



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 01:54 AM EDT

PDB ID : 6V4J
EMDB ID : EMD-21041
Title : Structure of TrkH-TrkA in complex with ATP
Authors : Zhou, M.; Zhang, H.
Deposited on : 2019-11-27
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

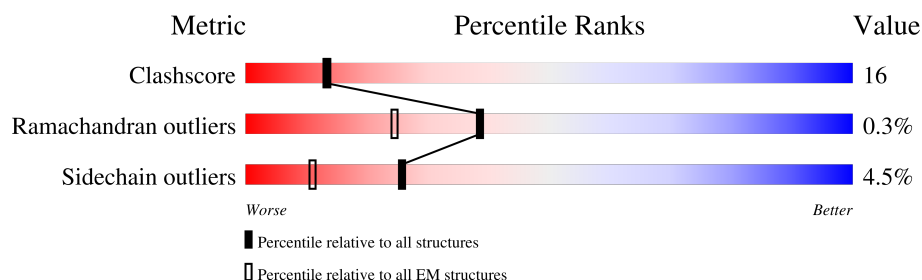
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

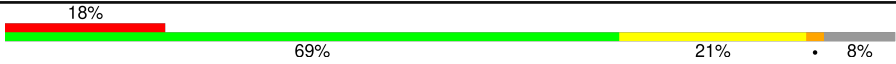

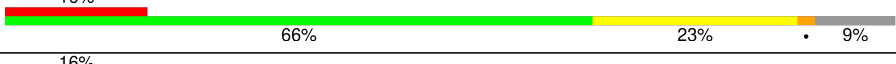



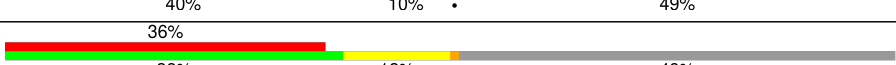
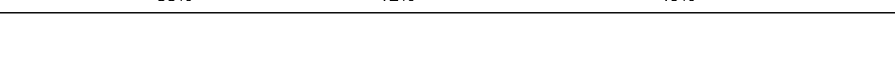
The reported resolution of this entry is 2.97 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	485	
1	B	485	
1	C	485	
1	D	485	
2	E	458	
2	F	458	
2	G	458	
2	H	458	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20637 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 Trk system potassium uptake protein TrkH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	447	Total	C	N	O	S	0	0
			3450	2320	538	575	17		
1	B	434	Total	C	N	O	S	0	0
			3354	2256	524	557	17		
1	C	442	Total	C	N	O	S	0	0
			3414	2297	532	568	17		
1	D	438	Total	C	N	O	S	0	0
			3390	2282	528	563	17		

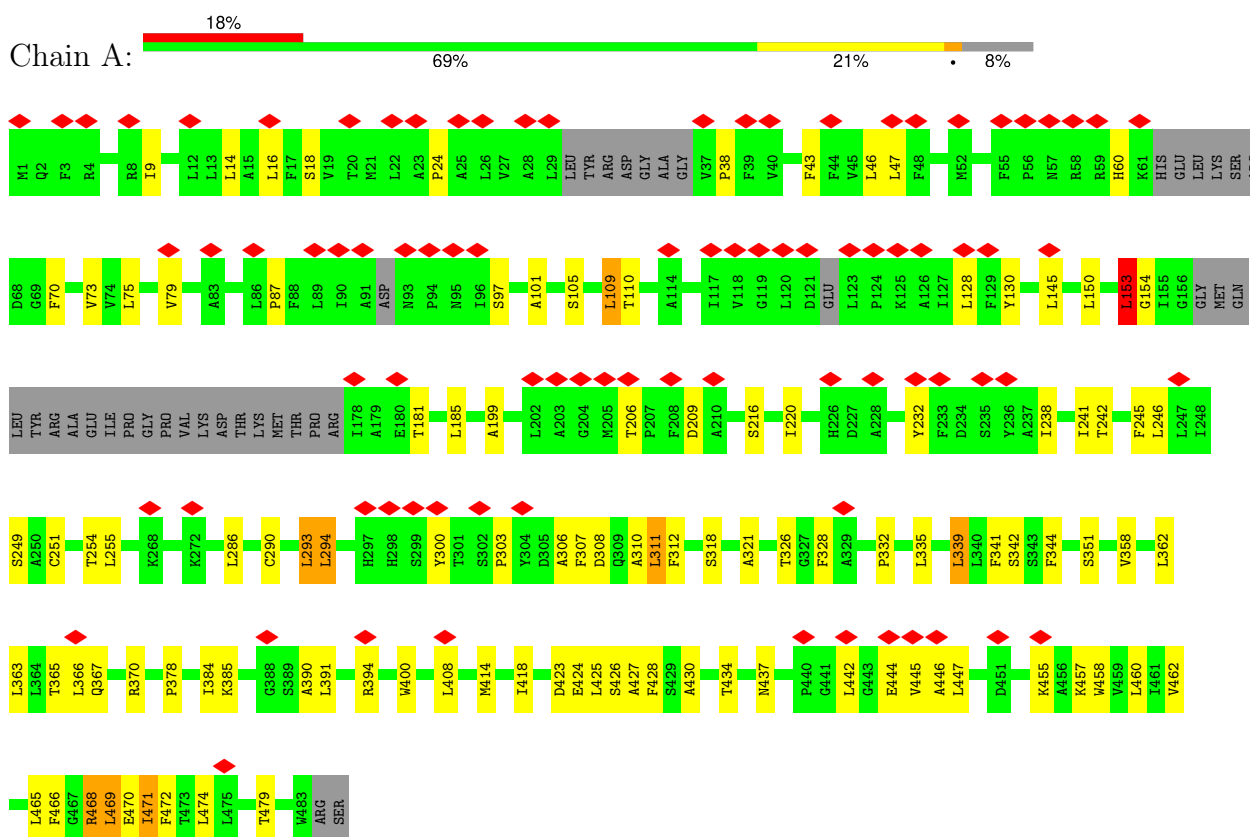
- Molecule 2 is a protein called Potassium uptake protein TrkA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	234	Total	C	N	O	S	0	0
			1748	1088	303	348	9		
2	F	234	Total	C	N	O	S	0	0
			1767	1099	307	351	10		
2	G	234	Total	C	N	O	S	0	0
			1753	1090	307	347	9		
2	H	234	Total	C	N	O	S	0	0
			1761	1094	307	351	9		

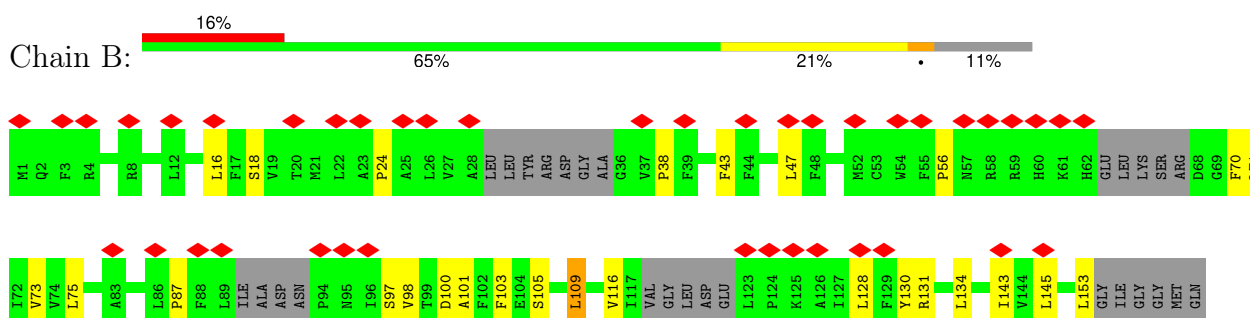
3 Residue-property plots

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.

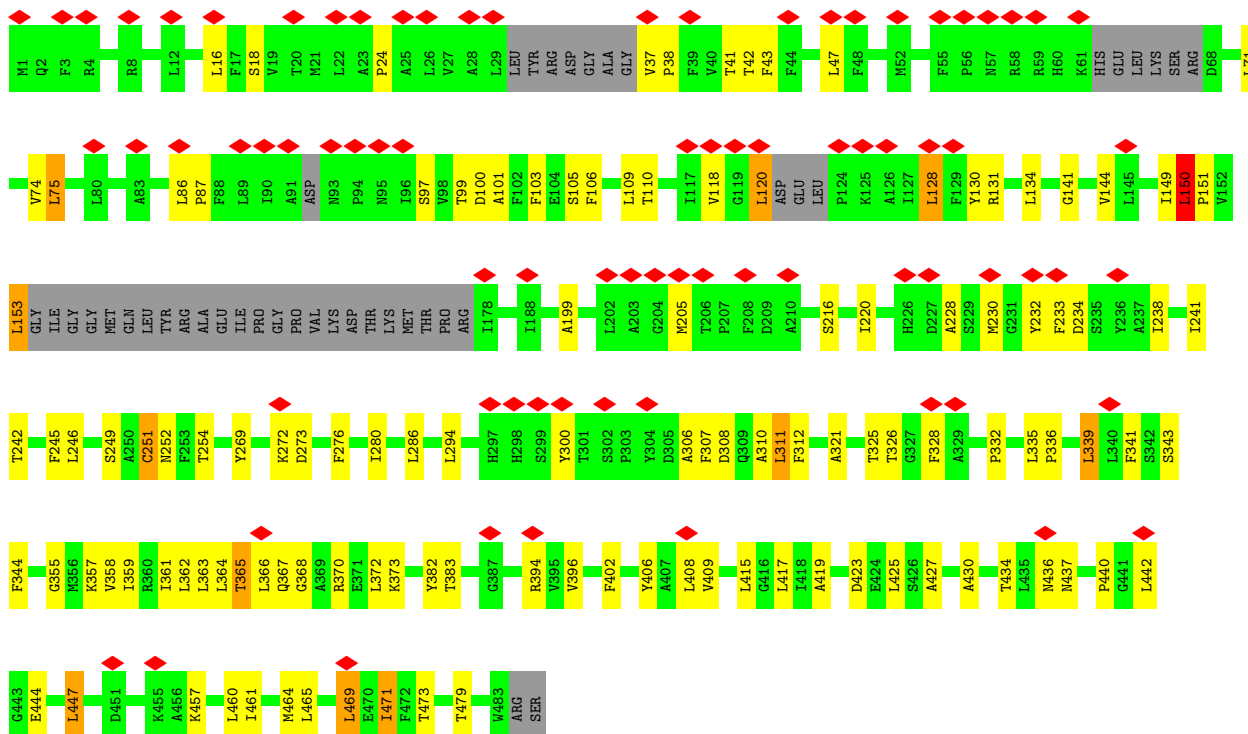
- Molecule 1: Trk system potassium uptake protein TrkH



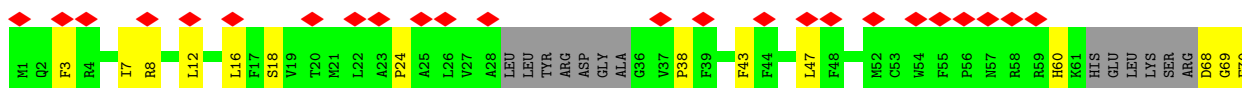
- Molecule 1: Trk system potassium uptake protein TrkH

