



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 02:17 AM UTC

PDB ID : 9OLX / pdb_00009olx
EMDB ID : EMD-70601
Title : Structure of a constitutively open human TRPC3 mutant in the inhibited state
Authors : Bell, B.; Baker, M.L.; Cordero-Morales, J.F.
Deposited on : 2025-05-13
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

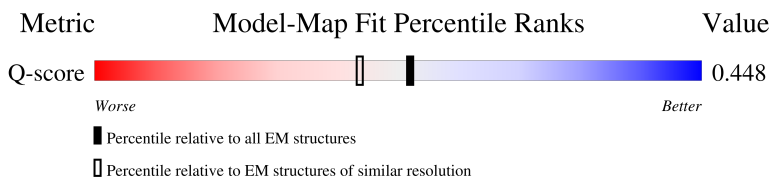
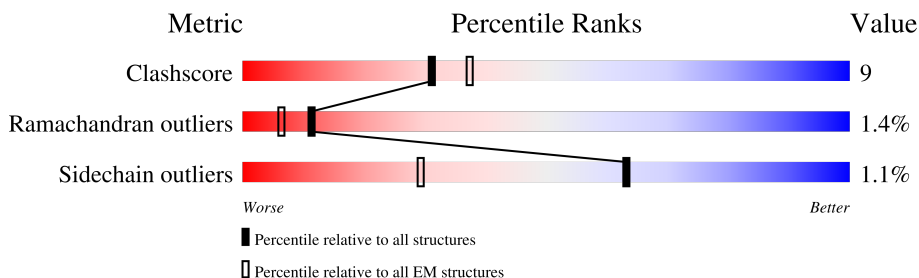
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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


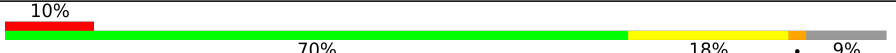
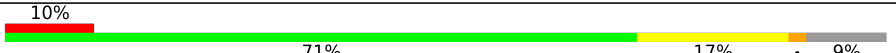
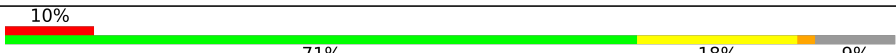
The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 $\leq 5\%$. 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	820	
1	B	820	
1	C	820	
1	D	820	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNL	A	903	-	-	X	-
2	UNL	B	902	-	-	X	-
2	UNL	B	903	-	-	X	-
2	UNL	C	902	-	-	X	-
2	UNL	C	903	-	-	X	-
2	UNL	D	901	-	-	X	-
2	UNL	D	904	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24592 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	745	Total	C	N	O	S	0	0
			5990	3890	970	1097	33		
1	B	745	Total	C	N	O	S	0	0
			5990	3890	970	1097	33		
1	C	745	Total	C	N	O	S	0	0
			5990	3890	970	1097	33		
1	D	745	Total	C	N	O	S	0	0
			5990	3890	970	1097	33		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	ALA	THR	engineered mutation	UNP Q13507
A	?	-	LEU	deletion	UNP Q13507
A	?	-	ASN	deletion	UNP Q13507
A	?	-	LEU	deletion	UNP Q13507
A	?	-	PHE	deletion	UNP Q13507
A	?	-	THR	deletion	UNP Q13507
A	?	-	GLN	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	ASN	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	ARG	deletion	UNP Q13507
A	?	-	VAL	deletion	UNP Q13507
A	?	-	PHE	deletion	UNP Q13507
A	?	-	GLU	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	HIS	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	PHE	deletion	UNP Q13507
A	?	-	ASN	deletion	UNP Q13507
A	?	-	SER	deletion	UNP Q13507
A	?	-	ILE	deletion	UNP Q13507
A	?	-	LEU	deletion	UNP Q13507

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP Q13507
A	?	-	GLN	deletion	UNP Q13507
A	?	-	PRO	deletion	UNP Q13507
A	?	-	THR	deletion	UNP Q13507
A	?	-	ARG	deletion	UNP Q13507
A	?	-	TYR	deletion	UNP Q13507
A	?	-	GLN	deletion	UNP Q13507
A	839	ILE	-	expression tag	UNP Q13507
A	840	SER	-	expression tag	UNP Q13507
A	841	SER	-	expression tag	UNP Q13507
A	842	LEU	-	expression tag	UNP Q13507
A	843	ARG	-	expression tag	UNP Q13507
A	844	TYR	-	expression tag	UNP Q13507
A	845	GLU	-	expression tag	UNP Q13507
A	846	LEU	-	expression tag	UNP Q13507
A	847	LEU	-	expression tag	UNP Q13507
A	848	GLU	-	expression tag	UNP Q13507
B	573	ALA	THR	engineered mutation	UNP Q13507
B	?	-	LEU	deletion	UNP Q13507
B	?	-	ASN	deletion	UNP Q13507
B	?	-	LEU	deletion	UNP Q13507
B	?	-	PHE	deletion	UNP Q13507
B	?	-	THR	deletion	UNP Q13507
B	?	-	GLN	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	ASN	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	ARG	deletion	UNP Q13507
B	?	-	VAL	deletion	UNP Q13507
B	?	-	PHE	deletion	UNP Q13507
B	?	-	GLU	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	HIS	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	PHE	deletion	UNP Q13507
B	?	-	ASN	deletion	UNP Q13507
B	?	-	SER	deletion	UNP Q13507
B	?	-	ILE	deletion	UNP Q13507
B	?	-	LEU	deletion	UNP Q13507
B	?	-	ASN	deletion	UNP Q13507
B	?	-	GLN	deletion	UNP Q13507
B	?	-	PRO	deletion	UNP Q13507

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q13507
B	?	-	ARG	deletion	UNP Q13507
B	?	-	TYR	deletion	UNP Q13507
B	?	-	GLN	deletion	UNP Q13507
B	839	ILE	-	expression tag	UNP Q13507
B	840	SER	-	expression tag	UNP Q13507
B	841	SER	-	expression tag	UNP Q13507
B	842	LEU	-	expression tag	UNP Q13507
B	843	ARG	-	expression tag	UNP Q13507
B	844	TYR	-	expression tag	UNP Q13507
B	845	GLU	-	expression tag	UNP Q13507
B	846	LEU	-	expression tag	UNP Q13507
B	847	LEU	-	expression tag	UNP Q13507
B	848	GLU	-	expression tag	UNP Q13507
C	573	ALA	THR	engineered mutation	UNP Q13507
C	?	-	LEU	deletion	UNP Q13507
C	?	-	ASN	deletion	UNP Q13507
C	?	-	LEU	deletion	UNP Q13507
C	?	-	PHE	deletion	UNP Q13507
C	?	-	THR	deletion	UNP Q13507
C	?	-	GLN	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	ASN	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	ARG	deletion	UNP Q13507
C	?	-	VAL	deletion	UNP Q13507
C	?	-	PHE	deletion	UNP Q13507
C	?	-	GLU	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	HIS	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	PHE	deletion	UNP Q13507
C	?	-	ASN	deletion	UNP Q13507
C	?	-	SER	deletion	UNP Q13507
C	?	-	ILE	deletion	UNP Q13507
C	?	-	LEU	deletion	UNP Q13507
C	?	-	ASN	deletion	UNP Q13507
C	?	-	GLN	deletion	UNP Q13507
C	?	-	PRO	deletion	UNP Q13507
C	?	-	THR	deletion	UNP Q13507
C	?	-	ARG	deletion	UNP Q13507
C	?	-	TYR	deletion	UNP Q13507

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLN	deletion	UNP Q13507
C	839	ILE	-	expression tag	UNP Q13507
C	840	SER	-	expression tag	UNP Q13507
C	841	SER	-	expression tag	UNP Q13507
C	842	LEU	-	expression tag	UNP Q13507
C	843	ARG	-	expression tag	UNP Q13507
C	844	TYR	-	expression tag	UNP Q13507
C	845	GLU	-	expression tag	UNP Q13507
C	846	LEU	-	expression tag	UNP Q13507
C	847	LEU	-	expression tag	UNP Q13507
C	848	GLU	-	expression tag	UNP Q13507
D	573	ALA	THR	engineered mutation	UNP Q13507
D	?	-	LEU	deletion	UNP Q13507
D	?	-	ASN	deletion	UNP Q13507
D	?	-	LEU	deletion	UNP Q13507
D	?	-	PHE	deletion	UNP Q13507
D	?	-	THR	deletion	UNP Q13507
D	?	-	GLN	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	ASN	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	ARG	deletion	UNP Q13507
D	?	-	VAL	deletion	UNP Q13507
D	?	-	PHE	deletion	UNP Q13507
D	?	-	GLU	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	HIS	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	PHE	deletion	UNP Q13507
D	?	-	ASN	deletion	UNP Q13507
D	?	-	SER	deletion	UNP Q13507
D	?	-	ILE	deletion	UNP Q13507
D	?	-	LEU	deletion	UNP Q13507
D	?	-	ASN	deletion	UNP Q13507
D	?	-	GLN	deletion	UNP Q13507
D	?	-	PRO	deletion	UNP Q13507
D	?	-	THR	deletion	UNP Q13507
D	?	-	ARG	deletion	UNP Q13507
D	?	-	TYR	deletion	UNP Q13507
D	?	-	GLN	deletion	UNP Q13507
D	839	ILE	-	expression tag	UNP Q13507
D	840	SER	-	expression tag	UNP Q13507

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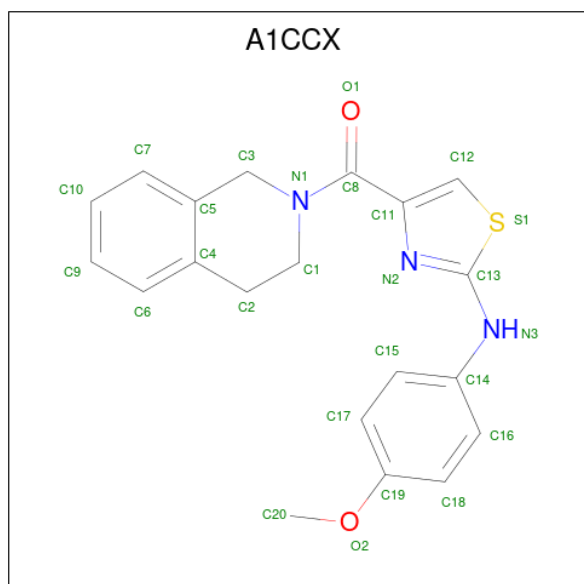
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Chain	Residue	Modelled	Actual	Comment	Reference
D	841	SER	-	expression tag	UNP Q13507
D	842	LEU	-	expression tag	UNP Q13507
D	843	ARG	-	expression tag	UNP Q13507
D	844	TYR	-	expression tag	UNP Q13507
D	845	GLU	-	expression tag	UNP Q13507
D	846	LEU	-	expression tag	UNP Q13507
D	847	LEU	-	expression tag	UNP Q13507
D	848	GLU	-	expression tag	UNP Q13507

- Molecule 2 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					AltConf
2	A	3	Total 132	C 102	N 3	O 24	P 3	0
2	B	3	Total 132	C 102	N 3	O 24	P 3	0
2	C	3	Total 132	C 102	N 3	O 24	P 3	0
2	D	3	Total 132	C 102	N 3	O 24	P 3	0

- Molecule 3 is (3,4-dihydroisoquinolin-2(1H)-yl)[2-(4-methoxyanilino)-1,3-thiazol-4-yl]methanone (CCD ID: A1CCX) (formula: C₂₀H₁₉N₃O₂S).

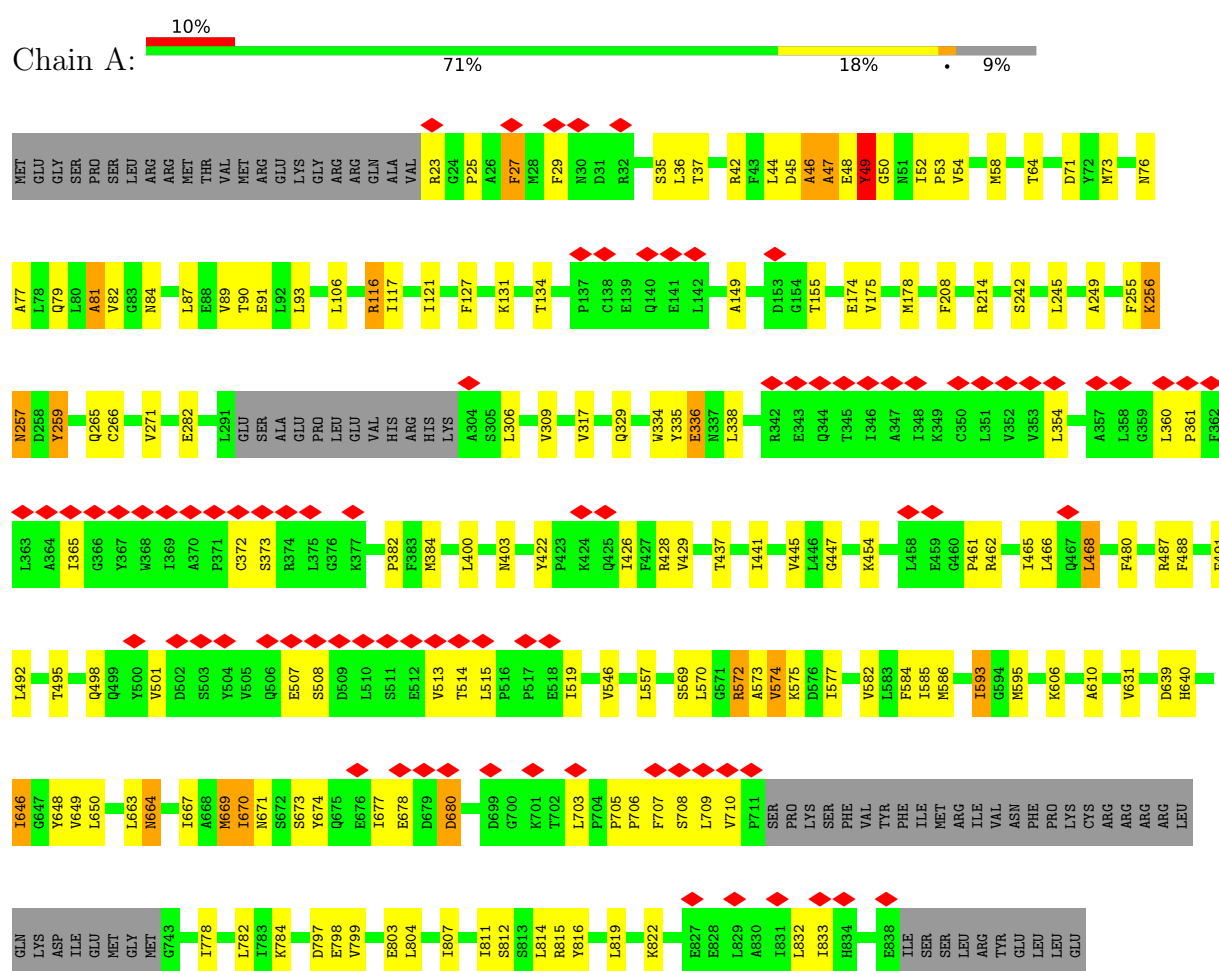


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 26	C 20	N 3	O 2	S 1	0
3	B	1	Total 26	C 20	N 3	O 2	S 1	0
3	C	1	Total 26	C 20	N 3	O 2	S 1	0
3	D	1	Total 26	C 20	N 3	O 2	S 1	0

