	2.58	0.44
1:B:639:HIS:O	1:B:663:ASN:ND2	2.50	0.44
1:D:52:MET:SD	1:D:118:LEU:HD12	2.57	0.44
1:F:162:LYS:HD3	1:F:246:LYS:HZ1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASP:OD1	1:B:292:ASP:N	2.33	0.44
1:C:61:THR:O	1:C:64:SER:OG	2.30	0.44
1:D:419:ARG:NH2	1:E:413:LEU:HD22	2.33	0.44
1:E:302:LEU:HD11	1:F:309:ARG:HG2	1.99	0.44
1:E:790:LEU:O	1:E:793:THR:CG2	2.33	0.44
1:F:256:GLU:OE1	1:F:256:GLU:N	2.43	0.44
3:A:902:POV:O22	4:B:901:CLR:H6	2.16	0.44
4:D:904:CLR:H211	4:D:904:CLR:H231	1.59	0.44
1:F:279:ILE:HD13	1:F:279:ILE:HA	1.76	0.44
1:F:343:MET:HB2	1:F:343:MET:HE2	1.78	0.44
1:C:118:LEU:HD22	1:C:123:LYS:HG3	1.99	0.44
1:C:324:PHE:HE1	4:C:901:CLR:H241	1.82	0.44
1:E:354:GLU:O	1:E:358:GLU:HG2	2.18	0.44
1:E:407:LEU:HD22	1:E:439:PRO:HG3	1.83	0.44
1:F:258:ASP:N	1:F:371:ASP:HB2	2.32	0.44
1:C:696:ASN:HA	1:D:640:ARG:HH22	1.81	0.44
1:D:364:ASP:OD2	1:D:397:VAL:N	2.42	0.44
2:D:901:P5S:H27	2:D:901:P5S:H30	1.41	0.44
1:E:552:LYS:HE2	1:F:516:LYS:HZ1	1.82	0.44
1:A:320:ILE:HG13	4:A:903:CLR:H12	1.99	0.44
1:C:418:GLN:H	1:C:418:GLN:HG3	1.61	0.44
1:D:639:HIS:O	1:D:663:ASN:ND2	2.51	0.44
1:F:639:HIS:O	1:F:663:ASN:ND2	2.51	0.44
2:F:901:P5S:H30	2:F:901:P5S:H27	1.44	0.44
1:A:164:PHE:CD1	1:A:389:ARG:HD2	2.53	0.43
1:A:416:LEU:O	1:A:420:LEU:HG	2.18	0.43
1:B:279:ILE:HD13	1:B:279:ILE:HA	1.83	0.43
1:B:403:ARG:CD	1:B:436:SER:HB3	2.46	0.43
1:D:32:SER:HA	1:D:35:MET:HE2	2.00	0.43
1:D:114:TYR:O	1:D:123:LYS:HE2	2.17	0.43
1:E:103:ARG:NH1	1:F:103:ARG:HE	2.15	0.43
1:F:236:GLU:HA	1:F:239:GLN:HG3	1.98	0.43
1:F:244:PHE:CE1	1:F:393:PHE:HA	2.42	0.43
1:F:323:SER:HB2	4:F:903:CLR:C11	2.48	0.43
1:D:19:ILE:HG22	1:D:379:ILE:HD12	1.99	0.43
2:D:901:P5S:H32	2:D:901:P5S:H29A	1.70	0.43
1:F:282:THR:HG21	1:F:326:ILE:HD11	2.00	0.43
1:F:375:MET:O	1:F:379:ILE:HG12	2.17	0.43
1:A:434:MET:HE3	1:B:463:PRO:HG2	1.99	0.43
1:B:58:LYS:HG3	1:B:99:TYR:HE1	1.83	0.43
1:C:370:ASN:OD1	1:C:370:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:THR:N	1:F:64:SER:O	2.35	0.43
1:A:353:PHE:HD1	1:A:356:ILE:HD13	1.83	0.43
1:E:333:GLY:O	1:E:337:MET:HG3	2.18	0.43
1:E:555:LEU:O	1:E:576:ASN:ND2	2.51	0.43
1:F:413:LEU:HD12	1:F:445:LEU:HD21	1.99	0.43
1:A:5:THR:OG1	1:F:6:GLU:OE2	2.32	0.43
1:A:45:LEU:HG	1:A:314:LEU:HD11	2.00	0.43
1:B:413:LEU:HA	1:B:413:LEU:HD12	1.70	0.43
1:B:789:ASP:OD1	1:B:790:LEU:N	2.50	0.43
2:C:903:P5S:H20	2:C:903:P5S:H1	1.82	0.43
1:D:348:LEU:HD23	1:D:374:PHE:HD1	1.84	0.43
1:D:365:ILE:HG12	1:D:395:SER:HB3	2.00	0.43
1:E:527:LEU:HD11	1:E:551:LEU:HD22	2.01	0.43
1:F:101:LEU:HD22	1:F:105:GLN:OE1	2.19	0.43
1:B:316:THR:O	1:B:320:ILE:HG23	2.18	0.43
1:C:527:LEU:HD11	1:C:551:LEU:HD22	2.01	0.43
1:F:322:ALA:O	1:F:326:ILE:HD13	2.19	0.43
1:F:323:SER:CB	4:F:903:CLR:C11	2.96	0.43
4:A:903:CLR:H183	4:A:903:CLR:H20	1.68	0.43
1:C:555:LEU:O	1:C:576:ASN:ND2	2.51	0.43
1:A:383:ASP:HB3	1:A:386:TYR:HD2	1.84	0.43
1:A:505:ILE:HD13	1:A:536:VAL:HG13	2.01	0.43
1:B:138:ALA:HA	2:B:903:P5S:H36B	2.00	0.43
4:C:902:CLR:H182	4:C:902:CLR:H8	1.80	0.43
1:B:168:TRP:CH2	1:B:398:SER:HB2	2.53	0.43
1:D:375:MET:O	1:D:379:ILE:HG12	2.19	0.43
1:E:58:LYS:HG3	1:E:99:TYR:HE1	1.84	0.43
1:A:10:PHE:O	1:A:141:ASN:ND2	2.52	0.43
1:A:255:GLU:HG2	1:A:369:LYS:HB2	2.01	0.43
1:A:258:ASP:HA	1:A:371:ASP:HB2	2.01	0.43
1:A:527:LEU:HD11	1:A:551:LEU:HD22	2.01	0.43
1:A:688:ARG:NE	1:F:800:GLU:HG3	2.34	0.43
1:B:11:ALA:HB2	1:B:137:LEU:HD13	2.00	0.43
1:B:715:ILE:HG21	1:B:720:ILE:CD1	2.49	0.43
2:E:901:P5S:H27	2:E:901:P5S:H30	1.43	0.43
4:A:903:CLR:H232	4:A:903:CLR:H211	1.51	0.42
1:B:19:ILE:H	1:B:19:ILE:HD12	1.84	0.42
1:B:419:ARG:NH2	1:C:413:LEU:HD13	2.34	0.42
1:C:719:ARG:NH2	1:D:639:HIS:O	2.52	0.42
1:D:275:PHE:CD1	1:D:333:GLY:HA3	2.54	0.42
1:F:584:LEU:HD12	1:F:584:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:PHE:O	1:B:357:ARG:HG3	2.18	0.42
1:D:46:GLN:HG3	1:D:50:ASP:HB3	2.01	0.42
1:F:19:ILE:HD12	1:F:19:ILE:H	1.84	0.42
1:A:354:GLU:HA	1:A:354:GLU:OE1	2.19	0.42
1:D:715:ILE:HG21	1:D:720:ILE:CD1	2.49	0.42
1:F:138:ALA:HA	2:F:901:P5S:H36B	1.99	0.42
1:A:584:LEU:O	1:A:584:LEU:CG	2.67	0.42
1:B:353:PHE:CE1	1:B:391:ALA:HB2	2.54	0.42
1:C:679:THR:CG2	1:C:703:ASP:OD2	2.67	0.42
1:F:407:LEU:CD2	1:F:439:PRO:HG3	2.48	0.42
1:F:159:ILE:HG22	1:F:390:PHE:HE1	1.84	0.42
1:A:295:CYS:SG	1:A:308:TYR:HB2	2.60	0.42
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.81	0.42
1:B:286:VAL:HG13	4:B:902:CLR:H12	2.01	0.42
1:C:302:LEU:HD11	1:D:309:ARG:HG2	2.01	0.42
1:D:2:ILE:HD11	1:E:41:PHE:HB2	2.01	0.42
1:E:38:ILE:HD11	1:E:325:TYR:HB2	2.02	0.42
1:E:323:SER:OG	4:E:904:CLR:H72	2.13	0.42
1:A:297:VAL:HG23	1:A:299:ILE:HG12	2.01	0.42
1:A:371:ASP:O	1:A:371:ASP:OD1	2.38	0.42
1:B:738:LEU:O	1:B:741:ASN:ND2	2.53	0.42
1:E:258:ASP:N	1:E:371:ASP:OD2	2.53	0.42
1:E:306:ARG:HG3	1:E:307:THR:HG23	2.01	0.42
1:F:738:LEU:O	1:F:741:ASN:ND2	2.53	0.42
1:B:323:SER:HB3	4:B:901:CLR:C12	2.49	0.42
1:D:7:LEU:C	1:D:9:TYR:H	2.23	0.42
1:C:295:CYS:SG	1:C:308:TYR:HB2	2.59	0.42
1:C:320:ILE:CG2	4:C:901:CLR:H6	2.50	0.42
1:D:3:PRO:HG2	1:D:6:GLU:OE2	2.20	0.42
2:F:901:P5S:H53	2:F:901:P5S:H50	1.62	0.42
1:A:290:LYS:HE2	1:A:290:LYS:HB3	1.91	0.42
1:A:600:ARG:CG	1:B:545:ARG:HH21	2.12	0.42
1:C:31:ILE:O	1:C:35:MET:HG3	2.20	0.42
1:D:348:LEU:HD23	1:D:374:PHE:CD1	2.54	0.42
1:E:236:GLU:HA	1:E:239:GLN:HG3	2.02	0.42
1:E:255:GLU:HG2	1:E:369:LYS:HB2	2.01	0.42
4:E:903:CLR:H182	4:E:903:CLR:H8	1.54	0.42
4:F:904:CLR:H162	4:F:904:CLR:H221	1.55	0.42
1:A:232:LEU:H	1:A:409:ASN:ND2	2.18	0.41
1:E:679:THR:CG2	1:E:703:ASP:OD2	2.68	0.41
4:E:904:CLR:H193	4:E:904:CLR:H111	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:715:ILE:HG21	1:F:720:ILE:CD1	2.49	0.41
1:B:19:ILE:HG22	1:B:379:ILE:HD12	2.02	0.41
1:A:92:THR:OG1	1:A:93:GLY:N	2.47	0.41
2:B:903:P5S:H27	2:B:903:P5S:H30	1.63	0.41
4:F:904:CLR:H111	4:F:904:CLR:H193	1.70	0.41
4:A:904:CLR:H221	4:A:904:CLR:H162	1.55	0.41
1:E:63:ASP:OD1	1:E:63:ASP:O	2.39	0.41
1:E:321:LEU:HD23	1:E:321:LEU:HA	1.88	0.41
1:E:353:PHE:CE1	1:E:391:ALA:HB2	2.55	0.41
1:A:578:GLY:N	1:A:600:ARG:O	2.45	0.41
1:D:121:PHE:HZ	1:D:282:THR:HG23	1.85	0.41
1:E:344:LEU:HA	1:E:344:LEU:HD23	1.80	0.41
1:A:395:SER:HG	1:A:398:SER:HG	1.59	0.41
3:A:902:POV:C25	1:B:320:ILE:HD12	2.51	0.41
1:C:505:ILE:HD13	1:C:536:VAL:HG13	2.01	0.41
1:E:296:THR:HG23	1:E:307:THR:HG22	2.02	0.41
1:E:505:ILE:HD13	1:E:536:VAL:HG13	2.01	0.41
1:F:154:GLU:HA	1:F:157:VAL:HG12	2.03	0.41
1:F:297:VAL:HG23	1:F:299:ILE:HG12	2.02	0.41
1:C:353:PHE:CE1	1:C:391:ALA:HB2	2.56	0.41
1:C:415:LYS:HA	1:C:418:GLN:CD	2.41	0.41
1:C:721:GLU:CD	1:D:686:LYS:NZ	2.74	0.41
1:D:349:LYS:HB3	1:D:370:ASN:HB3	2.01	0.41
1:E:138:ALA:HA	2:E:901:P5S:H36B	2.03	0.41
1:F:258:ASP:H	1:F:371:ASP:CB	2.29	0.41
4:F:903:CLR:H263	4:F:903:CLR:H231	1.81	0.41
1:A:370:ASN:N	1:A:370:ASN:OD1	2.53	0.41
1:A:679:THR:CG2	1:A:703:ASP:OD2	2.68	0.41
1:C:19:ILE:H	1:C:19:ILE:HD12	1.86	0.41
1:E:765:ARG:H	1:E:765:ARG:HG3	1.59	0.41
1:F:295:CYS:SG	1:F:308:TYR:HB2	2.61	0.41
1:F:296:THR:HG23	1:F:307:THR:HG22	2.02	0.41
1:F:348:LEU:HD23	1:F:374:PHE:HD1	1.86	0.41
2:F:901:P5S:H20	2:F:901:P5S:H39A	2.02	0.41
1:A:168:TRP:HA	1:A:171:ARG:HB3	2.02	0.41
1:A:340:LEU:HD12	1:A:340:LEU:HA	1.87	0.41
3:A:902:POV:H23A	4:B:901:CLR:H71	2.03	0.41
1:B:250:PHE:CE1	1:B:254:VAL:HG21	2.55	0.41
1:B:258:ASP:H	1:B:371:ASP:CB	2.32	0.41
1:C:260:VAL:HB	1:C:371:ASP:OD1	2.21	0.41
1:C:324:PHE:CE1	4:C:901:CLR:H241	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:MET:SD	1:D:463:PRO:CB	3.09	0.41
2:C:903:P5S:H30	2:C:903:P5S:H27	1.38	0.41
1:D:45:LEU:HD21	1:D:317:LEU:HD23	2.01	0.41
1:D:350:LYS:HE3	1:D:350:LYS:HB3	1.82	0.41
1:E:552:LYS:HE2	1:F:516:LYS:NZ	2.36	0.41
1:F:235:LYS:HZ3	1:F:239:GLN:HG2	1.84	0.41
1:F:353:PHE:HD1	1:F:356:ILE:HD13	1.84	0.41
1:B:40:VAL:O	1:B:44:THR:HG23	2.21	0.41
1:B:295:CYS:SG	1:B:308:TYR:HB2	2.61	0.41
1:C:13:THR:HG21	1:C:144:PHE:CD2	2.56	0.41
1:C:45:LEU:HG	1:C:314:LEU:HD21	2.04	0.41
1:D:11:ALA:HB2	1:D:137:LEU:HD13	2.03	0.41
1:D:738:LEU:O	1:D:741:ASN:ND2	2.53	0.41
1:E:156:PHE:HD1	1:E:250:PHE:HZ	1.69	0.41
2:A:901:P5S:H30	2:A:901:P5S:H27	1.33	0.40
1:B:346:ARG:HG2	1:B:346:ARG:O	2.20	0.40
1:D:236:GLU:O	1:D:239:GLN:HG2	2.21	0.40
1:D:279:ILE:CD1	1:D:329:VAL:HG12	2.37	0.40
1:D:364:ASP:CG	1:D:397:VAL:HG13	2.41	0.40
1:E:161:LEU:HD23	1:E:161:LEU:HA	1.86	0.40
1:E:411:TRP:HZ2	1:E:419:ARG:HH12	1.70	0.40
1:E:719:ARG:NH2	1:F:640:ARG:HG2	2.36	0.40
1:F:4:VAL:O	1:F:8:ARG:N	2.54	0.40
1:F:269:ILE:O	1:F:273:ILE:HG23	2.21	0.40
1:A:6:GLU:HB3	1:B:5:THR:OG1	2.21	0.40
4:C:901:CLR:H193	4:C:901:CLR:H111	1.83	0.40
1:D:320:ILE:HG22	4:D:903:CLR:H12	2.03	0.40
4:E:903:CLR:H162	4:E:903:CLR:H221	1.42	0.40
1:A:555:LEU:O	1:A:576:ASN:ND2	2.51	0.40
3:B:904:POV:H23A	4:C:901:CLR:H72	2.03	0.40
1:C:354:GLU:HA	1:C:357:ARG:HE	1.86	0.40
4:C:901:CLR:H8	4:C:901:CLR:H182	1.63	0.40
1:D:250:PHE:CE1	1:D:254:VAL:HG21	2.56	0.40
4:D:904:CLR:H162	4:D:904:CLR:H221	1.52	0.40
1:E:383:ASP:HB3	1:E:386:TYR:HD1	1.87	0.40
1:E:584:LEU:HD12	1:E:584:LEU:HA	1.84	0.40
4:E:904:CLR:H183	4:E:904:CLR:H20	1.75	0.40
1:F:354:GLU:OE1	1:F:357:ARG:NH1	2.50	0.40
1:B:7:LEU:HD12	1:B:134:LEU:HD21	2.03	0.40
1:B:118:LEU:HD21	1:B:122:ALA:HB3	2.03	0.40
1:B:370:ASN:C	1:B:372:PHE:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:ILE:HD13	1:F:159:ILE:HA	1.93	0.40
1:F:350:LYS:HD2	1:F:350:LYS:O	2.22	0.40
1:A:501:LYS:HZ3	1:B:489:ALA:CB	2.34	0.40
1:C:719:ARG:HH22	1:D:639:HIS:HB2	1.81	0.40
1:D:102:ASP:OD1	1:D:102:ASP:N	2.54	0.40
1:E:600:ARG:HH22	1:F:516:LYS:HB2	1.87	0.40
4:E:904:CLR:H221	4:E:904:CLR:H162	1.44	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	723/808 (90%)	680 (94%)	41 (6%)	2 (0%)	41 70
1	B	724/808 (90%)	697 (96%)	26 (4%)	1 (0%)	51 80
1	C	724/808 (90%)	689 (95%)	34 (5%)	1 (0%)	51 80
1	D	724/808 (90%)	691 (95%)	33 (5%)	0	100 100
1	E	724/808 (90%)	691 (95%)	32 (4%)	1 (0%)	51 80
1	F	724/808 (90%)	694 (96%)	28 (4%)	2 (0%)	41 70
All	All	4343/4848 (90%)	4142 (95%)	194 (4%)	7 (0%)	50 76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	584	LEU
1	F	413	LEU
1	A	585	ASN
1	B	585	ASN
1	C	585	ASN