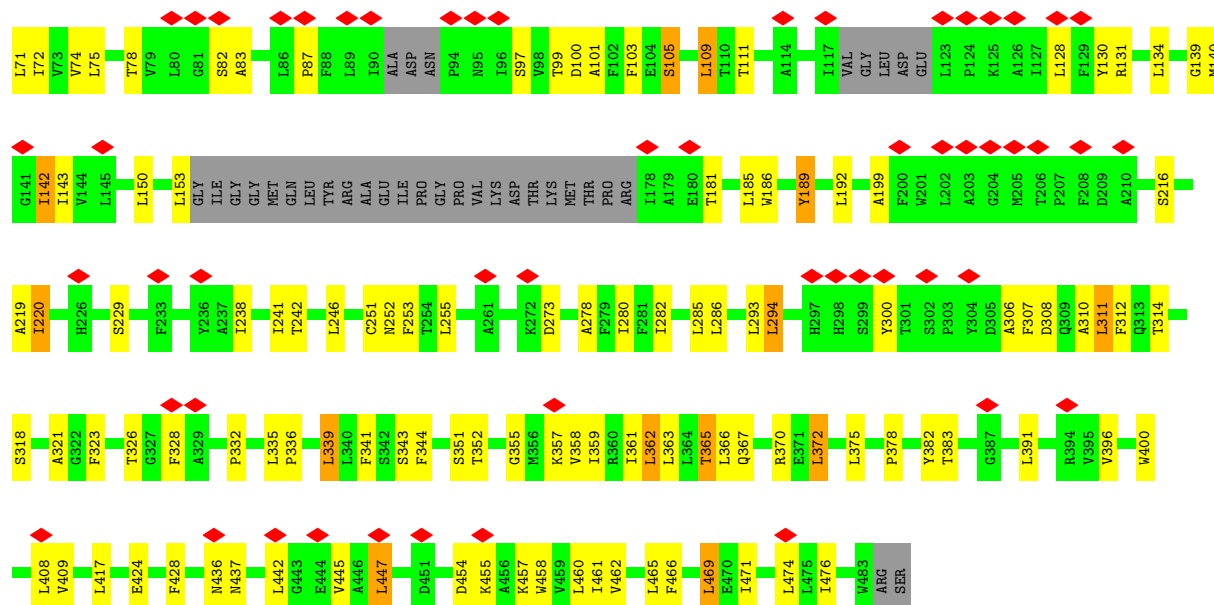


- Molecule 1: Trk system potassium uptake protein TrkH

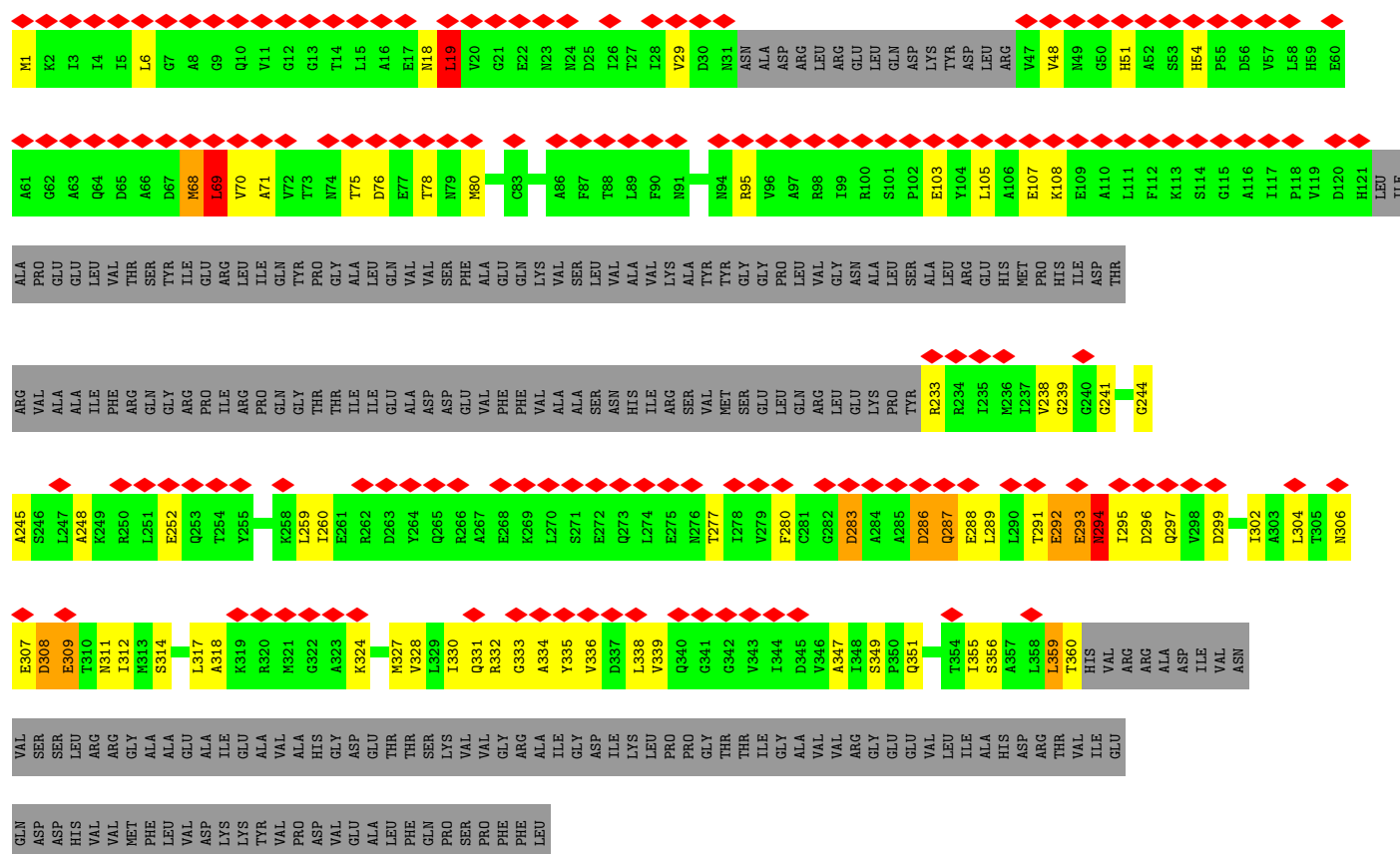
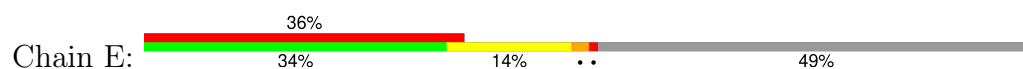


- Molecule 1: Trk system potassium uptake protein TrkH





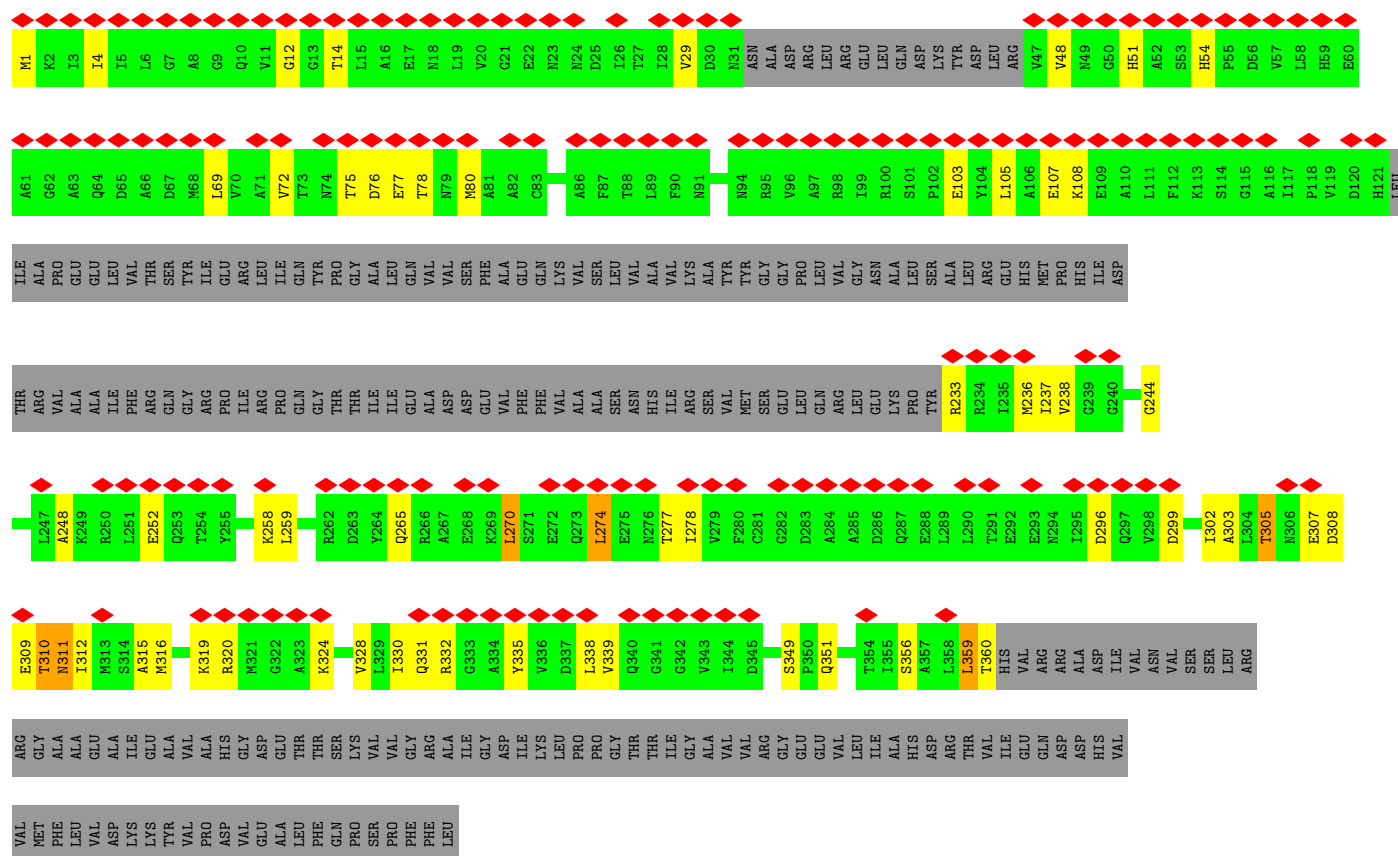
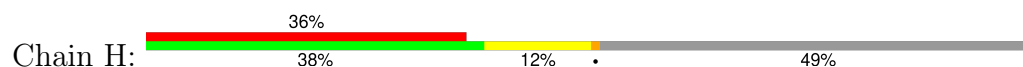
• Molecule 2: Potassium uptake protein TrkA



• Molecule 2: Potassium uptake protein TrkA



- Molecule 2: Potassium uptake protein TrkA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	273.24, 273.24, 273.24	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.242, 1.242, 1.242	Depositor

5 Model quality

5.1 Standard geometry

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	0.48	0/3546	0.94	20/4831 (0.4%)
1	B	0.46	0/3447	0.92	16/4692 (0.3%)
1	C	0.47	0/3510	0.90	13/4783 (0.3%)
1	D	0.46	0/3486	0.89	17/4748 (0.4%)
2	E	0.82	4/1763 (0.2%)	1.19	12/2388 (0.5%)
2	F	0.38	0/1782	0.72	2/2411 (0.1%)
2	G	0.36	0/1768	0.72	3/2394 (0.1%)
2	H	0.35	0/1776	0.73	2/2404 (0.1%)
All	All	0.49	4/21078 (0.0%)	0.90	85/28651 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
2	E	0	3
2	H	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	69	LEU	C-N	-27.42	0.70	1.34
2	E	68	MET	C-N	10.03	1.57	1.34
2	E	18	ASN	C-N	-8.95	1.13	1.34
2	E	19	LEU	C-N	6.59	1.49	1.34

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	68	MET	O-C-N	-28.54	77.04	122.70
2	E	68	MET	CA-C-N	20.00	161.19	117.20
2	E	68	MET	C-N-CA	16.50	162.96	121.70
2	E	18	ASN	C-N-CA	-13.95	86.82	121.70
2	E	18	ASN	O-C-N	13.00	143.50	122.70
1	A	447	LEU	CA-CB-CG	11.94	142.75	115.30
1	A	474	LEU	CA-CB-CG	10.56	139.59	115.30
2	E	19	LEU	O-C-N	-10.22	106.35	122.70
1	A	109	LEU	CA-CB-CG	9.95	138.19	115.30
2	E	18	ASN	CA-C-N	-9.28	96.79	117.20
1	D	447	LEU	CA-CB-CG	8.19	134.14	115.30
1	A	128	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	339	LEU	CB-CG-CD1	6.70	122.40	111.00
1	A	408	LEU	CA-CB-CG	6.66	130.62	115.30
1	B	109	LEU	CA-CB-CG	6.66	130.61	115.30
1	B	255	LEU	CA-CB-CG	6.64	130.58	115.30
1	B	128	LEU	CA-CB-CG	6.61	130.50	115.30
2	E	69	LEU	O-C-N	6.61	133.27	122.70
1	C	447	LEU	CB-CG-CD1	6.56	122.16	111.00
2	E	19	LEU	CA-C-N	6.50	131.51	117.20
1	B	363	LEU	CA-CB-CG	6.49	130.22	115.30
2	E	19	LEU	C-N-CA	6.47	137.89	121.70
1	A	474	LEU	CB-CG-CD1	-6.45	100.04	111.00
1	B	56	PRO	CA-N-CD	-6.40	102.54	111.50
1	D	128	LEU	CA-CB-CG	6.34	129.88	115.30
1	D	273	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	372	LEU	CA-CB-CG	6.22	129.60	115.30
2	F	270	LEU	CA-CB-CG	6.19	129.53	115.30
1	D	372	LEU	CA-CB-CG	6.17	129.49	115.30
2	G	270	LEU	CA-CB-CG	6.14	129.42	115.30
1	C	339	LEU	CB-CG-CD1	6.06	121.30	111.00
1	A	447	LEU	CB-CG-CD1	5.99	121.18	111.00
2	H	270	LEU	CA-CB-CG	5.99	129.07	115.30
2	H	274	LEU	CA-CB-CG	5.96	129.02	115.30
1	B	408	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	16	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	255	LEU	CA-CB-CG	5.92	128.91	115.30
1	C	153	LEU	CB-CG-CD1	5.90	121.03	111.00
1	C	47	LEU	CA-CB-CG	5.88	128.83	115.30
1	D	255	LEU	CA-CB-CG	5.85	128.75	115.30
1	B	474	LEU	CA-CB-CG	-5.84	101.88	115.30
1	A	286	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	16	LEU	CA-CB-CG	5.79	128.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	LEU	CB-CG-CD1	5.77	120.81	111.00
1	A	311	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	47	LEU	CA-CB-CG	5.76	128.56	115.30
1	C	408	LEU	CA-CB-CG	5.75	128.52	115.30
1	D	47	LEU	CA-CB-CG	5.74	128.51	115.30
1	B	311	LEU	CA-CB-CG	5.71	128.44	115.30
1	D	311	LEU	CA-CB-CG	5.71	128.42	115.30
1	C	372	LEU	CA-CB-CG	5.70	128.40	115.30
1	C	128	LEU	CB-CG-CD1	5.66	120.63	111.00
1	D	408	LEU	CA-CB-CG	5.64	128.27	115.30
1	C	311	LEU	CA-CB-CG	5.62	128.23	115.30
2	E	69	LEU	CA-C-N	-5.53	105.03	117.20
1	C	150	LEU	C-N-CD	5.51	139.97	128.40
1	C	153	LEU	CA-CB-CG	5.51	127.97	115.30
1	D	150	LEU	CA-CB-CG	5.44	127.82	115.30
1	D	16	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	153	LEU	CB-CG-CD1	5.40	120.18	111.00
1	D	286	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	286	LEU	CA-CB-CG	5.37	127.65	115.30
1	D	294	LEU	CA-CB-CG	5.36	127.62	115.30
2	G	310	THR	N-CA-C	-5.33	96.59	111.00
1	D	391	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	16	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	294	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	447	LEU	N-CA-CB	-5.30	99.81	110.40
2	G	359	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	472	PHE	CB-CG-CD1	-5.24	117.13	120.80
1	A	150	LEU	CB-CG-CD2	5.23	119.90	111.00
1	B	446	ALA	N-CA-C	-5.22	96.90	111.00
1	B	285	LEU	CA-CB-CG	5.22	127.31	115.30
2	F	358	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	335	LEU	CB-CG-CD2	5.17	119.78	111.00
1	A	335	LEU	CB-CG-CD2	5.12	119.70	111.00
1	A	150	LEU	N-CA-C	5.12	124.81	111.00
1	D	285	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	294	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	153	LEU	CA-CB-CG	5.10	127.03	115.30
1	D	12	LEU	CA-CB-CG	5.10	127.02	115.30
2	E	317	LEU	CA-CB-CG	5.09	127.00	115.30
1	B	339	LEU	CB-CG-CD1	5.08	119.64	111.00
1	C	335	LEU	CB-CG-CD2	5.08	119.64	111.00
1	C	286	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	275	GLU	Peptide
1	C	118	VAL	Peptide
1	C	251	CYS	Peptide
2	E	19	LEU	Mainchain
2	E	359	LEU	Peptide
2	E	68	MET	Mainchain
2	H	359	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3450	0	3527	85	0
1	B	3354	0	3426	88	0
1	C	3414	0	3485	90	0
1	D	3390	0	3465	90	0
2	E	1748	0	1745	110	0
2	F	1767	0	1780	74	0
2	G	1753	0	1756	73	0
2	H	1761	0	1763	99	0
All	All	20637	0	20947	661	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 16.

