



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:27 PM UTC

PDB ID : 8W8D / pdb_00008w8d
EMDB ID : EMD-37342
Title : Structural mechanism of inhibition of the Rho transcription termination factor
by Rof
Authors : Zhang, J.; Wang, C.
Deposited on : 2023-09-01
Resolution : 2.80 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:

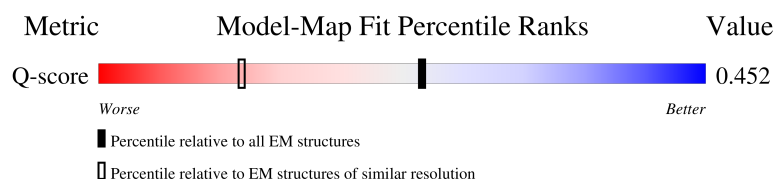
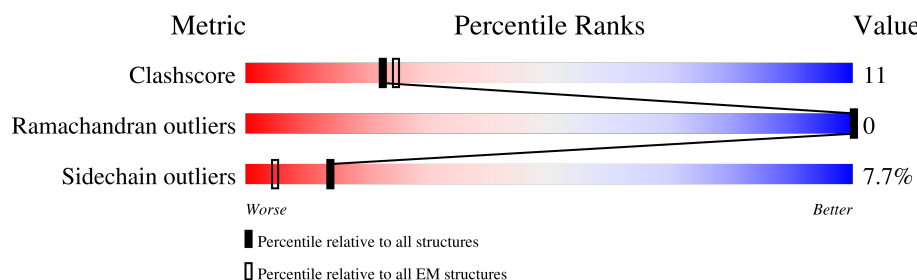
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.80 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	11806 (2.30 - 3.30)

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	419	
1	B	419	
1	C	419	
1	D	419	

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Mol	Chain	Length	Quality of chain
1	E	419	80% 16% .
1	F	419	75% 21% ..
2	a	84	12% 62% 21% 17%
2	b	84	33% 27% 24% . 14%
2	c	84	. 55% 17% 17% 12%
2	d	84	38% 32% 19% 5% 6%
2	e	84	. 67% 23% 11%
2	f	84	42% 61% 23% 17%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23063 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3261	2054	577	613	17		
1	B	412	Total	C	N	O	S	0	0
			3245	2044	574	610	17		
1	C	414	Total	C	N	O	S	0	0
			3261	2054	577	613	17		
1	D	414	Total	C	N	O	S	0	0
			3261	2054	577	613	17		
1	E	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	F	410	Total	C	N	O	S	0	0
			3222	2030	570	607	15		

- Molecule 2 is a protein called Protein rof.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	74	Total	C	N	O	S	0	0
			587	367	99	118	3		
2	e	75	Total	C	N	O	S	0	0
			596	372	101	120	3		
2	b	72	Total	C	N	O	S	0	0
			578	363	98	114	3		
2	a	70	Total	C	N	O	S	0	0
			559	347	94	115	3		
2	f	70	Total	C	N	O	S	0	0
			559	347	94	115	3		
2	d	79	Total	C	N	O	S	0	0
			625	390	105	127	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total	O	0
			3	3	

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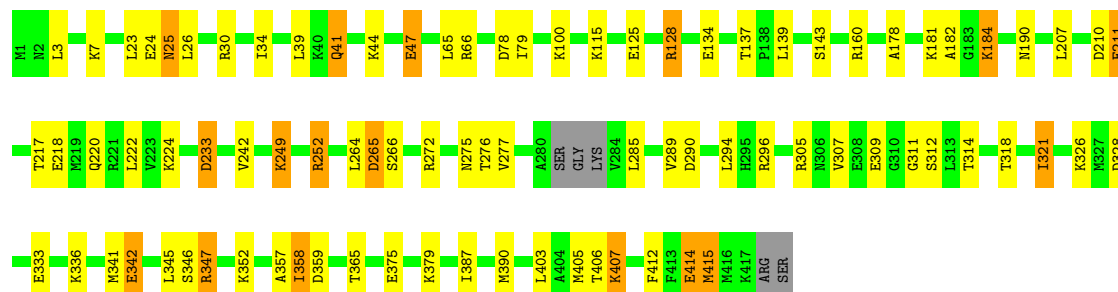
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Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total 1	O 1	0
3	C	3	Total 3	O 3	0
3	D	7	Total 7	O 7	0
3	E	8	Total 8	O 8	0
3	F	6	Total 6	O 6	0
3	a	1	Total 1	O 1	0