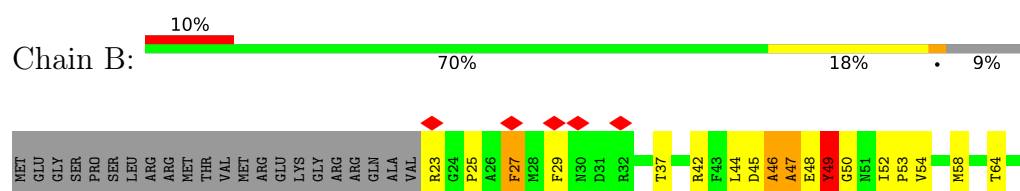
3 Residue-property plots

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

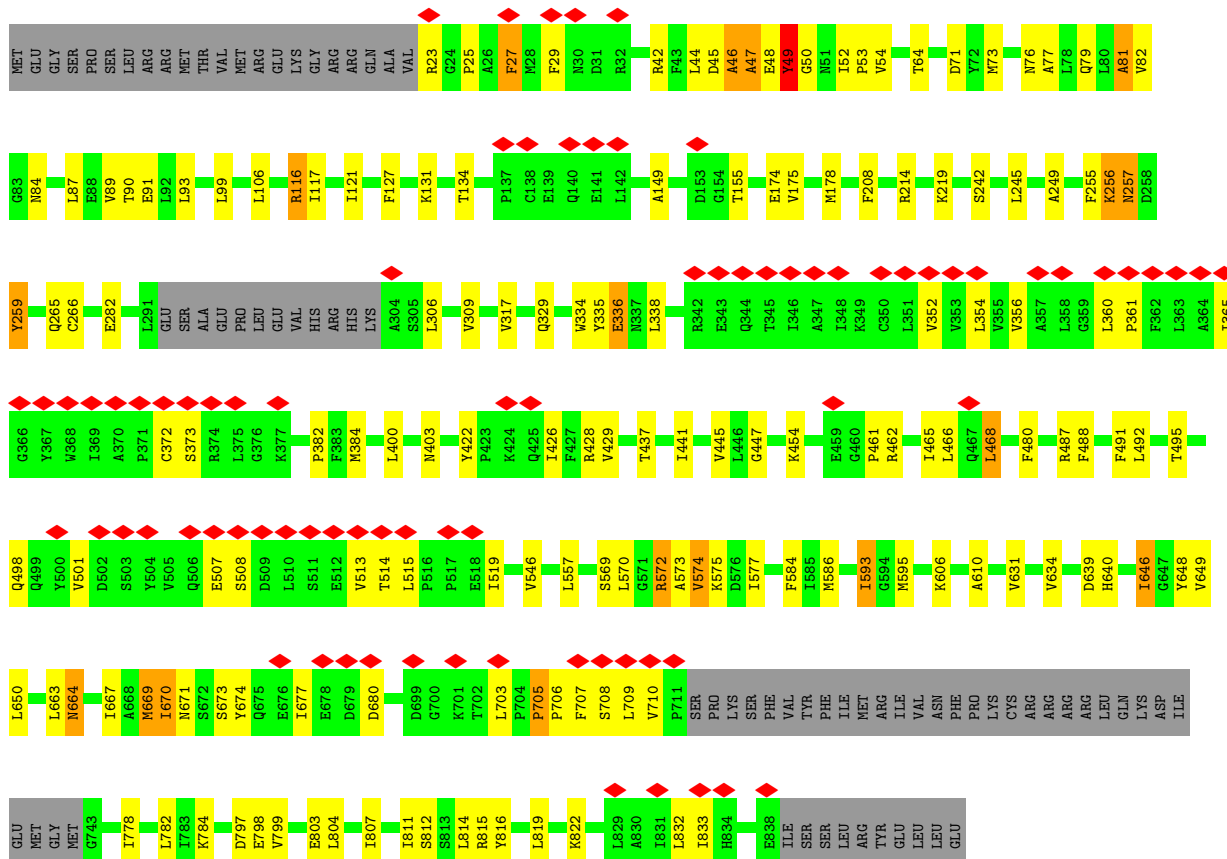
- Molecule 1: Short transient receptor potential channel 3



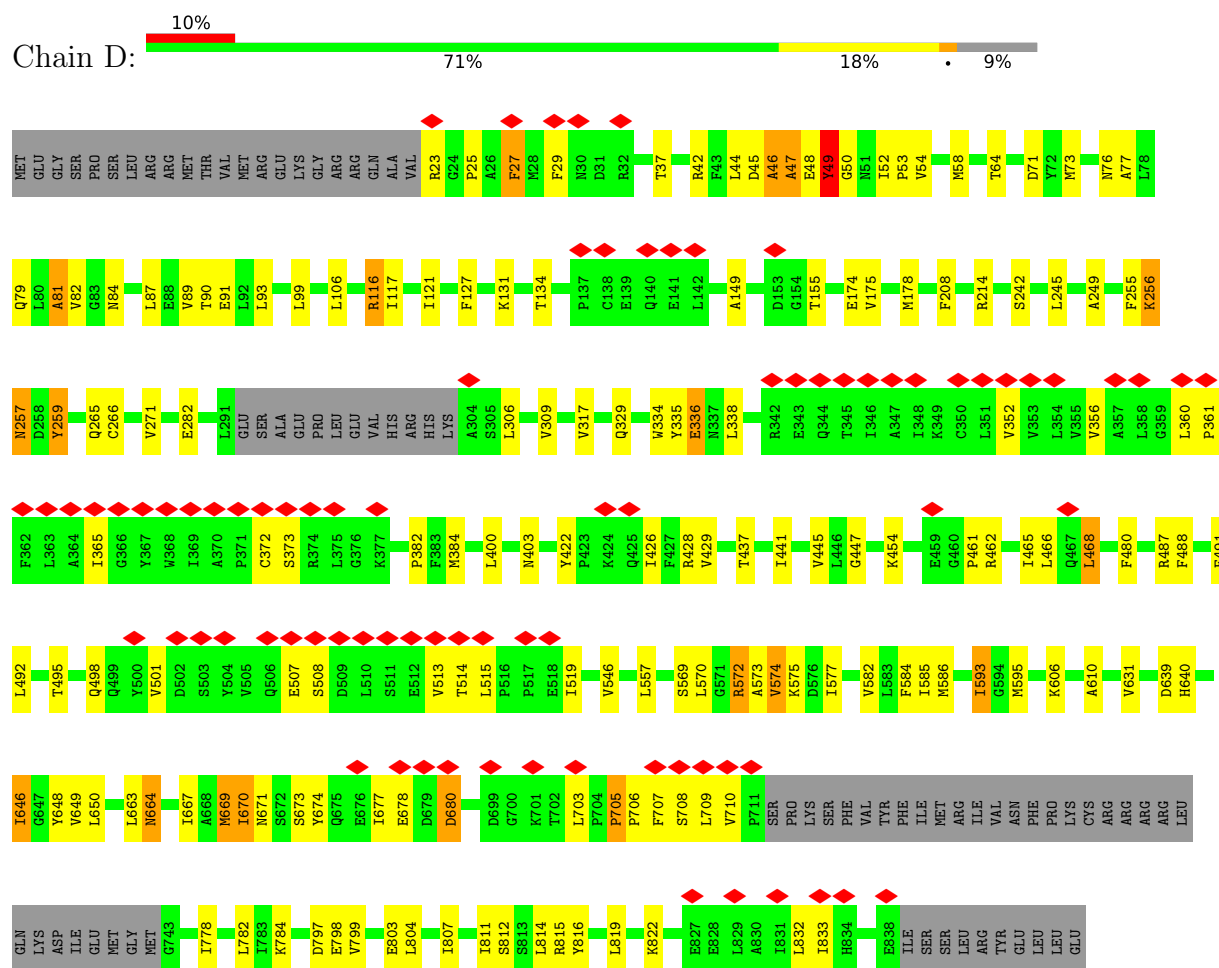
- Molecule 1: Short transient receptor potential channel 3



- Molecule 1: Short transient receptor potential channel 3



• Molecule 1: Short transient receptor potential channel 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	15296	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.468	Depositor
Minimum map value	-0.278	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.051	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, A1CCX

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	0.75	7/6121 (0.1%)	1.13	32/8284 (0.4%)
1	B	0.75	7/6121 (0.1%)	1.13	33/8284 (0.4%)
1	C	0.75	7/6121 (0.1%)	1.12	32/8284 (0.4%)
1	D	0.75	7/6121 (0.1%)	1.13	32/8284 (0.4%)
All	All	0.75	28/24484 (0.1%)	1.13	129/33136 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
All	All	0	28

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	461	PRO	N-CD	13.90	1.67	1.47
1	A	461	PRO	N-CD	13.88	1.67	1.47
1	B	461	PRO	N-CD	13.88	1.67	1.47
1	D	461	PRO	N-CD	13.88	1.67	1.47
1	A	25	PRO	N-CD	10.34	1.62	1.47
1	B	25	PRO	N-CD	10.34	1.62	1.47
1	D	25	PRO	N-CD	10.34	1.62	1.47
1	C	25	PRO	N-CD	10.33	1.62	1.47
1	A	573	ALA	C-O	8.70	1.35	1.24
1	B	573	ALA	C-O	8.70	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	573	ALA	C-O	8.70	1.35	1.24
1	D	573	ALA	C-O	8.70	1.35	1.24
1	B	640	HIS	C-O	7.67	1.34	1.23
1	C	640	HIS	C-O	7.67	1.34	1.23
1	A	640	HIS	C-O	7.62	1.34	1.23
1	D	640	HIS	C-O	7.61	1.34	1.23
1	B	569	SER	C-O	6.13	1.31	1.24
1	C	569	SER	C-O	6.13	1.31	1.24
1	A	569	SER	C-O	6.13	1.31	1.24
1	D	569	SER	C-O	6.13	1.31	1.24
1	A	259	TYR	C-O	-5.86	1.17	1.24
1	C	259	TYR	C-O	-5.86	1.17	1.24
1	D	259	TYR	C-O	-5.86	1.17	1.24
1	B	259	TYR	C-O	-5.79	1.17	1.24
1	C	91	GLU	C-O	5.41	1.30	1.24
1	A	91	GLU	C-O	5.39	1.30	1.24
1	B	91	GLU	C-O	5.39	1.30	1.24
1	D	91	GLU	C-O	5.31	1.30	1.24

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	336	GLU	N-CA-CB	17.18	139.52	110.49
1	B	336	GLU	N-CA-CB	17.16	139.50	110.49
1	A	336	GLU	N-CA-CB	17.16	139.49	110.49
1	C	336	GLU	N-CA-CB	17.14	139.46	110.49
1	B	50	GLY	N-CA-C	14.22	134.24	113.48
1	D	49	TYR	N-CA-CB	-10.31	93.06	110.49
1	A	49	TYR	N-CA-CB	-10.30	93.09	110.49
1	B	49	TYR	N-CA-CB	-10.30	93.09	110.49
1	C	49	TYR	N-CA-CB	-10.29	93.10	110.49
1	D	50	GLY	N-CA-C	8.90	134.29	113.18
1	A	50	GLY	N-CA-C	8.89	134.26	113.18
1	C	50	GLY	N-CA-C	8.88	134.24	113.18
1	D	84	ASN	N-CA-C	-8.07	97.44	110.20
1	A	84	ASN	N-CA-C	-8.06	97.47	110.20
1	B	84	ASN	N-CA-C	-8.06	97.47	110.20
1	C	84	ASN	N-CA-C	-8.06	97.47	110.20
1	B	27	PHE	CA-CB-CG	7.38	121.18	113.80
1	C	27	PHE	CA-CB-CG	7.37	121.17	113.80
1	A	27	PHE	CA-CB-CG	7.34	121.14	113.80
1	D	27	PHE	CA-CB-CG	7.33	121.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	VAL	CA-C-O	-7.05	113.62	120.95
1	B	574	VAL	CA-C-O	-7.05	113.62	120.95
1	D	574	VAL	CA-C-O	-7.05	113.62	120.95
1	D	208	PHE	CA-CB-CG	7.04	120.84	113.80
1	A	208	PHE	CA-CB-CG	7.03	120.83	113.80
1	B	208	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	208	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	574	VAL	CA-C-O	-7.03	113.64	120.95
1	A	89	VAL	N-CA-C	-6.75	103.94	110.42
1	D	89	VAL	N-CA-C	-6.75	103.94	110.42
1	B	89	VAL	N-CA-C	-6.75	103.94	110.42
1	C	89	VAL	N-CA-C	-6.74	103.95	110.42
1	A	49	TYR	N-CA-C	6.63	124.93	110.80
1	B	49	TYR	N-CA-C	6.63	124.93	110.80
1	D	49	TYR	N-CA-C	6.63	124.92	110.80
1	C	49	TYR	N-CA-C	6.62	124.90	110.80
1	A	584	PHE	CA-CB-CG	6.51	120.31	113.80
1	D	584	PHE	CA-CB-CG	6.51	120.31	113.80
1	B	584	PHE	CA-CB-CG	6.50	120.31	113.80
1	C	584	PHE	CA-CB-CG	6.50	120.31	113.80
1	A	680	ASP	N-CA-C	-6.47	104.86	112.89
1	B	680	ASP	N-CA-C	-6.47	104.86	112.89
1	D	680	ASP	N-CA-C	-6.47	104.86	112.89
1	C	680	ASP	N-CA-C	-6.45	104.90	112.89
1	B	259	TYR	CB-CA-C	6.09	120.89	110.79
1	C	259	TYR	CB-CA-C	6.08	120.88	110.79
1	A	71	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	71	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	259	TYR	CB-CA-C	6.06	120.85	110.79
1	C	71	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	259	TYR	CB-CA-C	6.06	120.85	110.79
1	C	480	PHE	CA-C-O	-6.05	114.46	120.82
1	B	71	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	480	PHE	CA-C-O	-6.00	114.51	120.82
1	B	480	PHE	CA-C-O	-6.00	114.51	120.82
1	D	480	PHE	CA-C-O	-6.00	114.51	120.82
1	C	329	GLN	CB-CA-C	-5.99	100.85	110.79
1	A	329	GLN	CB-CA-C	-5.97	100.88	110.79
1	D	329	GLN	CB-CA-C	-5.97	100.88	110.79
1	B	329	GLN	CB-CA-C	-5.96	100.90	110.79
1	B	705	PRO	N-CA-C	5.91	117.90	110.70
1	A	705	PRO	N-CA-C	5.89	117.88	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	705	PRO	N-CA-C	5.88	117.88	110.70
1	C	705	PRO	N-CA-C	5.87	117.86	110.70
1	B	422	TYR	CB-CA-C	5.84	116.80	108.68
1	D	422	TYR	CB-CA-C	5.84	116.79	108.68
1	A	422	TYR	CB-CA-C	5.83	116.78	108.68
1	C	422	TYR	CB-CA-C	5.81	116.75	108.68
1	C	646	ILE	N-CA-C	-5.80	104.70	110.62
1	A	646	ILE	N-CA-C	-5.80	104.71	110.62
1	B	646	ILE	N-CA-C	-5.80	104.71	110.62
1	D	646	ILE	N-CA-C	-5.80	104.71	110.62
1	D	365	ILE	CA-C-O	-5.78	115.04	121.17
1	A	365	ILE	CA-C-O	-5.75	115.08	121.17
1	B	365	ILE	CA-C-O	-5.75	115.08	121.17
1	C	365	ILE	CA-C-O	-5.75	115.08	121.17
1	C	574	VAL	N-CA-C	5.67	116.40	110.62
1	B	265	GLN	CB-CA-C	-5.65	101.07	110.68
1	A	265	GLN	CB-CA-C	-5.65	101.07	110.68
1	D	265	GLN	CB-CA-C	-5.65	101.07	110.68
1	A	574	VAL	N-CA-C	5.65	116.38	110.62
1	B	574	VAL	N-CA-C	5.65	116.38	110.62
1	C	265	GLN	CB-CA-C	-5.64	101.09	110.68
1	D	574	VAL	N-CA-C	5.62	116.35	110.62
1	D	336	GLU	N-CA-C	-5.48	99.13	110.80
1	A	336	GLU	N-CA-C	-5.47	99.16	110.80
1	C	336	GLU	N-CA-C	-5.46	99.16	110.80
1	B	336	GLU	N-CA-C	-5.45	99.18	110.80
1	B	259	TYR	CA-C-O	-5.39	114.83	120.55
1	A	259	TYR	CA-C-O	-5.38	114.84	120.55
1	C	259	TYR	CA-C-O	-5.38	114.84	120.55
1	D	259	TYR	CA-C-O	-5.38	114.84	120.55
1	B	90	THR	CA-C-O	-5.34	115.19	120.90
1	A	90	THR	CA-C-O	-5.32	115.21	120.90
1	D	90	THR	CA-C-O	-5.31	115.22	120.90
1	D	784	LYS	CA-C-O	-5.30	115.44	121.00
1	C	90	THR	CA-C-O	-5.29	115.24	120.90
1	A	784	LYS	CA-C-O	-5.28	115.45	121.00
1	B	784	LYS	CA-C-O	-5.28	115.45	121.00
1	B	81	ALA	CA-C-O	-5.25	115.05	121.67
1	C	784	LYS	CA-C-O	-5.24	115.50	121.00
1	D	81	ALA	CA-C-O	-5.23	115.08	121.67
1	A	81	ALA	CA-C-O	-5.22	115.09	121.67
1	C	81	ALA	CA-C-O	-5.21	115.11	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	778	ILE	N-CA-C	-5.19	105.33	110.62
1	B	778	ILE	N-CA-C	-5.19	105.33	110.62
1	D	778	ILE	N-CA-C	-5.19	105.33	110.62
1	C	778	ILE	N-CA-C	-5.18	105.34	110.62
1	B	259	TYR	N-CA-C	-5.16	105.66	111.28
1	D	79	GLN	N-CA-C	-5.16	106.99	113.28
1	A	79	GLN	N-CA-C	-5.14	107.01	113.28
1	C	79	GLN	N-CA-C	-5.14	107.01	113.28
1	D	87	LEU	CA-C-O	-5.14	114.53	120.24
1	A	87	LEU	CA-C-O	-5.14	114.54	120.24
1	C	87	LEU	CA-C-O	-5.14	114.54	120.24
1	B	87	LEU	CA-C-O	-5.13	114.54	120.24
1	A	259	TYR	N-CA-C	-5.13	105.69	111.28
1	B	79	GLN	N-CA-C	-5.13	107.02	113.28
1	C	259	TYR	N-CA-C	-5.13	105.69	111.28
1	D	259	TYR	N-CA-C	-5.13	105.69	111.28
1	A	454	LYS	CA-C-O	-5.08	115.67	121.00
1	B	454	LYS	CA-C-O	-5.08	115.67	121.00
1	D	454	LYS	CA-C-O	-5.08	115.67	121.00
1	C	454	LYS	CA-C-O	-5.03	115.72	121.00
1	B	265	GLN	N-CA-CB	5.02	117.59	110.06
1	C	265	GLN	N-CA-CB	5.01	117.58	110.06
1	B	335	TYR	CB-CA-C	5.01	120.39	110.42
1	A	265	GLN	N-CA-CB	5.01	117.57	110.06
1	D	265	GLN	N-CA-CB	5.01	117.57	110.06