All (661) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:332:ARG:HD2	2:G:335:TYR:CE2	1.24	1.65
2:G:332:ARG:HB3	2:G:335:TYR:CZ	1.33	1.59
2:G:332:ARG:CB	2:G:335:TYR:CZ	1.86	1.56
2:G:332:ARG:CD	2:G:335:TYR:HE2	0.94	1.56
1:A:425:LEU:HD23	1:A:444:GLU:CG	1.43	1.45
2:G:332:ARG:HB3	2:G:335:TYR:CE2	1.50	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:332:ARG:CB	2:G:335:TYR:CE2	1.98	1.44
2:F:107:GLU:CG	2:H:54:HIS:NE2	1.75	1.43
1:C:465:LEU:O	1:C:469:LEU:CD1	1.67	1.42
2:E:107:GLU:CG	2:G:54:HIS:NE2	1.77	1.41
2:E:69:LEU:CA	2:E:70:VAL:N	1.84	1.40
1:A:425:LEU:CD2	1:A:444:GLU:CG	1.99	1.40
1:A:425:LEU:CD2	1:A:444:GLU:OE2	1.67	1.38
2:E:54:HIS:NE2	2:G:107:GLU:CG	1.77	1.38
2:F:54:HIS:NE2	2:H:107:GLU:CG	1.75	1.38
2:E:69:LEU:C	2:E:70:VAL:CA	1.92	1.37
2:G:332:ARG:CG	2:G:335:TYR:CE2	2.08	1.34
1:A:425:LEU:HD23	1:A:444:GLU:CD	1.45	1.32
2:E:335:TYR:CE1	2:E:339:VAL:HG11	1.65	1.31
1:D:181:THR:HG22	1:D:185:LEU:CD1	1.59	1.30
2:G:332:ARG:CD	2:G:335:TYR:CE2	1.82	1.29
1:C:465:LEU:O	1:C:469:LEU:HD13	1.09	1.27
1:A:465:LEU:O	1:A:469:LEU:HD23	1.32	1.26
2:H:308:ASP:HB3	2:H:331:GLN:OE1	1.16	1.26
1:A:465:LEU:O	1:A:469:LEU:CD2	1.87	1.23
2:F:330:ILE:C	2:F:335:TYR:OH	1.78	1.22
2:E:335:TYR:CE1	2:E:339:VAL:CG1	2.26	1.19
2:F:107:GLU:HG3	2:H:54:HIS:NE2	1.54	1.19
2:H:335:TYR:CE1	2:H:338:LEU:CG	1.97	1.19
2:F:330:ILE:O	2:F:335:TYR:OH	1.61	1.18
2:E:107:GLU:HG3	2:G:54:HIS:NE2	1.57	1.18
2:E:306:ASN:O	2:E:307:GLU:HG3	1.39	1.16
2:E:69:LEU:O	2:E:70:VAL:N	1.79	1.16
2:G:309:GLU:O	2:G:312:ILE:N	1.77	1.16
2:H:335:TYR:HE1	2:H:338:LEU:CG	1.40	1.16
2:E:335:TYR:CD1	2:E:339:VAL:HG13	1.80	1.15
2:F:54:HIS:NE2	2:H:107:GLU:HG3	1.55	1.15
1:A:425:LEU:CD2	1:A:444:GLU:CD	2.04	1.15
1:A:425:LEU:HD21	1:A:444:GLU:OE2	1.48	1.13
2:E:54:HIS:NE2	2:G:107:GLU:HG3	1.57	1.13
2:E:330:ILE:CG2	2:E:335:TYR:CE2	2.32	1.13
1:B:442:LEU:O	1:B:445:VAL:HG13	1.49	1.12
2:G:309:GLU:O	2:G:310:THR:C	1.83	1.12
2:H:14:THR:CG2	2:H:332:ARG:NH2	2.12	1.12
1:D:142:ILE:CD1	1:D:352:THR:O	1.97	1.12
2:G:332:ARG:HB3	2:G:335:TYR:CE1	1.84	1.11
2:H:335:TYR:CE1	2:H:338:LEU:HG	1.72	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:335:TYR:CE1	2:H:338:LEU:CB	2.35	1.09
1:A:425:LEU:HD23	1:A:444:GLU:HG3	1.17	1.09
1:D:181:THR:HG22	1:D:185:LEU:HD11	1.35	1.09
2:E:330:ILE:HG21	2:E:335:TYR:CE2	1.88	1.09
2:G:332:ARG:HB2	2:G:335:TYR:OH	1.52	1.09
2:G:332:ARG:HB2	2:G:335:TYR:CZ	1.71	1.08
1:D:465:LEU:O	1:D:469:LEU:HG	1.51	1.08
2:H:14:THR:HG23	2:H:332:ARG:NH2	1.69	1.07
2:H:335:TYR:CE1	2:H:338:LEU:HB3	1.90	1.07
1:D:181:THR:HG22	1:D:185:LEU:HD13	1.30	1.05
1:D:363:LEU:O	1:D:367:GLN:HB2	1.57	1.04
2:F:308:ASP:OD1	2:F:330:ILE:HA	1.57	1.04
2:H:335:TYR:CD1	2:H:338:LEU:HB3	1.92	1.04
2:H:335:TYR:HE1	2:H:338:LEU:HG	0.90	1.04
1:D:142:ILE:HD11	1:D:352:THR:O	1.57	1.04
2:E:69:LEU:HD12	2:E:95:ARG:HG2	1.34	1.03
1:A:425:LEU:CD2	1:A:444:GLU:HG3	1.75	1.02
1:D:82:SER:O	1:D:83:ALA:HB3	1.55	1.01
1:C:469:LEU:HD13	1:C:469:LEU:H	1.25	1.01
2:H:14:THR:CG2	2:H:332:ARG:HH22	1.69	1.01
2:H:308:ASP:CB	2:H:331:GLN:OE1	2.10	1.00
2:G:332:ARG:HD2	2:G:335:TYR:CD2	1.97	0.99
2:E:306:ASN:O	2:E:307:GLU:CG	2.12	0.98
2:E:330:ILE:CG2	2:E:335:TYR:CD2	2.45	0.98
2:E:332:ARG:O	2:E:335:TYR:HD2	1.44	0.97
2:E:335:TYR:HE1	2:E:339:VAL:HG11	1.21	0.97
2:E:335:TYR:CD1	2:E:339:VAL:CG1	2.44	0.97
2:F:54:HIS:CD2	2:H:107:GLU:HG3	1.99	0.96
2:E:1:MET:CE	2:E:359:LEU:HD23	1.95	0.96
2:E:335:TYR:OH	2:E:347:ALA:HB1	1.66	0.95
1:C:465:LEU:O	1:C:469:LEU:HD11	1.66	0.95
2:F:107:GLU:HG3	2:H:54:HIS:CD2	2.00	0.95
2:E:54:HIS:CD2	2:G:107:GLU:HG3	2.01	0.94
2:H:309:GLU:OE1	2:H:312:ILE:HD12	1.67	0.94
1:A:425:LEU:CG	1:A:444:GLU:HG3	1.98	0.94
1:B:379:ARG:NH2	2:E:289:LEU:HD23	1.83	0.94
2:E:107:GLU:HG3	2:G:54:HIS:CD2	2.01	0.93
1:D:181:THR:CG2	1:D:185:LEU:CD1	2.46	0.93
2:H:1:MET:CE	2:H:359:LEU:HD23	1.98	0.93
2:E:330:ILE:HG21	2:E:335:TYR:CD2	2.05	0.92
1:D:181:THR:CG2	1:D:185:LEU:HD11	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:CD2	1:A:444:GLU:HG2	2.02	0.89
2:E:286:ASP:OD2	2:E:289:LEU:HB2	1.71	0.89
1:C:425:LEU:HD23	1:C:444:GLU:HG3	1.55	0.88
2:E:1:MET:HG2	2:E:359:LEU:HD21	1.55	0.88
2:F:54:HIS:NE2	2:H:107:GLU:HG2	1.86	0.88
2:H:1:MET:HG2	2:H:359:LEU:HD21	1.54	0.88
2:E:330:ILE:HG22	2:E:335:TYR:CD2	2.08	0.88
2:G:332:ARG:HB3	2:G:335:TYR:CD2	2.09	0.88
2:E:1:MET:CE	2:E:359:LEU:CD2	2.52	0.88
2:E:332:ARG:O	2:E:335:TYR:CD2	2.27	0.88
2:F:107:GLU:HG2	2:H:54:HIS:NE2	1.88	0.87
2:E:330:ILE:HG22	2:E:335:TYR:CE2	2.09	0.87
2:G:309:GLU:O	2:G:311:ASN:N	2.08	0.87
2:H:309:GLU:HA	2:H:312:ILE:HD12	1.57	0.87
1:A:363:LEU:O	1:A:367:GLN:HB2	1.74	0.87
1:B:447:LEU:HD12	1:B:447:LEU:H	1.39	0.87
2:F:1:MET:HE1	2:F:359:LEU:CD1	2.04	0.86
2:E:54:HIS:NE2	2:G:107:GLU:HG2	1.89	0.86
2:H:1:MET:CE	2:H:359:LEU:CD2	2.53	0.86
1:B:277:ARG:HH11	1:B:278:ALA:HA	1.40	0.85
2:E:107:GLU:HG2	2:G:54:HIS:NE2	1.89	0.85
1:D:82:SER:O	1:D:83:ALA:CB	2.20	0.85
2:E:335:TYR:HD1	2:E:339:VAL:HG13	1.33	0.85
2:G:308:ASP:O	2:G:311:ASN:HB2	1.77	0.84
1:A:469:LEU:HD23	1:A:469:LEU:H	1.42	0.84
2:H:1:MET:HE3	2:H:359:LEU:HD23	1.57	0.83
1:A:425:LEU:CG	1:A:444:GLU:CG	2.55	0.83
1:A:465:LEU:O	1:A:469:LEU:HD21	1.77	0.82
2:F:1:MET:CE	2:F:359:LEU:CD1	2.57	0.82
1:B:442:LEU:O	1:B:445:VAL:CG1	2.25	0.82
1:A:425:LEU:HD21	1:A:444:GLU:CG	2.05	0.82
1:D:142:ILE:HD12	1:D:352:THR:O	1.78	0.82
2:E:1:MET:HE3	2:E:359:LEU:HD23	1.60	0.81
2:H:14:THR:HG22	2:H:332:ARG:HH22	1.44	0.81
1:C:442:LEU:HD23	1:C:442:LEU:O	1.81	0.80
2:H:335:TYR:CD1	2:H:338:LEU:CB	2.62	0.80
2:E:283:ASP:OD2	2:E:283:ASP:N	2.15	0.80
2:F:1:MET:HE1	2:F:359:LEU:HD12	1.64	0.80
2:F:68:MET:CE	2:F:358:LEU:C	2.50	0.80
1:A:425:LEU:HD22	1:A:444:GLU:OE2	1.77	0.79
1:D:140:MET:HG2	1:D:189:TYR:CE2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HD23	1:B:444:GLU:HG3	1.64	0.79
2:G:332:ARG:NE	2:G:335:TYR:HE2	1.80	0.79
2:H:309:GLU:OE1	2:H:312:ILE:CD1	2.31	0.79
1:D:181:THR:O	1:D:185:LEU:HD13	1.83	0.78
2:E:19:LEU:HD21	2:E:355:ILE:HD13	1.63	0.78
2:G:309:GLU:CB	2:G:312:ILE:HD12	2.13	0.78
2:E:335:TYR:HE1	2:E:339:VAL:CG1	1.81	0.78
2:F:314:SER:O	2:F:317:LEU:N	2.16	0.78
2:H:14:THR:HG22	2:H:332:ARG:NH2	1.97	0.78
2:F:332:ARG:O	2:F:335:TYR:CE2	2.38	0.77
2:H:14:THR:HG23	2:H:332:ARG:HH22	1.33	0.77
1:D:465:LEU:O	1:D:469:LEU:CG	2.33	0.76
2:E:69:LEU:C	2:E:70:VAL:N	0.71	0.76
1:C:465:LEU:C	1:C:469:LEU:HD11	2.06	0.75
2:E:294:ASN:H	2:E:294:ASN:ND2	1.84	0.75
1:A:358:VAL:O	1:A:362:LEU:HB2	1.86	0.75
1:B:440:PRO:HG2	1:B:447:LEU:HB3	1.68	0.75
2:F:1:MET:CE	2:F:359:LEU:HD13	2.16	0.75
1:B:379:ARG:HH21	2:E:289:LEU:HD23	1.53	0.74
1:B:442:LEU:HD12	1:B:445:VAL:HG11	1.70	0.74
2:H:14:THR:CG2	2:H:332:ARG:HH21	2.02	0.73
1:C:465:LEU:C	1:C:469:LEU:CD1	2.56	0.73
2:E:283:ASP:HB2	2:E:286:ASP:HB3	1.70	0.73
1:C:294:LEU:HD11	1:C:306:ALA:HB1	1.71	0.73
2:E:330:ILE:HG21	2:E:335:TYR:CZ	2.23	0.73
2:F:54:HIS:CD2	2:H:107:GLU:CG	2.63	0.72
1:C:469:LEU:HD13	1:C:469:LEU:N	2.04	0.72
1:C:469:LEU:O	1:C:469:LEU:HD22	1.91	0.71
2:E:1:MET:HE2	2:E:359:LEU:CD2	2.20	0.71
1:B:358:VAL:O	1:B:362:LEU:HB2	1.90	0.71
1:B:440:PRO:CG	1:B:447:LEU:HB3	2.21	0.71
2:E:54:HIS:CD2	2:G:107:GLU:CG	2.65	0.70
1:A:465:LEU:C	1:A:469:LEU:HD21	2.12	0.70
2:E:1:MET:HE2	2:E:359:LEU:HD22	1.72	0.70
2:E:335:TYR:CE1	2:E:339:VAL:CG2	2.75	0.70
2:E:286:ASP:OD2	2:E:289:LEU:CB	2.40	0.70
2:F:237:ILE:HG22	2:F:302:ILE:HD12	1.73	0.70
2:E:335:TYR:HE1	2:E:339:VAL:HG21	1.56	0.70
2:F:80:MET:HE2	2:H:77:GLU:HG2	1.74	0.70
1:B:277:ARG:NH1	1:B:278:ALA:HA	2.07	0.69
1:C:370:ARG:HH21	1:C:383:THR:HA	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:O	1:B:367:GLN:HB2	1.93	0.69
1:D:181:THR:O	1:D:185:LEU:CD1	2.41	0.69
2:H:75:THR:HG22	2:H:78:THR:H	1.58	0.69
1:B:308:ASP:O	1:B:312:PHE:HB2	1.92	0.69
2:E:75:THR:HG22	2:E:78:THR:H	1.58	0.69
2:E:335:TYR:HE1	2:E:339:VAL:CG2	2.06	0.69
2:F:75:THR:HG22	2:F:78:THR:H	1.58	0.69
2:G:75:THR:HG22	2:G:78:THR:H	1.58	0.69
1:A:437:ASN:HB2	1:A:468:ARG:NH2	2.07	0.69
1:D:70:PHE:O	1:D:74:VAL:HG23	1.93	0.69
2:H:1:MET:SD	2:H:359:LEU:HD23	2.32	0.69
2:F:107:GLU:CG	2:H:54:HIS:CD2	2.64	0.69
2:E:335:TYR:CE1	2:E:339:VAL:HG21	2.28	0.68
2:G:309:GLU:C	2:G:311:ASN:N	2.40	0.68
2:E:1:MET:SD	2:E:359:LEU:HD23	2.34	0.68
2:H:1:MET:HG2	2:H:359:LEU:CD2	2.23	0.68
1:C:358:VAL:O	1:C:362:LEU:HB2	1.94	0.68
1:C:363:LEU:O	1:C:367:GLN:HB2	1.94	0.68
1:C:300:TYR:HB2	1:C:306:ALA:HB2	1.76	0.68
2:H:308:ASP:HB2	2:H:330:ILE:HA	1.75	0.68
1:D:306:ALA:O	1:D:310:ALA:HB3	1.94	0.68
1:A:306:ALA:O	1:A:310:ALA:HB3	1.93	0.67
1:B:442:LEU:HA	1:B:445:VAL:HG12	1.76	0.67
2:E:107:GLU:CG	2:G:54:HIS:CD2	2.65	0.67
1:D:326:THR:HG22	1:D:328:PHE:H	1.59	0.67
1:C:326:THR:HG22	1:C:328:PHE:H	1.60	0.67
2:E:69:LEU:O	2:E:70:VAL:CA	2.33	0.67
1:B:307:PHE:O	1:B:311:LEU:HB3	1.95	0.67
1:C:307:PHE:O	1:C:311:LEU:HB3	1.94	0.66
1:C:425:LEU:HD23	1:C:444:GLU:CG	2.26	0.66
1:A:425:LEU:HG	1:A:444:GLU:CG	2.24	0.66
1:A:307:PHE:O	1:A:311:LEU:HB3	1.95	0.66
1:D:74:VAL:O	1:D:78:THR:OG1	2.09	0.66
1:D:199:ALA:HB1	1:D:241:ILE:HG21	1.78	0.66
2:F:77:GLU:HG2	2:H:80:MET:HE2	1.76	0.66
2:E:1:MET:HG2	2:E:359:LEU:CD2	2.26	0.65
2:H:308:ASP:HB3	2:H:331:GLN:CD	2.10	0.65
1:C:308:ASP:O	1:C:312:PHE:HB2	1.96	0.65
1:C:306:ALA:O	1:C:310:ALA:HB3	1.96	0.65
1:B:276:PHE:O	1:B:280:ILE:HG12	1.97	0.64
1:B:294:LEU:HD11	1:B:306:ALA:HB1	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:GLU:OE1	1:C:444:GLU:HA	1.98	0.64
1:D:457:LYS:HA	1:D:460:LEU:HD12	1.79	0.64
1:A:426:SER:OG	1:A:446:ALA:HB3	1.96	0.64
1:D:220:ILE:CG1	1:D:321:ALA:O	2.45	0.64
1:A:425:LEU:HD21	1:A:444:GLU:HG2	1.75	0.64
2:H:310:THR:O	2:H:312:ILE:N	2.30	0.64
2:G:309:GLU:O	2:G:310:THR:O	2.15	0.64
1:B:444:GLU:OE2	1:B:444:GLU:HA	1.96	0.64
2:E:308:ASP:O	2:E:311:ASN:HB2	1.97	0.64
2:F:309:GLU:OE1	2:F:309:GLU:N	2.30	0.64
1:C:199:ALA:HB1	1:C:241:ILE:HG21	1.78	0.64
1:A:300:TYR:HB2	1:A:306:ALA:HB2	1.79	0.64
2:H:1:MET:HE2	2:H:359:LEU:HD22	1.79	0.64
1:B:306:ALA:O	1:B:310:ALA:HB3	1.98	0.64
1:D:300:TYR:HB2	1:D:306:ALA:HB2	1.78	0.64
1:A:442:LEU:HD13	1:A:442:LEU:O	1.98	0.63
1:A:251:CYS:O	1:A:351:SER:OG	2.17	0.63
1:B:300:TYR:HB2	1:B:306:ALA:HB2	1.80	0.63
1:C:457:LYS:HA	1:C:460:LEU:HD12	1.81	0.63
1:C:18:SER:HB3	1:C:43:PHE:HA	1.81	0.63
2:F:3:ILE:HD13	2:F:68:MET:HB3	1.79	0.63
1:D:294:LEU:HD11	1:D:306:ALA:HB1	1.79	0.63
2:F:1:MET:HE1	2:F:359:LEU:HD13	1.77	0.63
1:B:18:SER:HB3	1:B:43:PHE:HA	1.80	0.63
1:B:199:ALA:HB1	1:B:241:ILE:HG21	1.81	0.63
2:E:306:ASN:C	2:E:307:GLU:CG	2.67	0.62
2:G:332:ARG:CG	2:G:335:TYR:CD2	2.80	0.62
1:C:110:THR:HG21	1:C:464:MET:HG3	1.81	0.62
1:A:437:ASN:HB2	1:A:468:ARG:HH21	1.63	0.62
1:B:268:LYS:HB2	1:B:268:LYS:NZ	2.15	0.62
1:B:332:PRO:HD2	1:B:335:LEU:HD23	1.81	0.61
1:D:308:ASP:O	1:D:312:PHE:HB2	1.99	0.61
1:B:370:ARG:HH21	1:B:383:THR:HA	1.65	0.61
2:F:80:MET:HE1	2:H:77:GLU:HB3	1.82	0.61
2:H:1:MET:HE2	2:H:359:LEU:CD2	2.30	0.61
1:A:445:VAL:HG23	1:A:445:VAL:O	2.01	0.61
2:F:238:VAL:HG22	2:F:303:ALA:HA	1.82	0.61
2:F:308:ASP:OD2	2:F:335:TYR:HE1	1.83	0.61
2:G:332:ARG:CD	2:G:335:TYR:CD2	2.70	0.61
1:A:455:LYS:HA	1:A:458:TRP:HD1	1.66	0.61
1:A:457:LYS:HA	1:A:460:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD11	1:A:306:ALA:HB1	1.82	0.61
1:D:140:MET:CG	1:D:189:TYR:CE2	2.84	0.61
1:A:370:ARG:HD2	1:A:384:ILE:HG12	1.82	0.60
1:A:308:ASP:O	1:A:312:PHE:HB2	2.01	0.60
2:E:69:LEU:HA	2:E:70:VAL:N	2.06	0.60
2:G:332:ARG:HB3	2:G:335:TYR:CD1	2.33	0.60
1:A:425:LEU:HG	1:A:444:GLU:HG3	1.81	0.60
2:G:309:GLU:HA	2:G:312:ILE:HG13	1.84	0.60
2:G:332:ARG:NE	2:G:335:TYR:CE2	2.60	0.60
1:D:424:GLU:O	1:D:428:PHE:HB2	2.02	0.60
2:H:296:ASP:O	2:H:324:LYS:NZ	2.35	0.60
1:A:326:THR:HG22	1:A:328:PHE:H	1.67	0.60
2:F:77:GLU:HB3	2:H:80:MET:HE1	1.84	0.60
2:G:296:ASP:O	2:G:324:LYS:NZ	2.35	0.60
2:E:287:GLN:HG3	2:E:291:THR:HG23	1.83	0.59
2:G:233:ARG:N	2:G:299:ASP:OD2	2.35	0.59
2:E:296:ASP:O	2:E:324:LYS:NZ	2.35	0.59
1:D:111:THR:HG23	1:D:219:ALA:O	2.02	0.59
1:D:192:LEU:HD21	1:D:253:PHE:CE2	2.37	0.59
1:B:326:THR:HG22	1:B:328:PHE:H	1.67	0.59
1:D:192:LEU:HD21	1:D:253:PHE:HE2	1.67	0.59
2:H:72:VAL:O	2:H:72:VAL:HG23	2.02	0.59
2:H:233:ARG:N	2:H:299:ASP:OD2	2.36	0.59
1:D:111:THR:CG2	1:D:219:ALA:O	2.51	0.59
2:G:332:ARG:HG2	2:G:334:ALA:H	1.68	0.59
1:C:343:SER:OG	1:C:436:ASN:ND2	2.35	0.59
2:F:1:MET:HE3	2:F:359:LEU:HD13	1.85	0.59
2:G:332:ARG:CB	2:G:335:TYR:CE1	2.62	0.59
1:C:394:ARG:NH2	1:D:378:PRO:O	2.36	0.58
2:F:233:ARG:N	2:F:299:ASP:OD2	2.36	0.58
2:F:68:MET:CE	2:F:358:LEU:O	2.52	0.58
1:C:469:LEU:CD1	1:C:469:LEU:H	2.07	0.58
2:H:1:MET:CE	2:H:359:LEU:HD22	2.34	0.58
2:H:1:MET:HE3	2:H:359:LEU:CD2	2.27	0.58
1:D:343:SER:OG	1:D:436:ASN:ND2	2.36	0.58
1:D:307:PHE:O	1:D:311:LEU:HB3	2.04	0.58
1:D:220:ILE:HG13	1:D:321:ALA:O	2.03	0.58
1:D:363:LEU:O	1:D:367:GLN:CB	2.45	0.58
2:E:69:LEU:CD1	2:E:95:ARG:HG2	2.23	0.58
2:E:356:SER:O	2:E:360:THR:N	2.37	0.58
1:C:24:PRO:HG3	1:C:130:TYR:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:VAL:HB	1:B:447:LEU:HD11	1.86	0.57
1:D:18:SER:HB3	1:D:43:PHE:HA	1.85	0.57
2:E:309:GLU:HA	2:E:309:GLU:OE1	2.02	0.57
2:G:299:ASP:HA	2:G:324:LYS:HD2	1.86	0.57
1:B:442:LEU:HD12	1:B:445:VAL:CG1	2.34	0.57
2:H:311:ASN:O	2:H:315:ALA:HB2	2.05	0.57
2:H:356:SER:O	2:H:360:THR:N	2.37	0.57
1:A:24:PRO:HG3	1:A:130:TYR:HB2	1.86	0.57
2:H:335:TYR:CD2	2:H:339:VAL:HG13	2.40	0.57
1:D:306:ALA:O	1:D:310:ALA:CB	2.53	0.57
2:F:271:SER:HB2	2:F:279:VAL:HG11	1.87	0.56
2:E:294:ASN:H	2:E:294:ASN:HD22	1.50	0.56
2:E:299:ASP:HA	2:E:324:LYS:HD2	1.87	0.56
1:A:425:LEU:HG	1:A:444:GLU:HG2	1.87	0.56
2:G:335:TYR:CD2	2:G:335:TYR:N	2.73	0.56
2:H:1:MET:HE3	2:H:359:LEU:HA	1.87	0.56
1:A:378:PRO:O	1:B:394:ARG:NH2	2.39	0.56
1:D:24:PRO:HG3	1:D:130:TYR:HB2	1.88	0.56
2:E:233:ARG:N	2:E:299:ASP:OD2	2.39	0.56
1:A:199:ALA:HB1	1:A:241:ILE:HG21	1.88	0.56
1:B:100:ASP:OD1	1:B:457:LYS:NZ	2.37	0.56
2:E:1:MET:HE3	2:E:359:LEU:HA	1.88	0.56
2:E:69:LEU:C	2:E:70:VAL:HA	2.16	0.56
1:C:328:PHE:HD2	1:C:442:LEU:HD13	1.71	0.55
2:F:330:ILE:CA	2:F:335:TYR:OH	2.03	0.55
2:H:1:MET:SD	2:H:359:LEU:CD2	2.93	0.55
1:B:205:MET:HE3	1:B:238:ILE:HD11	1.88	0.55
2:H:299:ASP:HA	2:H:324:LYS:HD2	1.88	0.55
2:H:252:GLU:OE1	2:H:277:THR:OG1	2.23	0.55
2:H:319:LYS:NZ	2:H:324:LYS:O	2.38	0.55
1:A:425:LEU:HD21	1:A:444:GLU:CD	1.96	0.55
1:C:471:ILE:HD12	1:C:471:ILE:H	1.71	0.54
1:D:38:PRO:HB2	1:D:87:PRO:HB3	1.89	0.54
2:E:311:ASN:HB3	2:E:328:VAL:HG13	1.89	0.54
2:H:335:TYR:CE2	2:H:339:VAL:HG13	2.43	0.54
1:A:18:SER:HB3	1:A:43:PHE:HA	1.89	0.54
1:C:364:LEU:O	1:C:368:GLY:HA3	2.08	0.54
1:D:140:MET:HE3	1:D:189:TYR:CD2	2.42	0.54
2:F:309:GLU:CD	2:F:309:GLU:H	2.11	0.54
2:H:309:GLU:CD	2:H:312:ILE:HD12	2.28	0.54
2:F:299:ASP:HA	2:F:324:LYS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HD13	1:B:321:ALA:HB1	1.90	0.54
1:B:471:ILE:H	1:B:471:ILE:HD12	1.73	0.54