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Mol	Chain	Res	Type
1	E	585	ASN
1	F	585	ASN

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	678/748 (91%)	662 (98%)	16 (2%)	49 78
1	B	679/748 (91%)	673 (99%)	6 (1%)	78 92
1	C	679/748 (91%)	663 (98%)	16 (2%)	49 78
1	D	679/748 (91%)	663 (98%)	16 (2%)	49 78
1	E	679/748 (91%)	658 (97%)	21 (3%)	40 71
1	F	679/748 (91%)	663 (98%)	16 (2%)	49 78
All	All	4073/4488 (91%)	3982 (98%)	91 (2%)	54 80

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	143	TRP
1	A	175	GLU
1	A	236	GLU
1	A	241	LYS
1	A	250	PHE
1	A	275	PHE
1	A	281	TYR
1	A	346	ARG
1	A	367	ASP
1	A	411	TRP
1	A	413	LEU
1	A	415	LYS
1	A	418	GLN
1	A	583	VAL
1	A	719	ARG

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Mol	Chain	Res	Type
1	B	274	LYS
1	B	281	TYR
1	B	410	GLU
1	B	414	ASP
1	B	584	LEU
1	B	640	ARG
1	C	5	THR
1	C	51	LYS
1	C	235	LYS
1	C	241	LYS
1	C	281	TYR
1	C	306	ARG
1	C	331	PHE
1	C	346	ARG
1	C	412	THR
1	C	413	LEU
1	C	414	ASP
1	C	416	LEU
1	C	418	GLN
1	C	583	VAL
1	C	584	LEU
1	C	765	ARG
1	D	5	THR
1	D	51	LYS
1	D	102	ASP
1	D	235	LYS
1	D	249	LYS
1	D	275	PHE
1	D	281	TYR
1	D	298	ASP
1	D	343	MET
1	D	347	SER
1	D	410	GLU
1	D	412	THR
1	D	413	LEU
1	D	414	ASP
1	D	415	LYS
1	D	417	ARG
1	E	21	LYS
1	E	51	LYS
1	E	143	TRP
1	E	238	GLU

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Mol	Chain	Res	Type
1	E	239	GLN
1	E	241	LYS
1	E	253	HIS
1	E	265	MET
1	E	275	PHE
1	E	281	TYR
1	E	343	MET
1	E	346	ARG
1	E	371	ASP
1	E	410	GLU
1	E	411	TRP
1	E	412	THR
1	E	413	LEU
1	E	415	LYS
1	E	583	VAL
1	E	584	LEU
1	E	765	ARG
1	F	5	THR
1	F	63	ASP
1	F	165	ASP
1	F	235	LYS
1	F	239	GLN
1	F	275	PHE
1	F	281	TYR
1	F	350	LYS
1	F	357	ARG
1	F	410	GLU
1	F	413	LEU
1	F	414	ASP
1	F	415	LYS
1	F	417	ARG
1	F	467	GLN
1	F	584	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	ASN
1	A	418	GLN
1	B	409	ASN
1	C	404	GLN
1	C	418	GLN

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Mol	Chain	Res	Type
1	D	409	ASN
1	E	404	GLN
1	F	409	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

24 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	POV	B	904	-	37,37,51	1.12	2 (5%)	43,45,59	1.03	3 (6%)
4	CLR	B	902	-	31,31,31	0.92	2 (6%)	48,48,48	1.35	6 (12%)
2	P5S	E	901	-	52,53,53	0.93	2 (3%)	56,60,60	1.13	4 (7%)
2	P5S	F	901	-	52,53,53	0.91	2 (3%)	56,60,60	1.10	4 (7%)
4	CLR	D	903	-	31,31,31	0.99	2 (6%)	48,48,48	1.80	11 (22%)
2	P5S	B	903	-	52,53,53	0.92	2 (3%)	56,60,60	1.11	5 (8%)
4	CLR	C	901	-	31,31,31	1.05	2 (6%)	48,48,48	1.78	8 (16%)
4	CLR	C	902	-	31,31,31	0.92	2 (6%)	48,48,48	1.53	11 (22%)
4	CLR	D	904	-	31,31,31	0.91	2 (6%)	48,48,48	1.27	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CLR	E	904	-	31,31,31	0.86	2 (6%)	48,48,48	1.52	10 (20%)
4	CLR	F	904	-	31,31,31	0.91	2 (6%)	48,48,48	1.27	4 (8%)
3	POV	C	904	-	37,37,51	1.11	2 (5%)	43,45,59	1.03	3 (6%)
4	CLR	A	904	-	31,31,31	0.75	1 (3%)	48,48,48	1.26	5 (10%)
4	CLR	E	903	-	31,31,31	0.96	2 (6%)	48,48,48	2.02	13 (27%)
4	CLR	F	903	-	31,31,31	1.03	2 (6%)	48,48,48	2.06	15 (31%)
2	P5S	C	903	-	52,53,53	0.93	2 (3%)	56,60,60	1.15	5 (8%)
3	POV	F	902	-	37,37,51	1.12	2 (5%)	43,45,59	1.03	3 (6%)
3	POV	E	902	-	37,37,51	1.12	2 (5%)	43,45,59	1.03	3 (6%)
3	POV	D	902	-	37,37,51	1.12	2 (5%)	43,45,59	1.03	3 (6%)
4	CLR	A	903	-	31,31,31	1.06	3 (9%)	48,48,48	1.89	12 (25%)
3	POV	A	902	-	37,37,51	1.12	2 (5%)	43,45,59	1.03	3 (6%)
4	CLR	B	901	-	31,31,31	0.57	0	48,48,48	1.33	7 (14%)
2	P5S	A	901	-	52,53,53	0.95	2 (3%)	56,60,60	1.17	4 (7%)
2	P5S	D	901	-	52,53,53	0.92	2 (3%)	56,60,60	1.08	4 (7%)

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	POV	B	904	-	-	13/41/41/55	-
4	CLR	B	902	-	-	6/10/68/68	0/4/4/4
2	P5S	E	901	-	-	31/59/59/59	-
2	P5S	F	901	-	-	37/59/59/59	-
4	CLR	D	903	-	-	4/10/68/68	0/4/4/4
2	P5S	B	903	-	-	39/59/59/59	-
4	CLR	C	901	-	-	6/10/68/68	0/4/4/4
4	CLR	C	902	-	-	8/10/68/68	0/4/4/4
4	CLR	D	904	-	-	7/10/68/68	0/4/4/4
4	CLR	E	904	-	-	8/10/68/68	0/4/4/4
4	CLR	F	904	-	-	7/10/68/68	0/4/4/4
3	POV	C	904	-	-	13/41/41/55	-
4	CLR	A	904	-	-	9/10/68/68	0/4/4/4
4	CLR	E	903	-	-	7/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	F	903	-	-	7/10/68/68	0/4/4/4
2	P5S	C	903	-	-	30/59/59/59	-
3	POV	F	902	-	-	13/41/41/55	-
3	POV	E	902	-	-	13/41/41/55	-
3	POV	D	902	-	-	13/41/41/55	-
4	CLR	A	903	-	-	7/10/68/68	0/4/4/4
3	POV	A	902	-	-	13/41/41/55	-
4	CLR	B	901	-	-	1/10/68/68	0/4/4/4
2	P5S	A	901	-	-	28/59/59/59	-
2	P5S	D	901	-	-	40/59/59/59	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	902	POV	O31-C31	4.39	1.46	1.33
2	A	901	P5S	O37-C38	4.38	1.46	1.34
3	F	902	POV	O31-C31	4.37	1.46	1.33
3	B	904	POV	O31-C31	4.36	1.46	1.33
3	D	902	POV	O31-C31	4.36	1.46	1.33
3	C	904	POV	O31-C31	4.35	1.46	1.33
3	A	902	POV	O31-C31	4.35	1.46	1.33
2	C	903	P5S	O37-C38	4.29	1.46	1.34
2	E	901	P5S	O19-C17	4.27	1.45	1.33
3	B	904	POV	O21-C21	4.27	1.46	1.34
2	A	901	P5S	O19-C17	4.27	1.45	1.33
3	E	902	POV	O21-C21	4.26	1.46	1.34
3	F	902	POV	O21-C21	4.26	1.46	1.34
3	A	902	POV	O21-C21	4.25	1.46	1.34
3	D	902	POV	O21-C21	4.25	1.46	1.34
3	C	904	POV	O21-C21	4.23	1.46	1.34
2	C	903	P5S	O19-C17	4.20	1.45	1.33
2	D	901	P5S	O37-C38	4.18	1.46	1.34
2	F	901	P5S	O37-C38	4.18	1.46	1.34
2	B	903	P5S	O37-C38	4.18	1.46	1.34
2	F	901	P5S	O19-C17	4.14	1.45	1.33
2	D	901	P5S	O19-C17	4.14	1.45	1.33
2	B	903	P5S	O19-C17	4.13	1.45	1.33
2	E	901	P5S	O37-C38	4.12	1.45	1.34
4	F	903	CLR	C10-C9	-2.79	1.51	1.56
4	D	903	CLR	C10-C9	-2.74	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	904	CLR	C10-C9	-2.65	1.51	1.56
4	C	901	CLR	C10-C9	-2.62	1.51	1.56
4	C	901	CLR	C13-C14	-2.60	1.50	1.55
4	F	904	CLR	C10-C9	-2.57	1.51	1.56
4	B	902	CLR	C10-C9	-2.54	1.51	1.56
4	C	902	CLR	C13-C14	-2.54	1.50	1.55
4	F	903	CLR	C13-C14	-2.52	1.50	1.55
4	A	903	CLR	C10-C9	-2.49	1.51	1.56
4	A	903	CLR	C13-C14	-2.46	1.50	1.55
4	E	903	CLR	C13-C14	-2.45	1.50	1.55
4	D	903	CLR	C13-C14	-2.43	1.50	1.55
4	E	904	CLR	C13-C14	-2.36	1.50	1.55
4	E	903	CLR	C10-C9	-2.19	1.52	1.56
4	B	902	CLR	C13-C14	-2.15	1.50	1.55
4	C	902	CLR	C10-C9	-2.12	1.52	1.56
4	A	904	CLR	C10-C9	-2.11	1.52	1.56
4	F	904	CLR	C13-C14	-2.10	1.51	1.55
4	D	904	CLR	C13-C14	-2.08	1.51	1.55
4	E	904	CLR	C10-C9	-2.05	1.52	1.56
4	A	903	CLR	C13-C17	-2.02	1.51	1.55

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	903	CLR	C13-C14-C8	-6.13	105.30	114.38
4	A	903	CLR	C1-C2-C3	5.62	117.67	110.47
4	F	903	CLR	C13-C14-C8	-5.57	106.13	114.38
4	A	903	CLR	C13-C17-C20	-5.45	110.95	119.49
4	F	903	CLR	C13-C17-C20	-5.44	110.96	119.49
4	D	903	CLR	C13-C14-C8	-5.39	106.40	114.38
4	E	903	CLR	C13-C17-C20	-5.26	111.25	119.49
4	C	901	CLR	C13-C14-C8	-5.22	106.65	114.38
4	C	901	CLR	C13-C17-C20	-5.01	111.63	119.49
2	A	901	P5S	O37-C38-C39	4.99	122.26	111.50
2	C	903	P5S	O37-C38-C39	4.92	122.09	111.50
4	A	903	CLR	C4-C5-C10	4.67	122.63	116.42
4	E	903	CLR	C8-C7-C6	-4.51	106.26	112.73
2	B	903	P5S	O37-C38-C39	4.36	120.90	111.50
4	E	904	CLR	C8-C7-C6	-4.35	106.48	112.73
2	F	901	P5S	O37-C38-C39	4.34	120.86	111.50
2	D	901	P5S	O37-C38-C39	4.31	120.80	111.50
4	F	903	CLR	C4-C5-C10	4.26	122.08	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	901	P5S	O37-C38-C39	4.19	120.53	111.50
4	D	903	CLR	C14-C8-C9	-4.08	103.63	109.09
4	E	903	CLR	C17-C13-C14	3.87	104.66	100.07
4	F	903	CLR	C17-C13-C14	3.83	104.61	100.07
4	D	903	CLR	C7-C8-C9	3.81	114.33	109.71
4	E	903	CLR	C14-C8-C9	-3.78	104.03	109.09
4	F	903	CLR	C11-C9-C10	-3.64	108.28	113.08
4	C	902	CLR	C8-C7-C6	-3.60	107.56	112.73
4	C	901	CLR	C3-C4-C5	-3.55	106.00	112.03
3	B	904	POV	O21-C21-C22	3.55	119.14	111.50
3	A	902	POV	O21-C21-C22	3.54	119.13	111.50
3	F	902	POV	O21-C21-C22	3.54	119.12	111.50
4	C	901	CLR	C7-C8-C9	3.54	114.00	109.71
3	D	902	POV	O21-C21-C22	3.54	119.12	111.50
3	C	904	POV	O21-C21-C22	3.53	119.12	111.50
3	E	902	POV	O21-C21-C22	3.53	119.11	111.50
4	D	903	CLR	C17-C13-C14	3.52	104.24	100.07
4	F	903	CLR	C14-C8-C9	-3.52	104.38	109.09
4	D	903	CLR	C13-C17-C20	-3.47	114.05	119.49
4	B	901	CLR	C12-C11-C9	3.43	119.06	113.11
4	F	904	CLR	C13-C17-C20	-3.39	114.17	119.49
3	D	902	POV	O31-C31-C32	3.38	122.52	111.91
3	A	902	POV	O31-C31-C32	3.37	122.50	111.91
3	B	904	POV	O31-C31-C32	3.37	122.48	111.91
3	F	902	POV	O31-C31-C32	3.37	122.48	111.91
3	E	902	POV	O31-C31-C32	3.36	122.45	111.91
3	C	904	POV	O31-C31-C32	3.36	122.44	111.91
4	A	904	CLR	C4-C5-C10	3.35	120.87	116.42
4	B	902	CLR	C13-C17-C20	-3.30	114.31	119.49
4	F	904	CLR	C11-C9-C10	-3.26	108.79	113.08
4	D	904	CLR	C13-C17-C20	-3.25	114.39	119.49
4	E	904	CLR	C13-C17-C20	-3.23	114.43	119.49
4	A	904	CLR	C13-C17-C20	-3.10	114.64	119.49
4	C	901	CLR	C17-C13-C14	3.08	103.72	100.07
4	C	901	CLR	C14-C8-C9	-3.05	105.01	109.09
2	A	901	P5S	O19-C17-C20	3.05	121.47	111.91
4	C	902	CLR	C13-C17-C20	-3.03	114.74	119.49
2	E	901	P5S	O19-C17-C20	3.02	121.38	111.91
4	F	903	CLR	C7-C8-C9	2.99	113.33	109.71
4	C	902	CLR	C3-C4-C5	-2.97	106.99	112.03
4	D	904	CLR	C11-C9-C10	-2.96	109.18	113.08
4	B	902	CLR	C10-C9-C8	-2.93	108.35	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	902	CLR	C12-C11-C9	2.90	118.14	113.11
4	A	903	CLR	C10-C5-C6	-2.90	118.47	122.90
4	F	903	CLR	C1-C10-C5	2.85	113.98	108.75
4	D	903	CLR	C3-C4-C5	-2.84	107.20	112.03
4	D	904	CLR	C10-C9-C8	-2.83	108.50	112.73
4	C	902	CLR	C13-C14-C8	-2.79	110.24	114.38
4	B	902	CLR	C11-C9-C10	-2.79	109.40	113.08
2	C	903	P5S	O19-C17-C20	2.79	120.66	111.91
2	F	901	P5S	O19-C17-C20	2.77	120.59	111.91
4	C	902	CLR	C10-C9-C8	-2.75	108.61	112.73
4	E	903	CLR	C4-C5-C10	2.72	120.04	116.42
4	F	903	CLR	C2-C3-C4	-2.72	106.57	110.31
4	E	903	CLR	C11-C9-C10	-2.70	109.53	113.08
2	B	903	P5S	O19-C17-C20	2.69	120.35	111.91
4	E	904	CLR	C13-C14-C8	-2.65	110.45	114.38
4	F	904	CLR	C19-C10-C9	-2.63	108.55	111.68
4	E	903	CLR	C19-C10-C9	-2.62	108.56	111.68
4	A	903	CLR	C13-C14-C8	-2.62	110.50	114.38
4	C	901	CLR	C11-C9-C10	-2.62	109.63	113.08
4	E	903	CLR	C7-C6-C5	-2.61	120.25	125.06
4	D	903	CLR	C4-C5-C10	2.61	119.88	116.42
4	E	904	CLR	C19-C10-C9	-2.58	108.61	111.68
4	C	902	CLR	C19-C10-C9	-2.56	108.63	111.68
4	D	904	CLR	C19-C10-C9	-2.55	108.64	111.68
4	B	901	CLR	C19-C10-C5	-2.52	104.26	108.34
4	B	902	CLR	C19-C10-C9	-2.52	108.67	111.68
4	B	901	CLR	C19-C10-C9	2.50	114.66	111.68
4	D	903	CLR	C2-C3-C4	-2.49	106.89	110.31
4	C	902	CLR	C11-C9-C10	-2.46	109.84	113.08
4	A	904	CLR	C4-C5-C6	-2.45	117.07	120.61
4	A	903	CLR	C19-C10-C9	-2.44	108.78	111.68
4	A	903	CLR	C9-C10-C5	-2.42	105.85	109.65
4	F	903	CLR	C19-C10-C9	-2.42	108.79	111.68
2	D	901	P5S	O19-C17-C20	2.42	119.50	111.91
4	E	904	CLR	C11-C9-C10	-2.40	109.92	113.08
4	E	904	CLR	C10-C9-C8	-2.39	109.15	112.73
4	B	901	CLR	C4-C5-C10	2.37	119.56	116.42
4	E	904	CLR	C12-C11-C9	2.36	117.21	113.11
4	F	904	CLR	C10-C9-C8	-2.34	109.23	112.73
4	F	903	CLR	C16-C17-C13	2.32	106.64	103.84
4	A	903	CLR	C10-C9-C8	-2.32	109.25	112.73
4	A	904	CLR	C17-C13-C14	2.32	102.82	100.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	902	POV	O31-C31-O32	-2.30	117.78	123.59
3	D	902	POV	O31-C31-O32	-2.30	117.78	123.59
3	B	904	POV	O31-C31-O32	-2.30	117.80	123.59
4	B	901	CLR	C15-C14-C8	-2.29	115.30	119.08
4	A	904	CLR	C8-C7-C6	-2.29	109.44	112.73
3	E	902	POV	O31-C31-O32	-2.29	117.82	123.59
3	A	902	POV	O31-C31-O32	-2.29	117.82	123.59
3	C	904	POV	O31-C31-O32	-2.28	117.83	123.59
2	C	903	P5S	OXT-C-O	-2.28	118.91	124.09
4	C	902	CLR	C1-C2-C3	2.27	113.38	110.47
4	E	903	CLR	C7-C8-C9	2.27	112.46	109.71
4	B	901	CLR	C12-C13-C14	-2.25	103.77	107.27
4	A	903	CLR	C11-C9-C10	-2.25	110.11	113.08
2	A	901	P5S	O37-C38-O47	-2.24	118.29	123.70
4	A	903	CLR	C17-C13-C14	2.23	102.71	100.07
2	C	903	P5S	O37-C38-O47	-2.22	118.34	123.70
4	F	903	CLR	C8-C7-C6	-2.19	109.59	112.73
4	C	902	CLR	C17-C13-C14	2.18	102.66	100.07
2	F	901	P5S	OXT-C-O	-2.18	119.14	124.09
4	E	904	CLR	C4-C5-C6	-2.17	117.48	120.61
2	A	901	P5S	OXT-C-O	-2.17	119.16	124.09
4	E	904	CLR	C3-C4-C5	-2.16	108.36	112.03
2	D	901	P5S	OXT-C-O	-2.15	119.21	124.09
4	F	903	CLR	C23-C22-C20	-2.14	108.88	115.03
4	E	903	CLR	C9-C10-C5	2.12	112.98	109.65
4	E	904	CLR	C17-C13-C14	2.12	102.59	100.07
2	E	901	P5S	OG-CB-CA	2.11	109.89	108.06
4	F	903	CLR	C10-C5-C6	-2.10	119.69	122.90
4	A	903	CLR	C8-C7-C6	-2.10	109.71	112.73
4	F	903	CLR	C11-C12-C13	-2.10	109.18	112.78
2	B	903	P5S	OXT-C-O	-2.09	119.33	124.09
4	B	901	CLR	C13-C17-C20	2.09	122.77	119.49
2	B	903	P5S	O37-C38-O47	-2.09	118.65	123.70
2	E	901	P5S	OXT-C-O	-2.08	119.36	124.09
4	B	902	CLR	C1-C10-C9	2.07	111.62	108.73
4	C	901	CLR	C7-C6-C5	-2.07	121.25	125.06
4	D	903	CLR	C7-C6-C5	-2.06	121.26	125.06
4	B	902	CLR	C8-C7-C6	-2.06	109.78	112.73
4	E	903	CLR	C2-C3-C4	-2.06	107.48	110.31
2	F	901	P5S	O37-C38-O47	-2.05	118.74	123.70
4	E	903	CLR	C23-C22-C20	-2.05	109.15	115.03
2	D	901	P5S	O37-C38-O47	-2.03	118.80	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	902	CLR	C18-C13-C17	-2.02	107.95	111.71
4	D	903	CLR	C11-C9-C10	-2.02	110.42	113.08
4	A	903	CLR	C7-C6-C5	-2.02	121.34	125.06
2	B	903	P5S	C2-O37-C38	-2.01	112.84	117.79
4	D	904	CLR	C18-C13-C17	-2.01	107.97	111.71
4	D	903	CLR	C11-C12-C13	-2.01	109.34	112.78
2	C	903	P5S	OXT-C-CA	2.01	120.22	113.38