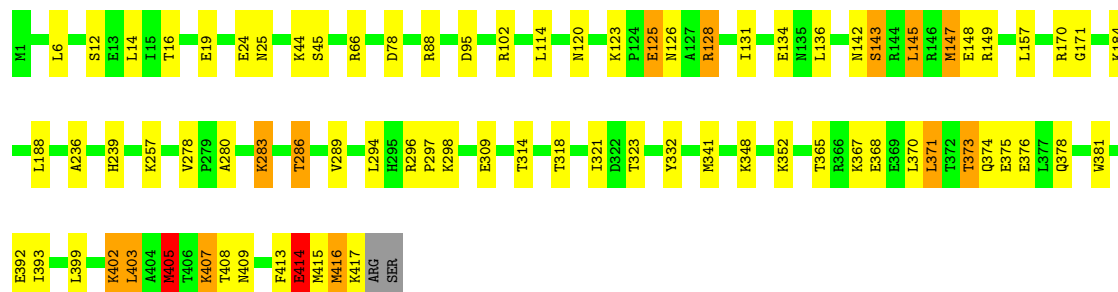
• Molecule 1: Transcription termination factor Rho

Chain D: 78% 17% . .



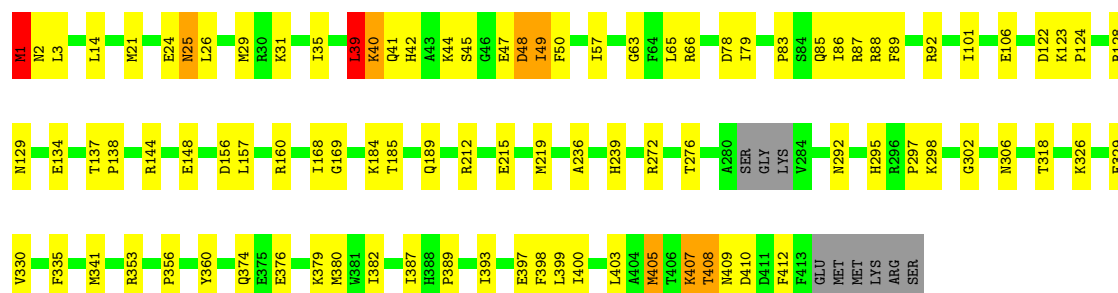
• Molecule 1: Transcription termination factor Rho

Chain E: 80% 16% .



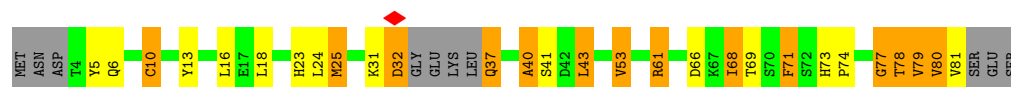
• Molecule 1: Transcription termination factor Rho

Chain F: 75% 21% . .



• Molecule 2: Protein rof

Chain c: 55% 17% 17% 12%

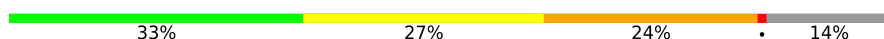


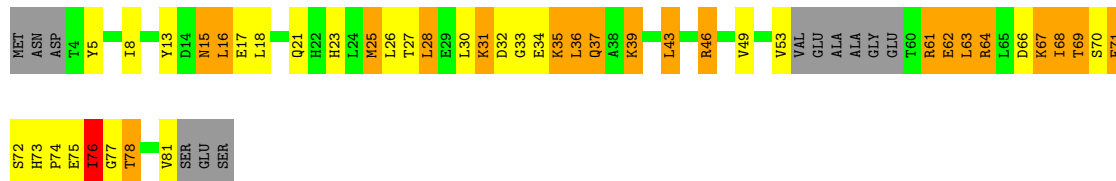
- Molecule 2: Protein rof

Chain e: 



- Molecule 2: Protein rof

Chain b: 



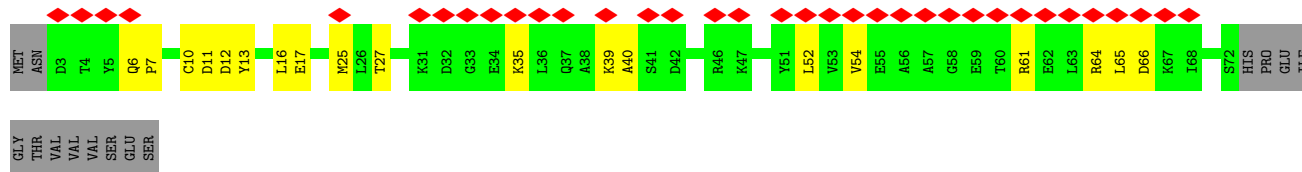
- Molecule 2: Protein rof

Chain a: 