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	214	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	42	ARG	Sidechain
1	A	487	ARG	Sidechain
1	A	639	ASP	Mainchain
1	A	664	ASN	Mainchain
1	B	116	ARG	Sidechain
1	B	214	ARG	Sidechain
1	B	23	ARG	Sidechain
1	B	42	ARG	Sidechain
1	B	487	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	639	ASP	Mainchain
1	B	664	ASN	Mainchain
1	C	116	ARG	Sidechain
1	C	214	ARG	Sidechain
1	C	23	ARG	Sidechain
1	C	42	ARG	Sidechain
1	C	487	ARG	Sidechain
1	C	639	ASP	Mainchain
1	C	664	ASN	Mainchain
1	D	116	ARG	Sidechain
1	D	214	ARG	Sidechain
1	D	23	ARG	Sidechain
1	D	42	ARG	Sidechain
1	D	487	ARG	Sidechain
1	D	639	ASP	Mainchain
1	D	664	ASN	Mainchain

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	5990	0	6037	126	0
1	B	5990	0	6037	129	0
1	C	5990	0	6037	126	0
1	D	5990	0	6037	130	0
2	A	132	0	0	7	0
2	B	132	0	0	9	0
2	C	132	0	0	8	0
2	D	132	0	0	9	0
3	A	26	0	0	2	0
3	B	26	0	0	1	0
3	C	26	0	0	2	0
3	D	26	0	0	1	0
All	All	24592	0	24148	427	0