There are no chirality outliers.

All (360) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	P5S	O37-C2-C3-O16
2	A	901	P5S	C3-O16-P12-O13
2	A	901	P5S	O18-C17-O19-C1
2	A	901	P5S	C20-C17-O19-C1
2	A	901	P5S	C39-C38-O37-C2
2	A	901	P5S	O47-C38-O37-C2
2	B	903	P5S	O-C-CA-CB
2	B	903	P5S	OXT-C-CA-CB
2	B	903	P5S	N-CA-CB-OG
2	B	903	P5S	CA-CB-OG-P12
2	B	903	P5S	CB-OG-P12-O13
2	B	903	P5S	O47-C38-O37-C2
2	C	903	P5S	N-CA-CB-OG
2	C	903	P5S	C3-O16-P12-O13
2	C	903	P5S	C3-O16-P12-O15
2	C	903	P5S	O18-C17-O19-C1
2	C	903	P5S	C20-C17-O19-C1
2	C	903	P5S	O47-C38-O37-C2
2	D	901	P5S	O-C-CA-CB
2	D	901	P5S	OXT-C-CA-CB
2	D	901	P5S	C-CA-CB-OG
2	D	901	P5S	N-CA-CB-OG
2	D	901	P5S	CB-OG-P12-O13
2	D	901	P5S	C3-O16-P12-OG
2	D	901	P5S	C3-O16-P12-O15
2	D	901	P5S	C39-C38-O37-C2
2	E	901	P5S	C-CA-CB-OG
2	E	901	P5S	N-CA-CB-OG
2	E	901	P5S	CB-OG-P12-O13
2	E	901	P5S	CB-OG-P12-O15

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Mol	Chain	Res	Type	Atoms
2	E	901	P5S	O18-C17-O19-C1
2	E	901	P5S	C20-C17-O19-C1
2	E	901	P5S	C39-C38-O37-C2
2	F	901	P5S	O-C-CA-N
2	F	901	P5S	O-C-CA-CB
2	F	901	P5S	OXT-C-CA-CB
2	F	901	P5S	O37-C2-C3-O16
2	F	901	P5S	C-CA-CB-OG
2	F	901	P5S	N-CA-CB-OG
2	F	901	P5S	CB-OG-P12-O13
2	F	901	P5S	CB-OG-P12-O15
2	F	901	P5S	O47-C38-O37-C2
4	D	903	CLR	C22-C23-C24-C25
3	A	902	POV	O32-C31-O31-C3
3	B	904	POV	O32-C31-O31-C3
3	C	904	POV	O32-C31-O31-C3
3	D	902	POV	O32-C31-O31-C3
3	E	902	POV	O32-C31-O31-C3
3	F	902	POV	O32-C31-O31-C3
4	E	904	CLR	C16-C17-C20-C21
4	F	904	CLR	C16-C17-C20-C21
4	B	902	CLR	C13-C17-C20-C21
4	C	902	CLR	C13-C17-C20-C21
4	D	904	CLR	C13-C17-C20-C21
4	E	904	CLR	C13-C17-C20-C21
4	F	904	CLR	C13-C17-C20-C21
2	D	901	P5S	O47-C38-O37-C2
2	E	901	P5S	O47-C38-O37-C2
3	A	902	POV	C32-C31-O31-C3
3	B	904	POV	C32-C31-O31-C3
3	C	904	POV	C32-C31-O31-C3
3	D	902	POV	C32-C31-O31-C3
3	E	902	POV	C32-C31-O31-C3
3	F	902	POV	C32-C31-O31-C3
2	B	903	P5S	C39-C38-O37-C2
2	C	903	P5S	C39-C38-O37-C2
2	F	901	P5S	C39-C38-O37-C2
4	A	903	CLR	C21-C20-C22-C23
4	A	904	CLR	C21-C20-C22-C23
4	B	902	CLR	C21-C20-C22-C23
4	C	902	CLR	C21-C20-C22-C23
4	D	904	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
4	E	904	CLR	C21-C20-C22-C23
4	F	903	CLR	C21-C20-C22-C23
4	F	904	CLR	C21-C20-C22-C23
4	B	902	CLR	C16-C17-C20-C21
4	C	902	CLR	C16-C17-C20-C21
4	D	904	CLR	C16-C17-C20-C21
4	A	904	CLR	C13-C17-C20-C21
4	A	903	CLR	C13-C17-C20-C22
4	A	904	CLR	C13-C17-C20-C22
4	B	902	CLR	C13-C17-C20-C22
4	C	902	CLR	C13-C17-C20-C22
4	D	904	CLR	C13-C17-C20-C22
4	E	904	CLR	C13-C17-C20-C22
4	F	904	CLR	C13-C17-C20-C22
4	A	904	CLR	C16-C17-C20-C21
4	A	903	CLR	C13-C17-C20-C21
4	C	902	CLR	C16-C17-C20-C22
4	F	904	CLR	C16-C17-C20-C22
4	B	902	CLR	C17-C20-C22-C23
4	D	904	CLR	C17-C20-C22-C23
2	B	903	P5S	C29-C30-C31-C32
2	D	901	P5S	C44-C45-C46-C48
2	A	901	P5S	C44-C45-C46-C48
2	F	901	P5S	C44-C45-C46-C48
4	E	904	CLR	C16-C17-C20-C22
4	A	904	CLR	C17-C20-C22-C23
4	E	903	CLR	C17-C20-C22-C23
4	E	904	CLR	C17-C20-C22-C23
4	F	904	CLR	C17-C20-C22-C23
2	C	903	P5S	C44-C45-C46-C48
4	D	904	CLR	C16-C17-C20-C22
4	C	902	CLR	C17-C20-C22-C23
2	A	901	P5S	C27-C28-C29-C30
2	B	903	P5S	OXT-C-CA-N
2	D	901	P5S	OXT-C-CA-N
2	F	901	P5S	OXT-C-CA-N
2	F	901	P5S	C20-C17-O19-C1
4	B	902	CLR	C16-C17-C20-C22
2	C	903	P5S	C27-C28-C29-C30
4	E	903	CLR	C21-C20-C22-C23
2	F	901	P5S	C29-C30-C31-C32
2	F	901	P5S	O18-C17-O19-C1

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Mol	Chain	Res	Type	Atoms
2	D	901	P5S	C17-C20-C21-C22
4	F	903	CLR	C17-C20-C22-C23
2	E	901	P5S	C27-C28-C29-C30
2	D	901	P5S	C27-C28-C29-C30
4	A	903	CLR	C20-C22-C23-C24
4	F	903	CLR	C20-C22-C23-C24
2	B	903	P5S	C17-C20-C21-C22
2	C	903	P5S	C38-C39-C40-C41
2	F	901	P5S	C38-C39-C40-C41
2	A	901	P5S	C38-C39-C40-C41
2	B	903	P5S	C38-C39-C40-C41
2	F	901	P5S	C27-C28-C29-C30
4	A	904	CLR	C16-C17-C20-C22
4	E	903	CLR	C22-C23-C24-C25
2	A	901	P5S	C3-O16-P12-OG
2	C	903	P5S	C3-O16-P12-OG
2	E	901	P5S	CB-OG-P12-O16
2	F	901	P5S	CB-OG-P12-O16
4	B	901	CLR	C21-C20-C22-C23
2	D	901	P5S	C29-C30-C31-C32
4	A	904	CLR	C20-C22-C23-C24
2	E	901	P5S	C38-C39-C40-C41
2	B	903	P5S	C23-C24-C25-C26
4	A	903	CLR	C17-C20-C22-C23
2	D	901	P5S	C26-C27-C28-C29
2	E	901	P5S	C51-C52-C53-C54
2	F	901	P5S	C51-C52-C53-C54
4	D	903	CLR	C23-C24-C25-C27
2	A	901	P5S	C52-C53-C54-C55
2	E	901	P5S	C31-C32-C33-C34
2	B	903	P5S	C45-C46-C48-C49
2	E	901	P5S	C52-C53-C54-C55
2	C	903	P5S	C52-C53-C54-C55
2	E	901	P5S	C26-C27-C28-C29
2	D	901	P5S	C39-C40-C41-C42
2	F	901	P5S	C25-C26-C27-C28
2	B	903	P5S	C20-C21-C22-C23
3	D	902	POV	C33-C34-C35-C36
2	A	901	P5S	C26-C27-C28-C29
3	A	902	POV	C33-C34-C35-C36
3	B	904	POV	C33-C34-C35-C36
3	C	904	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	E	902	POV	C33-C34-C35-C36
3	F	902	POV	C33-C34-C35-C36
2	C	903	P5S	C26-C27-C28-C29
2	D	901	P5S	C22-C23-C24-C25
2	D	901	P5S	C25-C26-C27-C28
2	F	901	P5S	C52-C53-C54-C55
2	D	901	P5S	C38-C39-C40-C41
2	B	903	P5S	C22-C23-C24-C25
2	B	903	P5S	C42-C43-C44-C45
2	F	901	P5S	C26-C27-C28-C29
4	D	903	CLR	C20-C22-C23-C24
2	A	901	P5S	C25-C26-C27-C28
2	A	901	P5S	C51-C52-C53-C54
2	E	901	P5S	C39-C40-C41-C42
4	D	903	CLR	C23-C24-C25-C26
2	F	901	P5S	C50-C51-C52-C53
2	C	903	P5S	C25-C26-C27-C28
2	A	901	P5S	C48-C49-C50-C51
4	A	903	CLR	C16-C17-C20-C21
2	A	901	P5S	C31-C32-C33-C34
2	B	903	P5S	C52-C53-C54-C55
2	B	903	P5S	C20-C17-O19-C1
2	C	903	P5S	C48-C49-C50-C51
2	E	901	P5S	C45-C46-C48-C49
2	E	901	P5S	C23-C24-C25-C26
2	B	903	P5S	C-CA-CB-OG
4	A	903	CLR	C16-C17-C20-C22
2	C	903	P5S	C31-C32-C33-C34
2	C	903	P5S	O37-C2-C3-O16
2	C	903	P5S	C51-C52-C53-C54
2	B	903	P5S	C41-C42-C43-C44
2	D	901	P5S	C31-C32-C33-C34
2	D	901	P5S	C48-C49-C50-C51
2	A	901	P5S	C22-C23-C24-C25
2	D	901	P5S	C20-C21-C22-C23
2	E	901	P5S	C44-C45-C46-C48
2	A	901	P5S	C42-C43-C44-C45
2	E	901	P5S	C25-C26-C27-C28
2	B	903	P5S	C25-C26-C27-C28
2	B	903	P5S	CB-OG-P12-O16
2	C	903	P5S	C1-C2-C3-O16
2	F	901	P5S	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
4	E	903	CLR	C13-C17-C20-C21
2	B	903	P5S	C43-C44-C45-C46
2	E	901	P5S	C46-C48-C49-C50
3	B	904	POV	C24-C25-C26-C27
3	A	902	POV	C24-C25-C26-C27
3	C	904	POV	C24-C25-C26-C27
3	D	902	POV	C24-C25-C26-C27
3	E	902	POV	C24-C25-C26-C27
3	F	902	POV	C24-C25-C26-C27
2	D	901	P5S	C46-C48-C49-C50
2	F	901	P5S	C46-C48-C49-C50
2	B	903	P5S	C26-C27-C28-C29
2	F	901	P5S	O19-C1-C2-C3
3	A	902	POV	C1-C2-C3-O31
3	B	904	POV	C1-C2-C3-O31
3	C	904	POV	C1-C2-C3-O31
3	D	902	POV	C1-C2-C3-O31
3	E	902	POV	C1-C2-C3-O31
3	F	902	POV	C1-C2-C3-O31
2	D	901	P5S	O19-C17-C20-C21
2	E	901	P5S	C48-C49-C50-C51
2	B	903	P5S	O18-C17-O19-C1
4	E	903	CLR	C13-C17-C20-C22
2	F	901	P5S	C48-C49-C50-C51
2	E	901	P5S	C40-C41-C42-C43
2	E	901	P5S	C41-C42-C43-C44
4	C	901	CLR	C13-C17-C20-C21
4	F	903	CLR	C13-C17-C20-C21
2	D	901	P5S	C53-C54-C55-C56
4	F	904	CLR	C20-C22-C23-C24
2	B	903	P5S	C1-C2-C3-O16
2	D	901	P5S	C1-C2-C3-O16
2	F	901	P5S	C1-C2-C3-O16
2	B	903	P5S	C24-C25-C26-C27
2	B	903	P5S	C31-C32-C33-C34
2	D	901	P5S	C33-C34-C35-C36
4	E	904	CLR	C23-C24-C25-C26
4	E	904	CLR	C23-C24-C25-C27
2	D	901	P5S	CB-OG-P12-O16
4	C	902	CLR	C23-C24-C25-C27
2	F	901	P5S	C31-C32-C33-C34
2	F	901	P5S	O19-C1-C2-O37