2:E:1:MET:SD	2:E:359:LEU:CD2	2.95	0.54
2:F:305:THR:OG1	2:F:311:ASN:ND2	2.41	0.54
1:D:220:ILE:HG12	1:D:321:ALA:O	2.07	0.54
1:A:14:LEU:HD23	1:A:46:LEU:HD22	1.90	0.54
1:B:343:SER:OG	1:B:436:ASN:ND2	2.41	0.53
2:E:252:GLU:OE1	2:E:277:THR:OG1	2.24	0.53
1:B:442:LEU:HA	1:B:445:VAL:CG1	2.38	0.53
1:B:38:PRO:HB2	1:B:87:PRO:HB3	1.91	0.53
1:C:440:PRO:HG3	1:C:447:LEU:HD22	1.90	0.53
1:C:469:LEU:HD22	1:C:469:LEU:C	2.28	0.53
1:A:306:ALA:O	1:A:310:ALA:CB	2.55	0.53
1:A:469:LEU:HD23	1:A:469:LEU:N	2.17	0.53
1:A:307:PHE:O	1:A:311:LEU:CB	2.57	0.53
1:D:370:ARG:HH21	1:D:383:THR:HA	1.73	0.53
2:E:239:GLY:HA3	2:E:304:LEU:HB2	1.91	0.53
2:F:94:ASN:ND2	2:F:358:LEU:O	2.41	0.53
2:G:319:LYS:NZ	2:G:324:LYS:O	2.40	0.53
2:H:309:GLU:HA	2:H:312:ILE:CD1	2.35	0.53
1:C:238:ILE:O	1:C:242:THR:OG1	2.18	0.53
1:D:229:SER:HB2	1:D:323:PHE:HD1	1.73	0.53
1:C:269:TYR:HA	1:C:272:LYS:HB3	1.91	0.53
1:C:409:VAL:HG11	1:C:471:ILE:HG21	1.90	0.53
1:C:150:LEU:HA	1:C:153:LEU:O	2.10	0.52
2:E:259:LEU:O	2:E:280:PHE:N	2.43	0.52
2:G:305:THR:OG1	2:G:311:ASN:ND2	2.32	0.52
1:B:251:CYS:O	1:B:351:SER:OG	2.25	0.52
1:D:139:GLY:O	1:D:142:ILE:HG22	2.09	0.52
2:E:69:LEU:O	2:E:70:VAL:HA	2.07	0.52
2:G:349:SER:OG	2:G:351:GLN:OE1	2.28	0.52
2:F:335:TYR:HB2	2:F:338:LEU:HB3	1.90	0.52
1:C:38:PRO:HB2	1:C:87:PRO:HB3	1.92	0.52
1:D:358:VAL:O	1:D:362:LEU:HB3	2.09	0.52
1:A:385:LYS:HA	1:A:391:LEU:HD12	1.92	0.52
1:B:307:PHE:O	1:B:311:LEU:CB	2.57	0.52
1:C:307:PHE:O	1:C:311:LEU:CB	2.58	0.52
1:B:341:PHE:HA	1:B:344:PHE:HD2	1.75	0.52
2:F:252:GLU:OE1	2:F:277:THR:OG1	2.26	0.52
2:E:308:ASP:OD1	2:E:308:ASP:N	2.44	0.51
2:F:307:GLU:HB3	2:F:310:THR:HG22	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:311:ASN:HB3	2:H:328:VAL:HG13	1.93	0.51
1:B:97:SER:O	1:B:101:ALA:N	2.38	0.51
1:B:224:SER:OG	1:B:226:HIS:O	2.28	0.51
2:E:244:GLY:O	2:E:248:ALA:CB	2.59	0.51
2:H:244:GLY:O	2:H:248:ALA:CB	2.58	0.51
1:A:245:PHE:O	1:A:249:SER:OG	2.23	0.51
1:B:379:ARG:CZ	2:E:289:LEU:HD23	2.40	0.51
1:D:140:MET:CE	1:D:189:TYR:CD2	2.93	0.51
2:F:51:HIS:HE2	2:H:103:GLU:HB3	1.76	0.51
2:E:314:SER:O	2:E:318:ALA:N	2.41	0.51
2:G:241:GLY:O	2:G:245:ALA:N	2.40	0.51
1:B:440:PRO:HB2	1:B:447:LEU:HB3	1.93	0.51
1:D:355:GLY:H	1:D:357:LYS:HZ1	1.58	0.51
1:A:394:ARG:NH2	1:B:378:PRO:O	2.40	0.51
1:B:424:GLU:O	1:B:428:PHE:HB2	2.11	0.51
1:D:97:SER:O	1:D:101:ALA:N	2.38	0.51
2:E:349:SER:OG	2:E:351:GLN:OE1	2.29	0.51
2:G:332:ARG:HB3	2:G:335:TYR:CG	2.46	0.51
2:G:356:SER:O	2:G:360:THR:N	2.43	0.51
2:H:349:SER:OG	2:H:351:GLN:OE1	2.29	0.51
1:B:358:VAL:O	1:B:362:LEU:CB	2.57	0.50
1:C:306:ALA:O	1:C:310:ALA:CB	2.58	0.50
1:B:306:ALA:O	1:B:310:ALA:CB	2.58	0.50
1:D:186:TRP:HA	1:D:186:TRP:CE3	2.46	0.50
1:A:358:VAL:O	1:A:362:LEU:CB	2.59	0.50
2:F:80:MET:CE	2:H:77:GLU:HB3	2.41	0.50
1:B:466:PHE:CG	1:B:471:ILE:HG23	2.47	0.50
2:F:77:GLU:HB3	2:H:80:MET:CE	2.42	0.50
2:E:335:TYR:HE1	2:E:339:VAL:CB	2.25	0.50
1:A:425:LEU:CG	1:A:444:GLU:HG2	2.34	0.50
1:C:328:PHE:CD2	1:C:442:LEU:HD13	2.46	0.50
1:C:341:PHE:HA	1:C:344:PHE:HD2	1.76	0.50
1:C:205:MET:HE1	1:C:238:ILE:HD11	1.94	0.49
2:F:244:GLY:O	2:F:248:ALA:CB	2.60	0.49
1:A:97:SER:O	1:A:101:ALA:N	2.40	0.49
1:C:358:VAL:O	1:C:362:LEU:CB	2.59	0.49
1:C:442:LEU:HD23	1:C:442:LEU:C	2.31	0.49
2:E:335:TYR:CD1	2:E:335:TYR:C	2.85	0.49
1:C:97:SER:O	1:C:101:ALA:N	2.41	0.49
1:D:362:LEU:HG	1:D:366:LEU:HD22	1.95	0.49
1:A:363:LEU:O	1:A:367:GLN:CB	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ALA:HB1	1:C:325:THR:HG23	1.95	0.49
1:A:437:ASN:CB	1:A:468:ARG:HH21	2.26	0.49
1:B:238:ILE:O	1:B:242:THR:OG1	2.20	0.49
2:H:238:VAL:HG22	2:H:303:ALA:HA	1.95	0.49
2:G:309:GLU:HA	2:G:312:ILE:CG1	2.42	0.49
2:H:236:MET:HA	2:H:258:LYS:HB2	1.95	0.49
1:C:233:PHE:HE2	1:C:238:ILE:HD12	1.78	0.49
2:H:237:ILE:HG22	2:H:302:ILE:HD12	1.94	0.49
1:B:268:LYS:HB2	1:B:268:LYS:HZ3	1.77	0.48
2:G:252:GLU:OE1	2:G:277:THR:OG1	2.26	0.48
2:H:274:LEU:HD13	2:H:277:THR:HB	1.94	0.48
1:B:24:PRO:HG3	1:B:130:TYR:HB2	1.95	0.48
2:E:335:TYR:O	2:E:338:LEU:N	2.45	0.48
2:F:80:MET:CE	2:H:77:GLU:CG	2.91	0.48
2:E:302:ILE:HA	2:E:327:MET:HB2	1.94	0.48
2:H:308:ASP:H	2:H:331:GLN:HE22	1.61	0.48
1:D:341:PHE:HA	1:D:344:PHE:HD2	1.77	0.48
2:E:29:VAL:HG22	2:E:48:VAL:HB	1.95	0.48
2:F:29:VAL:HG22	2:F:48:VAL:HB	1.95	0.48
2:G:309:GLU:HA	2:G:312:ILE:CD1	2.44	0.48
2:E:1:MET:HE3	2:E:359:LEU:CD2	2.33	0.48
2:E:51:HIS:HE2	2:G:103:GLU:HB3	1.79	0.48
1:D:251:CYS:O	1:D:351:SER:OG	2.32	0.48
1:D:370:ARG:NH2	1:D:382:TYR:O	2.44	0.48
1:B:440:PRO:CB	1:B:447:LEU:HB3	2.44	0.48
1:C:328:PHE:CD2	1:C:442:LEU:CD1	2.96	0.48
2:F:68:MET:HE3	2:F:358:LEU:C	2.33	0.48
1:B:445:VAL:HB	1:B:447:LEU:CD1	2.44	0.48
1:C:120:LEU:HD21	1:C:128:LEU:HD23	1.94	0.48
2:F:103:GLU:HB3	2:H:51:HIS:HE2	1.78	0.48
2:F:332:ARG:HG2	2:F:334:ALA:H	1.79	0.48
2:G:335:TYR:O	2:G:338:LEU:N	2.45	0.48
2:H:12:GLY:CA	2:H:72:VAL:HG21	2.43	0.48
1:A:238:ILE:O	1:A:242:THR:OG1	2.18	0.48
2:F:77:GLU:CG	2:H:80:MET:HE2	2.44	0.48
1:A:430:ALA:O	1:A:434:THR:OG1	2.18	0.47
1:B:335:LEU:HD13	1:B:335:LEU:HA	1.81	0.47
1:C:359:ILE:O	1:C:363:LEU:HB2	2.14	0.47
1:D:100:ASP:OD1	1:D:457:LYS:NZ	2.45	0.47
2:E:331:GLN:O	2:E:351:GLN:NE2	2.40	0.47
2:F:80:MET:CE	2:H:77:GLU:HG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:GLU:HB3	2:G:51:HIS:HE2	1.79	0.47
1:A:109:LEU:HD23	1:A:110:THR:HG23	1.97	0.47
2:E:312:ILE:HD11	2:E:330:ILE:HD11	1.95	0.47
2:E:241:GLY:O	2:E:245:ALA:N	2.45	0.47
2:F:80:MET:HE2	2:H:77:GLU:CG	2.43	0.47
2:G:311:ASN:O	2:G:315:ALA:HB2	2.15	0.47
2:F:307:GLU:N	2:F:307:GLU:OE2	2.48	0.47
1:D:103:PHE:HA	1:D:461:ILE:HD11	1.97	0.47
1:D:307:PHE:O	1:D:311:LEU:CB	2.62	0.47
2:H:258:LYS:HG2	2:H:278:ILE:HD11	1.96	0.47
1:B:268:LYS:NZ	1:B:268:LYS:CB	2.73	0.47
1:B:425:LEU:CD2	1:B:444:GLU:HG3	2.41	0.47
1:D:142:ILE:HG23	1:D:143:ILE:HG23	1.97	0.47
2:E:291:THR:O	2:E:292:GLU:O	2.33	0.47
1:B:210:ALA:O	1:B:214:SER:OG	2.31	0.46
2:F:77:GLU:CG	2:H:80:MET:CE	2.93	0.46
2:G:309:GLU:O	2:G:311:ASN:CA	2.64	0.46
2:H:1:MET:CG	2:H:359:LEU:CD2	2.92	0.46
2:G:309:GLU:CA	2:G:312:ILE:HD12	2.45	0.46
1:D:8:ARG:HH21	1:D:60:HIS:HB2	1.81	0.46
2:G:271:SER:HB2	2:G:279:VAL:HG11	1.96	0.46
1:C:245:PHE:O	1:C:249:SER:OG	2.26	0.46
2:E:238:VAL:HG12	2:E:260:ILE:HB	1.98	0.46
2:F:77:GLU:HA	2:F:80:MET:HE3	1.97	0.46
2:G:29:VAL:HG22	2:G:48:VAL:HB	1.95	0.46
2:H:29:VAL:HG22	2:H:48:VAL:HB	1.95	0.46
1:B:105:SER:O	1:B:109:LEU:HB2	2.16	0.46
1:C:141:GLY:O	1:C:144:VAL:HG22	2.15	0.46
1:C:71:LEU:O	1:C:75:LEU:HB2	2.15	0.46
1:D:3:PHE:O	1:D:7:ILE:HG13	2.15	0.46
1:A:362:LEU:HG	1:A:366:LEU:HD13	1.97	0.46
1:B:474:LEU:HD23	1:B:474:LEU:HA	1.77	0.46
2:H:305:THR:HG23	2:H:311:ASN:HD21	1.80	0.46
1:D:314:THR:O	1:D:318:SER:HB2	2.16	0.46
2:F:259:LEU:HD13	2:F:270:LEU:HD21	1.98	0.46
1:D:409:VAL:HG11	1:D:471:ILE:HG21	1.98	0.46
1:B:277:ARG:HD3	1:B:277:ARG:C	2.36	0.45
1:C:373:LYS:O	1:C:382:TYR:OH	2.22	0.45
1:D:278:ALA:O	1:D:282:ILE:HG13	2.16	0.45
2:E:294:ASN:O	2:E:297:GLN:N	2.36	0.45
1:A:423:ASP:OD1	1:A:427:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HD13	1:A:442:LEU:C	2.37	0.45
2:E:293:GLU:O	2:E:295:ILE:N	2.49	0.45
2:F:314:SER:O	2:F:315:ALA:C	2.54	0.45
1:B:363:LEU:HD21	1:B:396:VAL:HG23	1.98	0.45
1:C:363:LEU:HD21	1:C:396:VAL:HG23	1.97	0.45
1:D:72:ILE:N	1:D:72:ILE:HD13	2.32	0.45
2:G:238:VAL:HG22	2:G:303:ALA:HA	1.99	0.45
1:B:442:LEU:CA	1:B:445:VAL:HG12	2.47	0.45
1:A:465:LEU:HB3	1:A:469:LEU:HD21	1.99	0.45
1:A:471:ILE:HD12	1:A:471:ILE:H	1.81	0.45
2:H:77:GLU:HA	2:H:80:MET:HE3	1.97	0.45
1:A:181:THR:HG22	1:A:185:LEU:HG	1.98	0.44
2:G:330:ILE:CG2	2:G:335:TYR:HD1	2.29	0.44
1:C:361:ILE:O	1:C:365:THR:OG1	2.34	0.44
1:B:275:GLU:O	1:B:275:GLU:HG2	2.17	0.44
1:D:252:ASN:C	1:D:253:PHE:HD1	2.21	0.44
1:D:465:LEU:O	1:D:469:LEU:CD2	2.65	0.44
1:B:181:THR:HG22	1:B:185:LEU:HG	2.00	0.44
1:C:364:LEU:O	1:C:368:GLY:CA	2.65	0.44
2:E:293:GLU:OE2	2:E:293:GLU:HA	2.16	0.44
1:C:100:ASP:OD1	1:C:457:LYS:NZ	2.45	0.44
1:C:230:MET:HE3	1:C:230:MET:HB2	1.63	0.44
1:D:442:LEU:O	1:D:445:VAL:HG22	2.18	0.44
1:C:120:LEU:HD21	1:C:128:LEU:CD2	2.48	0.44
1:D:229:SER:HB2	1:D:323:PHE:CD1	2.51	0.44
2:E:335:TYR:OH	2:E:347:ALA:CB	2.52	0.44
2:G:311:ASN:HB3	2:G:328:VAL:HG13	1.99	0.44
2:G:330:ILE:HG23	2:G:335:TYR:HD1	1.83	0.44
2:H:335:TYR:CE2	2:H:339:VAL:CG1	3.00	0.44
1:A:153:LEU:HD13	1:A:154:GLY:H	1.83	0.44
1:A:318:SER:HG	1:A:342:SER:HG	1.64	0.44
1:D:355:GLY:H	1:D:357:LYS:NZ	2.14	0.44
2:H:316:MET:O	2:H:320:ARG:HG2	2.18	0.44
1:A:9:ILE:HD11	1:A:60:HIS:CE1	2.53	0.44
1:B:277:ARG:HD3	1:B:278:ALA:N	2.32	0.44
1:C:103:PHE:HA	1:C:461:ILE:HD11	1.99	0.44
1:C:415:LEU:O	1:C:419:ALA:HB2	2.18	0.44
2:G:316:MET:O	2:G:320:ARG:HG2	2.18	0.44
2:H:309:GLU:O	2:H:312:ILE:HB	2.18	0.44
1:D:417:LEU:HD23	1:D:417:LEU:HA	1.87	0.43
1:C:469:LEU:CD1	1:C:469:LEU:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:THR:HG21	1:B:372:LEU:HD21	2.00	0.43
1:C:149:ILE:HG13	1:C:149:ILE:O	2.18	0.43
1:D:361:ILE:O	1:D:365:THR:OG1	2.34	0.43
1:A:38:PRO:HB2	1:A:87:PRO:HB3	1.99	0.43
1:B:370:ARG:NH2	1:B:382:TYR:O	2.48	0.43
1:B:379:ARG:HH21	2:E:289:LEU:CD2	2.27	0.43
1:D:238:ILE:O	1:D:242:THR:OG1	2.16	0.43
1:A:206:THR:HG23	1:A:209:ASP:H	1.84	0.43
1:A:466:PHE:CG	1:A:471:ILE:HG23	2.54	0.43
1:C:276:PHE:O	1:C:280:ILE:HB	2.19	0.43
1:A:341:PHE:HA	1:A:344:PHE:HD2	1.83	0.43
1:A:468:ARG:HA	1:A:468:ARG:HD3	1.32	0.43
2:F:241:GLY:O	2:F:245:ALA:N	2.48	0.43
2:H:4:ILE:HB	2:H:69:LEU:HD12	1.99	0.43
2:H:310:THR:C	2:H:312:ILE:H	2.22	0.43
1:D:131:ARG:HA	1:D:134:LEU:HD12	2.01	0.43
1:B:425:LEU:HD23	1:B:444:GLU:CG	2.44	0.43
1:C:37:VAL:O	1:C:41:THR:OG1	2.33	0.43
1:C:355:GLY:H	1:C:357:LYS:NZ	2.17	0.43
2:E:1:MET:CG	2:E:359:LEU:CD2	2.95	0.43
1:C:75:LEU:HD22	1:C:75:LEU:HA	1.90	0.43
1:D:474:LEU:HD23	1:D:474:LEU:HA	1.76	0.43
2:F:76:ASP:O	2:F:80:MET:HG3	2.19	0.43
1:A:424:GLU:O	1:A:428:PHE:HB2	2.19	0.42
1:B:457:LYS:HA	1:B:460:LEU:HD12	2.00	0.42
1:C:150:LEU:O	1:C:151:PRO:C	2.55	0.42
1:C:332:PRO:O	1:C:336:PRO:HD2	2.19	0.42
2:G:117:ILE:HA	2:G:118:PRO:HD3	1.89	0.42
2:H:308:ASP:O	2:H:311:ASN:HB2	2.19	0.42
1:C:430:ALA:O	1:C:434:THR:OG1	2.20	0.42
2:E:76:ASP:O	2:E:80:MET:HG3	2.20	0.42
2:E:244:GLY:O	2:E:248:ALA:HB2	2.18	0.42
2:F:235:ILE:HB	2:F:257:VAL:HA	2.00	0.42
1:A:110:THR:HG21	1:A:465:LEU:HD23	2.00	0.42
1:B:363:LEU:O	1:B:367:GLN:CB	2.66	0.42
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.84	0.42
1:C:362:LEU:HG	1:C:366:LEU:HD13	2.00	0.42
2:F:68:MET:HE3	2:F:358:LEU:O	2.18	0.42
1:C:469:LEU:C	1:C:469:LEU:CD2	2.87	0.42
2:G:6:LEU:HB2	2:G:71:ALA:HA	2.01	0.42
2:H:259:LEU:HD13	2:H:270:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:THR:HG22	1:C:86:LEU:HD23	2.02	0.42
2:E:304:LEU:HD23	2:E:304:LEU:HA	1.85	0.42
2:F:105:LEU:HA	2:F:108:LYS:HB3	2.02	0.42
1:A:70:PHE:HA	1:A:73:VAL:HG22	2.02	0.42
1:D:280:ILE:HD13	1:D:280:ILE:HA	1.92	0.42
2:E:105:LEU:HA	2:E:108:LYS:HB3	2.02	0.42
2:F:54:HIS:CD2	2:H:107:GLU:CD	2.61	0.42
2:F:77:GLU:HG2	2:H:77:GLU:N	2.34	0.42
2:G:76:ASP:O	2:G:80:MET:HG3	2.19	0.42
2:G:309:GLU:HA	2:G:312:ILE:HD12	2.02	0.42
2:H:76:ASP:O	2:H:80:MET:HG3	2.19	0.42
1:C:402:PHE:O	1:C:406:TYR:HB2	2.20	0.42
1:C:479:THR:HG21	1:D:372:LEU:HD11	2.02	0.42
1:D:358:VAL:O	1:D:362:LEU:CB	2.68	0.42
1:B:103:PHE:HA	1:B:461:ILE:HD11	2.01	0.42
1:B:362:LEU:HG	1:B:366:LEU:HD13	2.00	0.42
2:E:287:GLN:HE21	2:E:287:GLN:HB2	1.61	0.42
1:B:402:PHE:O	1:B:406:TYR:HB2	2.20	0.42
2:H:244:GLY:O	2:H:248:ALA:HB2	2.19	0.42
1:A:220:ILE:HD13	1:A:321:ALA:HB1	2.01	0.42
1:A:303:PRO:O	1:A:307:PHE:HB3	2.19	0.42
1:B:116:VAL:O	1:B:448:HIS:HB3	2.20	0.42
1:B:370:ARG:NH2	1:B:383:THR:HA	2.34	0.42
1:D:332:PRO:O	1:D:336:PRO:HD2	2.19	0.42
2:F:295:ILE:HG12	2:F:321:MET:HG3	2.02	0.42
2:H:105:LEU:HA	2:H:108:LYS:HB3	2.01	0.42
1:C:241:ILE:HD13	1:C:241:ILE:HA	1.91	0.41
2:F:244:GLY:O	2:F:248:ALA:HB2	2.19	0.41
2:E:335:TYR:CD1	2:E:335:TYR:O	2.73	0.41
2:G:105:LEU:HA	2:G:108:LYS:HB3	2.02	0.41
1:B:332:PRO:O	1:B:336:PRO:HD2	2.21	0.41
1:C:109:LEU:HD13	1:C:134:LEU:HD22	2.03	0.41
1:D:466:PHE:CE1	1:D:474:LEU:HD12	2.56	0.41
2:E:333:GLY:O	2:E:336:VAL:HG23	2.20	0.41
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.89	0.41
1:A:385:LYS:HE2	1:A:390:ALA:HA	2.02	0.41
1:C:131:ARG:HA	1:C:134:LEU:HD12	2.02	0.41
1:C:373:LYS:HB3	1:C:373:LYS:HE3	1.86	0.41
2:E:6:LEU:HB2	2:E:71:ALA:HA	2.01	0.41
2:F:6:LEU:HB2	2:F:71:ALA:HA	2.01	0.41
1:A:293:LEU:HD11	1:A:332:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PHE:HA	1:B:73:VAL:HG22	2.03	0.41
1:B:214:SER:O	1:B:218:ILE:HG13	2.21	0.41
1:D:359:ILE:HA	1:D:362:LEU:HD22	2.02	0.41
1:D:454:ASP:HA	1:D:457:LYS:HB2	2.02	0.41
1:D:455:LYS:O	1:D:458:TRP:HB2	2.21	0.41
1:A:43:PHE:O	1:A:47:LEU:HB2	2.20	0.41
1:D:69:GLY:HA2	1:D:72:ILE:HG12	2.02	0.41
1:B:364:LEU:O	1:B:368:GLY:HA3	2.21	0.41
1:C:141:GLY:O	1:C:144:VAL:CG2	2.68	0.41
1:D:68:ASP:OD1	1:D:68:ASP:N	2.53	0.41
1:D:68:ASP:O	1:D:71:LEU:HB3	2.21	0.41
1:D:220:ILE:HD13	1:D:323:PHE:CD2	2.55	0.41
2:E:54:HIS:CD2	2:G:107:GLU:CD	2.62	0.41
2:F:1:MET:CE	2:F:359:LEU:HD12	2.39	0.41
2:F:302:ILE:HG23	2:F:327:MET:HB2	2.02	0.41
2:G:332:ARG:HD3	2:G:334:ALA:HB3	2.02	0.41
1:A:43:PHE:O	1:A:47:LEU:CB	2.69	0.41
1:A:414:MET:O	1:A:418:ILE:HG13	2.21	0.41
1:C:74:VAL:HG22	1:C:473:THR:HG22	2.02	0.41
1:C:417:LEU:HA	1:C:417:LEU:HD23	1.86	0.41
2:E:287:GLN:C	2:E:289:LEU:N	2.73	0.41
2:E:330:ILE:HG21	2:E:335:TYR:CG	2.53	0.41
2:G:310:THR:O	2:G:312:ILE:N	2.54	0.41
1:C:415:LEU:O	1:C:419:ALA:CB	2.69	0.40
1:D:476:ILE:HD12	1:D:476:ILE:HA	1.94	0.40
1:B:131:ARG:HA	1:B:134:LEU:HD12	2.03	0.40
1:D:105:SER:O	1:D:109:LEU:HB2	2.22	0.40
2:F:77:GLU:N	2:H:77:GLU:HG2	2.35	0.40
1:B:440:PRO:HB2	1:B:447:LEU:HA	2.04	0.40
1:C:220:ILE:HD13	1:C:321:ALA:HB1	2.02	0.40
1:D:359:ILE:O	1:D:363:LEU:HB2	2.22	0.40
2:F:309:GLU:N	2:F:309:GLU:CD	2.73	0.40
1:B:385:LYS:HE2	1:B:385:LYS:HB3	1.92	0.40
1:C:106:PHE:CE1	1:C:465:LEU:HD11	2.57	0.40
1:B:71:LEU:O	1:B:75:LEU:HB2	2.22	0.40
1:B:220:ILE:HD11	1:B:323:PHE:CD2	2.56	0.40
1:B:361:ILE:O	1:B:365:THR:OG1	2.37	0.40
1:C:149:ILE:O	1:C:149:ILE:CG1	2.70	0.40
1:C:423:ASP:OD1	1:C:427:ALA:N	2.53	0.40
2:H:307:GLU:OE1	2:H:310:THR:OG1	2.33	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	435/485 (90%)	415 (95%)	20 (5%)	0	100	100
1	B	420/485 (87%)	408 (97%)	11 (3%)	1 (0%)	44	74
1	C	430/485 (89%)	415 (96%)	14 (3%)	1 (0%)	44	74
1	D	426/485 (88%)	411 (96%)	14 (3%)	1 (0%)	44	74
2	E	228/458 (50%)	210 (92%)	14 (6%)	4 (2%)	7	29
2	F	228/458 (50%)	221 (97%)	7 (3%)	0	100	100
2	G	228/458 (50%)	214 (94%)	13 (6%)	1 (0%)	30	63
2	H	228/458 (50%)	215 (94%)	12 (5%)	1 (0%)	30	63
All	All	2623/3772 (70%)	2509 (96%)	105 (4%)	9 (0%)	38	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	69	LEU
2	E	294	ASN
2	H	311	ASN
2	E	292	GLU
2	G	311	ASN
1	C	437	ASN
2	E	334	ALA
1	B	437	ASN
1	D	437	ASN