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

All (427) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:LYS:NZ	2:B:902:UNL:O31	1.63	1.31
1:C:575:LYS:NZ	2:C:902:UNL:O31	1.63	1.30
1:A:575:LYS:NZ	2:A:902:UNL:O31	1.63	1.27
1:D:575:LYS:NZ	2:D:904:UNL:O31	1.63	1.26
1:A:76:ASN:OD1	1:A:77:ALA:N	1.98	0.96
1:D:76:ASN:OD1	1:D:77:ALA:N	1.98	0.95
1:B:76:ASN:OD1	1:B:77:ALA:N	1.98	0.95
1:C:76:ASN:OD1	1:C:77:ALA:N	1.98	0.94
1:A:822:LYS:HZ3	1:B:822:LYS:HZ3	1.28	0.80
1:C:822:LYS:HD2	1:D:822:LYS:HE2	1.66	0.78
1:A:822:LYS:HE2	1:D:822:LYS:HD2	1.66	0.78
1:B:822:LYS:HD2	1:C:822:LYS:HE2	1.66	0.77
1:A:822:LYS:HZ3	1:D:822:LYS:HZ3	1.30	0.76
1:A:822:LYS:HD2	1:B:822:LYS:HE2	1.66	0.76
1:C:822:LYS:HZ3	1:D:822:LYS:HZ3	1.33	0.75
1:A:426:ILE:HD11	1:A:501:VAL:HG21	1.70	0.73
1:D:426:ILE:HD11	1:D:501:VAL:HG21	1.70	0.73
1:B:426:ILE:HD11	1:B:501:VAL:HG21	1.70	0.73
1:C:671:ASN:HB2	1:D:674:TYR:CE1	2.24	0.73
1:B:671:ASN:HB2	1:C:674:TYR:CE1	2.24	0.72
1:B:822:LYS:HZ3	1:C:822:LYS:HZ3	1.35	0.72
1:A:674:TYR:CE1	1:D:671:ASN:HB2	2.24	0.72
1:C:426:ILE:HD11	1:C:501:VAL:HG21	1.70	0.72
1:A:671:ASN:HB2	1:B:674:TYR:CE1	2.24	0.71
1:A:45:ASP:OD1	1:A:93:LEU:HD11	1.91	0.70
1:B:45:ASP:OD1	1:B:93:LEU:HD11	1.91	0.70
1:D:45:ASP:OD1	1:D:93:LEU:HD11	1.91	0.70
1:C:45:ASP:OD1	1:C:93:LEU:HD11	1.91	0.70
1:D:515:LEU:HD22	1:D:519:ILE:HG21	1.74	0.70
1:B:574:VAL:HG11	2:B:902:UNL:C36	2.22	0.70
1:C:515:LEU:HD22	1:C:519:ILE:HG21	1.74	0.70
1:A:574:VAL:HG11	2:A:902:UNL:C36	2.22	0.70
1:C:574:VAL:HG11	2:C:902:UNL:C36	2.22	0.70
1:D:574:VAL:HG11	2:D:904:UNL:C36	2.22	0.69
1:B:515:LEU:HD22	1:B:519:ILE:HG21	1.74	0.69
1:A:515:LEU:HD22	1:A:519:ILE:HG21	1.74	0.67
1:B:338:LEU:CD1	1:B:384:MET:HE3	2.25	0.67
1:B:282:GLU:HB3	1:B:782:LEU:HD11	1.77	0.67
1:C:338:LEU:CD1	1:C:384:MET:HE3	2.25	0.67
1:A:822:LYS:NZ	1:D:822:LYS:HZ3	1.94	0.66
1:D:282:GLU:HB3	1:D:782:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:CD1	1:A:384:MET:HE3	2.25	0.66
1:C:282:GLU:HB3	1:C:782:LEU:HD11	1.77	0.66
1:A:149:ALA:HA	1:A:155:THR:HG22	1.78	0.66
1:B:149:ALA:HA	1:B:155:THR:HG22	1.78	0.66
1:C:670:ILE:HD11	1:D:670:ILE:HD12	1.78	0.65
1:D:338:LEU:CD1	1:D:384:MET:HE3	2.25	0.65
1:C:822:LYS:HZ3	1:D:822:LYS:NZ	1.95	0.65
1:A:282:GLU:HB3	1:A:782:LEU:HD11	1.77	0.65
1:A:670:ILE:CD1	1:D:670:ILE:HD11	2.27	0.65
1:A:670:ILE:HD12	1:D:670:ILE:HD11	1.78	0.65
1:B:670:ILE:HD11	1:C:670:ILE:HD12	1.78	0.65
1:C:670:ILE:HD11	1:D:670:ILE:CD1	2.27	0.65
1:A:670:ILE:HD11	1:B:670:ILE:HD12	1.78	0.65
1:B:670:ILE:HD11	1:C:670:ILE:CD1	2.27	0.64
1:C:149:ALA:HA	1:C:155:THR:HG22	1.78	0.64
1:D:149:ALA:HA	1:D:155:THR:HG22	1.78	0.64
1:A:670:ILE:HD11	1:B:670:ILE:CD1	2.27	0.63
1:A:822:LYS:HZ3	1:B:822:LYS:NZ	1.96	0.63
1:A:822:LYS:CD	1:B:822:LYS:HE2	2.28	0.63
1:B:822:LYS:CD	1:C:822:LYS:HE2	2.29	0.63
1:A:822:LYS:HE2	1:D:822:LYS:CD	2.29	0.62
1:C:822:LYS:CD	1:D:822:LYS:HE2	2.29	0.62
1:C:82:VAL:HG13	1:C:117:ILE:HG21	1.83	0.61
1:A:82:VAL:HG13	1:A:117:ILE:HG21	1.83	0.61
1:A:804:LEU:HD22	1:B:799:VAL:HG21	1.84	0.60
1:D:82:VAL:HG13	1:D:117:ILE:HG21	1.83	0.60
1:B:804:LEU:HD22	1:C:799:VAL:HG21	1.84	0.59
1:C:338:LEU:HD11	1:C:384:MET:HE3	1.85	0.59
1:B:82:VAL:HG13	1:B:117:ILE:HG21	1.83	0.59
1:A:338:LEU:HD11	1:A:384:MET:HE3	1.85	0.59
1:A:822:LYS:NZ	1:B:822:LYS:NZ	2.51	0.59
1:B:822:LYS:HZ3	1:C:822:LYS:NZ	1.99	0.59
1:A:799:VAL:HG21	1:D:804:LEU:HD22	1.84	0.58
1:C:804:LEU:HD22	1:D:799:VAL:HG21	1.84	0.58
1:B:663:LEU:HD23	1:C:669:MET:HE3	1.85	0.57
1:B:822:LYS:NZ	1:C:822:LYS:NZ	2.51	0.57
1:C:822:LYS:NZ	1:D:822:LYS:NZ	2.51	0.57
1:A:669:MET:HE3	1:D:663:LEU:HD23	1.85	0.57
1:A:822:LYS:NZ	1:D:822:LYS:NZ	2.51	0.57
1:B:338:LEU:HD11	1:B:384:MET:HE3	1.85	0.57
1:C:663:LEU:HD23	1:D:669:MET:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HG3	1:C:131:LYS:O	2.05	0.57
1:D:400:LEU:HD11	1:D:546:VAL:HG22	1.86	0.57
1:A:663:LEU:HD23	1:B:669:MET:HE3	1.85	0.57
1:A:400:LEU:HD11	1:A:546:VAL:HG22	1.86	0.57
1:D:338:LEU:HD11	1:D:384:MET:HE3	1.85	0.56
1:D:429:VAL:HG21	1:D:498:GLN:HB2	1.88	0.56
1:B:400:LEU:HD11	1:B:546:VAL:HG22	1.86	0.56
1:B:429:VAL:HG21	1:B:498:GLN:HB2	1.88	0.56
1:A:822:LYS:HE2	1:D:822:LYS:HG3	1.88	0.56
1:A:822:LYS:HG3	1:B:822:LYS:HE2	1.88	0.56
1:A:429:VAL:HG21	1:A:498:GLN:HB2	1.88	0.56
1:C:429:VAL:HG21	1:C:498:GLN:HB2	1.88	0.56
1:C:822:LYS:HG3	1:D:822:LYS:HE2	1.88	0.56
1:B:822:LYS:HG3	1:C:822:LYS:HE2	1.88	0.56
1:D:131:LYS:O	1:D:131:LYS:HG3	2.05	0.56
1:C:400:LEU:HD11	1:C:546:VAL:HG22	1.86	0.55
1:D:372:CYS:SG	1:D:373:SER:N	2.78	0.55
1:A:131:LYS:HG3	1:A:131:LYS:O	2.05	0.55
1:B:131:LYS:O	1:B:131:LYS:HG3	2.05	0.55
1:A:664:ASN:HA	1:A:667:ILE:HD12	1.89	0.55
1:A:586:MET:HE1	1:B:557:LEU:HD11	1.89	0.55
1:B:833:ILE:HD12	1:C:832:LEU:HB2	1.89	0.54
1:D:488:PHE:CE1	1:D:492:LEU:HD11	2.42	0.54
1:B:372:CYS:SG	1:B:373:SER:N	2.78	0.54
1:D:664:ASN:HA	1:D:667:ILE:HD12	1.89	0.54
1:B:488:PHE:CE1	1:B:492:LEU:HD11	2.42	0.54
2:C:903:UNL:C33	2:C:903:UNL:C2	2.85	0.54
1:C:833:ILE:HD12	1:D:832:LEU:HB2	1.89	0.54
1:A:833:ILE:HD12	1:B:832:LEU:HB2	1.89	0.54
2:B:903:UNL:C2	2:B:903:UNL:C33	2.85	0.54
1:A:557:LEU:HD11	1:D:586:MET:HE1	1.89	0.54
1:B:664:ASN:HA	1:B:667:ILE:HD12	1.89	0.54
1:C:64:THR:O	1:C:64:THR:HG23	2.08	0.54
1:A:64:THR:HG23	1:A:64:THR:O	2.08	0.53
1:A:174:GLU:HG3	1:A:178:MET:HE2	1.91	0.53
1:A:488:PHE:CE1	1:A:492:LEU:HD11	2.42	0.53
2:A:903:UNL:C33	2:A:903:UNL:C2	2.85	0.53
1:D:174:GLU:HG3	1:D:178:MET:HE2	1.91	0.53
1:A:832:LEU:HB2	1:D:833:ILE:HD12	1.89	0.53
1:C:488:PHE:CE1	1:C:492:LEU:HD11	2.42	0.53
2:D:901:UNL:C2	2:D:901:UNL:C33	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:THR:HG23	1:B:64:THR:O	2.08	0.53
1:C:372:CYS:SG	1:C:373:SER:N	2.78	0.53
1:D:709:LEU:HD12	1:D:710:VAL:HG13	1.91	0.53
1:C:586:MET:HE1	1:D:557:LEU:HD11	1.89	0.53
1:C:174:GLU:HG3	1:C:178:MET:HE2	1.91	0.53
1:B:174:GLU:HG3	1:B:178:MET:HE2	1.91	0.53
1:B:586:MET:HE1	1:C:557:LEU:HD11	1.89	0.53
1:C:664:ASN:HA	1:C:667:ILE:HD12	1.89	0.53
1:D:64:THR:HG23	1:D:64:THR:O	2.08	0.53
1:A:507:GLU:HG2	1:A:513:VAL:CG2	2.40	0.52
1:A:709:LEU:HD12	1:A:710:VAL:HG13	1.91	0.52
1:C:507:GLU:HG2	1:C:513:VAL:CG2	2.40	0.52
1:B:709:LEU:HD12	1:B:710:VAL:HG13	1.91	0.52
1:D:507:GLU:HG2	1:D:513:VAL:CG2	2.40	0.51
1:C:709:LEU:HD12	1:C:710:VAL:HG13	1.91	0.51
1:A:631:VAL:HG12	1:A:631:VAL:O	2.10	0.51
1:B:507:GLU:HG2	1:B:513:VAL:CG2	2.40	0.51
1:A:815:ARG:HA	1:B:814:LEU:HD21	1.93	0.51
1:B:631:VAL:HG12	1:B:631:VAL:O	2.10	0.51
1:C:703:LEU:HD13	1:C:707:PHE:HB2	1.93	0.51
1:A:804:LEU:HD23	1:B:803:GLU:HB3	1.93	0.51
1:B:804:LEU:HD23	1:C:803:GLU:HB3	1.93	0.51
1:C:631:VAL:HG12	1:C:631:VAL:O	2.10	0.50
1:D:631:VAL:HG12	1:D:631:VAL:O	2.10	0.50
1:D:703:LEU:HD13	1:D:707:PHE:HB2	1.93	0.50
1:A:814:LEU:HD21	1:D:815:ARG:HA	1.93	0.50
1:B:815:ARG:HA	1:C:814:LEU:HD21	1.93	0.50
1:C:815:ARG:HA	1:D:814:LEU:HD21	1.93	0.50
1:A:703:LEU:HD13	1:A:707:PHE:HB2	1.93	0.49
1:B:703:LEU:HD13	1:B:707:PHE:HB2	1.93	0.49
1:C:804:LEU:HD23	1:D:803:GLU:HB3	1.93	0.49
1:B:674:TYR:N	1:B:674:TYR:CD1	2.79	0.49
1:D:465:ILE:HG22	1:D:466:LEU:HG	1.94	0.49
1:A:803:GLU:HB3	1:D:804:LEU:HD23	1.93	0.49
1:B:465:ILE:HG22	1:B:466:LEU:HG	1.94	0.49
1:C:674:TYR:N	1:C:674:TYR:CD1	2.79	0.49
1:A:245:LEU:HD21	1:A:259:TYR:O	2.13	0.48
1:C:465:ILE:HG22	1:C:466:LEU:HG	1.94	0.48
1:D:245:LEU:HD21	1:D:259:TYR:O	2.13	0.48
1:A:465:ILE:HG22	1:A:466:LEU:HG	1.94	0.48
1:A:674:TYR:N	1:A:674:TYR:CD1	2.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:904:A1CCX:C16	2:D:904:UNL:C17	2.91	0.48
1:D:674:TYR:N	1:D:674:TYR:CD1	2.79	0.48
1:C:249:ALA:HB2	1:C:259:TYR:HB3	1.96	0.48
1:A:249:ALA:HB2	1:A:259:TYR:HB3	1.96	0.48
1:A:822:LYS:CG	1:B:822:LYS:HE2	2.44	0.48
3:A:904:A1CCX:C16	2:B:902:UNL:C17	2.91	0.48
1:D:131:LYS:HB2	1:D:134:THR:HG23	1.96	0.48
1:A:46:ALA:O	1:A:47:ALA:C	2.57	0.48
1:C:46:ALA:O	1:C:47:ALA:C	2.57	0.48
1:D:46:ALA:O	1:D:47:ALA:C	2.57	0.48
3:B:904:A1CCX:C16	2:C:902:UNL:C17	2.91	0.48
1:C:245:LEU:HD21	1:C:259:TYR:O	2.13	0.48
2:A:902:UNL:C17	3:D:902:A1CCX:C16	2.91	0.48
1:A:48:GLU:HG2	1:B:116:ARG:HD3	1.96	0.47
1:B:822:LYS:CG	1:C:822:LYS:HE2	2.44	0.47
1:B:48:GLU:HG2	1:C:116:ARG:HD3	1.97	0.47
1:B:245:LEU:HD21	1:B:259:TYR:O	2.13	0.47
1:A:131:LYS:HB2	1:A:134:THR:HG23	1.96	0.47
1:A:703:LEU:HD21	1:A:710:VAL:HG23	1.96	0.47
1:C:48:GLU:HG2	1:D:116:ARG:HD3	1.96	0.47
1:C:488:PHE:O	1:C:492:LEU:HD13	2.15	0.47
1:A:822:LYS:HE2	1:D:822:LYS:CG	2.44	0.47
1:B:131:LYS:HB2	1:B:134:THR:HG23	1.96	0.47
1:D:249:ALA:HB2	1:D:259:TYR:HB3	1.96	0.47
1:A:116:ARG:HD3	1:D:48:GLU:HG2	1.97	0.47
1:A:428:ARG:HA	1:A:428:ARG:HD2	1.66	0.47
1:C:822:LYS:CG	1:D:822:LYS:HE2	2.44	0.47
1:D:703:LEU:HD21	1:D:710:VAL:HG23	1.96	0.47
1:B:804:LEU:HD22	1:C:799:VAL:CG2	2.45	0.47
1:A:799:VAL:CG2	1:D:804:LEU:HD22	2.45	0.46
1:B:249:ALA:HB2	1:B:259:TYR:HB3	1.96	0.46
1:B:703:LEU:HD21	1:B:710:VAL:HG23	1.96	0.46
1:B:46:ALA:O	1:B:47:ALA:C	2.57	0.46
1:C:131:LYS:HB2	1:C:134:THR:HG23	1.96	0.46
1:D:488:PHE:O	1:D:492:LEU:HD13	2.15	0.46
1:A:372:CYS:SG	1:A:373:SER:N	2.78	0.46
1:D:99:LEU:HD12	1:D:99:LEU:HA	1.84	0.46
1:C:428:ARG:HA	1:C:428:ARG:HD2	1.66	0.46
1:B:488:PHE:O	1:B:492:LEU:HD13	2.15	0.46
1:C:703:LEU:HD21	1:C:710:VAL:HG23	1.96	0.46
1:C:491:PHE:O	1:C:495:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:PHE:O	1:A:492:LEU:HD13	2.15	0.46
1:A:804:LEU:HD22	1:B:799:VAL:CG2	2.45	0.46
1:B:491:PHE:O	1:B:495:THR:HG23	2.16	0.45
1:A:491:PHE:O	1:A:495:THR:HG23	2.16	0.45
1:D:491:PHE:O	1:D:495:THR:HG23	2.16	0.45
1:A:798:GLU:OE2	1:D:798:GLU:OE1	2.34	0.45
1:A:249:ALA:HB2	1:A:259:TYR:CB	2.47	0.45
1:B:249:ALA:HB2	1:B:259:TYR:CB	2.47	0.45
1:B:428:ARG:HD2	1:B:428:ARG:HA	1.66	0.45
1:B:798:GLU:OE1	1:C:798:GLU:OE2	2.34	0.45
1:B:49:TYR:CD1	1:B:816:TYR:CZ	3.05	0.45
1:C:804:LEU:HD22	1:D:799:VAL:CG2	2.45	0.45
1:C:249:ALA:HB2	1:C:259:TYR:CB	2.47	0.45
1:A:646:ILE:HD13	2:A:903:UNL:C37	2.47	0.45
1:A:798:GLU:OE1	1:B:798:GLU:OE2	2.34	0.45
1:C:462:ARG:HD3	1:C:462:ARG:HA	1.75	0.44
1:C:798:GLU:OE1	1:D:798:GLU:OE2	2.34	0.44
1:B:49:TYR:CD1	1:B:812:SER:HB2	2.52	0.44
1:D:249:ALA:HB2	1:D:259:TYR:CB	2.47	0.44
1:A:106:LEU:HD22	1:A:127:PHE:CE2	2.53	0.44
1:D:256:LYS:O	1:D:257:ASN:C	2.61	0.44
1:D:428:ARG:HA	1:D:428:ARG:HD2	1.66	0.44
1:A:667:ILE:HG21	1:B:673:SER:CB	2.48	0.44
1:B:354:LEU:HD12	1:B:354:LEU:HA	1.81	0.44
1:D:106:LEU:HD22	1:D:127:PHE:CE2	2.53	0.44
1:A:49:TYR:CD1	1:A:812:SER:HB2	2.52	0.44
1:B:667:ILE:HG21	1:C:673:SER:CB	2.48	0.44
1:B:822:LYS:HA	1:B:822:LYS:HD3	1.86	0.44
1:C:106:LEU:HD22	1:C:127:PHE:CE2	2.53	0.44
1:C:256:LYS:O	1:C:257:ASN:C	2.61	0.44
1:C:670:ILE:HD11	1:D:670:ILE:HD13	2.00	0.44
1:B:462:ARG:HA	1:B:462:ARG:HD3	1.75	0.44
1:B:646:ILE:HD13	2:B:903:UNL:C37	2.47	0.44
1:D:646:ILE:HD13	2:D:901:UNL:C37	2.48	0.44
1:A:49:TYR:CD1	1:A:816:TYR:CZ	3.05	0.44
1:B:593:ILE:HD12	1:B:593:ILE:HA	1.80	0.44
1:C:46:ALA:HB2	1:C:81:ALA:HB2	2.00	0.44
1:C:49:TYR:CD1	1:C:812:SER:HB2	2.52	0.44
1:C:646:ILE:HD13	2:C:903:UNL:C37	2.48	0.44
1:C:667:ILE:HG21	1:D:673:SER:CB	2.48	0.44
1:D:822:LYS:HA	1:D:822:LYS:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ILE:HD13	1:D:670:ILE:HD11	2.00	0.43
1:B:106:LEU:HD22	1:B:127:PHE:CE2	2.53	0.43
1:D:49:TYR:CD1	1:D:812:SER:HB2	2.52	0.43
1:A:447:GLY:HA3	1:A:708:SER:HB2	2.00	0.43
1:C:49:TYR:CD1	1:C:816:TYR:CZ	3.05	0.43
1:C:447:GLY:HA3	1:C:708:SER:HB2	2.01	0.43
1:C:822:LYS:HA	1:C:822:LYS:HD3	1.86	0.43
1:D:403:ASN:HD22	1:D:437:THR:HG22	1.83	0.43
1:A:256:LYS:O	1:A:257:ASN:C	2.61	0.43
1:B:403:ASN:HD22	1:B:437:THR:HG22	1.83	0.43
1:B:706:PRO:O	1:B:707:PHE:C	2.62	0.43
1:A:706:PRO:O	1:A:707:PHE:C	2.62	0.43
1:B:572:ARG:HH22	1:B:677:ILE:HD12	1.84	0.43
1:D:46:ALA:HB2	1:D:81:ALA:HB2	2.00	0.43
1:B:256:LYS:O	1:B:257:ASN:C	2.61	0.43
1:D:49:TYR:CD1	1:D:816:TYR:CZ	3.05	0.43
1:D:52:ILE:N	1:D:53:PRO:CD	2.82	0.43
1:A:673:SER:CB	1:D:667:ILE:HG21	2.48	0.43
1:B:447:GLY:HA3	1:B:708:SER:HB2	2.00	0.43
1:C:52:ILE:N	1:C:53:PRO:CD	2.82	0.43
1:C:593:ILE:HD12	1:C:593:ILE:HA	1.79	0.43
1:D:572:ARG:HH22	1:D:677:ILE:HD12	1.84	0.43
1:A:175:VAL:HA	1:A:178:MET:HE3	2.00	0.43
1:B:46:ALA:HB2	1:B:81:ALA:HB2	2.00	0.43
1:A:670:ILE:HD11	1:B:670:ILE:HD13	2.00	0.43
1:C:175:VAL:HA	1:C:178:MET:HE3	2.00	0.43
1:C:403:ASN:HD22	1:C:437:THR:HG22	1.83	0.43
1:D:447:GLY:HA3	1:D:708:SER:HB2	2.01	0.43
1:A:514:THR:HG23	1:A:514:THR:O	2.19	0.43
1:A:593:ILE:HD12	1:A:593:ILE:HA	1.80	0.43
1:C:664:ASN:HB3	1:D:570:LEU:HD22	2.01	0.43
1:D:507:GLU:HG3	1:D:508:SER:H	1.84	0.43
1:C:49:TYR:HB3	1:C:816:TYR:CE2	2.54	0.43
1:C:242:SER:HB2	1:C:266:CYS:HB2	2.01	0.43
1:C:572:ARG:HH22	1:C:677:ILE:HD12	1.84	0.43
1:D:49:TYR:HB3	1:D:816:TYR:CE2	2.54	0.43
1:A:572:ARG:HH22	1:A:677:ILE:HD12	1.84	0.42
1:C:44:LEU:HD22	1:C:54:VAL:CG1	2.49	0.42
1:A:27:PHE:CZ	1:A:73:MET:HE2	2.54	0.42
1:A:403:ASN:HD22	1:A:437:THR:HG22	1.83	0.42
1:A:488:PHE:HE1	1:A:492:LEU:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ILE:N	1:B:53:PRO:CD	2.82	0.42
1:B:664:ASN:HB3	1:C:570:LEU:HD22	2.01	0.42
1:C:27:PHE:CZ	1:C:73:MET:HE2	2.54	0.42
1:D:175:VAL:HA	1:D:178:MET:HE3	2.00	0.42
1:D:400:LEU:HD21	1:D:546:VAL:HG13	2.01	0.42
1:D:574:VAL:HG21	2:D:904:UNL:C37	2.49	0.42
1:A:46:ALA:HB2	1:A:81:ALA:HB2	2.00	0.42
1:A:49:TYR:HB3	1:A:816:TYR:CE2	2.54	0.42
1:A:317:VAL:O	1:A:317:VAL:HG13	2.20	0.42
1:B:175:VAL:HA	1:B:178:MET:HE3	2.00	0.42
1:B:306:LEU:HD23	1:B:309:VAL:HG21	2.02	0.42
1:C:574:VAL:HG21	2:C:902:UNL:C37	2.49	0.42
1:D:606:LYS:HE3	1:D:610:ALA:HB3	2.01	0.42
1:B:49:TYR:HB3	1:B:816:TYR:CE2	2.54	0.42
1:B:492:LEU:HD12	1:B:492:LEU:N	2.34	0.42
1:D:44:LEU:HD22	1:D:54:VAL:CG1	2.49	0.42
1:A:462:ARG:HA	1:A:462:ARG:HD3	1.75	0.42
1:A:507:GLU:HG3	1:A:508:SER:H	1.84	0.42
1:C:649:VAL:HG21	2:C:903:UNL:C38	2.50	0.42
1:C:706:PRO:O	1:C:707:PHE:C	2.62	0.42
1:D:317:VAL:HG13	1:D:317:VAL:O	2.20	0.42
1:D:492:LEU:N	1:D:492:LEU:HD12	2.34	0.42
1:A:242:SER:HB2	1:A:266:CYS:HB2	2.01	0.42
1:B:582:VAL:HA	1:B:585:ILE:HG12	2.02	0.42
1:C:317:VAL:HG13	1:C:317:VAL:O	2.20	0.42
1:D:338:LEU:HD12	1:D:384:MET:HE3	2.02	0.42
1:A:52:ILE:N	1:A:53:PRO:CD	2.82	0.42
1:A:400:LEU:HD21	1:A:546:VAL:HG13	2.01	0.42
1:A:582:VAL:HA	1:A:585:ILE:HG12	2.02	0.42
1:B:44:LEU:HD22	1:B:54:VAL:CG1	2.49	0.42
1:B:331:LEU:HD23	1:B:331:LEU:HA	1.94	0.42
1:B:649:VAL:HG21	2:B:903:UNL:C38	2.50	0.42
1:C:514:THR:O	1:C:514:THR:HG23	2.19	0.42
1:D:27:PHE:CZ	1:D:73:MET:HE2	2.54	0.42
1:D:242:SER:HB2	1:D:266:CYS:HB2	2.01	0.42
1:A:106:LEU:HD13	1:A:121:ILE:HB	2.01	0.42
1:A:570:LEU:HD22	1:D:664:ASN:HB3	2.01	0.42
1:A:577:ILE:HG12	1:A:669:MET:HE2	2.02	0.42
1:A:664:ASN:HB3	1:B:570:LEU:HD22	2.01	0.42
1:B:242:SER:HB2	1:B:266:CYS:HB2	2.01	0.42
1:B:514:THR:HG23	1:B:514:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:VAL:HG21	2:B:902:UNL:C37	2.49	0.42
1:C:488:PHE:HE1	1:C:492:LEU:HD11	1.84	0.42
1:D:106:LEU:HD13	1:D:121:ILE:HB	2.01	0.42
1:D:514:THR:HG23	1:D:514:THR:O	2.19	0.42
1:A:606:LYS:HE3	1:A:610:ALA:HB3	2.01	0.42
1:B:488:PHE:HE1	1:B:492:LEU:HD11	1.85	0.42
1:C:306:LEU:HD23	1:C:309:VAL:HG21	2.02	0.42
1:C:400:LEU:HD21	1:C:546:VAL:HG13	2.01	0.42
1:C:507:GLU:HG3	1:C:508:SER:H	1.84	0.42
1:A:574:VAL:HG21	2:A:902:UNL:C37	2.50	0.42
1:A:649:VAL:HG21	2:A:903:UNL:C38	2.50	0.42
1:B:106:LEU:HD13	1:B:121:ILE:HB	2.01	0.42
1:B:507:GLU:HG3	1:B:508:SER:H	1.84	0.42
1:C:807:ILE:O	1:C:811:ILE:HG12	2.20	0.42
1:A:44:LEU:HD22	1:A:54:VAL:CG1	2.49	0.41
1:B:27:PHE:CZ	1:B:73:MET:HE2	2.54	0.41
1:C:99:LEU:HD12	1:C:99:LEU:HA	1.84	0.41
1:B:255:PHE:O	1:B:256:LYS:C	2.63	0.41
1:B:317:VAL:HG13	1:B:317:VAL:O	2.20	0.41
1:C:360:LEU:HB3	1:C:361:PRO:HD3	2.03	0.41
1:D:649:VAL:HG21	2:D:901:UNL:C38	2.50	0.41
1:A:306:LEU:HD23	1:A:309:VAL:HG21	2.02	0.41
1:A:814:LEU:HD23	1:A:814:LEU:HA	1.96	0.41
1:C:219:LYS:HE3	1:C:219:LYS:HB2	1.64	0.41
1:A:574:VAL:HA	1:A:577:ILE:HD12	2.02	0.41
1:A:678:GLU:C	1:A:680:ASP:N	2.77	0.41
1:B:606:LYS:HE3	1:B:610:ALA:HB3	2.01	0.41
1:C:577:ILE:HG12	1:C:669:MET:HE2	2.02	0.41
1:D:255:PHE:O	1:D:256:LYS:C	2.63	0.41
1:D:593:ILE:HD12	1:D:593:ILE:HA	1.80	0.41
1:D:706:PRO:O	1:D:707:PHE:C	2.62	0.41
1:A:255:PHE:O	1:A:256:LYS:C	2.63	0.41
1:A:360:LEU:HB3	1:A:361:PRO:HD3	2.03	0.41
1:B:360:LEU:HB3	1:B:361:PRO:HD3	2.03	0.41
1:B:805:LYS:HE3	1:B:805:LYS:HB3	1.91	0.41
1:C:334:TRP:CE3	1:C:382:PRO:HB2	2.56	0.41
1:D:306:LEU:HD23	1:D:309:VAL:HG21	2.02	0.41
1:A:35:SER:O	1:A:36:LEU:C	2.63	0.41
1:B:807:ILE:O	1:B:811:ILE:HG12	2.20	0.41
1:C:492:LEU:HD12	1:C:492:LEU:N	2.34	0.41
1:D:334:TRP:CE3	1:D:382:PRO:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.81	0.41
1:A:492:LEU:N	1:A:492:LEU:HD12	2.34	0.41
1:C:575:LYS:HZ3	2:C:902:UNL:C33	2.33	0.41
1:A:674:TYR:OH	1:D:670:ILE:HG13	2.21	0.41
1:A:833:ILE:HD12	1:B:832:LEU:HD13	2.02	0.41
1:B:37:THR:O	1:B:58:MET:HE1	2.21	0.41
1:B:400:LEU:HD21	1:B:546:VAL:HG13	2.01	0.41
1:B:441:ILE:O	1:B:445:VAL:HG23	2.21	0.41
1:B:678:GLU:C	1:B:680:ASP:N	2.78	0.41
1:C:441:ILE:O	1:C:445:VAL:HG23	2.21	0.41
1:D:360:LEU:HB3	1:D:361:PRO:HD3	2.03	0.41
1:D:677:ILE:O	1:D:677:ILE:HG23	2.21	0.41
1:A:37:THR:O	1:A:58:MET:HE1	2.21	0.41
1:A:441:ILE:O	1:A:445:VAL:HG23	2.21	0.41
1:B:352:VAL:O	1:B:356:VAL:HG23	2.21	0.41
1:B:574:VAL:HA	1:B:577:ILE:HD12	2.02	0.41
1:B:577:ILE:HG12	1:B:669:MET:HE2	2.02	0.41
1:B:595:MET:HE1	1:B:650:LEU:HB3	2.03	0.41
1:C:255:PHE:O	1:C:256:LYS:C	2.63	0.41
1:C:352:VAL:O	1:C:356:VAL:HG23	2.21	0.41
1:C:606:LYS:HE3	1:C:610:ALA:HB3	2.01	0.41
1:D:37:THR:O	1:D:58:MET:HE1	2.21	0.41
1:D:574:VAL:HA	1:D:577:ILE:HD12	2.02	0.41
1:D:582:VAL:HA	1:D:585:ILE:HG12	2.02	0.41
1:D:814:LEU:HD23	1:D:814:LEU:HA	1.96	0.41
1:A:832:LEU:HD13	1:D:833:ILE:HD12	2.02	0.41
1:C:634:VAL:O	1:C:634:VAL:HG12	2.21	0.41
1:D:577:ILE:HG12	1:D:669:MET:HE2	2.02	0.41
1:D:678:GLU:C	1:D:680:ASP:N	2.78	0.41
1:A:334:TRP:CE3	1:A:382:PRO:HB2	2.56	0.40
1:A:595:MET:HE1	1:A:650:LEU:HB3	2.03	0.40
1:A:670:ILE:HG13	1:B:674:TYR:OH	2.21	0.40
1:A:807:ILE:O	1:A:811:ILE:HG12	2.20	0.40
1:C:705:PRO:N	1:C:706:PRO:HD2	2.36	0.40
1:C:833:ILE:HD12	1:D:832:LEU:HD13	2.02	0.40
1:D:271:VAL:HG12	1:D:271:VAL:O	2.21	0.40
1:B:833:ILE:HD12	1:C:832:LEU:HD13	2.02	0.40
1:C:106:LEU:HD13	1:C:121:ILE:HB	2.01	0.40
1:D:441:ILE:O	1:D:445:VAL:HG23	2.21	0.40
1:D:807:ILE:O	1:D:811:ILE:HG12	2.20	0.40
1:A:271:VAL:O	1:A:271:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:VAL:O	1:B:271:VAL:HG12	2.21	0.40
1:C:677:ILE:HG23	1:C:677:ILE:O	2.21	0.40
1:D:352:VAL:O	1:D:356:VAL:HG23	2.21	0.40
1:D:705:PRO:N	1:D:706:PRO:HD2	2.36	0.40
1:B:334:TRP:CE3	1:B:382:PRO:HB2	2.56	0.40
1:C:354:LEU:HD12	1:C:354:LEU:HA	1.81	0.40
1:C:595:MET:HE1	1:C:650:LEU:HB3	2.03	0.40
3:C:904:A1CCX:C10	2:D:903:UNL:C47	3.00	0.40
1:D:462:ARG:HA	1:D:462:ARG:HD3	1.75	0.40
1:D:574:VAL:CG1	2:D:904:UNL:C36	2.97	0.40
1:D:595:MET:HE1	1:D:650:LEU:HB3	2.03	0.40
3:A:904:A1CCX:C10	2:B:901:UNL:C47	3.00	0.40
1:B:598:LEU:HD12	1:B:598:LEU:HA	1.96	0.40
1:B:670:ILE:HG13	1:C:674:TYR:OH	2.21	0.40
1:B:705:PRO:N	1:B:706:PRO:HD2	2.36	0.40
2:B:903:UNL:C31	2:B:903:UNL:O3P	2.70	0.40
1:C:663:LEU:CD2	1:D:669:MET:HE3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/820 (90%)	684 (93%)	45 (6%)	10 (1%)	9	33
1	B	739/820 (90%)	684 (93%)	45 (6%)	10 (1%)	9	33
1	C	739/820 (90%)	684 (93%)	45 (6%)	10 (1%)	9	33
1	D	739/820 (90%)	684 (93%)	45 (6%)	10 (1%)	9	33
All	All	2956/3280 (90%)	2736 (93%)	180 (6%)	40 (1%)	11	33