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Mol	Chain	Res	Type	Atoms
4	C	901	CLR	C13-C17-C20-C22
4	F	903	CLR	C13-C17-C20-C22
2	B	903	P5S	O-C-CA-N
2	D	901	P5S	O-C-CA-N
2	A	901	P5S	C28-C29-C30-C31
2	B	903	P5S	C50-C51-C52-C53
2	C	903	P5S	C45-C46-C48-C49
2	D	901	P5S	C2-C3-O16-P12
2	C	903	P5S	C42-C43-C44-C45
3	A	902	POV	C32-C33-C34-C35
3	B	904	POV	C32-C33-C34-C35
3	C	904	POV	C32-C33-C34-C35
3	F	902	POV	C32-C33-C34-C35
3	D	902	POV	C32-C33-C34-C35
3	E	902	POV	C32-C33-C34-C35
2	F	901	P5S	C28-C29-C30-C31
2	C	903	P5S	C39-C40-C41-C42
2	D	901	P5S	C23-C24-C25-C26
2	A	901	P5S	C33-C34-C35-C36
2	F	901	P5S	C21-C22-C23-C24
2	B	903	P5S	O19-C1-C2-C3
2	B	903	P5S	O37-C2-C3-O16
2	D	901	P5S	O37-C2-C3-O16
4	E	903	CLR	C16-C17-C20-C21
2	E	901	P5S	C33-C34-C35-C36
2	F	901	P5S	C33-C34-C35-C36
2	A	901	P5S	CA-CB-OG-P12
2	C	903	P5S	CA-CB-OG-P12
2	D	901	P5S	CA-CB-OG-P12
2	F	901	P5S	CA-CB-OG-P12
2	A	901	P5S	C24-C25-C26-C27
2	D	901	P5S	C24-C25-C26-C27
2	B	903	P5S	C33-C34-C35-C36
2	A	901	P5S	N-CA-CB-OG
4	C	901	CLR	C22-C23-C24-C25
2	E	901	P5S	C3-O16-P12-OG
2	A	901	P5S	C3-O16-P12-O15
2	D	901	P5S	C3-O16-P12-O13
4	C	902	CLR	C23-C24-C25-C26
2	A	901	P5S	C1-C2-C3-O16
2	B	903	P5S	O19-C17-C20-C21
2	F	901	P5S	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
2	E	901	P5S	C28-C29-C30-C31
4	E	903	CLR	C16-C17-C20-C22
2	B	903	P5S	O19-C1-C2-O37
2	C	903	P5S	C33-C34-C35-C36
4	D	904	CLR	C20-C22-C23-C24
2	E	901	P5S	C21-C22-C23-C24
2	B	903	P5S	C28-C29-C30-C31
2	C	903	P5S	C28-C29-C30-C31
2	B	903	P5S	C46-C48-C49-C50
4	C	901	CLR	C16-C17-C20-C21
3	B	904	POV	C22-C23-C24-C25
3	E	902	POV	C22-C23-C24-C25
3	A	902	POV	C22-C23-C24-C25
3	C	904	POV	C22-C23-C24-C25
3	D	902	POV	C22-C23-C24-C25
3	F	902	POV	C22-C23-C24-C25
4	F	903	CLR	C16-C17-C20-C21
3	A	902	POV	O21-C2-C3-O31
3	B	904	POV	O21-C2-C3-O31
3	C	904	POV	O21-C2-C3-O31
3	D	902	POV	O21-C2-C3-O31
3	E	902	POV	O21-C2-C3-O31
3	F	902	POV	O21-C2-C3-O31
2	B	903	P5S	C3-O16-P12-OG
2	E	901	P5S	C50-C51-C52-C53
2	D	901	P5S	C40-C41-C42-C43
4	C	901	CLR	C16-C17-C20-C22
4	F	903	CLR	C16-C17-C20-C22
2	B	903	P5S	C27-C28-C29-C30
2	A	901	P5S	C-CA-CB-OG
2	C	903	P5S	C-CA-CB-OG
2	C	903	P5S	C22-C23-C24-C25
2	D	901	P5S	O18-C17-C20-C21
2	D	901	P5S	C28-C29-C30-C31
3	A	902	POV	C210-C211-C212-C213
3	B	904	POV	C210-C211-C212-C213
3	C	904	POV	C210-C211-C212-C213
3	D	902	POV	C210-C211-C212-C213
3	E	902	POV	C210-C211-C212-C213
3	F	902	POV	C210-C211-C212-C213
4	A	904	CLR	C23-C24-C25-C26
3	A	902	POV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
3	B	904	POV	C31-C32-C33-C34
3	D	902	POV	C31-C32-C33-C34
3	E	902	POV	C31-C32-C33-C34
3	F	902	POV	C31-C32-C33-C34
3	C	904	POV	C31-C32-C33-C34
2	D	901	P5S	O19-C1-C2-C3
2	A	901	P5S	C23-C24-C25-C26
2	C	903	P5S	C41-C42-C43-C44
3	A	902	POV	C27-C28-C29-C210
3	B	904	POV	C27-C28-C29-C210
3	C	904	POV	C27-C28-C29-C210
3	D	902	POV	C27-C28-C29-C210
3	E	902	POV	C27-C28-C29-C210
3	F	902	POV	C27-C28-C29-C210
4	C	901	CLR	C17-C20-C22-C23
3	A	902	POV	O21-C21-C22-C23
3	D	902	POV	O21-C21-C22-C23
3	B	904	POV	O21-C21-C22-C23
3	C	904	POV	O21-C21-C22-C23
3	E	902	POV	O21-C21-C22-C23
3	F	902	POV	O21-C21-C22-C23
2	C	903	P5S	C23-C24-C25-C26
4	A	904	CLR	C23-C24-C25-C27
2	E	901	P5S	CA-CB-OG-P12
2	D	901	P5S	C45-C46-C48-C49
2	E	901	P5S	O-C-CA-CB
3	B	904	POV	O22-C21-C22-C23
3	A	902	POV	O22-C21-C22-C23
3	D	902	POV	O22-C21-C22-C23
3	E	902	POV	O22-C21-C22-C23
2	F	901	P5S	C42-C43-C44-C45
3	C	904	POV	O22-C21-C22-C23
3	F	902	POV	O22-C21-C22-C23
2	A	901	P5S	C45-C46-C48-C49
2	F	901	P5S	C23-C24-C25-C26
2	C	903	P5S	C24-C25-C26-C27

There are no ring outliers.

22 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	904	POV	2	0

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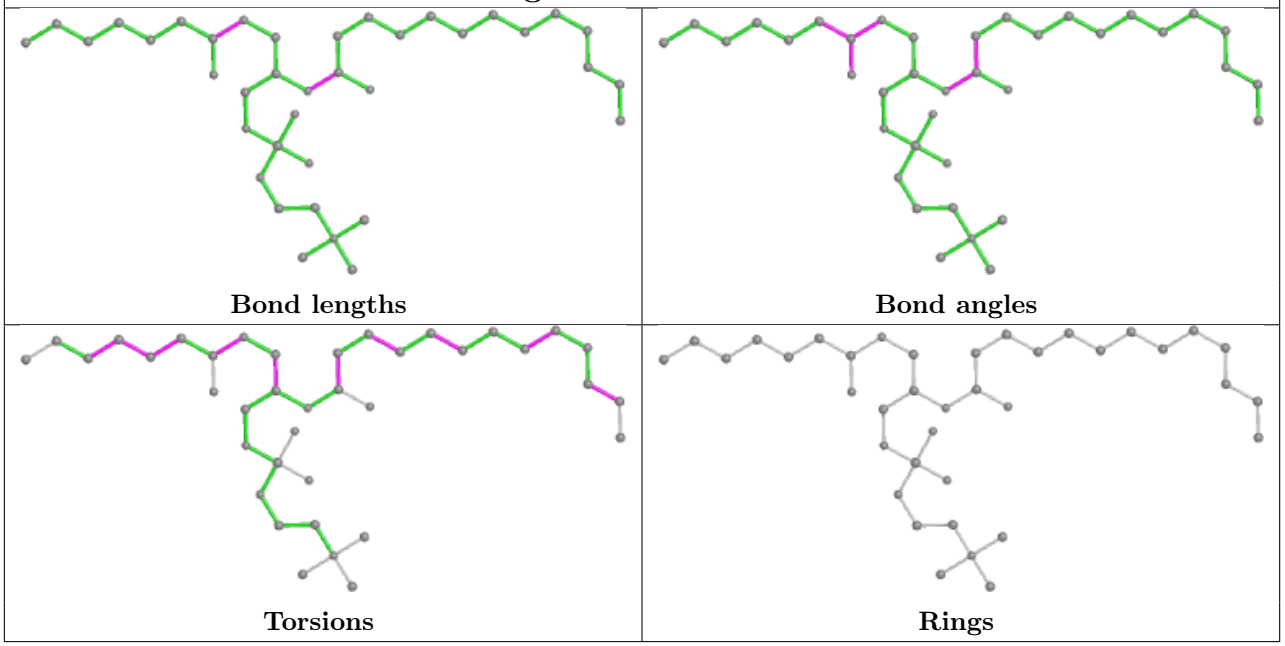
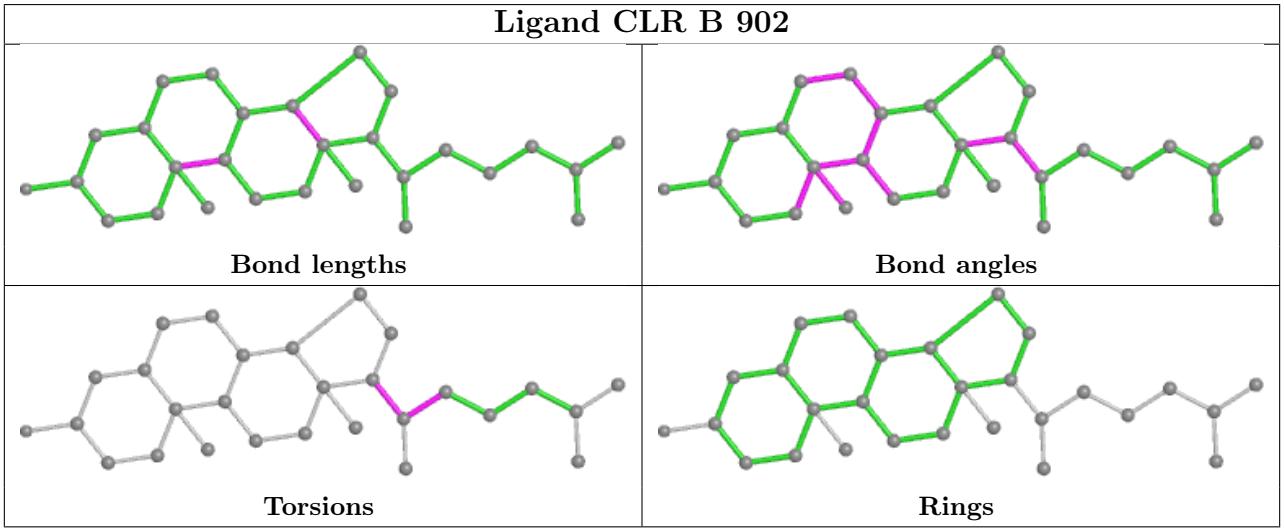
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	902	CLR	5	0
2	E	901	P5S	2	0
2	F	901	P5S	6	0
4	D	903	CLR	12	0
2	B	903	P5S	2	0
4	C	901	CLR	11	0
4	C	902	CLR	2	0
4	D	904	CLR	8	0
4	E	904	CLR	16	0
4	F	904	CLR	8	0
3	C	904	POV	1	0
4	A	904	CLR	2	0
4	E	903	CLR	10	0
4	F	903	CLR	9	0
2	C	903	P5S	4	0
3	F	902	POV	1	0
4	A	903	CLR	16	0
3	A	902	POV	5	0
4	B	901	CLR	9	0
2	A	901	P5S	1	0
2	D	901	P5S	3	0

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

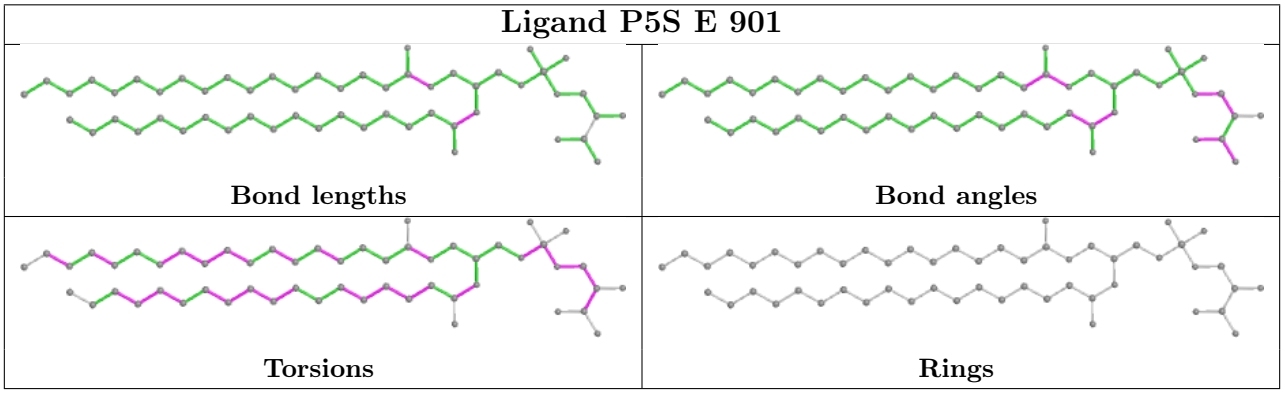
Ligand POV B 904



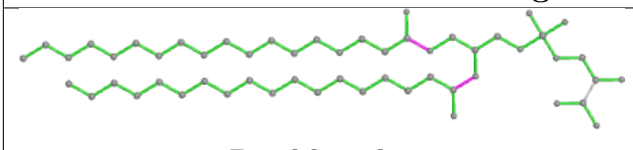
Ligand CLR B 902

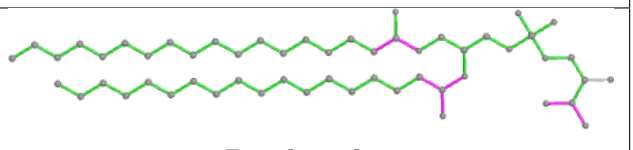


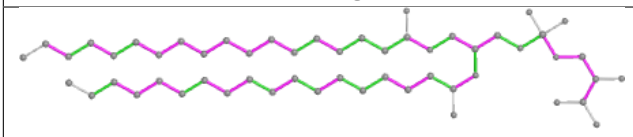
Ligand P5S E 901

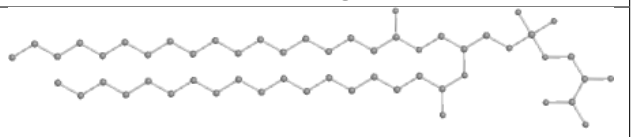


Ligand P5S F 901

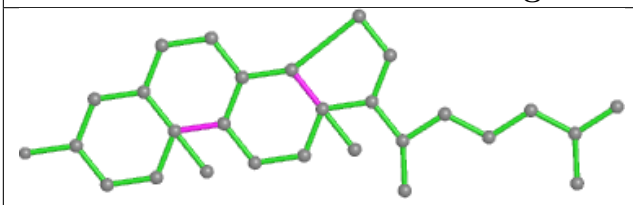

Bond lengths

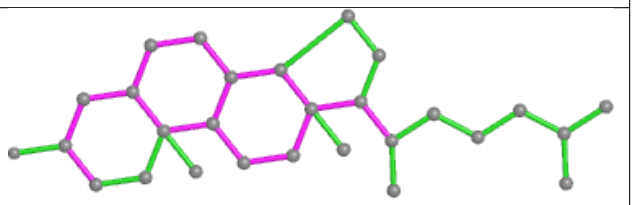

Bond angles

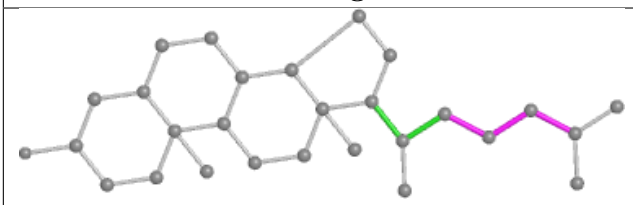

Torsions

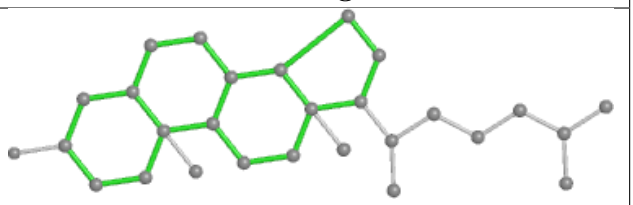

Rings

Ligand CLR D 903

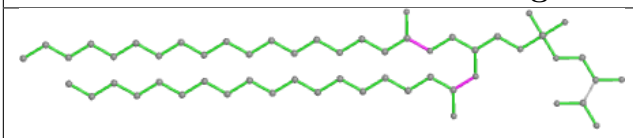

Bond lengths


Bond angles


Torsions


Rings

Ligand P5S B 903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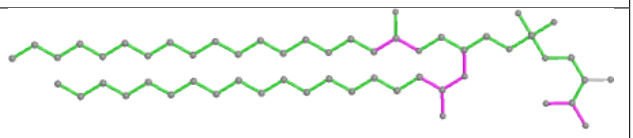
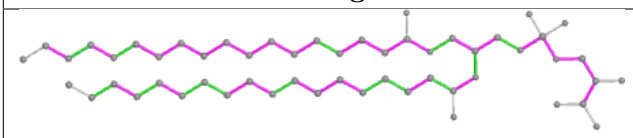
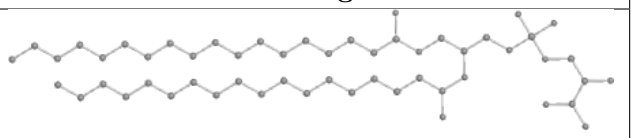
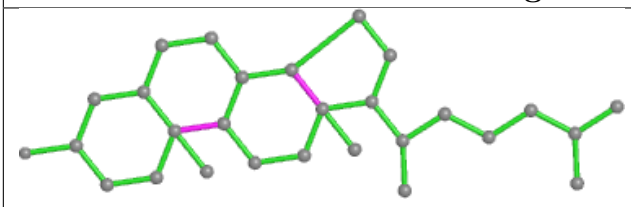

Bond angles

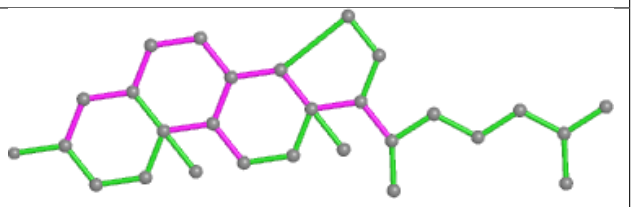

Torsions


Rings

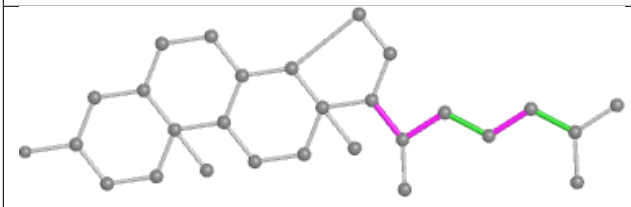
Ligand CLR C 901



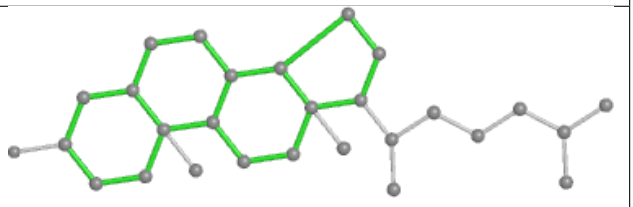
Bond lengths



Bond angles

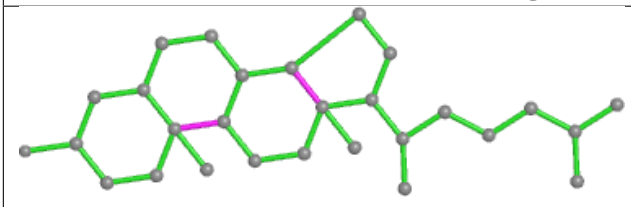


Torsions



Rings

Ligand CLR C 902



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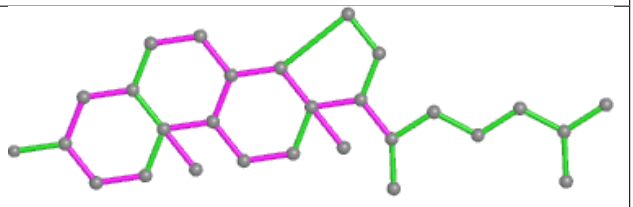
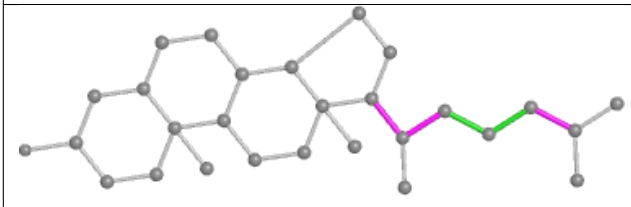
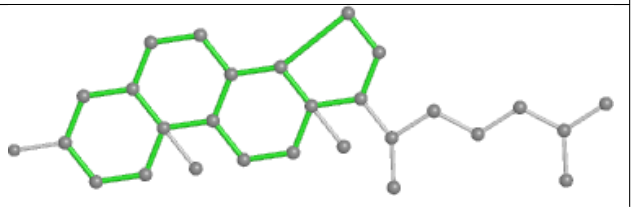