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	363/395 (92%)	344 (95%)	19 (5%)	19	50
1	B	353/395 (89%)	334 (95%)	19 (5%)	18	48
1	C	359/395 (91%)	342 (95%)	17 (5%)	22	53
1	D	357/395 (90%)	337 (94%)	20 (6%)	17	47
2	E	185/378 (49%)	177 (96%)	8 (4%)	25	56
2	F	190/378 (50%)	180 (95%)	10 (5%)	19	49
2	G	186/378 (49%)	184 (99%)	2 (1%)	70	86
2	H	188/378 (50%)	185 (98%)	3 (2%)	58	81
All	All	2181/3092 (70%)	2083 (96%)	98 (4%)	26	55

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	79	VAL
1	A	105	SER
1	A	145	LEU
1	A	153	LEU
1	A	216	SER
1	A	232	TYR
1	A	246	LEU
1	A	254	THR
1	A	290	CYS
1	A	293	LEU
1	A	339	LEU
1	A	365	THR
1	A	400	TRP
1	A	462	VAL
1	A	468	ARG
1	A	469	LEU
1	A	470	GLU
1	A	471	ILE
1	B	98	VAL
1	B	143	ILE
1	B	145	LEU
1	B	153	LEU
1	B	216	SER
1	B	246	LEU