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ALA
1	A	256	LYS
1	A	336	GLU
1	B	46	ALA
1	B	256	LYS
1	B	336	GLU
1	C	46	ALA
1	C	256	LYS
1	C	336	GLU
1	D	46	ALA
1	D	256	LYS
1	D	336	GLU
1	A	335	TYR
1	A	468	LEU
1	B	335	TYR
1	B	468	LEU
1	C	335	TYR
1	C	468	LEU
1	D	335	TYR
1	D	468	LEU
1	A	49	TYR
1	B	49	TYR
1	C	49	TYR
1	D	49	TYR
1	A	257	ASN
1	A	648	TYR
1	A	797	ASP
1	B	257	ASN
1	B	648	TYR
1	B	797	ASP
1	C	257	ASN
1	C	648	TYR
1	C	797	ASP
1	D	257	ASN
1	D	648	TYR
1	D	797	ASP
1	A	47	ALA
1	B	47	ALA
1	C	47	ALA
1	D	47	ALA

5.3.2 Protein sidechains ⓘ

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	656/726 (90%)	649 (99%)	7 (1%)	65	76
1	B	656/726 (90%)	649 (99%)	7 (1%)	65	76
1	C	656/726 (90%)	649 (99%)	7 (1%)	65	76
1	D	656/726 (90%)	649 (99%)	7 (1%)	65	76
All	All	2624/2904 (90%)	2596 (99%)	28 (1%)	63	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	468	LEU
1	A	572	ARG
1	A	593	ILE
1	A	669	MET
1	A	670	ILE
1	A	819	LEU
1	B	29	PHE
1	B	468	LEU
1	B	572	ARG
1	B	593	ILE
1	B	669	MET
1	B	670	ILE
1	B	819	LEU
1	C	29	PHE
1	C	468	LEU
1	C	572	ARG
1	C	593	ILE
1	C	669	MET
1	C	670	ILE
1	C	819	LEU
1	D	29	PHE
1	D	468	LEU
1	D	572	ARG

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Mol	Chain	Res	Type
1	D	593	ILE
1	D	669	MET
1	D	670	ILE
1	D	819	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	403	ASN
1	A	671	ASN
1	B	403	ASN
1	B	470	ASN
1	B	671	ASN
1	C	403	ASN
1	C	470	ASN
1	C	671	ASN
1	D	403	ASN
1	D	470	ASN
1	D	671	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are unknown - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1CCX	B	904	-	29,29,29	4.95	21 (72%)	38,40,40	3.56	13 (34%)
3	A1CCX	D	902	-	29,29,29	4.94	21 (72%)	38,40,40	3.58	13 (34%)
3	A1CCX	A	904	-	29,29,29	4.95	21 (72%)	38,40,40	3.57	13 (34%)
3	A1CCX	C	904	-	29,29,29	4.95	21 (72%)	38,40,40	3.57	13 (34%)

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	A1CCX	B	904	-	-	1/14/23/23	0/4/4/4
3	A1CCX	D	902	-	-	1/14/23/23	0/4/4/4
3	A1CCX	A	904	-	-	1/14/23/23	0/4/4/4
3	A1CCX	C	904	-	-	1/14/23/23	0/4/4/4

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	904	A1CCX	C16-C14	8.68	1.53	1.39
3	C	904	A1CCX	C16-C14	8.68	1.53	1.39
3	D	902	A1CCX	C16-C14	8.68	1.53	1.39
3	A	904	A1CCX	C16-C14	8.66	1.53	1.39
3	A	904	A1CCX	C1-N1	-8.64	1.31	1.47
3	B	904	A1CCX	C1-N1	-8.63	1.31	1.47
3	D	902	A1CCX	C1-N1	-8.62	1.31	1.47
3	C	904	A1CCX	C1-N1	-8.61	1.31	1.47
3	D	902	A1CCX	C17-C15	8.19	1.52	1.38
3	A	904	A1CCX	C17-C15	8.17	1.52	1.38
3	C	904	A1CCX	C17-C15	8.17	1.52	1.38
3	B	904	A1CCX	C17-C15	8.12	1.51	1.38
3	B	904	A1CCX	C10-C9	7.12	1.53	1.38
3	C	904	A1CCX	C10-C9	7.10	1.53	1.38
3	A	904	A1CCX	C10-C9	7.08	1.53	1.38
3	D	902	A1CCX	C10-C9	7.08	1.53	1.38
3	A	904	A1CCX	C7-C5	6.60	1.50	1.39
3	B	904	A1CCX	C7-C5	6.60	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	904	A1CCX	C7-C5	6.59	1.50	1.39
3	D	902	A1CCX	C7-C5	6.58	1.50	1.39
3	A	904	A1CCX	C3-C5	6.31	1.65	1.51
3	C	904	A1CCX	C3-C5	6.31	1.65	1.51
3	D	902	A1CCX	C3-C5	6.31	1.65	1.51
3	B	904	A1CCX	C3-C5	6.28	1.65	1.51
3	A	904	A1CCX	C12-C11	6.09	1.47	1.36
3	B	904	A1CCX	C12-C11	6.05	1.47	1.36
3	D	902	A1CCX	C12-C11	6.05	1.47	1.36
3	B	904	A1CCX	C13-S1	-6.03	1.65	1.74
3	C	904	A1CCX	C13-S1	-6.03	1.65	1.74
3	C	904	A1CCX	C12-C11	6.01	1.47	1.36
3	D	902	A1CCX	C13-S1	-5.98	1.65	1.74
3	A	904	A1CCX	C13-S1	-5.92	1.66	1.74
3	A	904	A1CCX	C6-C4	5.90	1.49	1.39
3	B	904	A1CCX	C6-C4	5.90	1.49	1.39
3	A	904	A1CCX	C18-C19	5.89	1.49	1.38
3	B	904	A1CCX	C18-C19	5.89	1.49	1.38
3	C	904	A1CCX	C18-C19	5.89	1.49	1.38
3	D	902	A1CCX	C18-C19	5.89	1.49	1.38
3	C	904	A1CCX	C6-C4	5.87	1.49	1.39
3	D	902	A1CCX	C6-C4	5.83	1.49	1.39
3	D	902	A1CCX	C13-N3	5.46	1.45	1.36
3	D	902	A1CCX	C1-C2	-5.46	1.41	1.51
3	C	904	A1CCX	C13-N3	5.45	1.45	1.36
3	A	904	A1CCX	C1-C2	-5.44	1.41	1.51
3	B	904	A1CCX	C1-C2	-5.44	1.41	1.51
3	A	904	A1CCX	C13-N3	5.43	1.44	1.36
3	B	904	A1CCX	C13-N3	5.43	1.44	1.36
3	C	904	A1CCX	C1-C2	-5.41	1.41	1.51
3	B	904	A1CCX	C18-C16	-5.18	1.30	1.38
3	C	904	A1CCX	C18-C16	-5.18	1.30	1.38
3	A	904	A1CCX	C18-C16	-5.12	1.30	1.38
3	D	902	A1CCX	C18-C16	-5.12	1.30	1.38
3	A	904	A1CCX	C8-N1	5.09	1.43	1.34
3	B	904	A1CCX	C8-N1	5.09	1.43	1.34
3	C	904	A1CCX	C8-N1	5.06	1.43	1.34
3	D	902	A1CCX	C8-N1	5.06	1.43	1.34
3	A	904	A1CCX	C15-C14	-4.88	1.31	1.39
3	C	904	A1CCX	C15-C14	-4.88	1.31	1.39
3	B	904	A1CCX	C15-C14	-4.84	1.31	1.39
3	D	902	A1CCX	C15-C14	-4.81	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	904	A1CCX	C9-C6	-4.25	1.31	1.38
3	B	904	A1CCX	C9-C6	-4.24	1.31	1.38
3	A	904	A1CCX	C9-C6	-4.22	1.31	1.38
3	D	902	A1CCX	C9-C6	-4.18	1.31	1.38
3	A	904	A1CCX	C17-C19	-3.64	1.31	1.38
3	B	904	A1CCX	C17-C19	-3.64	1.31	1.38
3	C	904	A1CCX	C17-C19	-3.64	1.31	1.38
3	D	902	A1CCX	C17-C19	-3.64	1.31	1.38
3	A	904	A1CCX	O1-C8	-3.54	1.15	1.23
3	D	902	A1CCX	O1-C8	-3.54	1.15	1.23
3	B	904	A1CCX	O1-C8	-3.50	1.15	1.23
3	C	904	A1CCX	O1-C8	-3.50	1.15	1.23
3	A	904	A1CCX	C3-N1	-3.44	1.41	1.46
3	B	904	A1CCX	C3-N1	-3.44	1.41	1.46
3	C	904	A1CCX	C3-N1	-3.43	1.41	1.46
3	D	902	A1CCX	C3-N1	-3.43	1.41	1.46
3	A	904	A1CCX	C10-C7	-3.38	1.33	1.38
3	B	904	A1CCX	C10-C7	-3.35	1.33	1.38
3	D	902	A1CCX	C10-C7	-3.32	1.33	1.38
3	C	904	A1CCX	C10-C7	-3.29	1.33	1.38
3	A	904	A1CCX	C14-N3	2.28	1.46	1.41
3	B	904	A1CCX	C14-N3	2.28	1.46	1.41
3	C	904	A1CCX	C14-N3	2.28	1.46	1.41
3	D	902	A1CCX	C14-N3	2.24	1.46	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	A1CCX	C2-C1-N1	15.34	125.85	110.03
3	A	904	A1CCX	C2-C1-N1	15.28	125.78	110.03
3	C	904	A1CCX	C2-C1-N1	15.25	125.75	110.03
3	B	904	A1CCX	C2-C1-N1	15.19	125.69	110.03
3	B	904	A1CCX	C5-C3-N1	7.69	123.19	111.56
3	C	904	A1CCX	C5-C3-N1	7.68	123.19	111.56
3	D	902	A1CCX	C5-C3-N1	7.68	123.19	111.56
3	A	904	A1CCX	C5-C3-N1	7.67	123.17	111.56
3	B	904	A1CCX	C1-C2-C4	5.63	121.06	111.34
3	C	904	A1CCX	C1-C2-C4	5.62	121.04	111.34
3	D	902	A1CCX	C1-C2-C4	5.61	121.03	111.34
3	A	904	A1CCX	C1-C2-C4	5.60	121.01	111.34
3	A	904	A1CCX	C8-C11-N2	5.13	132.68	123.70
3	A	904	A1CCX	C12-C11-N2	-5.13	108.38	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	A1CCX	C12-C11-N2	-5.12	108.39	115.43
3	D	902	A1CCX	C8-C11-N2	5.12	132.66	123.70
3	C	904	A1CCX	C12-C11-N2	-5.11	108.40	115.43
3	B	904	A1CCX	C8-C11-N2	5.11	132.64	123.70
3	C	904	A1CCX	C8-C11-N2	5.11	132.64	123.70
3	B	904	A1CCX	C12-C11-N2	-5.10	108.41	115.43
3	B	904	A1CCX	O1-C8-C11	-4.69	111.38	118.65
3	C	904	A1CCX	O1-C8-C11	-4.69	111.38	118.65
3	A	904	A1CCX	O1-C8-C11	-4.67	111.41	118.65
3	D	902	A1CCX	O1-C8-C11	-4.67	111.41	118.65
3	D	902	A1CCX	C2-C4-C5	-3.47	113.36	120.77
3	A	904	A1CCX	C2-C4-C5	-3.46	113.38	120.77
3	B	904	A1CCX	C2-C4-C5	-3.44	113.43	120.77
3	C	904	A1CCX	C2-C4-C5	-3.44	113.43	120.77
3	A	904	A1CCX	C14-N3-C13	-3.20	122.63	129.46
3	B	904	A1CCX	C14-N3-C13	-3.20	122.63	129.46
3	D	902	A1CCX	C14-N3-C13	-3.19	122.65	129.46
3	C	904	A1CCX	C14-N3-C13	-3.18	122.67	129.46
3	D	902	A1CCX	S1-C13-N2	2.61	118.43	115.69
3	B	904	A1CCX	S1-C13-N2	2.60	118.42	115.69
3	C	904	A1CCX	S1-C13-N2	2.60	118.42	115.69
3	A	904	A1CCX	S1-C13-N2	2.60	118.42	115.69
3	B	904	A1CCX	C3-C5-C7	2.32	126.18	119.86
3	D	902	A1CCX	C3-C5-C7	2.32	126.16	119.86
3	A	904	A1CCX	C3-C5-C7	2.31	126.15	119.86
3	C	904	A1CCX	C3-C5-C7	2.31	126.13	119.86
3	C	904	A1CCX	C2-C4-C6	2.24	125.72	121.05
3	D	902	A1CCX	C2-C4-C6	2.24	125.72	121.05
3	A	904	A1CCX	C2-C4-C6	2.24	125.72	121.05
3	B	904	A1CCX	C2-C4-C6	2.23	125.72	121.05
3	A	904	A1CCX	O1-C8-N1	-2.23	119.15	122.67
3	D	902	A1CCX	O1-C8-N1	-2.22	119.16	122.67
3	B	904	A1CCX	O1-C8-N1	-2.21	119.17	122.67
3	C	904	A1CCX	O1-C8-N1	-2.21	119.17	122.67
3	B	904	A1CCX	C12-S1-C13	2.19	90.10	88.40
3	C	904	A1CCX	C12-S1-C13	2.16	90.08	88.40
3	A	904	A1CCX	C12-S1-C13	2.14	90.06	88.40
3	D	902	A1CCX	C12-S1-C13	2.14	90.06	88.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