Bond angles

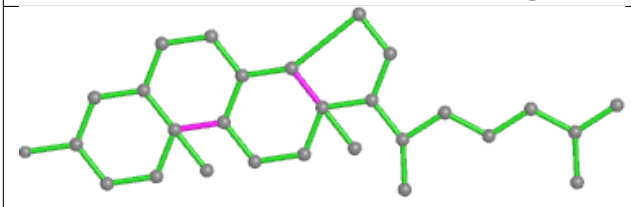


Torsions



Rings

Ligand CLR D 904



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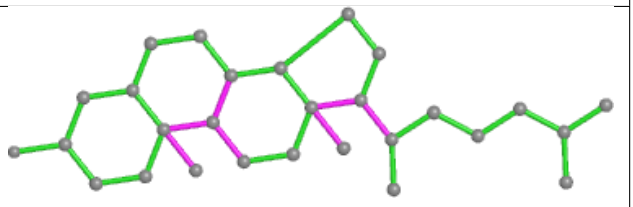
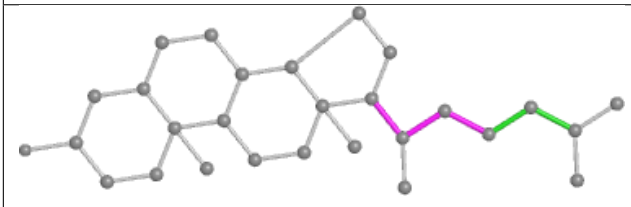


Bond angles



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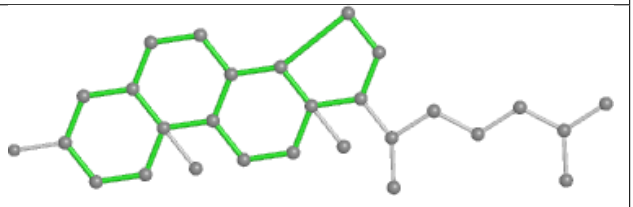
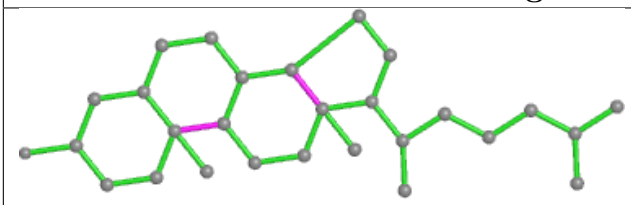


Rings

Ligand CLR E 904



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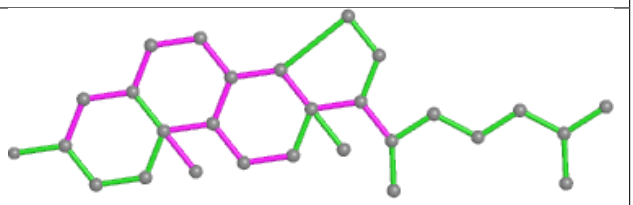

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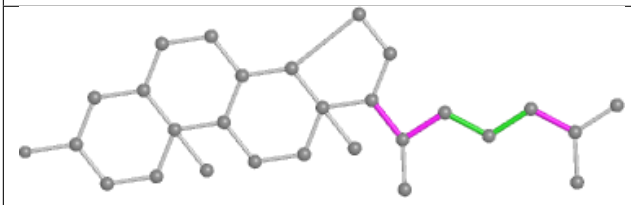

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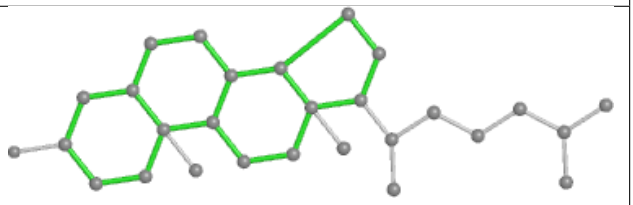
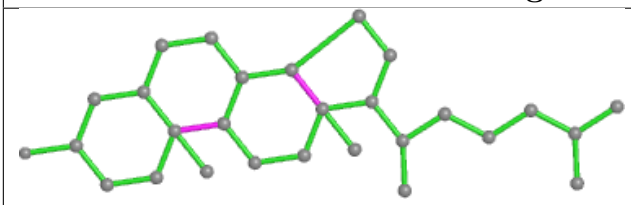
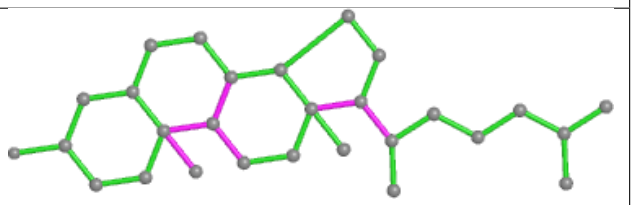


Rings

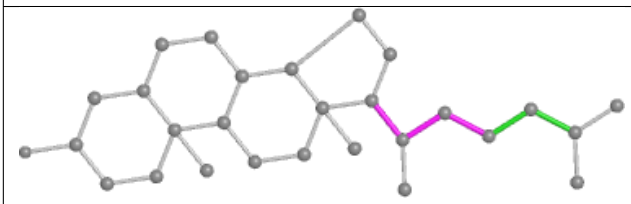
Ligand CLR F 904



Bond lengths



Bond angles



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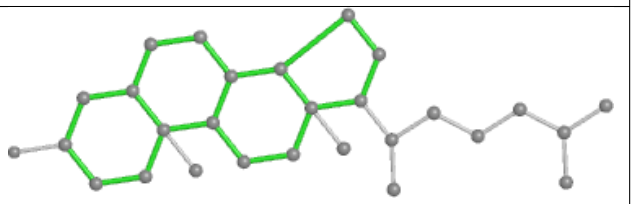
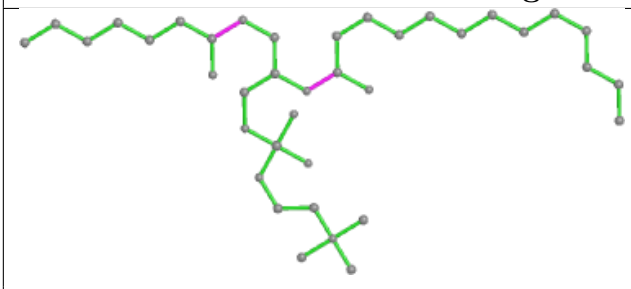
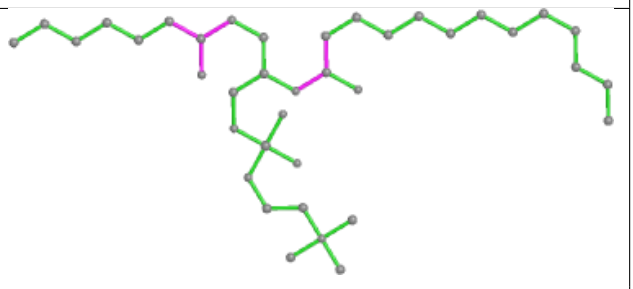