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Mol	Chain	Res	Type
1	B	268	LYS
1	B	277	ARG
1	B	290	CYS
1	B	293	LEU
1	B	339	LEU
1	B	365	THR
1	B	379	ARG
1	B	447	LEU
1	B	453	ASN
1	B	455	LYS
1	B	462	VAL
1	B	471	ILE
1	B	473	THR
1	C	75	LEU
1	C	99	THR
1	C	105	SER
1	C	120	LEU
1	C	150	LEU
1	C	216	SER
1	C	232	TYR
1	C	234	ASP
1	C	246	LEU
1	C	251	CYS
1	C	252	ASN
1	C	254	THR
1	C	273	ASP
1	C	339	LEU
1	C	365	THR
1	C	469	LEU
1	C	471	ILE
1	D	75	LEU
1	D	99	THR
1	D	105	SER
1	D	109	LEU
1	D	142	ILE
1	D	153	LEU
1	D	189	TYR
1	D	216	SER
1	D	220	ILE
1	D	246	LEU
1	D	293	LEU
1	D	339	LEU

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Mol	Chain	Res	Type
1	D	362	LEU
1	D	365	THR
1	D	375	LEU
1	D	396	VAL
1	D	400	TRP
1	D	447	LEU
1	D	462	VAL
1	D	469	LEU
2	E	283	ASP
2	E	286	ASP
2	E	287	GLN
2	E	288	GLU
2	E	293	GLU
2	E	294	ASN
2	E	308	ASP
2	E	309	GLU
2	F	238	VAL
2	F	242	ASN
2	F	305	THR
2	F	306	ASN
2	F	307	GLU
2	F	309	GLU
2	F	335	TYR
2	F	354	THR
2	F	358	LEU
2	F	360	THR
2	G	335	TYR
2	G	359	LEU
2	H	265	GLN
2	H	305	THR
2	H	310	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	377	HIS
1	A	448	HIS
1	B	57	ASN
1	B	60	HIS
1	B	436	ASN
1	B	448	HIS

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Mol	Chain	Res	Type
1	B	453	ASN
1	C	60	HIS
1	C	313	GLN
1	C	436	ASN
1	D	377	HIS
1	D	436	ASN
1	D	448	HIS
2	E	287	GLN
2	E	294	ASN
2	F	94	ASN
2	F	311	ASN
2	G	311	ASN
2	H	265	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	18:ASN	C	19:LEU	N	1.13
1	E	69:LEU	C	70:VAL	N	0.71

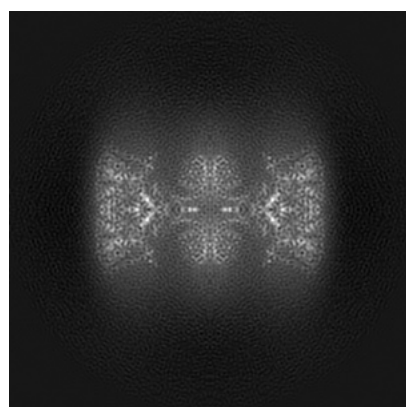
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21041. These allow visual inspection of the internal detail of the map and identification of artifacts.