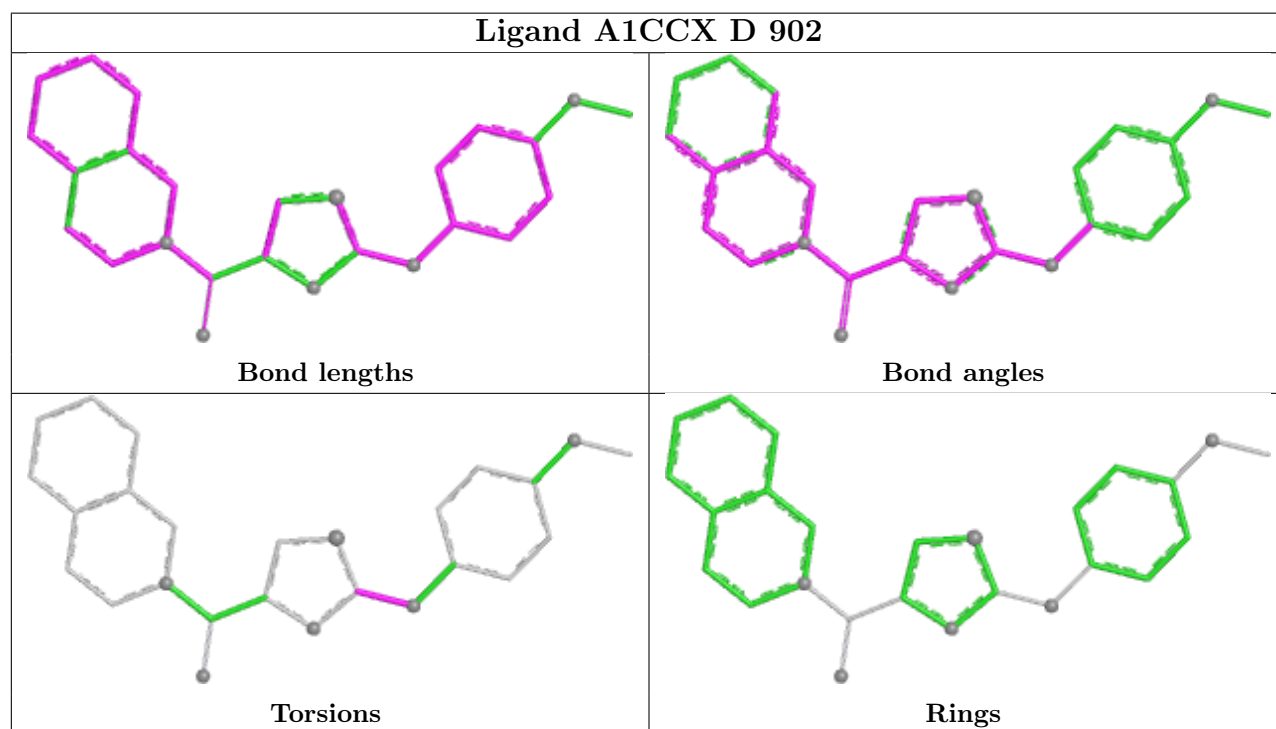
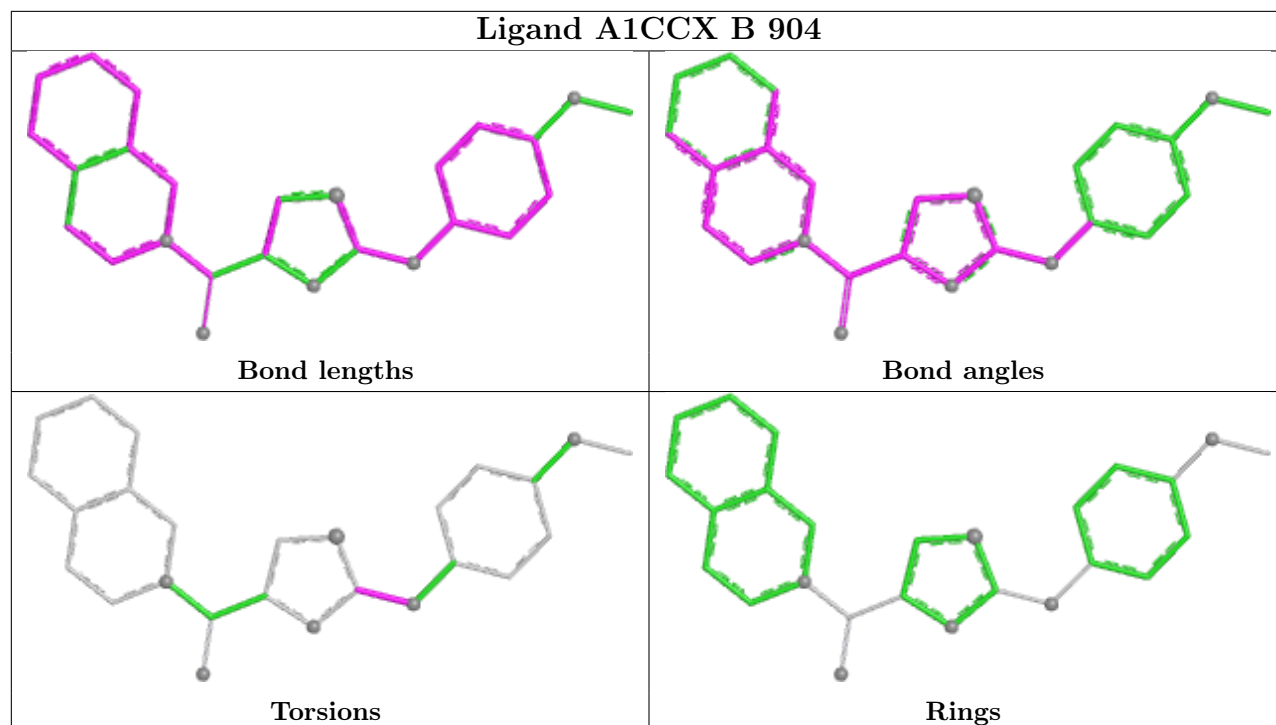
Mol	Chain	Res	Type	Atoms
3	A	904	A1CCX	N2-C13-N3-C14
3	B	904	A1CCX	N2-C13-N3-C14
3	C	904	A1CCX	N2-C13-N3-C14
3	D	902	A1CCX	N2-C13-N3-C14

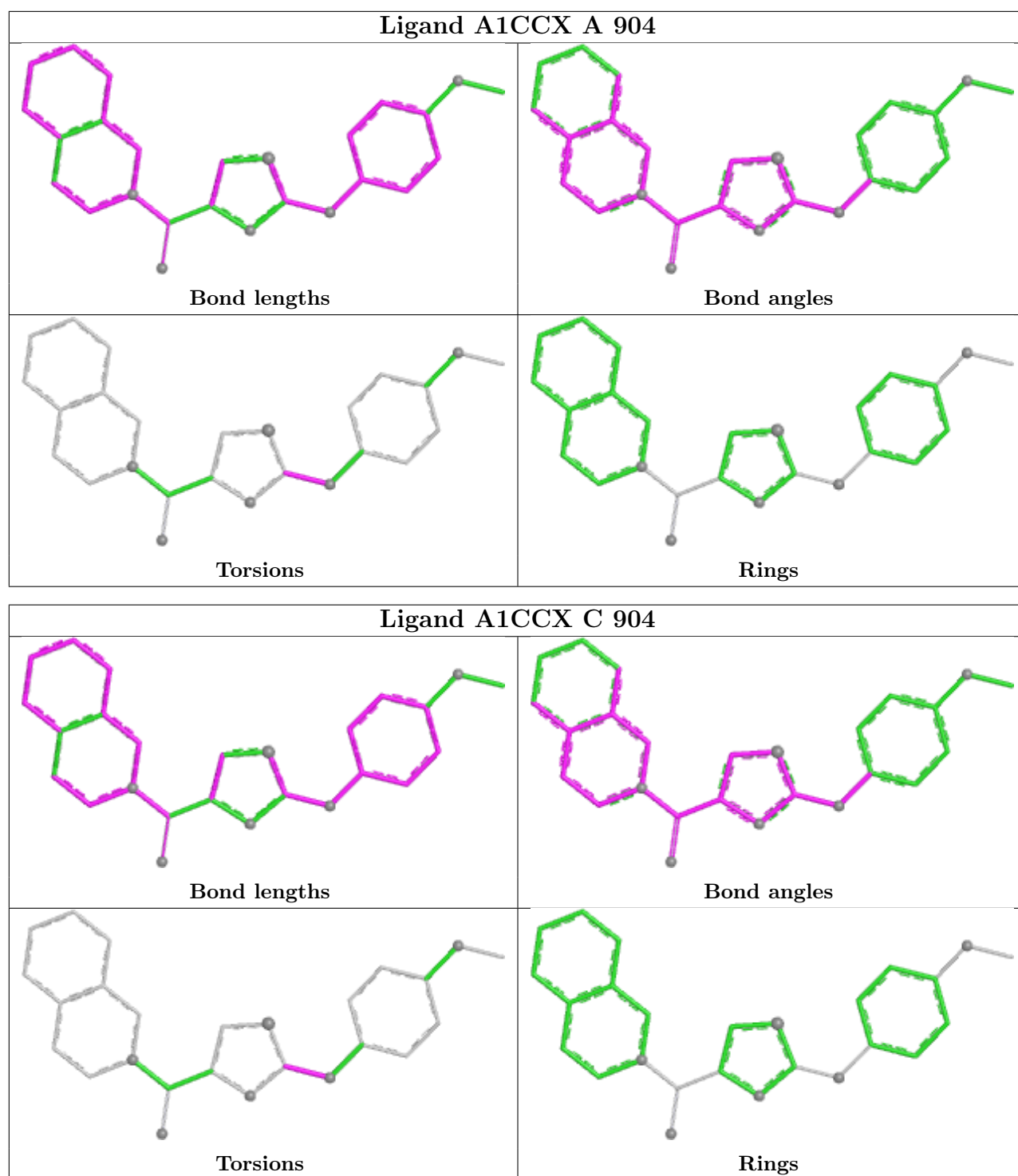
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	904	A1CCX	1	0
3	D	902	A1CCX	1	0
3	A	904	A1CCX	2	0
3	C	904	A1CCX	2	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 than 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.





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.

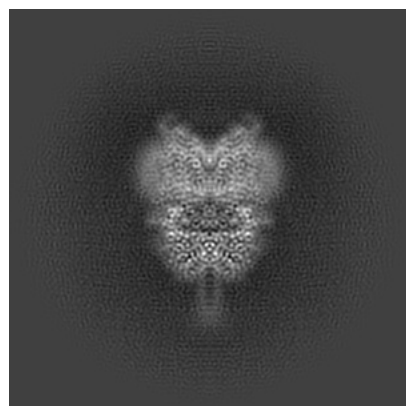
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70601. These allow visual inspection of the internal detail of the map and identification of artifacts.

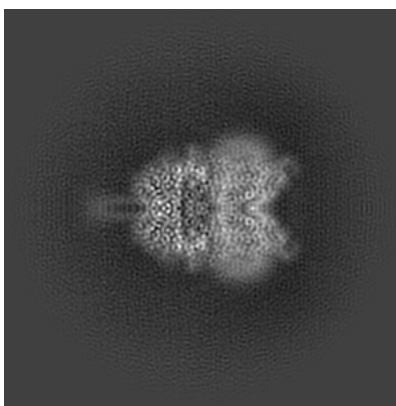
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

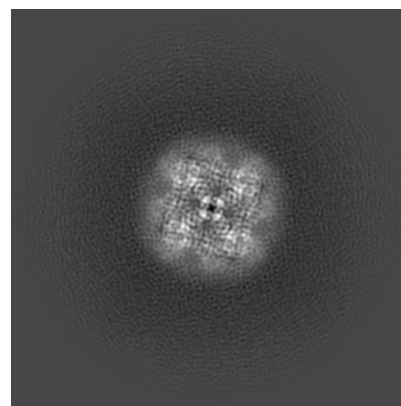
6.1.1 Primary map



X

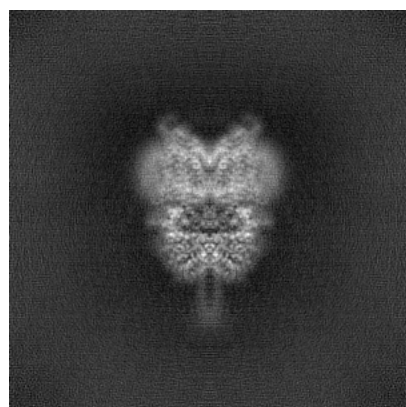


Y

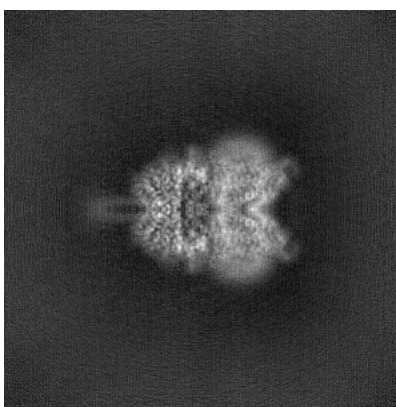


Z

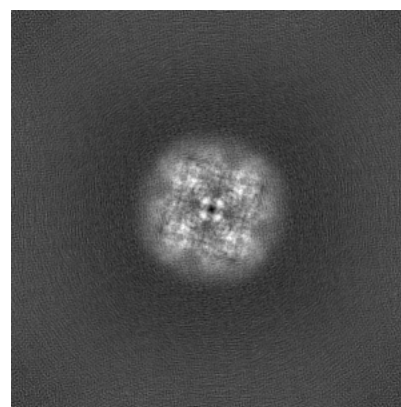
6.1.2 Raw map



X



Y

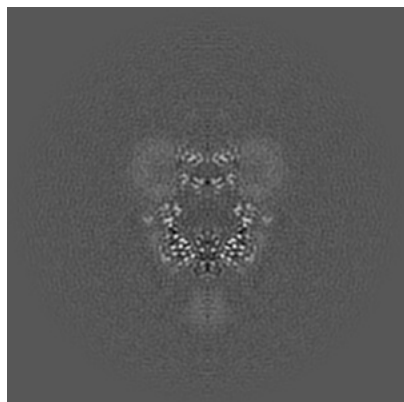


Z

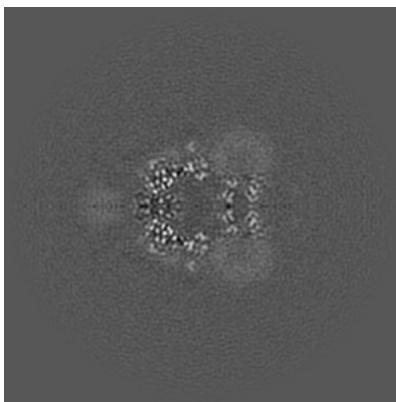
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

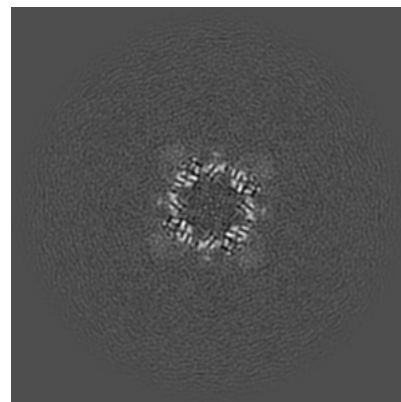
6.2.1 Primary map



X Index: 150

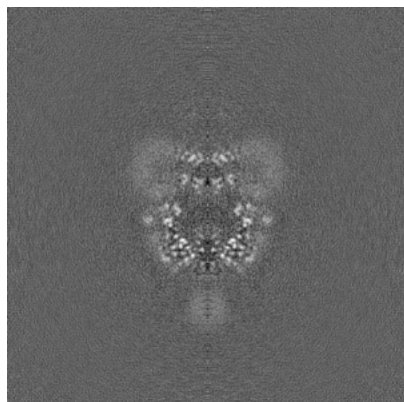


Y Index: 150

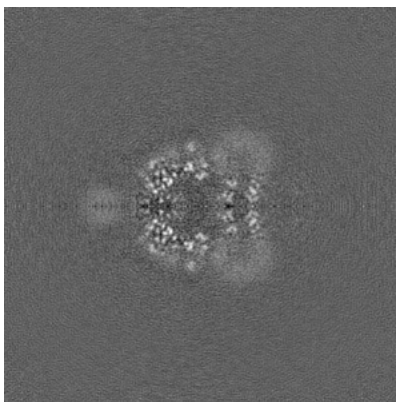


Z Index: 150

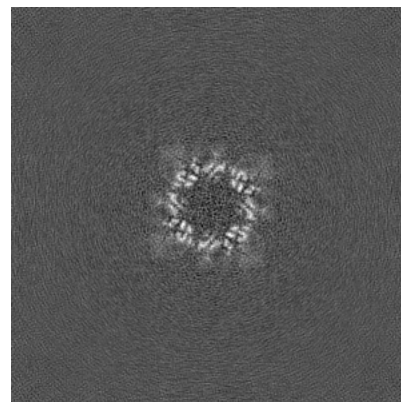
6.2.2 Raw map



X Index: 150



Y Index: 150

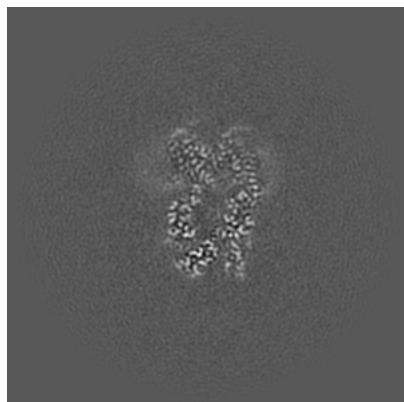


Z Index: 150

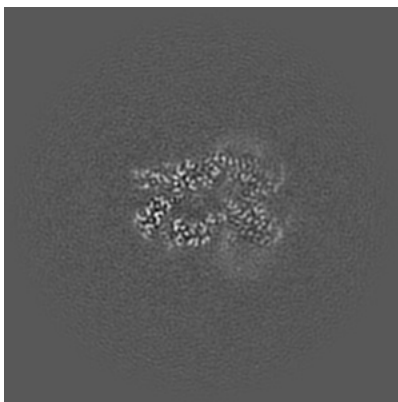
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