Rings

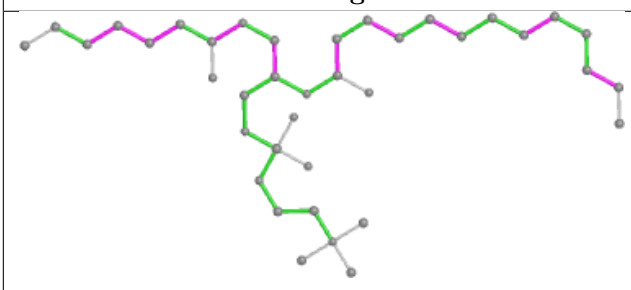
Ligand POV C 904



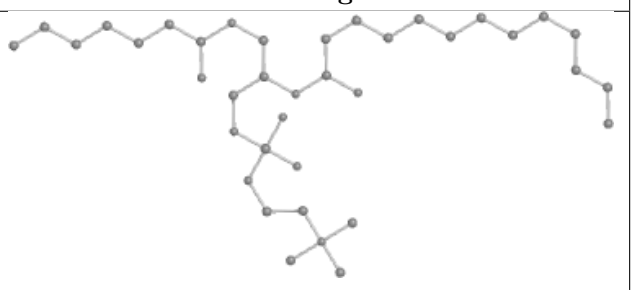
Bond lengths



Bond angles

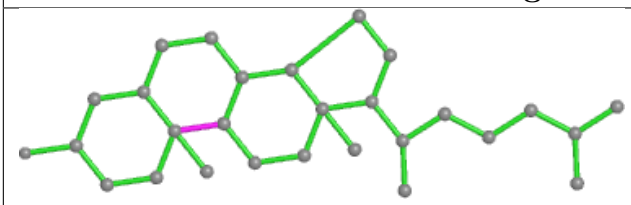


Torsions

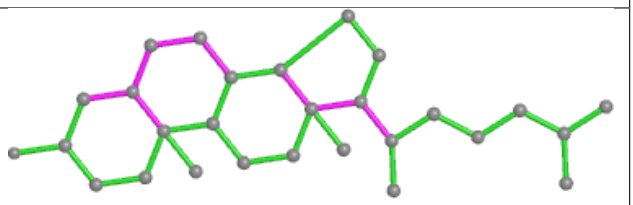


Rings

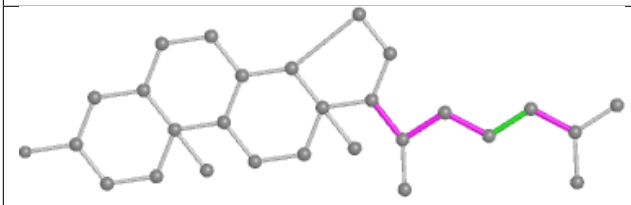
Ligand CLR A 904



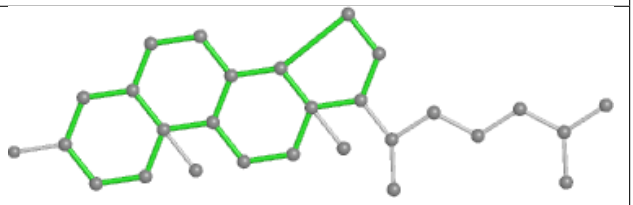
Bond lengths



Bond angles

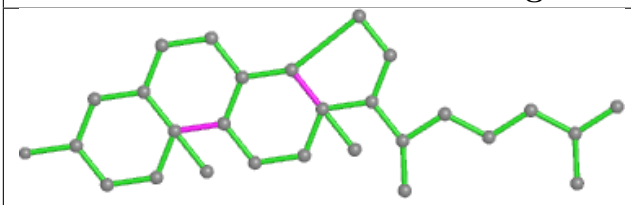


Torsions

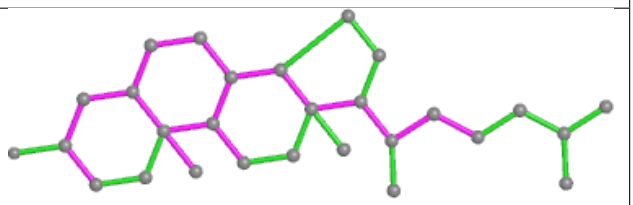


Rings

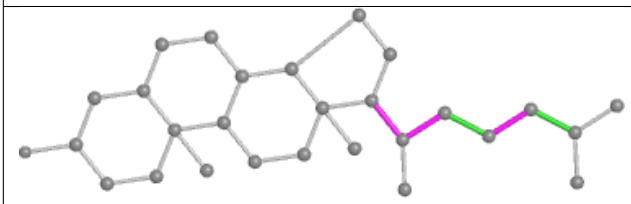
Ligand CLR E 903



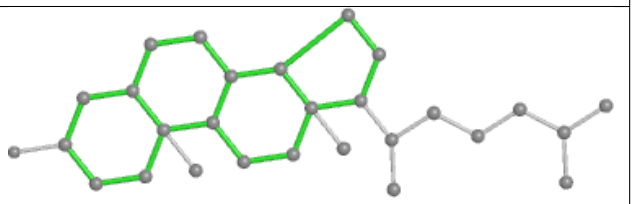
Bond lengths



Bond angles

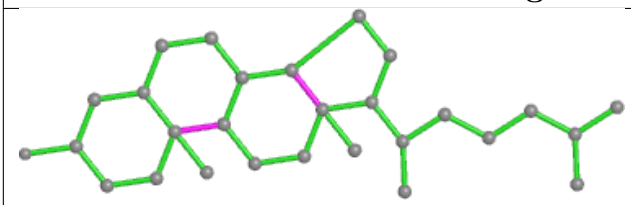


Torsions

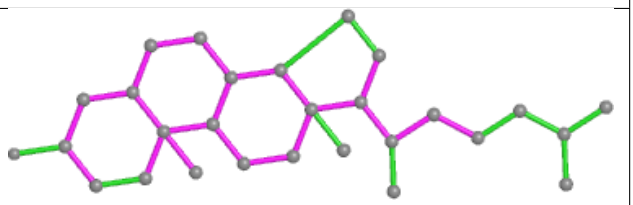


Rings

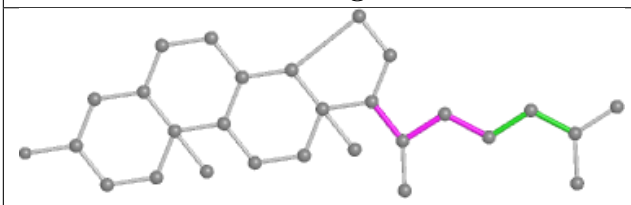
Ligand CLR F 903



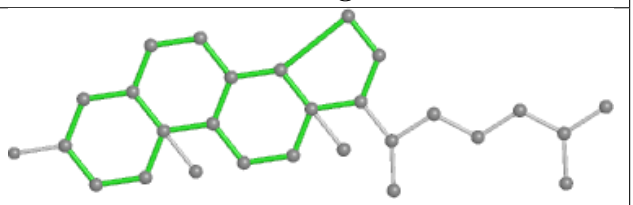
Bond lengths



Bond angles

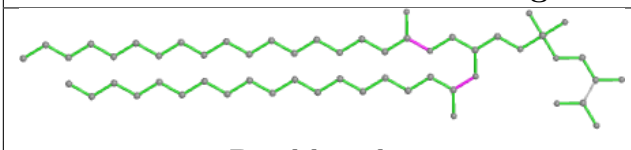


Torsions

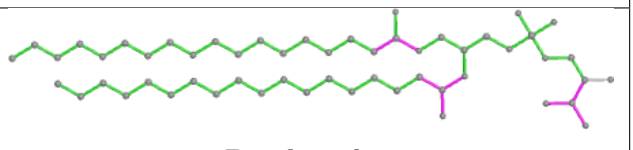


Rings

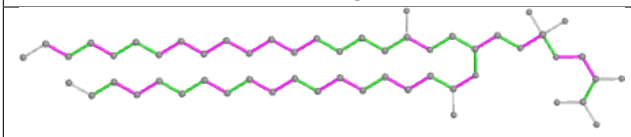
Ligand P5S C 903



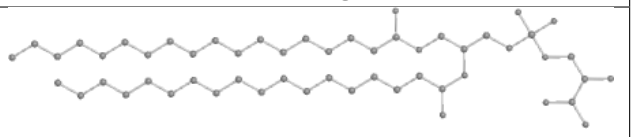
Bond lengths



Bond angles

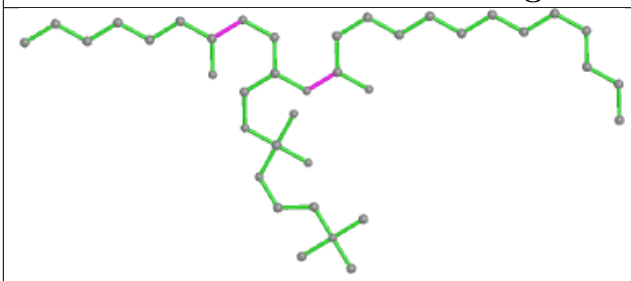


Torsions

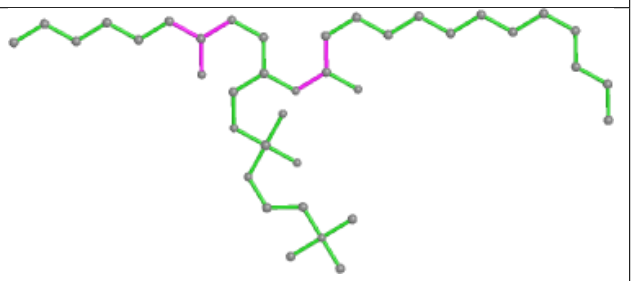


Rings

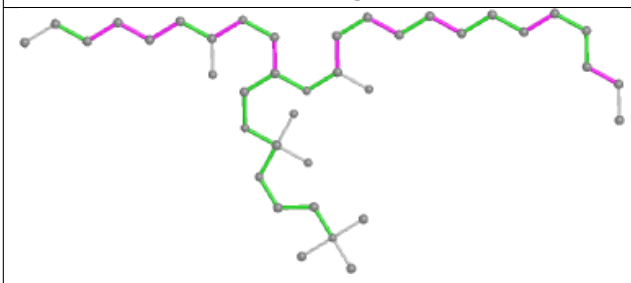
Ligand POV F 902



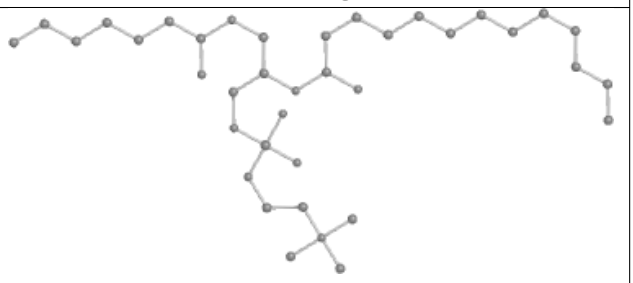
Bond lengths



Bond angles

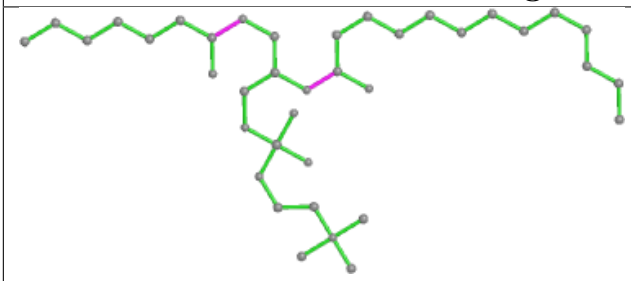


Torsions

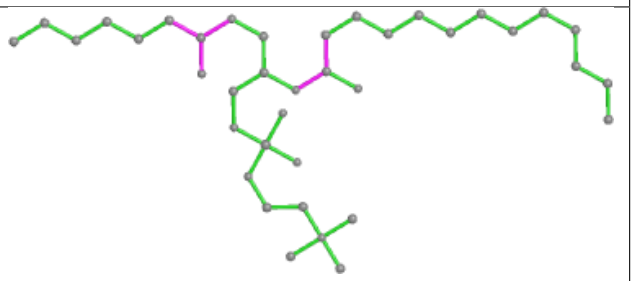


Rings

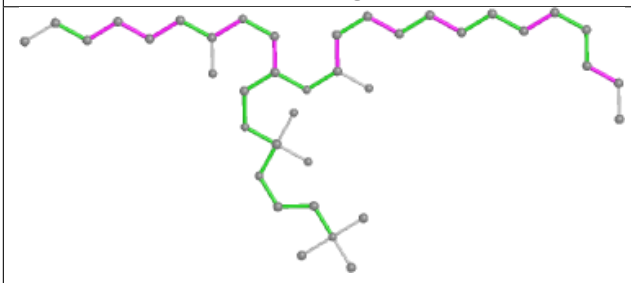
Ligand POV E 902



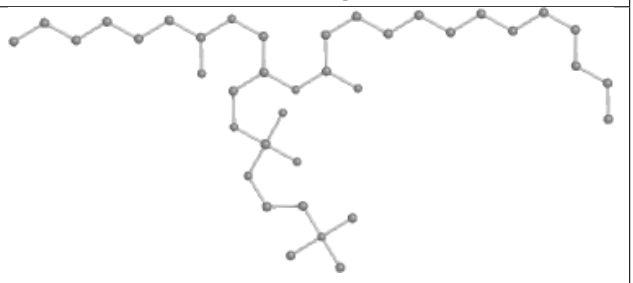
Bond lengths



Bond angles

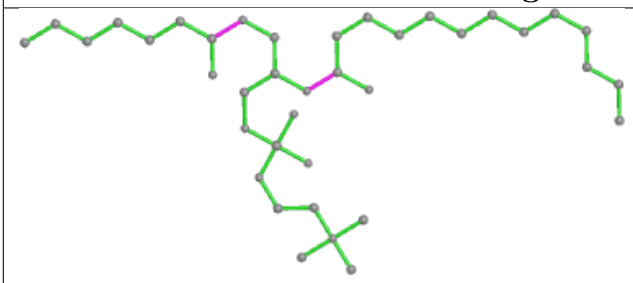


Torsions

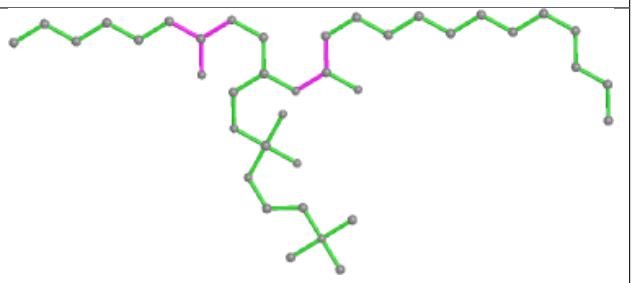


Rings

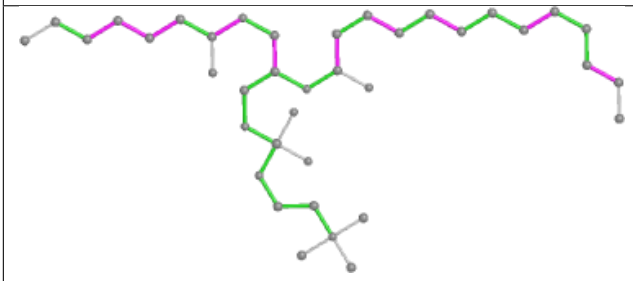
Ligand POV D 902



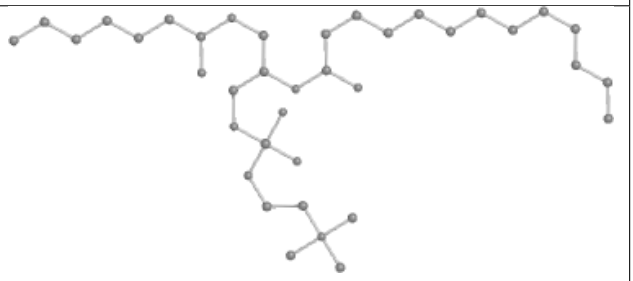
Bond lengths



Bond angles

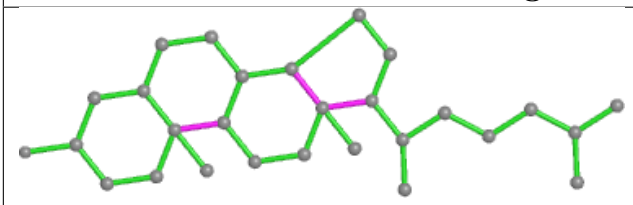


Torsions

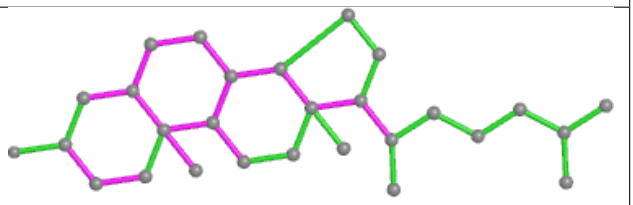


Rings

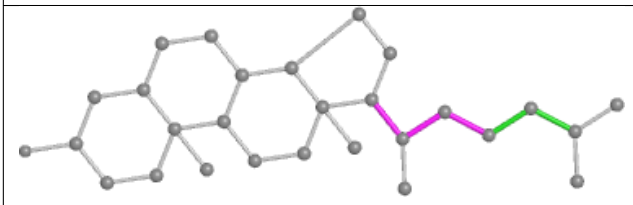
Ligand CLR A 903



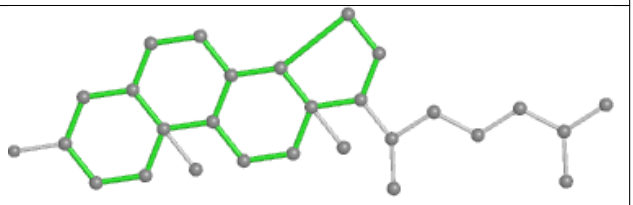
Bond lengths



Bond angles

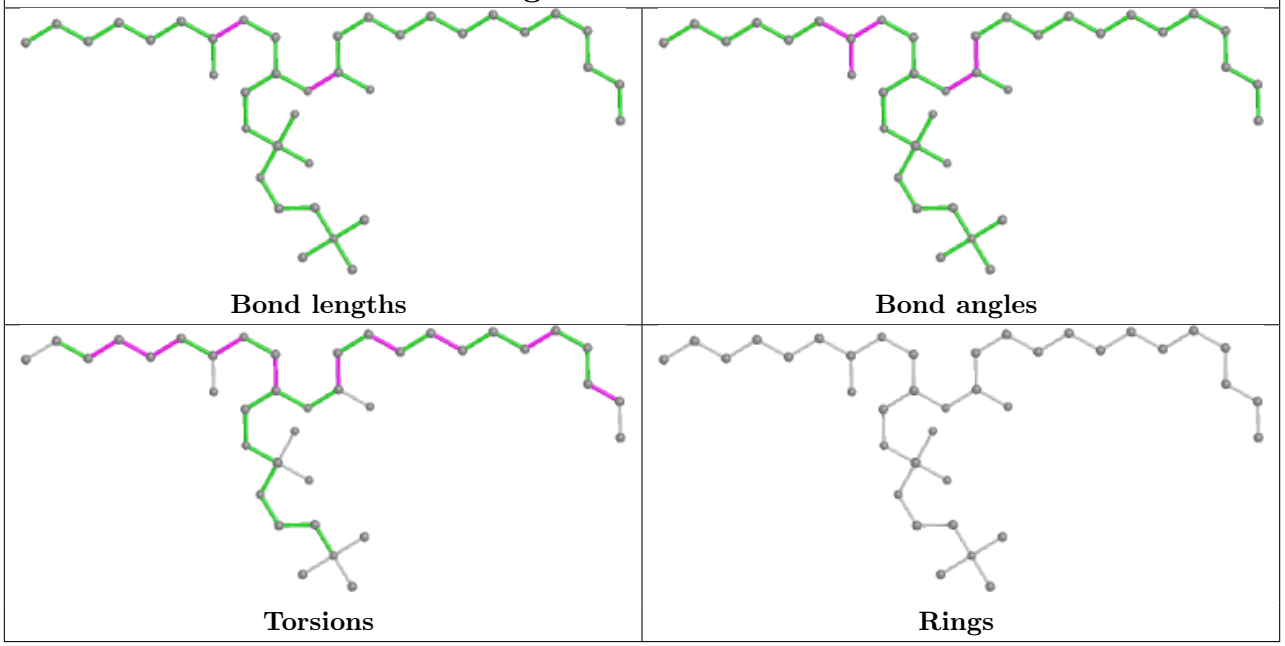


Torsions

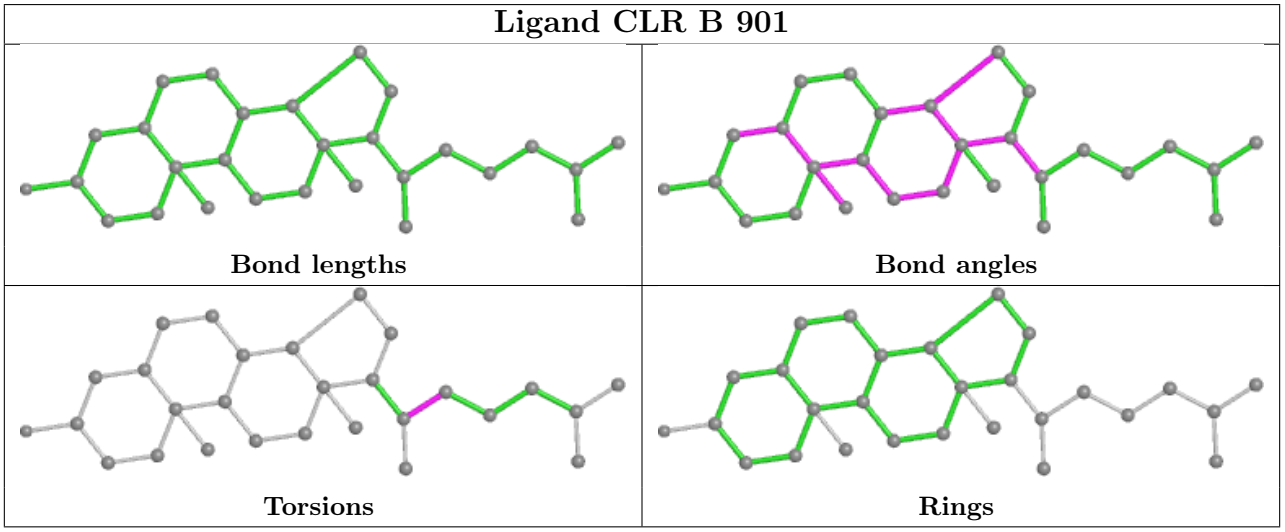


Rings

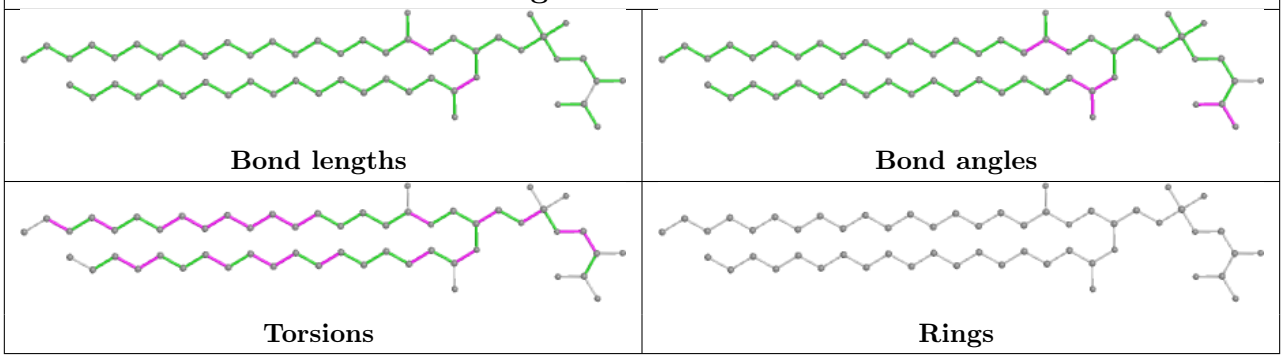
Ligand POV A 902



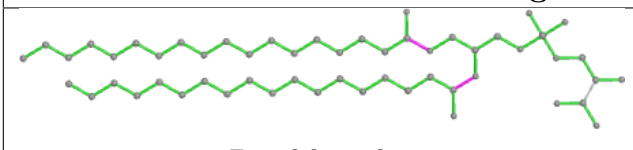
Ligand CLR B 901



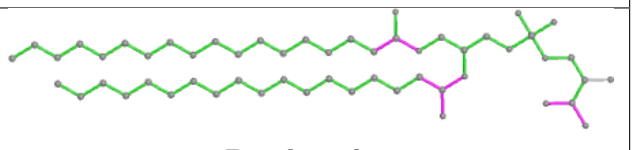
Ligand P5S A 901



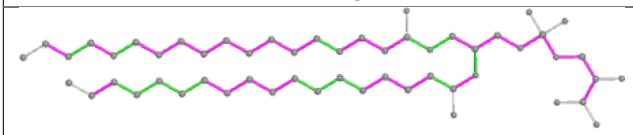
Ligand P5S D 901



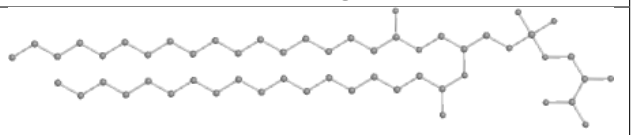
Bond lengths



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.

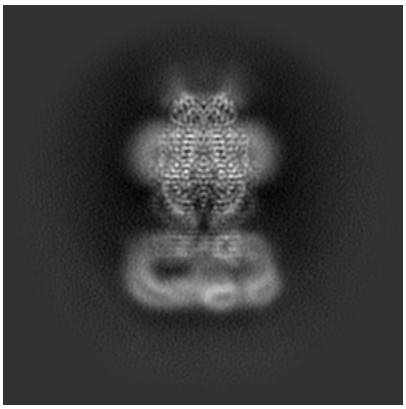
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33527. These allow visual inspection of the internal detail of the map and identification of artifacts.

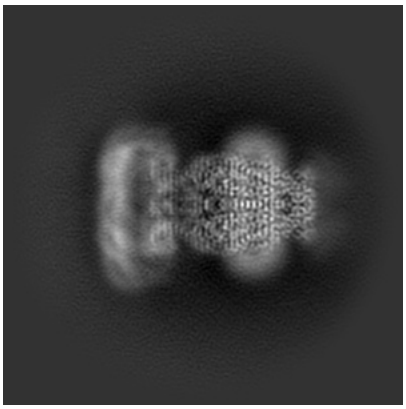
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

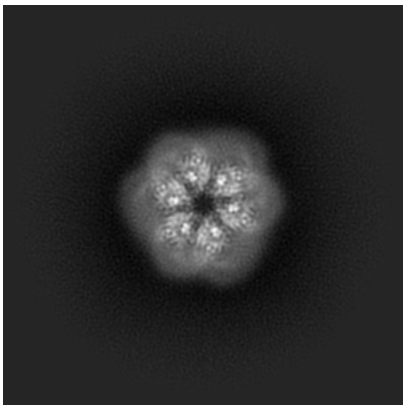
6.1.1 Primary map



X

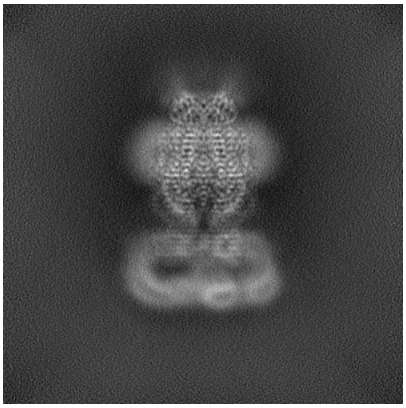


Y

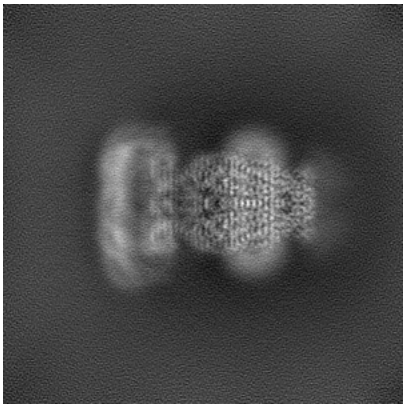


Z

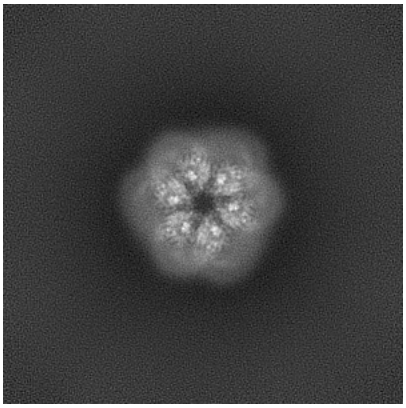
6.1.2 Raw map



X



Y

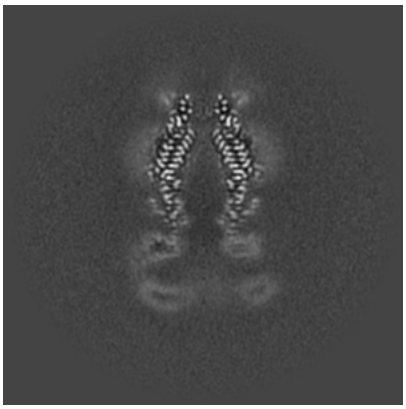


Z

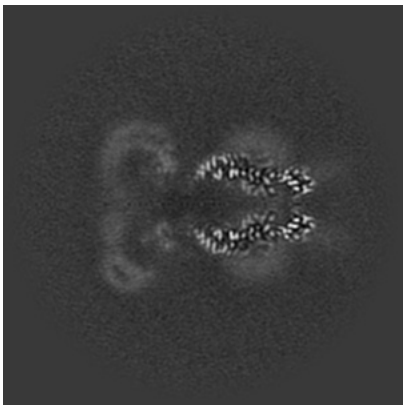
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