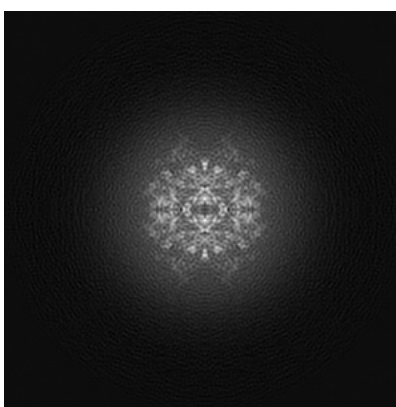
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

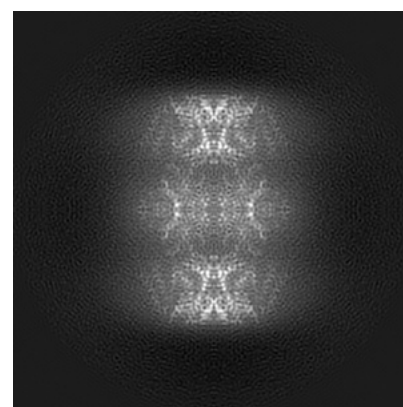
6.1.1 Primary map



X



Y

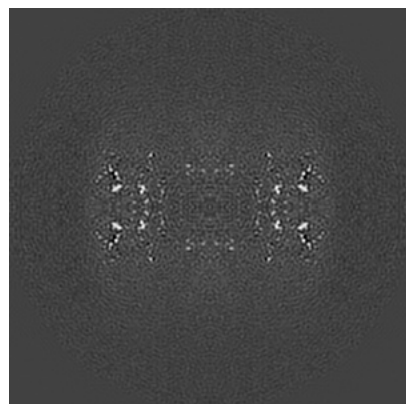


Z

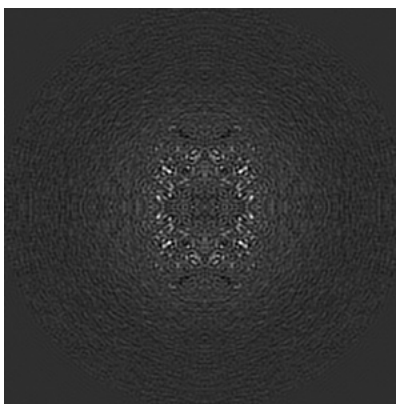
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

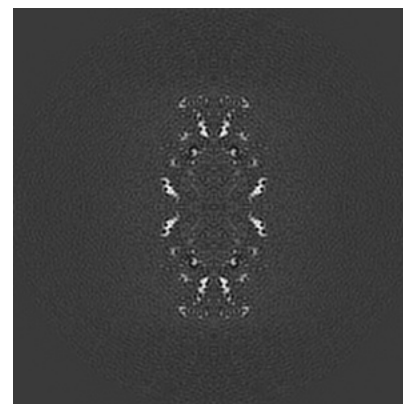
6.2.1 Primary map



X Index: 110



Y Index: 110

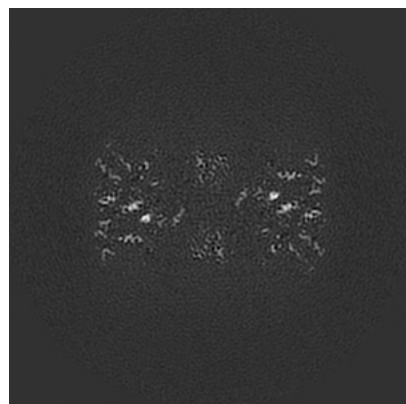


Z Index: 110

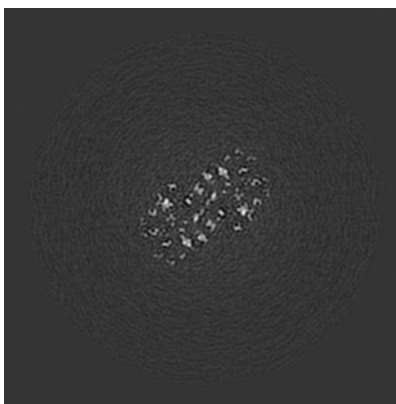
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

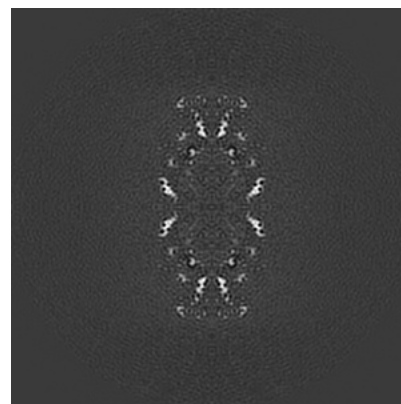
6.3.1 Primary map



X Index: 116



Y Index: 55

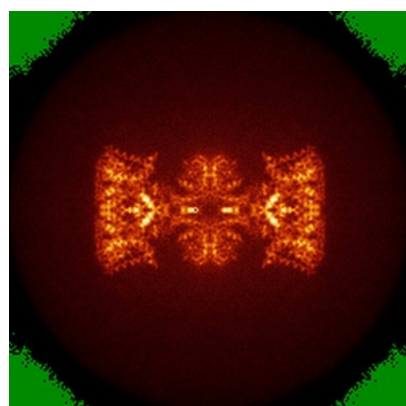


Z Index: 110

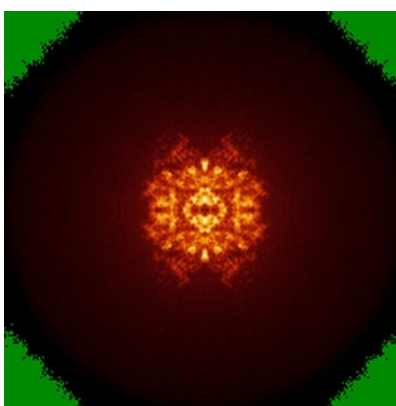
The images above show the largest variance slices of the map in three orthogonal directions.

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

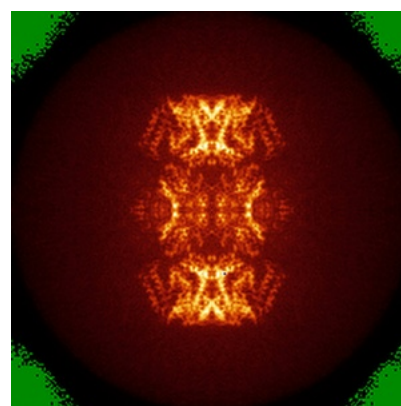
6.4.1 Primary map



X



Y

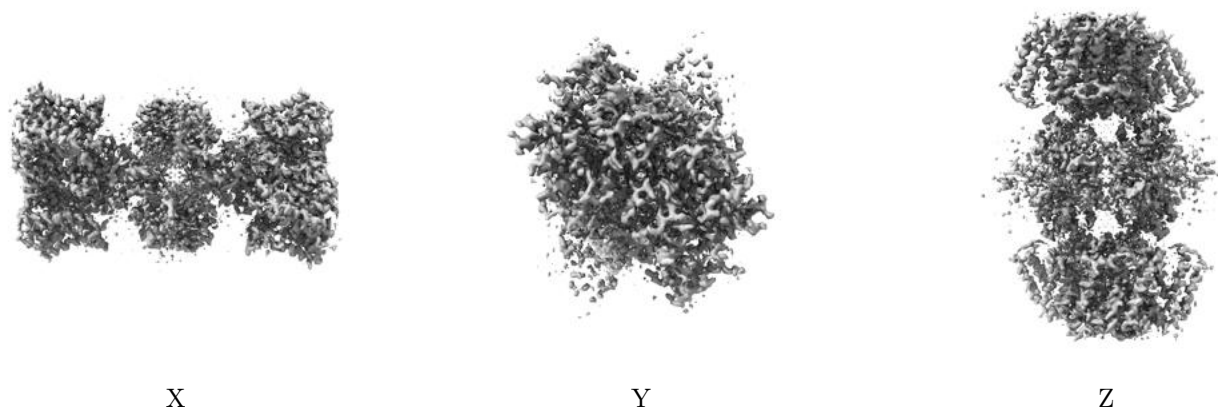


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

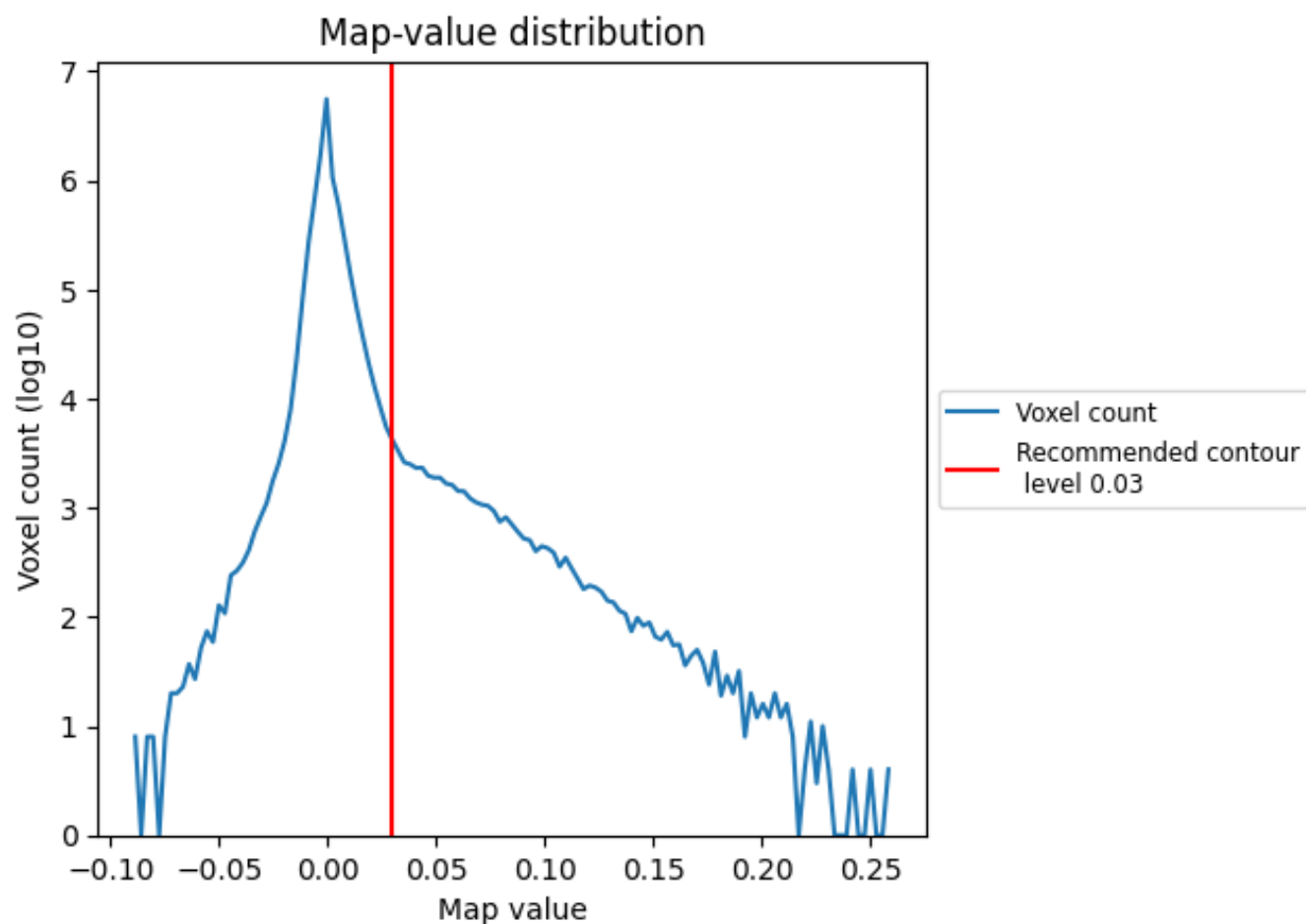
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

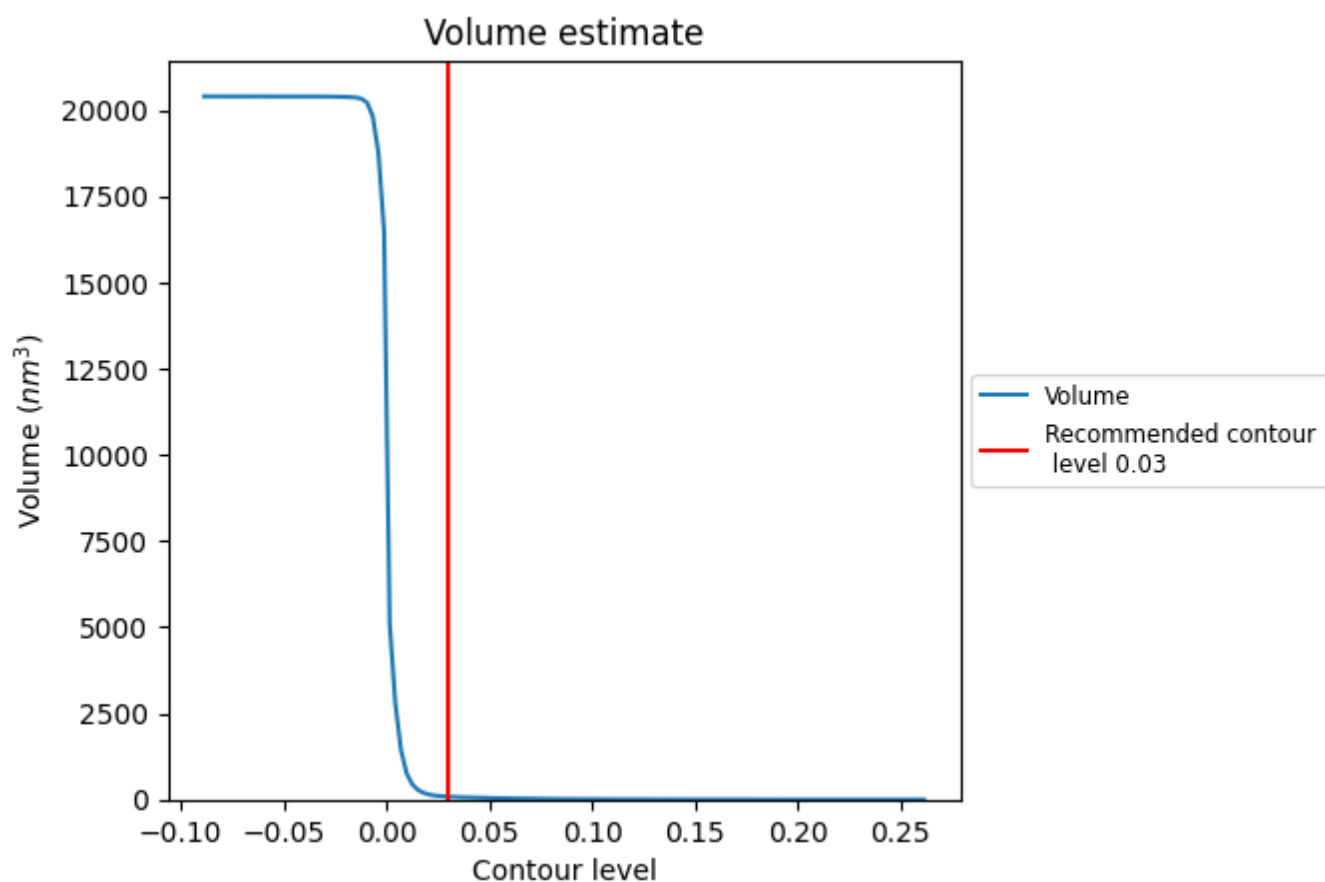
This section contains the results of statistical analysis of the map.