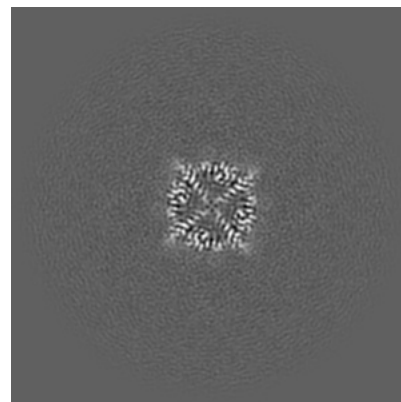
6.3.1 Primary map



X Index: 133

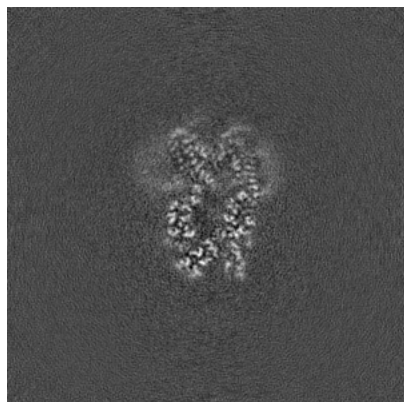


Y Index: 167

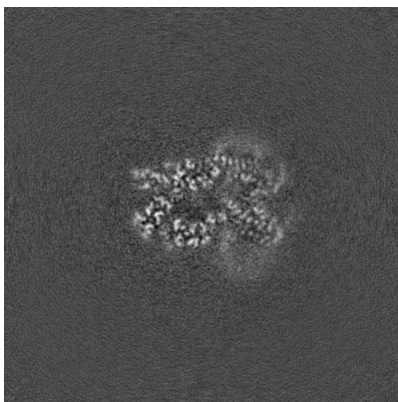


Z Index: 131

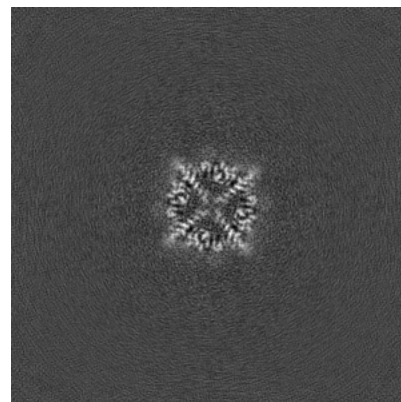
6.3.2 Raw map



X Index: 133



Y Index: 167

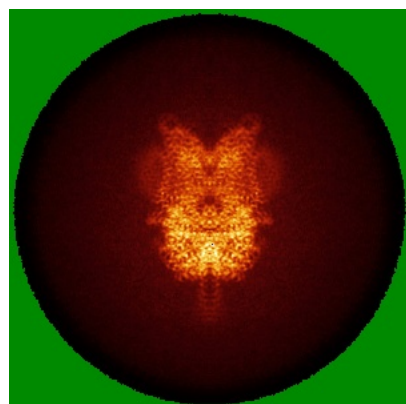


Z Index: 131

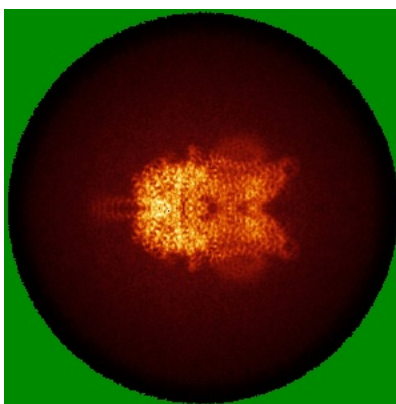
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

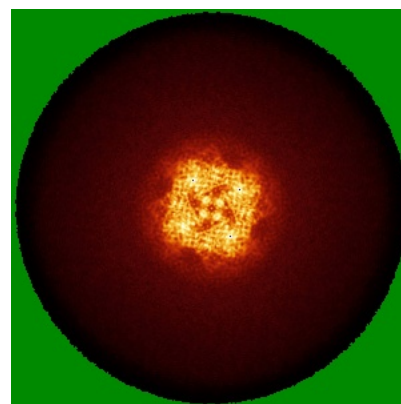
6.4.1 Primary map



X

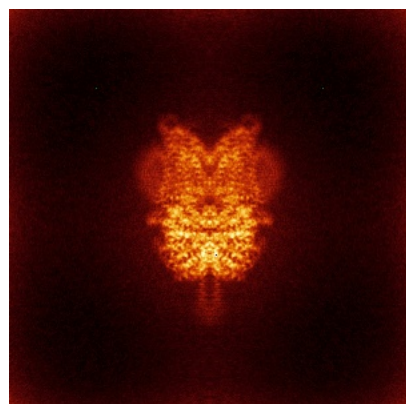


Y

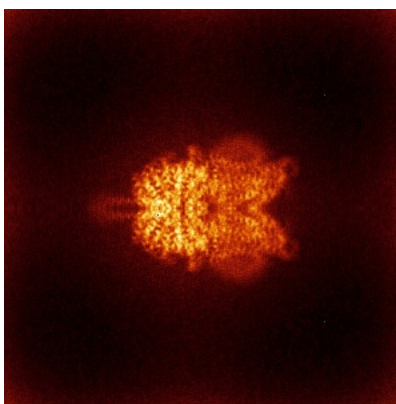


Z

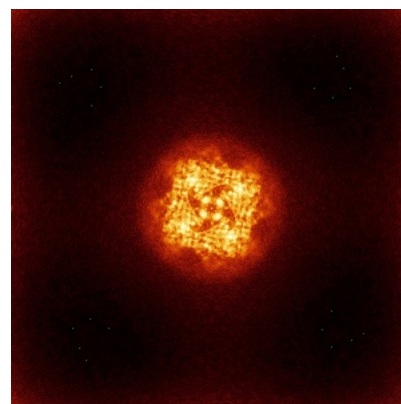
6.4.2 Raw map



X



Y

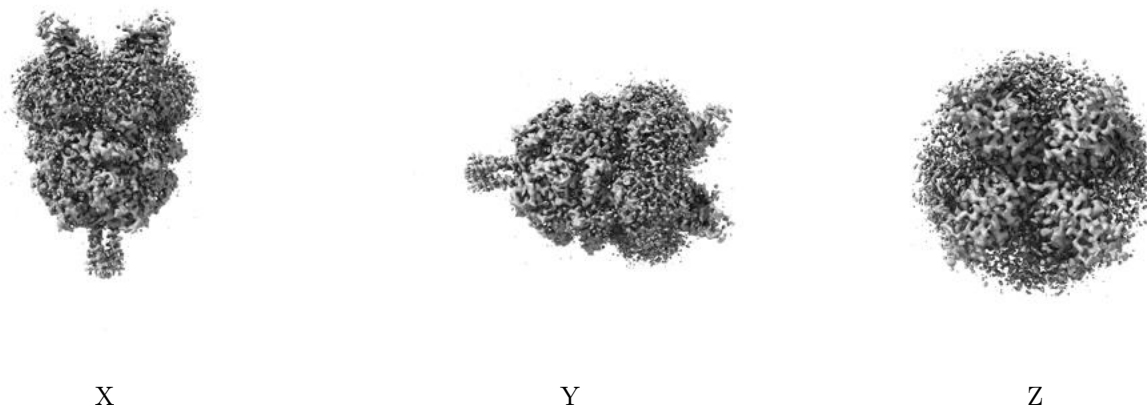


Z

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.

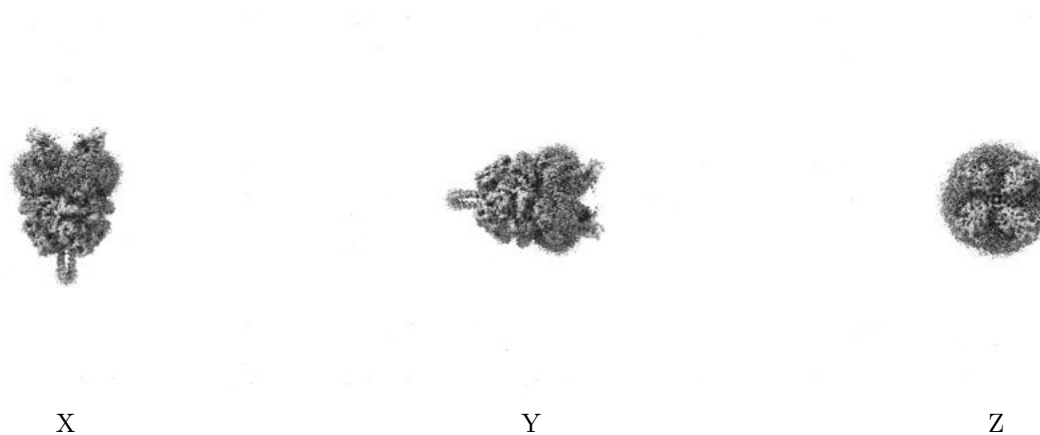
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.051. 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



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.

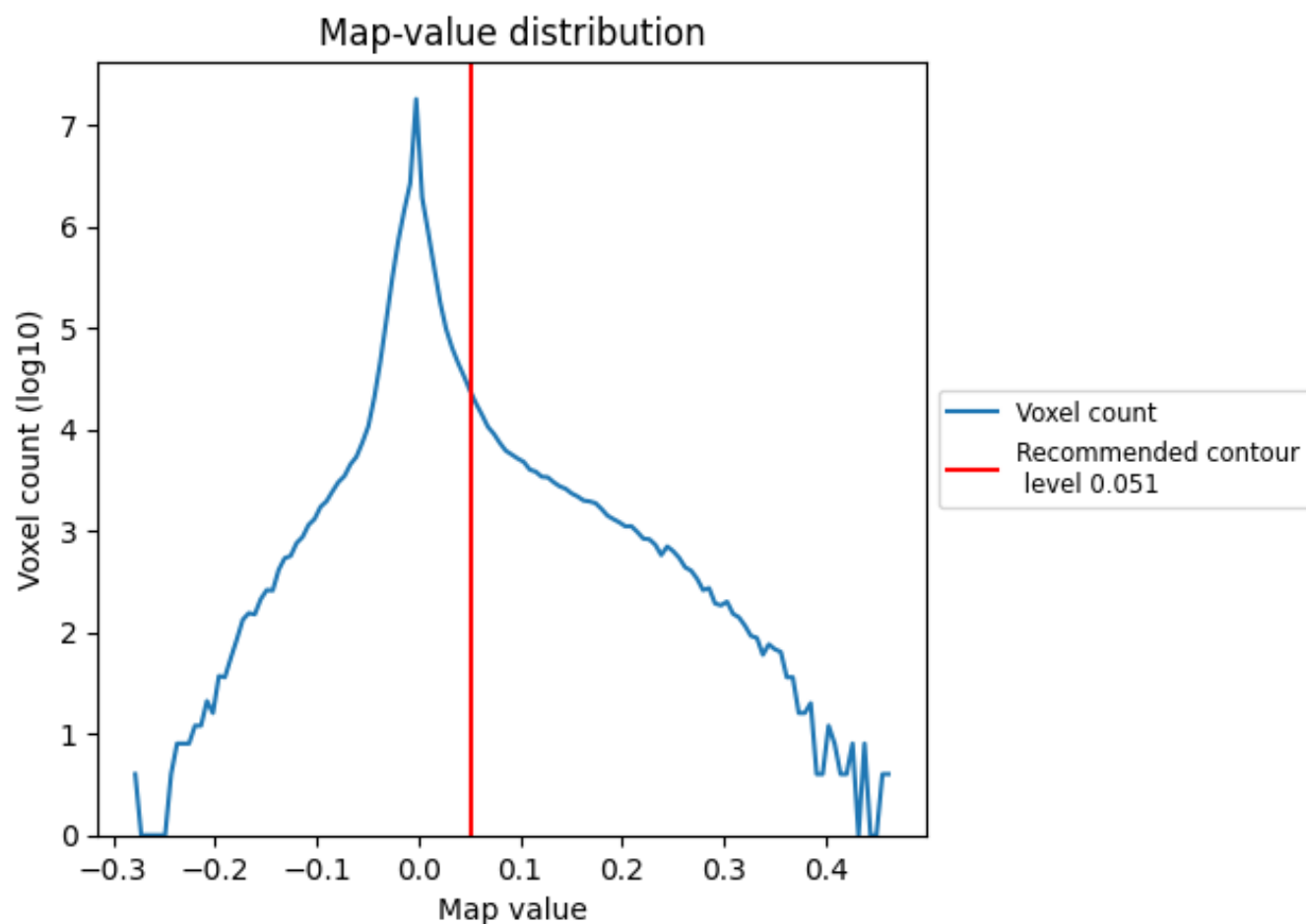
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

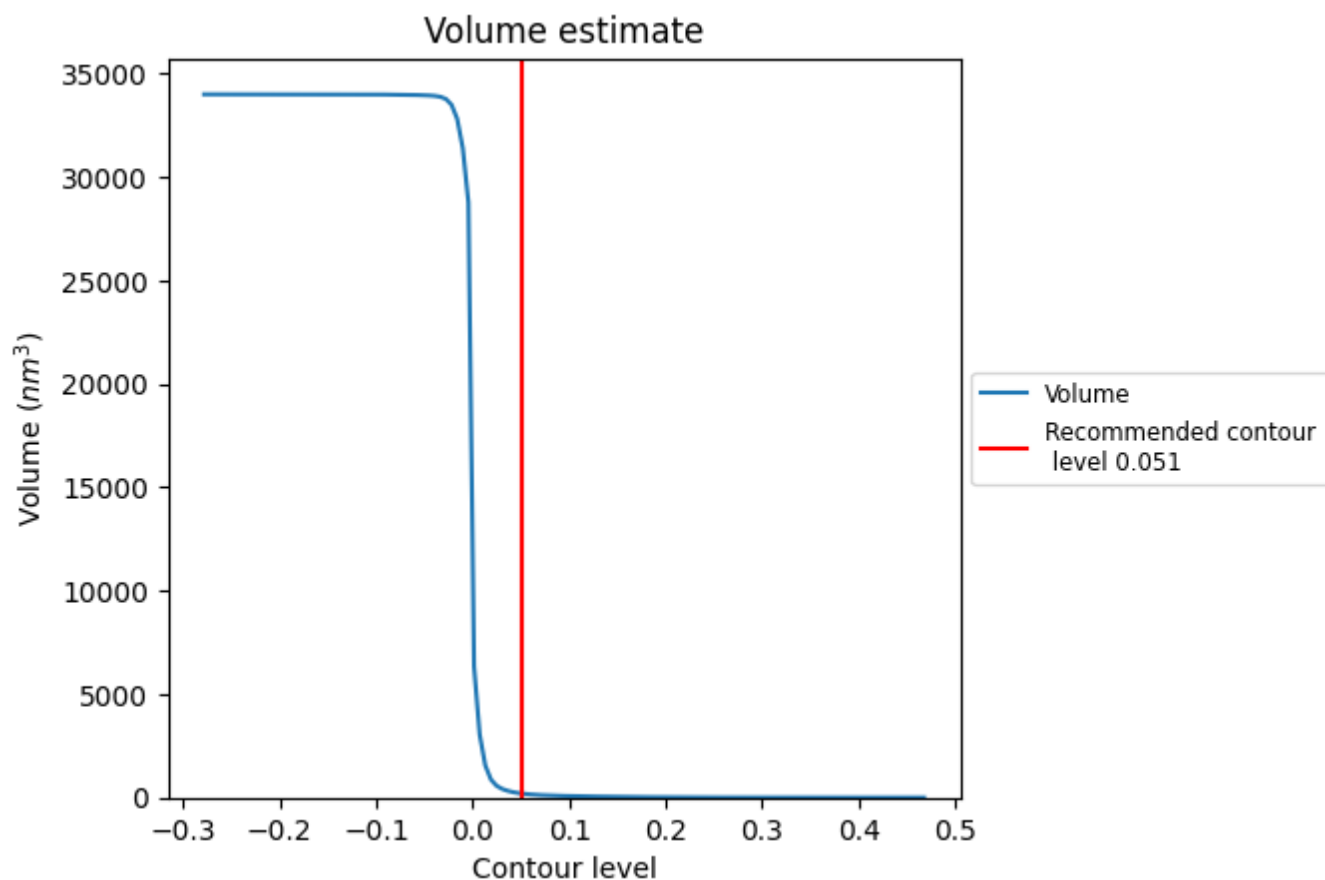
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