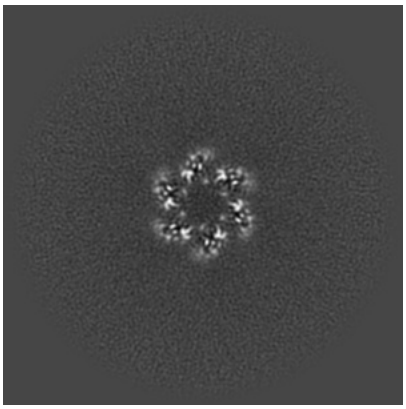
6.2.1 Primary map



X Index: 150

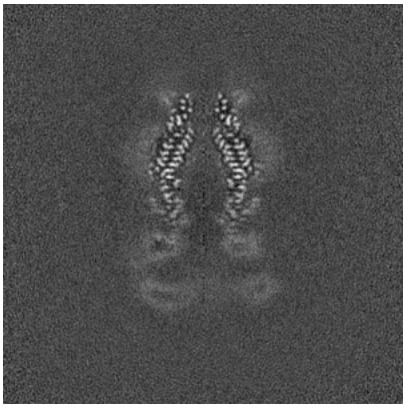


Y Index: 150

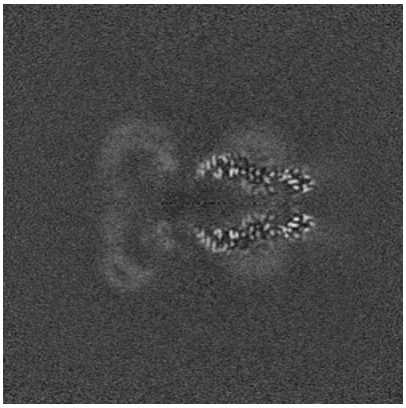


Z Index: 150

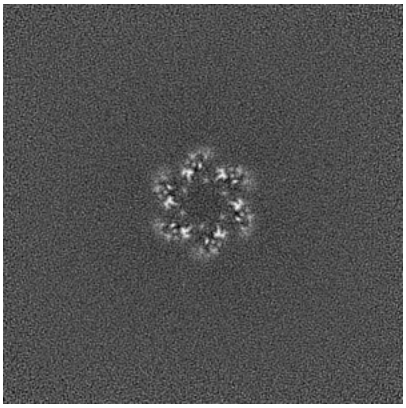
6.2.2 Raw map



X Index: 150



Y Index: 150

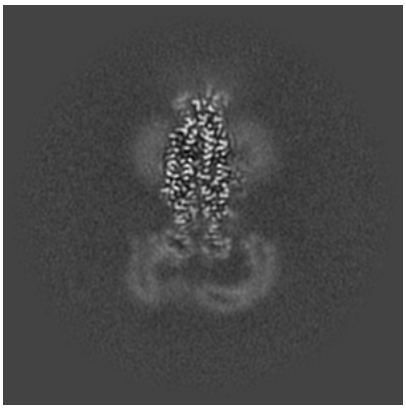


Z Index: 150

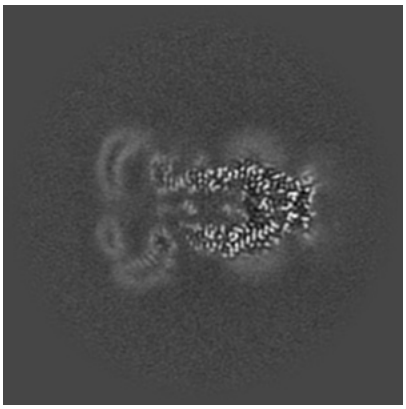
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

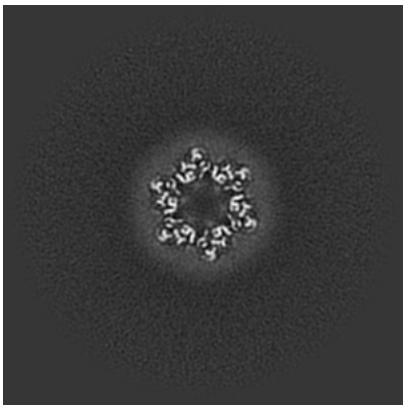
6.3.1 Primary map



X Index: 129

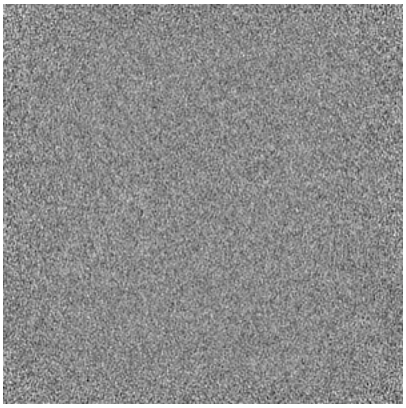


Y Index: 164

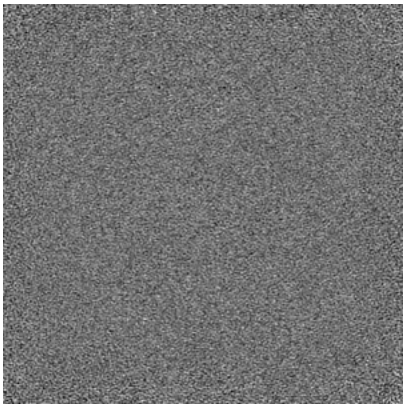


Z Index: 171

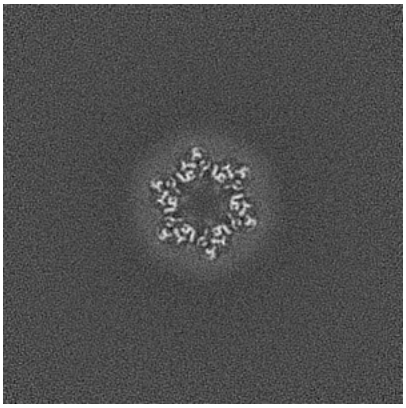
6.3.2 Raw map



X Index: 0



Y Index: 0

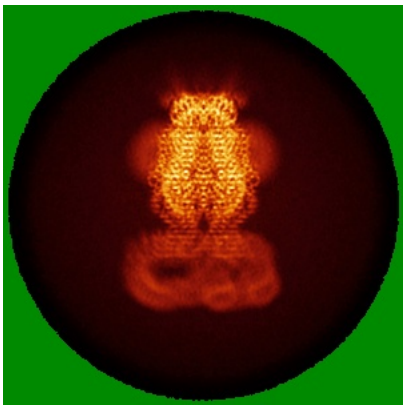


Z Index: 171

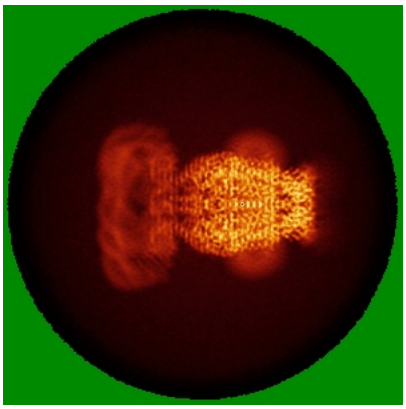
The images above show the largest variance slices of the map in three orthogonal directions.

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

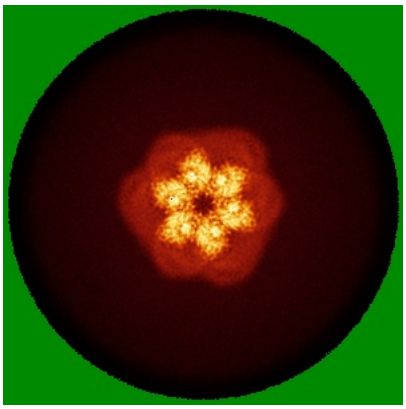
6.4.1 Primary map



X

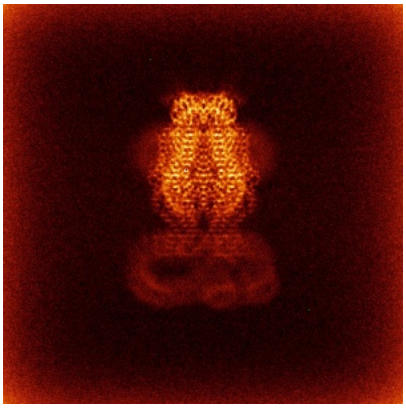


Y

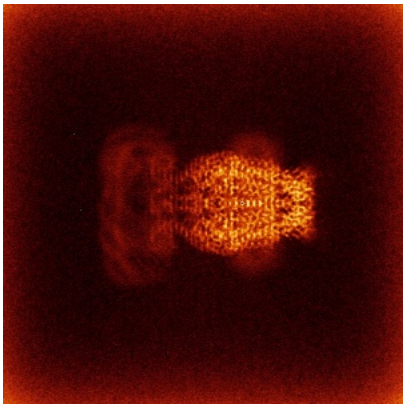


Z

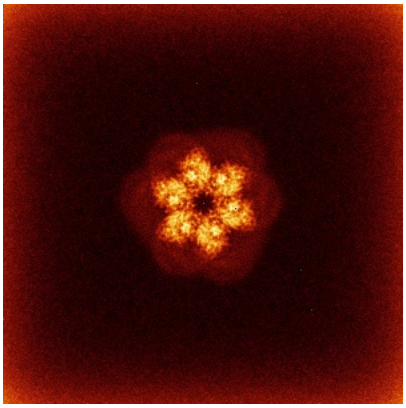
6.4.2 Raw map



X



Y

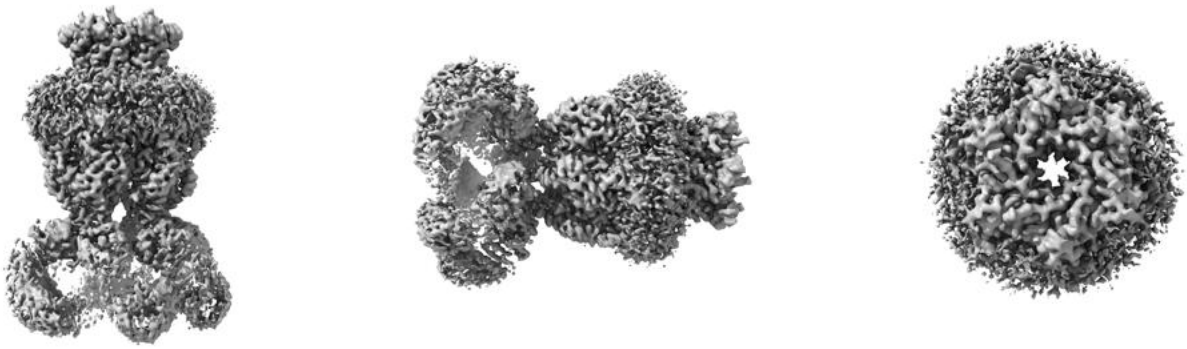


Z

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)

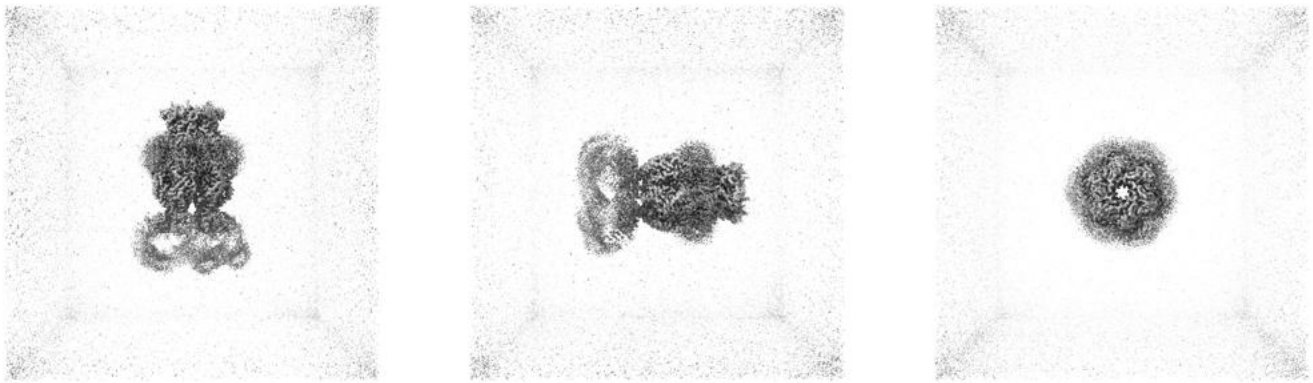
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

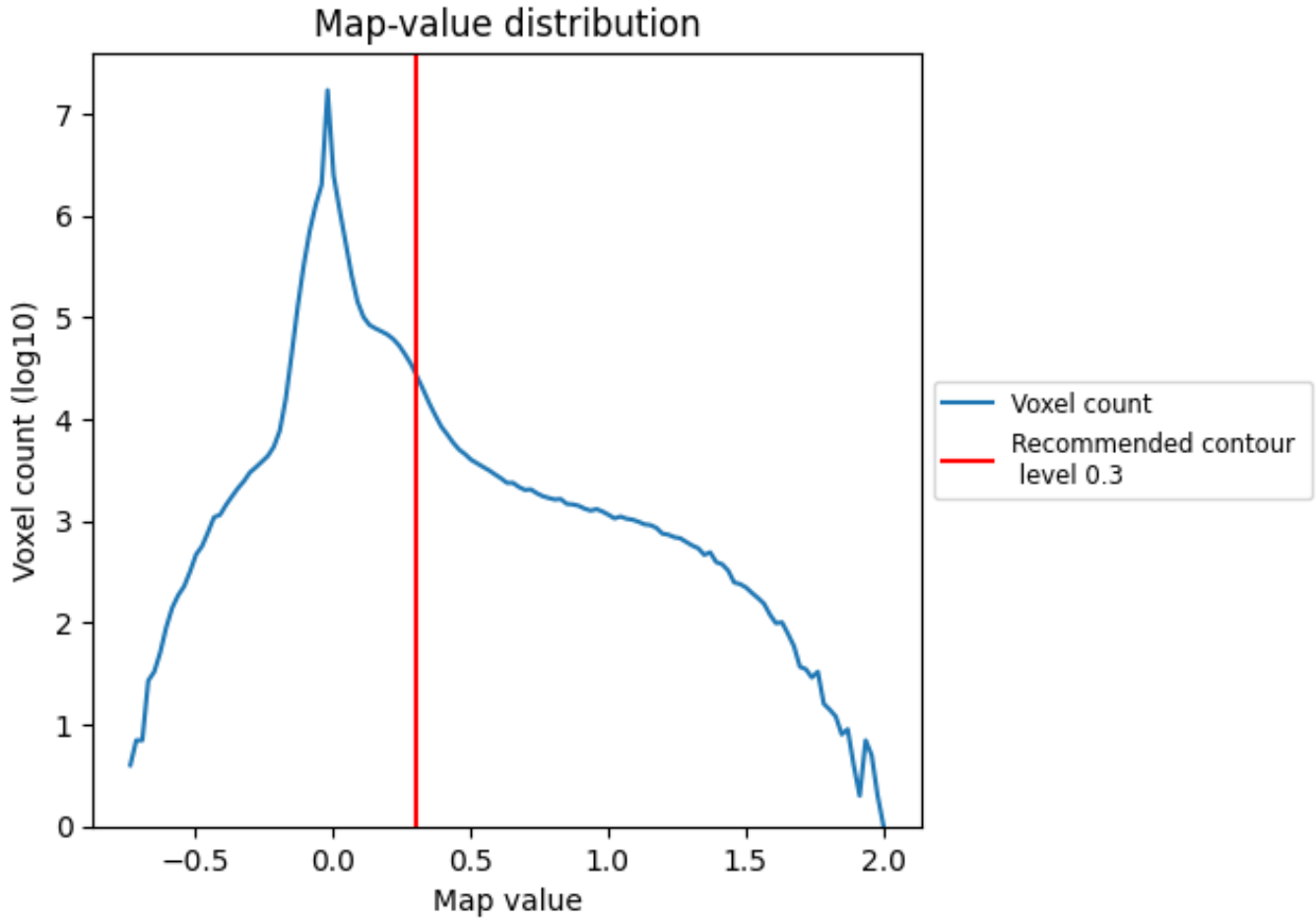
6.6 Mask visualisation (i)

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

7 Map analysis

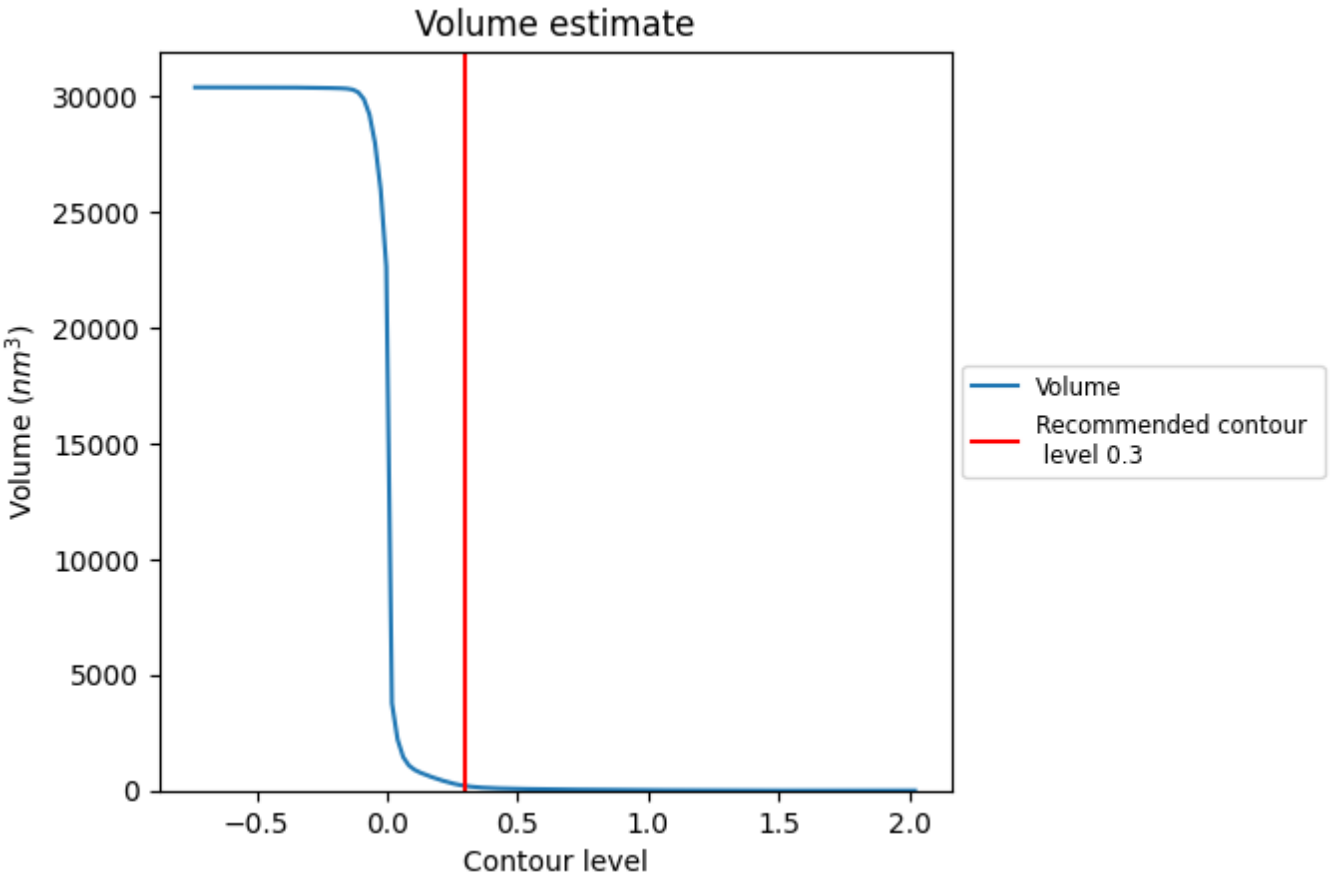
This section contains the results of statistical analysis of the map.