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.

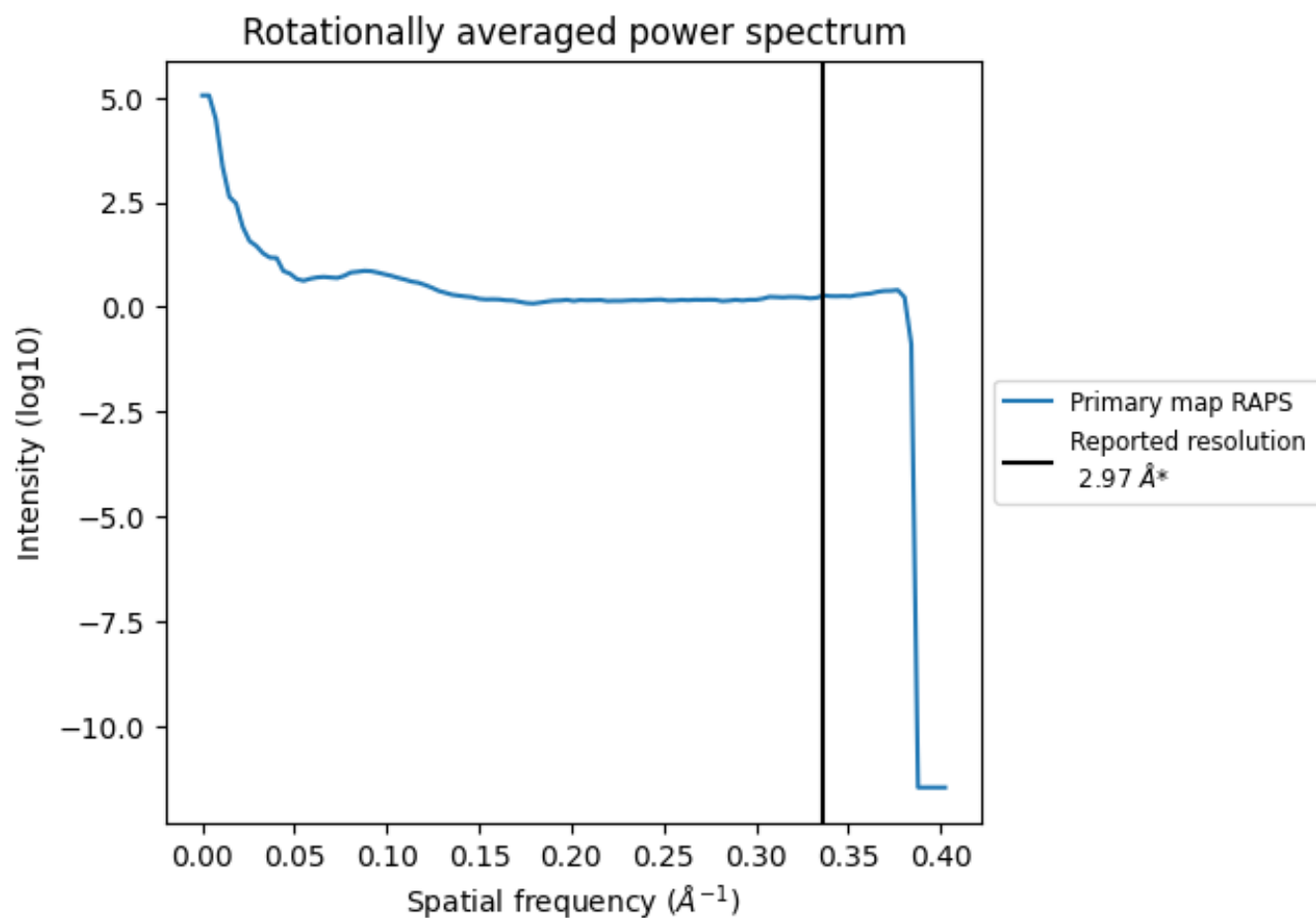
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 83 nm³; this corresponds to an approximate mass of 75 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 0.337 Å⁻¹

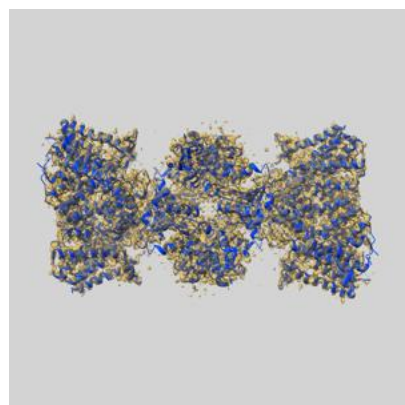
8 Fourier-Shell correlation ⓘ

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

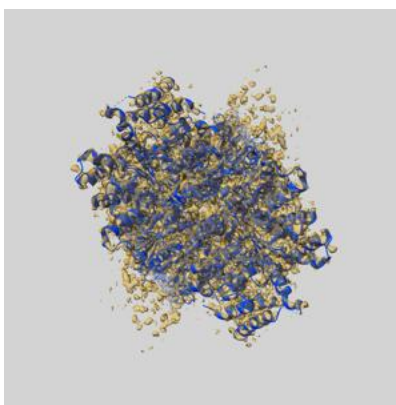
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21041 and PDB model 6V4J. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

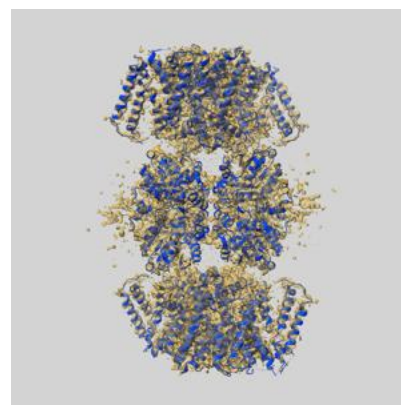
9.1 Map-model overlay [i](#)



X



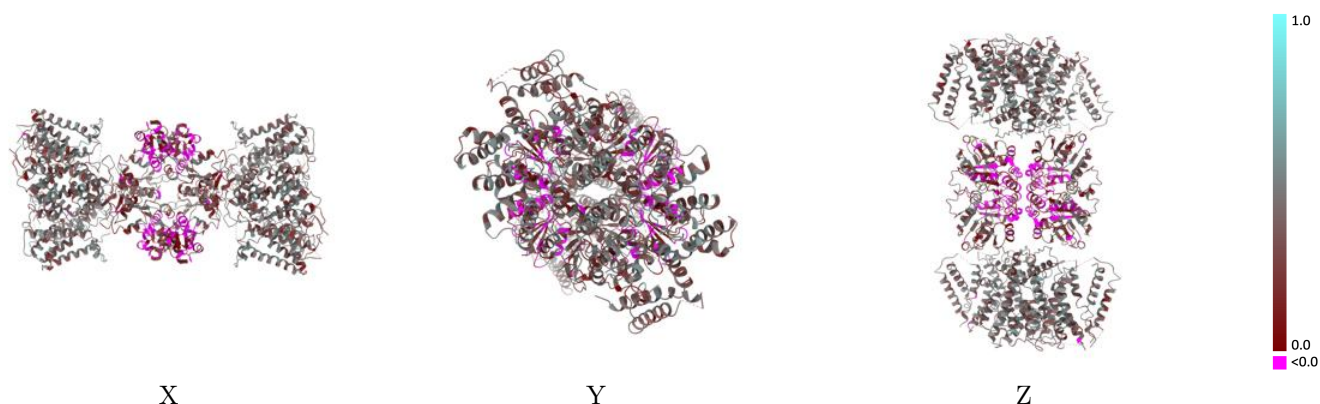
Y



Z

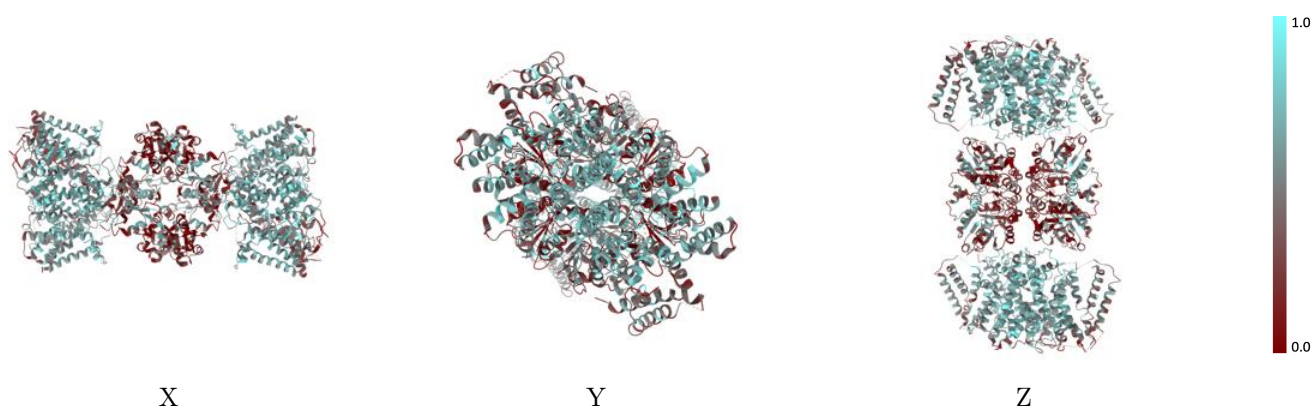
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



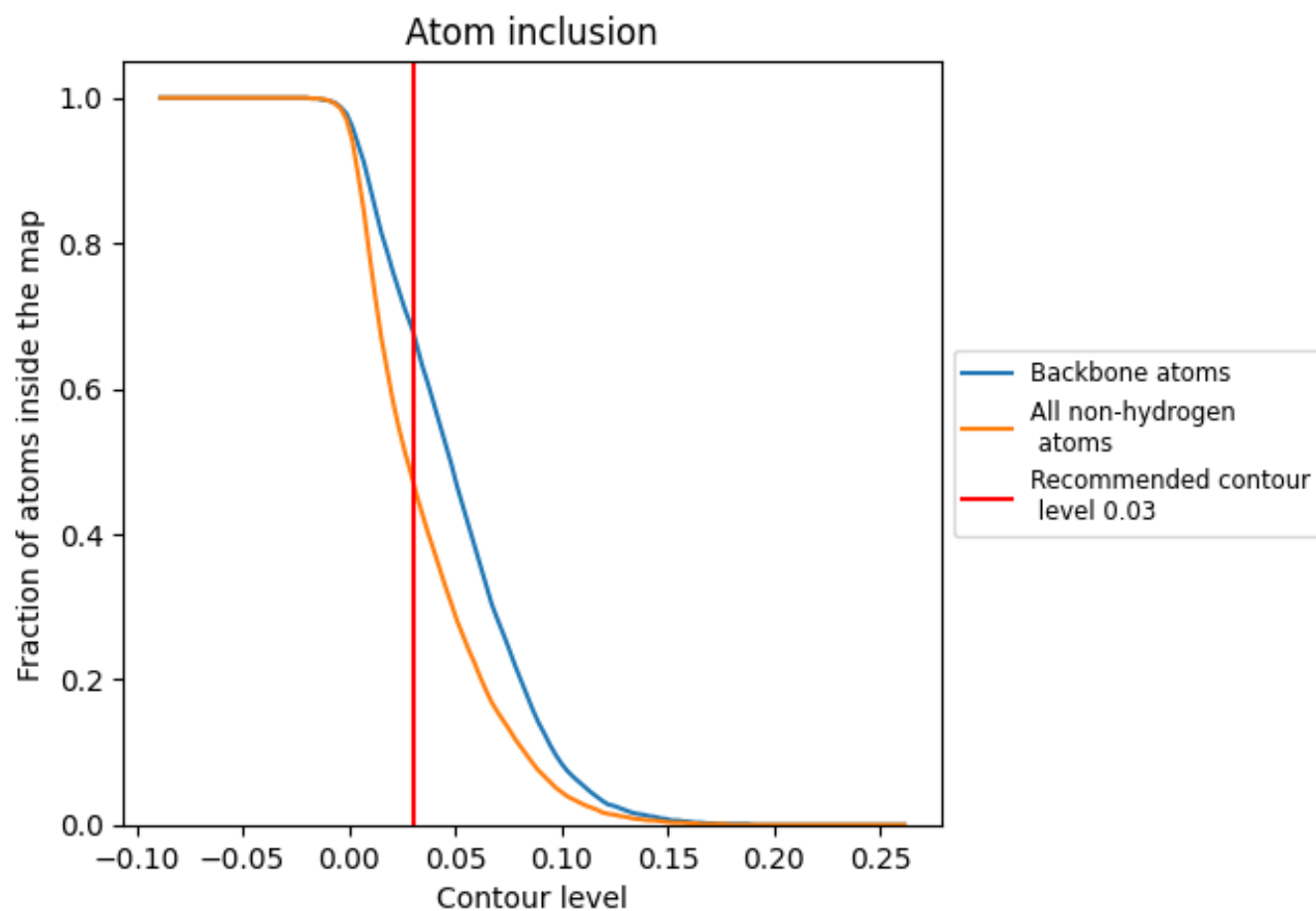
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 47% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4740	<div></div> 0.3370
A	<div></div> 0.5720	<div></div> 0.4190
B	<div></div> 0.5800	<div></div> 0.4180
C	<div></div> 0.5720	<div></div> 0.4210
D	<div></div> 0.5780	<div></div> 0.4190
E	<div></div> 0.2820	<div></div> 0.1800
F	<div></div> 0.2730	<div></div> 0.1700
G	<div></div> 0.2760	<div></div> 0.1750
H	<div></div> 0.2770	<div></div> 0.1790

1.0

0.0

<0.0