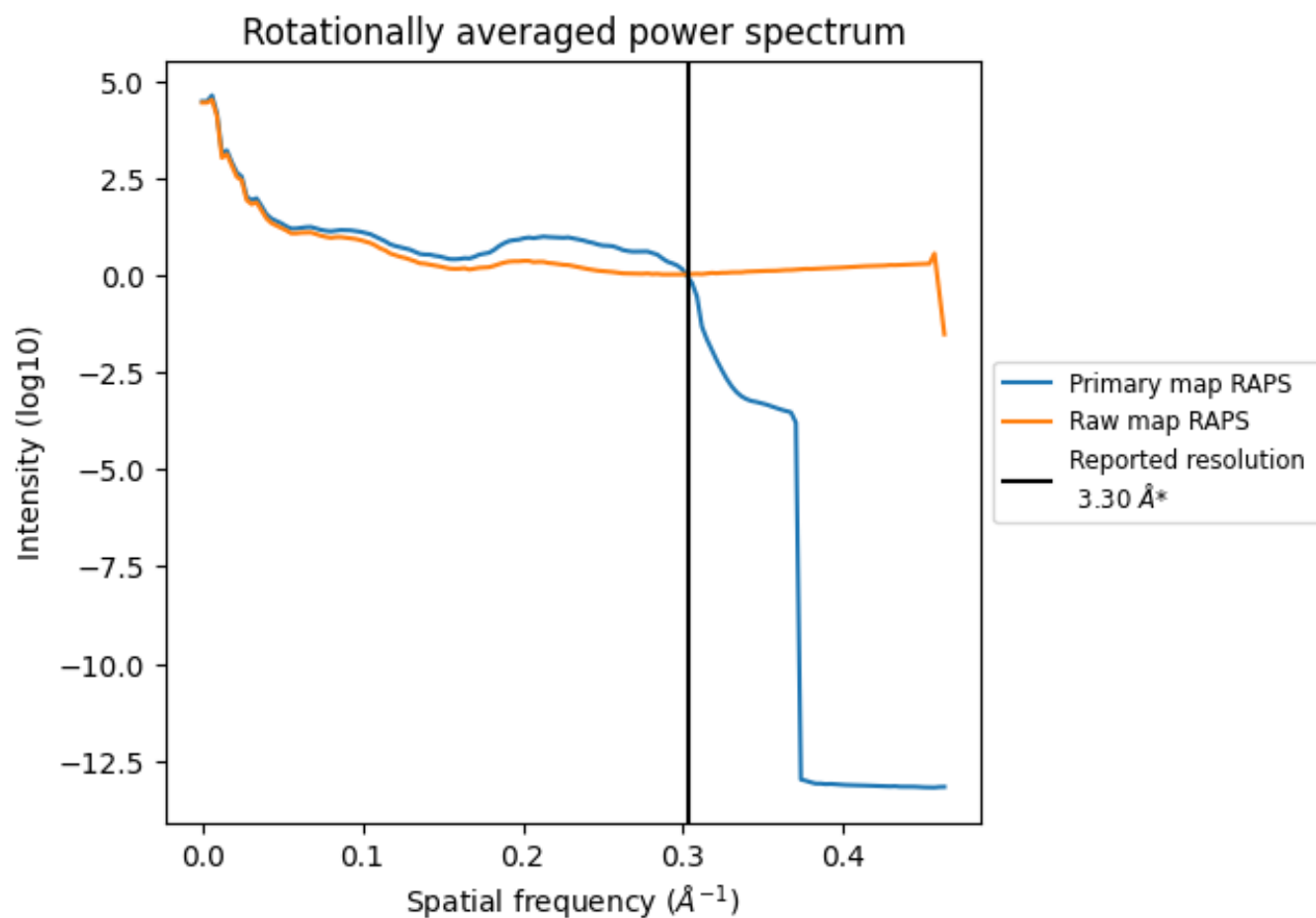
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 175 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 ⓘ

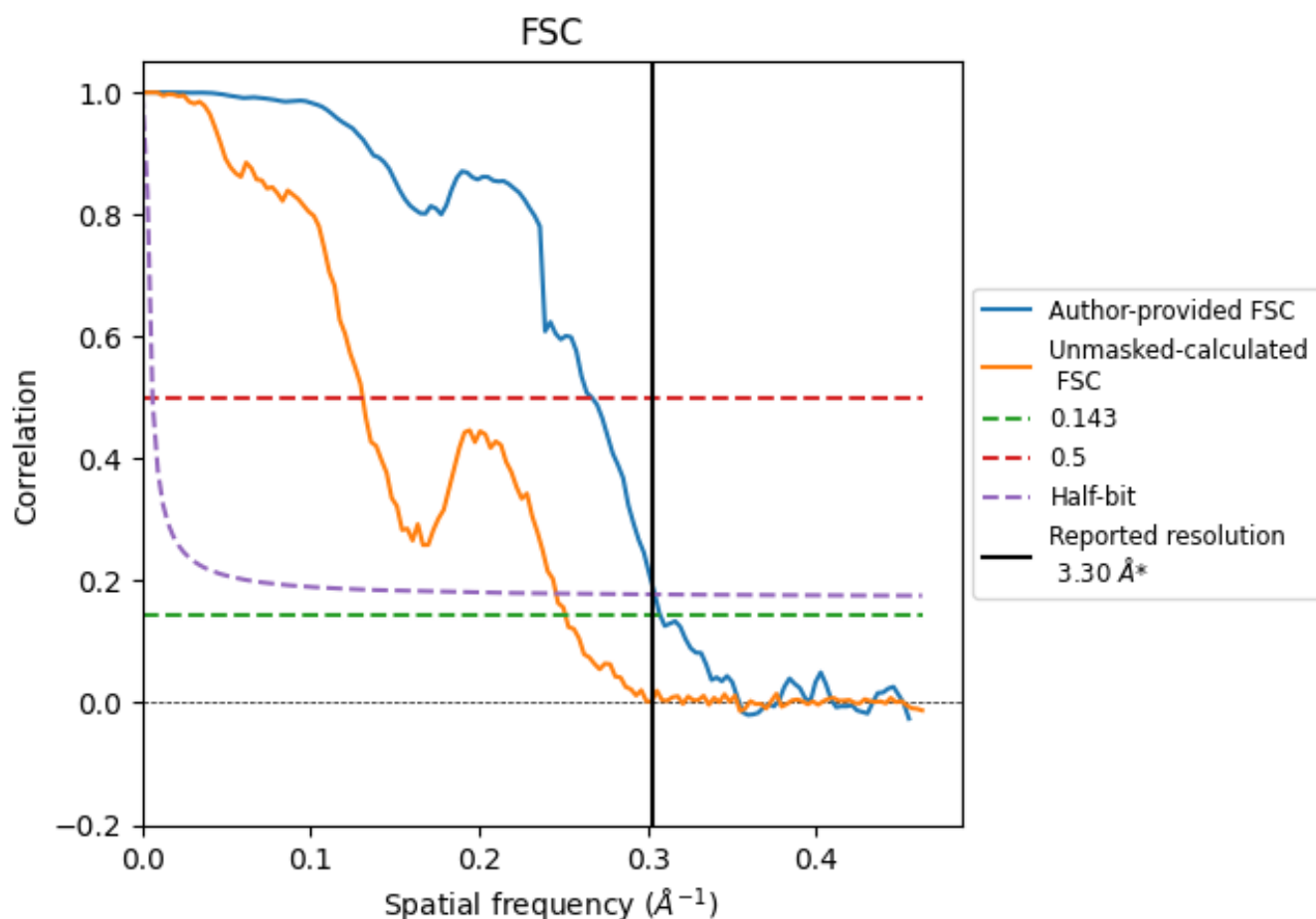


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

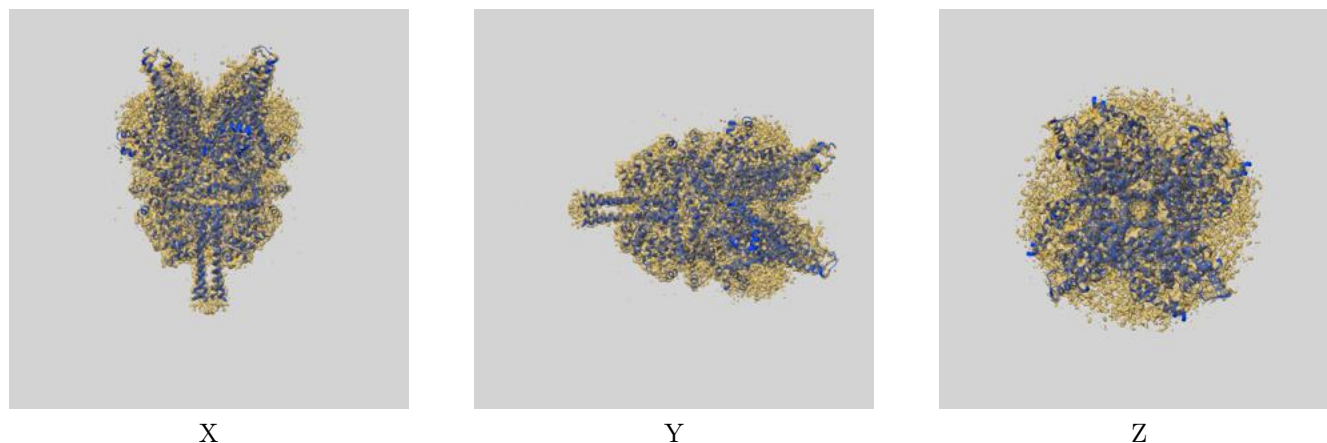
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.75	3.29
Unmasked-calculated*	3.98	7.64	4.07

*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 3.98 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

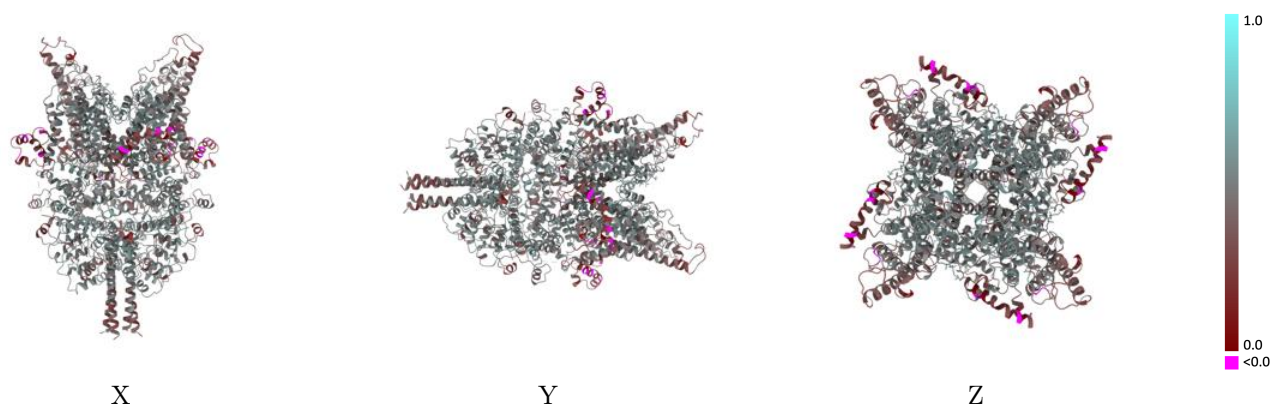
This section contains information regarding the fit between EMDB map EMD-70601 and PDB model 9OLX. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



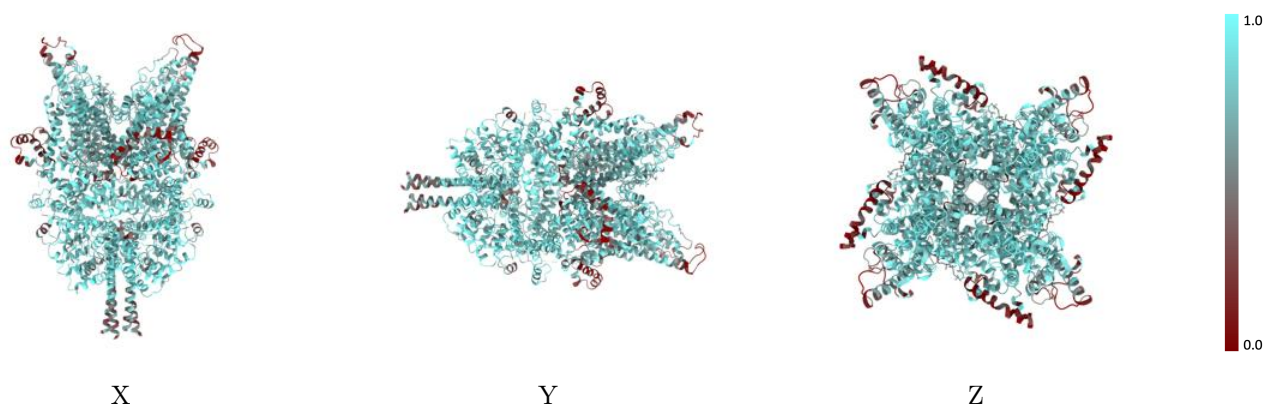
The images above show the 3D surface view of the map at the recommended contour level 0.051 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



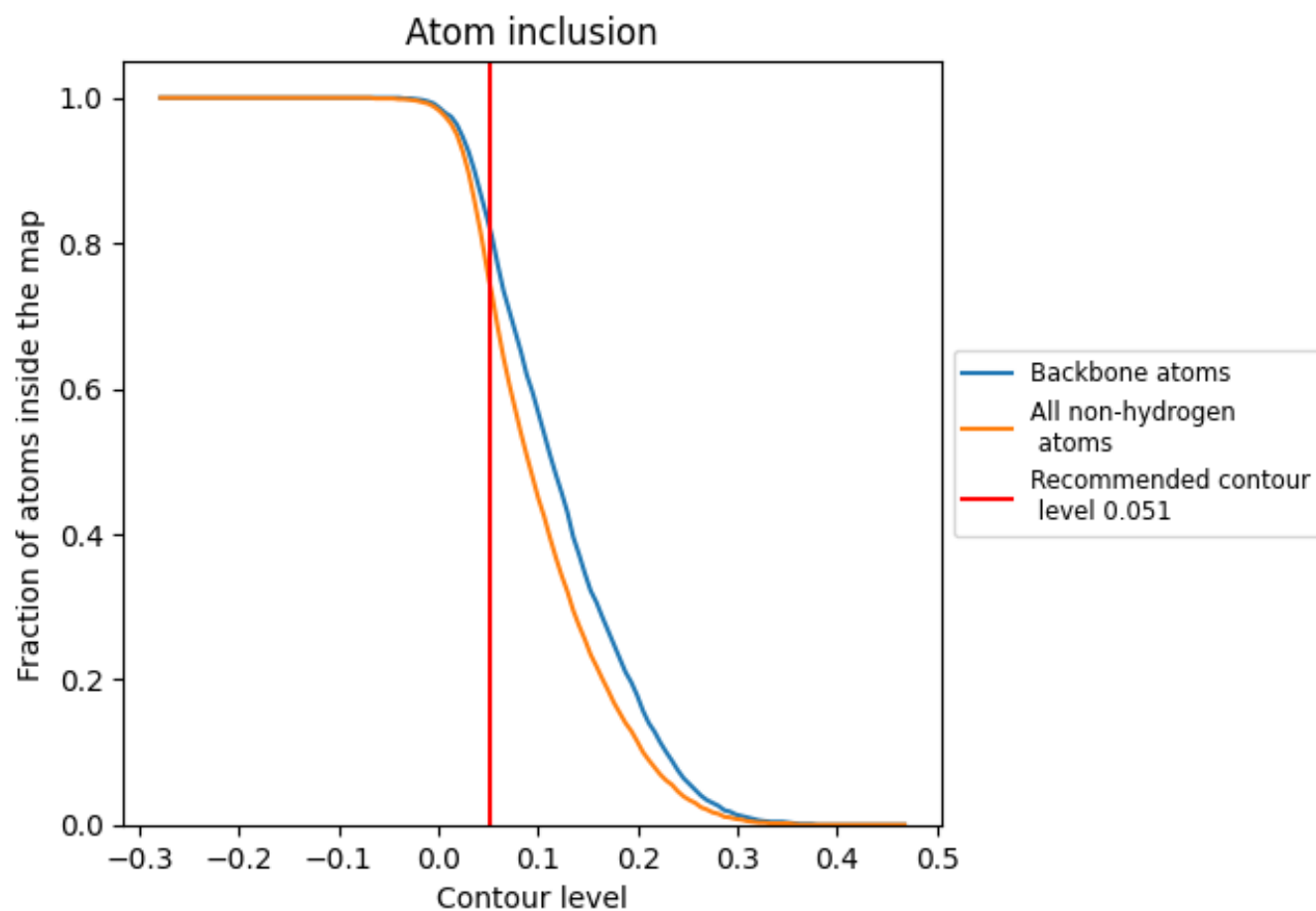
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.051).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.051) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7490	<div></div> 0.4480
A	<div></div> 0.7490	<div></div> 0.4480
B	<div></div> 0.7490	<div></div> 0.4480
C	<div></div> 0.7490	<div></div> 0.4480
D	<div></div> 0.7500	<div></div> 0.4480