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.

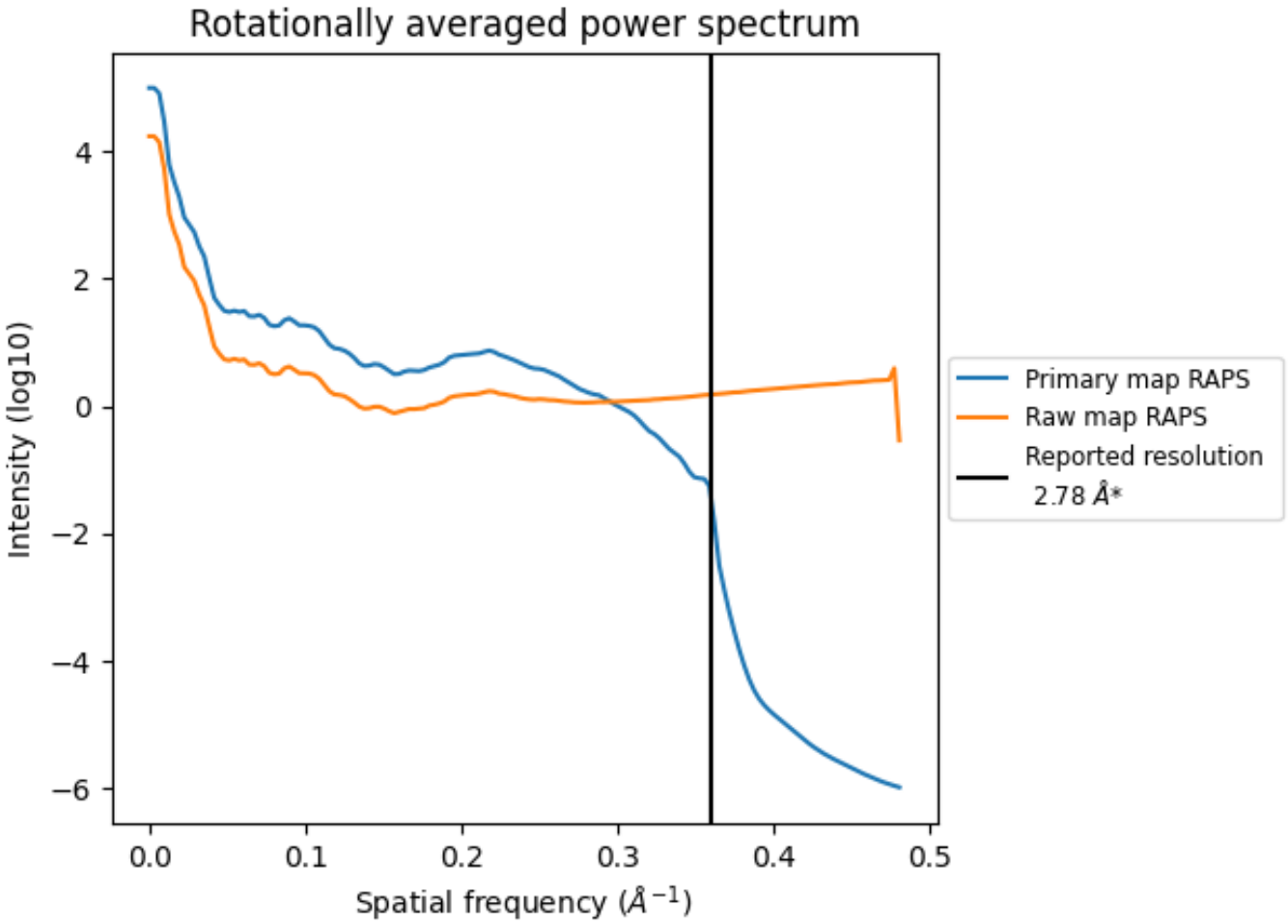
7.2 Volume estimate



The volume at the recommended contour level is 201 nm^3; this corresponds to an approximate mass of 182 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)

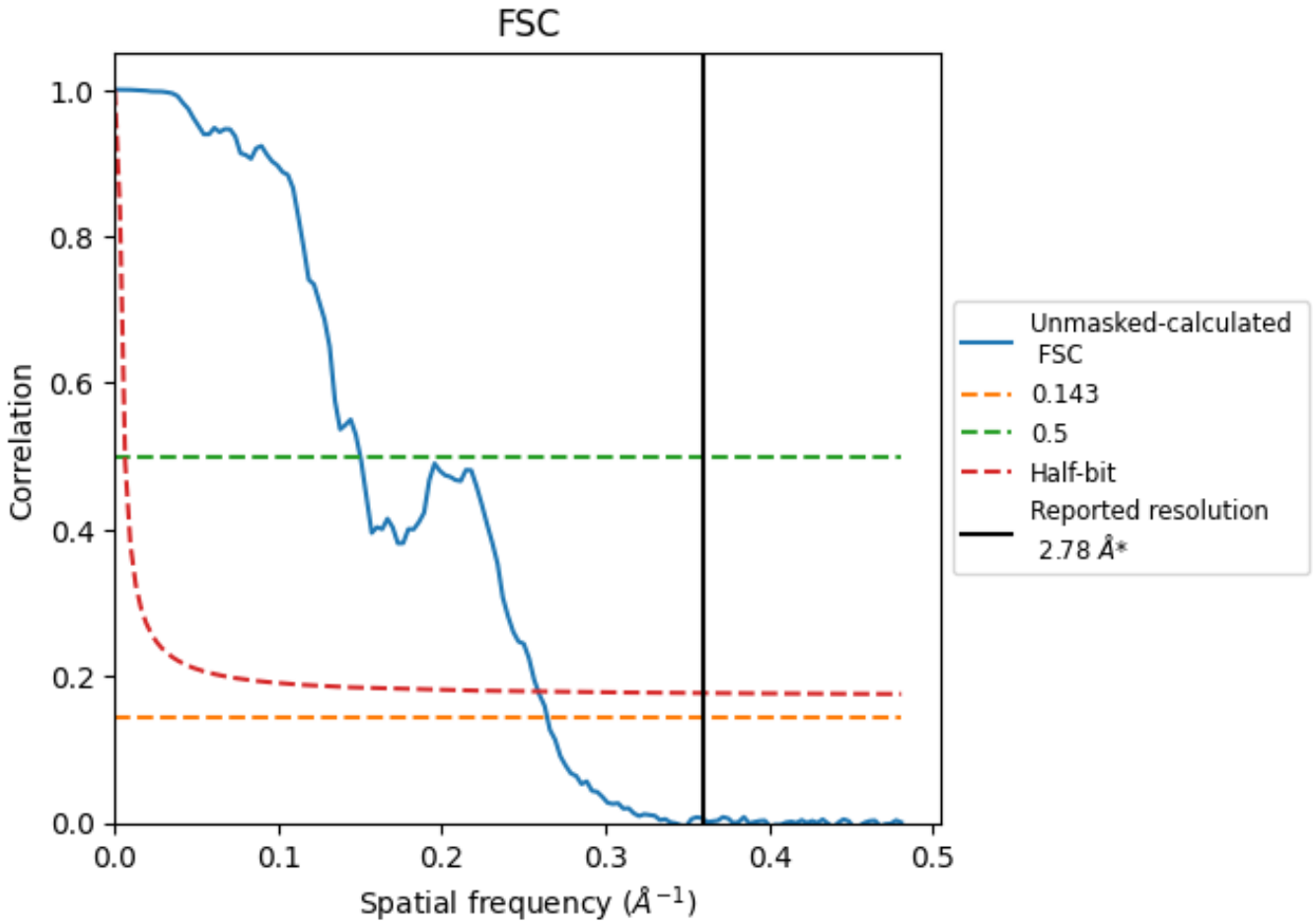


*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

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 0.360 $Å^{-1}$

8.2 Resolution estimates (i)

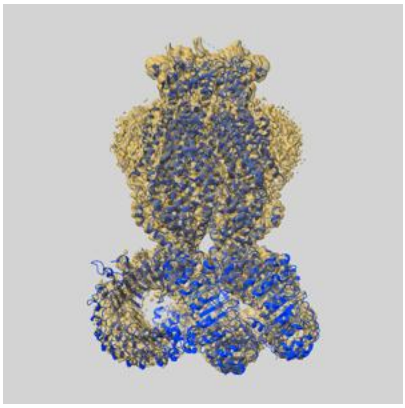
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	6.66	3.86

*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 3.78 differs from the reported value 2.78 by more than 10 %

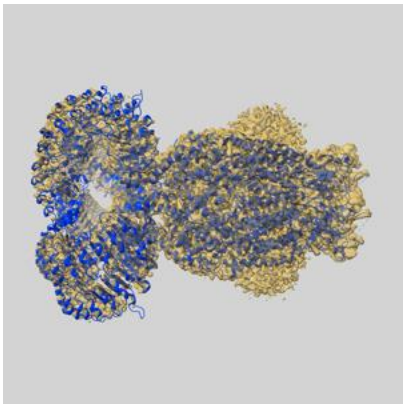
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33527 and PDB model 7XZH. Per-residue inclusion information can be found in section 3 on page 7.

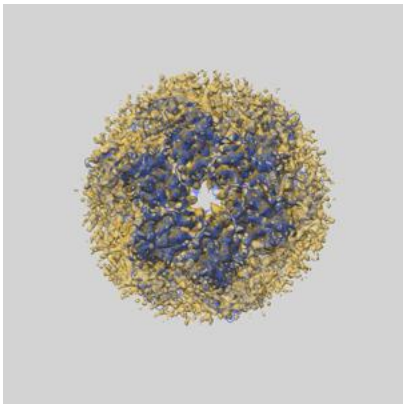
9.1 Map-model overlay



X



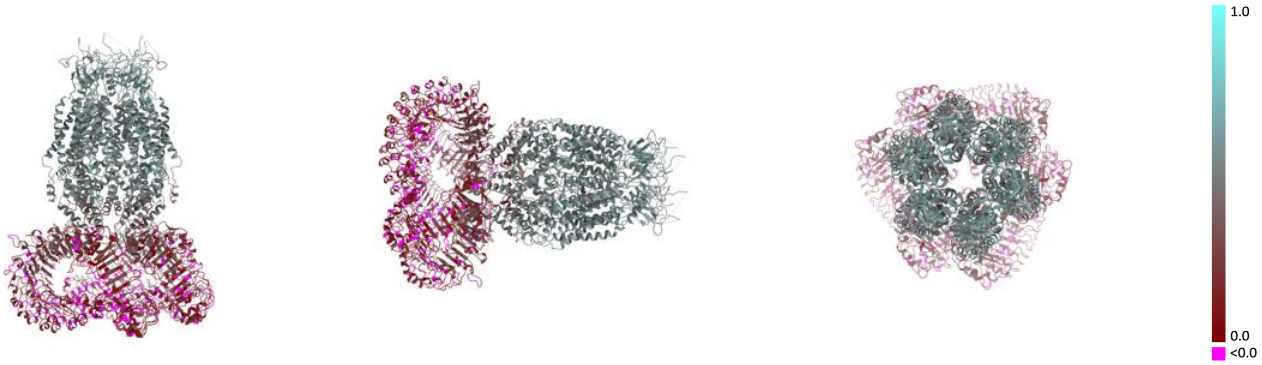
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

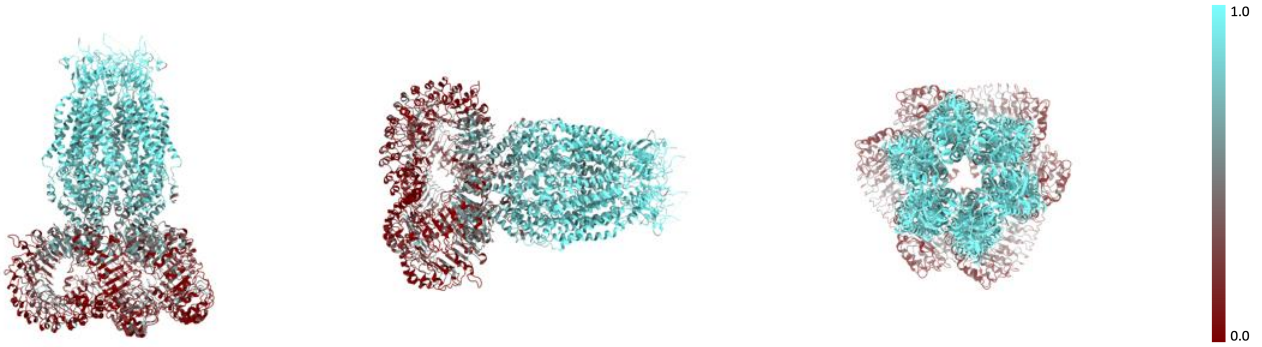
9.2 Q-score mapped to coordinate model (i)



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.

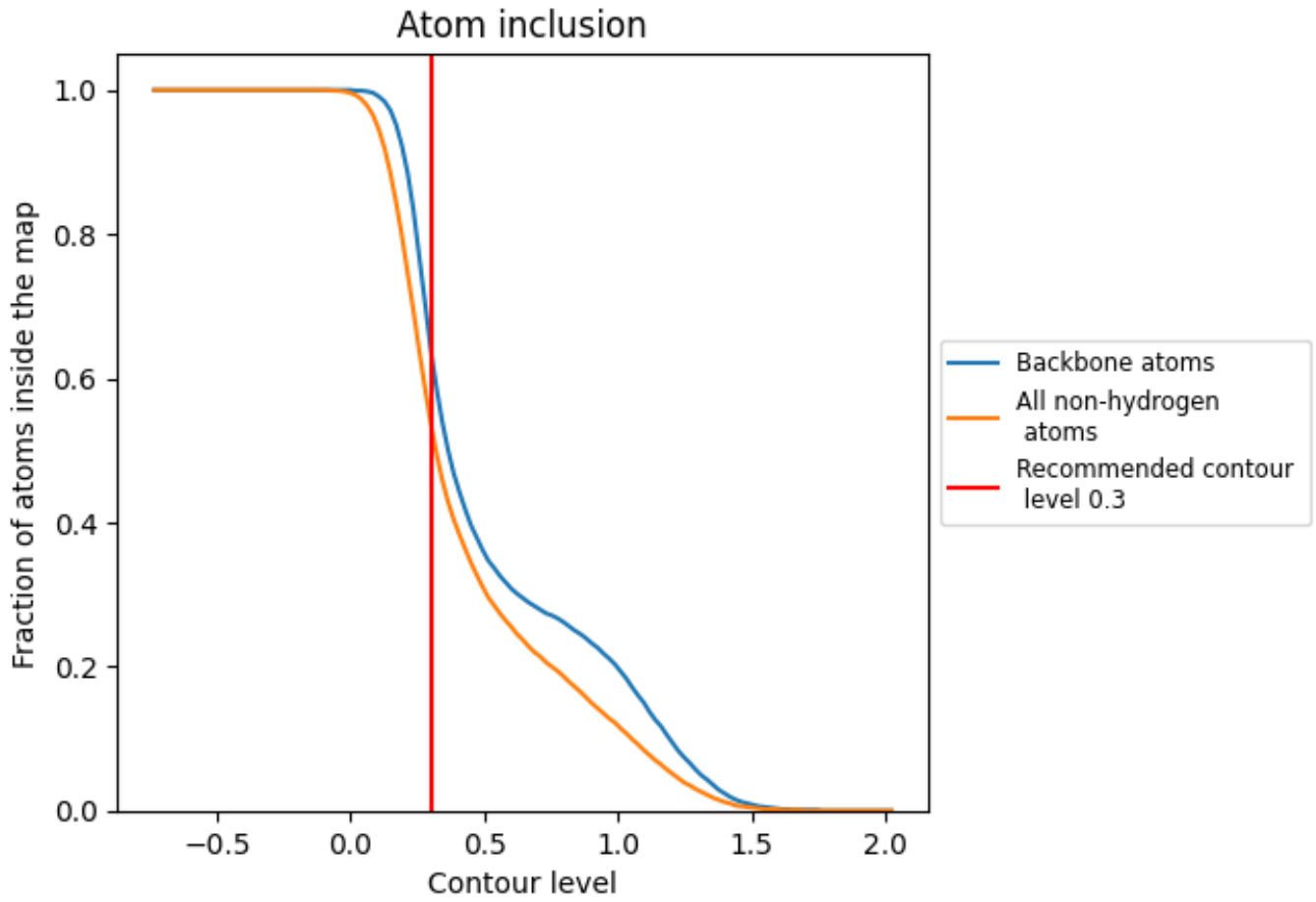
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 54% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5360	0.3220
A	0.5300	0.3100
B	0.5420	0.3360
C	0.5330	0.3110
D	0.5380	0.3310
E	0.5320	0.3140
F	0.5410	0.3320