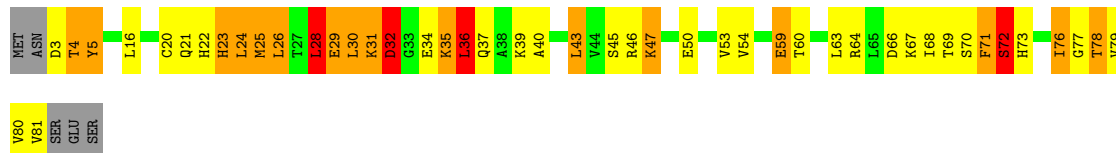
- Molecule 2: Protein rof

Chain f: 



- Molecule 2: Protein rof

Chain d: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1099028	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00451	Depositor
Map size ($\text{\AA}$)	357.00003, 357.00003, 357.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.19, 1.19, 1.19	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	0.27	0/3309	0.42	1/4456 (0.0%)
1	B	0.30	0/3292	0.68	11/4431 (0.2%)
1	C	0.32	0/3309	0.55	4/4456 (0.1%)
1	D	0.71	0/3309	0.95	14/4456 (0.3%)
1	E	0.43	0/3329	0.68	5/4483 (0.1%)
1	F	0.30	0/3269	0.66	16/4405 (0.4%)
2	a	0.11	0/565	0.40	0/762
2	b	0.96	0/585	1.41	8/790 (1.0%)
2	c	0.97	0/594	1.18	4/804 (0.5%)
2	d	0.95	0/633	1.60	14/857 (1.6%)
2	e	0.29	0/604	0.51	0/816
2	f	0.11	0/565	0.38	0/762
All	All	0.47	0/23363	0.75	77/31478 (0.2%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	GLY	N-CA-C	17.60	138.09	115.21
1	F	405	MET	N-CA-C	17.17	137.83	111.56
2	d	78	THR	N-CA-C	14.68	132.31	110.30
1	B	149	ARG	CB-CA-C	-13.57	87.64	110.44
1	B	10	PRO	CA-N-CD	-12.39	94.66	112.00
2	d	37	GLN	N-CA-C	12.06	125.24	110.41
1	E	409	ASN	N-CA-C	-11.65	99.20	113.41
1	E	147	MET	N-CA-C	-10.88	96.94	110.65
1	D	265	ASP	N-CA-C	10.81	123.07	111.28
1	F	405	MET	CB-CA-C	-10.61	91.18	111.03
1	B	144	ARG	N-CA-C	10.11	124.49	110.24
2	b	69	THR	N-CA-C	-10.08	89.32	110.80
2	b	76	ILE	N-CA-C	9.93	130.00	109.34
2	b	77	GLY	N-CA-C	9.57	127.45	113.48
1	C	134	GLU	N-CA-C	-9.28	102.53	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	31	LYS	CB-CA-C	-9.11	90.61	111.83
2	b	34	GLU	N-CA-CB	-9.07	96.33	110.85
2	d	31	LYS	N-CA-C	-8.98	97.24	109.54
2	c	78	THR	N-CA-CB	8.73	125.11	111.24
2	d	37	GLN	N-CA-CB	-8.45	98.81	110.38
1	C	133	PHE	N-CA-C	8.02	121.12	111.82
2	d	28	LEU	N-CA-C	7.88	119.78	111.03
2	c	40	ALA	CB-CA-C	7.88	123.78	109.37
2	d	36	LEU	N-CA-C	-7.84	97.23	107.73
1	B	144	ARG	CB-CA-C	-7.79	97.16	109.70
1	F	45	SER	CB-CA-C	-7.73	95.61	111.22
2	c	77	GLY	N-CA-C	-7.67	95.00	113.18
1	E	414	GLU	N-CA-C	-7.51	104.09	113.18
2	b	33	GLY	N-CA-C	7.40	126.47	115.08
2	b	68	ILE	CB-CA-C	7.34	123.34	111.29
1	D	24	GLU	N-CA-C	-7.33	98.71	109.63
2	d	31	LYS	CA-C-N	7.33	131.68	121.79
2	d	31	LYS	C-N-CA	7.33	131.68	121.79
1	E	405	MET	N-CA-C	-7.28	104.43	113.38
1	F	40	LYS	N-CA-CB	-7.25	99.45	110.33
1	D	359	ASP	N-CA-C	-7.17	99.54	110.30
1	D	181	LYS	N-CA-C	7.17	121.61	112.86
1	C	406	THR	CB-CA-C	-7.11	97.90	111.48
1	D	182	ALA	N-CA-CB	-6.96	100.33	110.70
1	B	143	SER	N-CA-C	6.90	121.42	111.56
1	D	24	GLU	CB-CA-C	-6.75	100.09	113.45
1	D	311	GLY	CA-C-O	-6.63	117.68	122.45
1	F	39	LEU	CB-CA-C	6.59	124.22	110.32
1	D	47	GLU	N-CA-C	6.51	120.23	111.24
1	B	153	SER	CB-CA-C	-6.42	100.75	113.45
2	d	5	TYR	N-CA-C	6.31	119.80	111.28
2	d	28	LEU	N-CA-CB	-6.22	100.96	109.98
1	F	1	MET	CA-C-N	6.21	131.24	121.56
1	F	1	MET	C-N-CA	6.21	131.24	121.56
2	d	72	SER	CB-CA-C	6.20	117.42	109.80
1	D	182	ALA	N-CA-C	6.19	119.77	112.72
1	D	359	ASP	CB-CA-C	6.14	118.59	110.06
1	F	40	LYS	N-CA-C	6.14	120.94	112.90
1	F	45	SER	N-CA-C	-6.01	101.03	109.69
1	D	358	ILE	N-CA-C	5.99	116.31	107.15
1	B	155	GLU	N-CA-CB	-5.95	102.01	110.81
1	C	133	PHE	CB-CA-C	-5.89	99.36	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	SER	N-CA-C	-5.83	98.37	110.80
2	b	76	ILE	CB-CA-C	-5.81	101.77	111.29
1	F	45	SER	CA-C-N	5.79	128.94	122.69
1	F	45	SER	C-N-CA	5.79	128.94	122.69
2	c	40	ALA	N-CA-C	-5.79	100.75	109.95
1	D	357	ALA	N-CA-C	5.67	119.40	111.74
1	F	389	PRO	CA-N-CD	-5.59	104.17	112.00
2	b	34	GLU	N-CA-C	5.54	118.77	109.95
1	B	10	PRO	N-CD-CG	-5.48	94.98	103.20
1	F	129	ASN	CB-CA-C	-5.46	110.26	116.54
1	D	358	ILE	N-CA-CB	-5.43	105.47	111.66
1	B	149	ARG	N-CA-C	5.34	120.98	113.02
2	d	73	HIS	N-CA-C	-5.34	99.59	108.23
1	A	128	ARG	N-CA-C	-5.32	108.04	114.75
1	F	389	PRO	N-CD-CG	-5.11	95.53	103.20
1	B	156	ASP	N-CA-C	-5.10	107.12	113.19
1	F	405	MET	CA-C-N	5.07	129.74	122.23
1	F	405	MET	C-N-CA	5.07	129.74	122.23
2	d	32	ASP	O-C-N	5.06	124.58	120.83
1	E	149	ARG	N-CA-C	-5.03	107.22	113.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3261	0	3337	87	0
1	B	3245	0	3319	55	0
1	C	3261	0	3337	41	0
1	D	3261	0	3337	50	0
1	E	3280	0	3358	47	0
1	F	3222	0	3295	85	0
2	a	559	0	549	14	0
2	b	578	0	577	67	0
2	c	587	0	579	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	625	0	617	41	0
2	e	596	0	587	13	0
2	f	559	0	549	14	0
3	A	3	0	0	1	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	7	0	0	0	0
3	E	8	0	0	0	0
3	F	6	0	0	1	0
3	a	1	0	0	0	0
All	All	23063	0	23441	525	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 11.

All (525) 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:F:379:LYS:HD3	1:F:412:PHE:CZ	1.24	1.62
1:F:379:LYS:CD	1:F:412:PHE:CZ	2.09	1.35
1:F:379:LYS:HD3	1:F:412:PHE:CE2	1.58	1.35
2:b:31:LYS:HA	2:b:69:THR:OG1	1.32	1.26
2:b:73:HIS:CD2	2:b:74:PRO:HD2	1.68	1.26
1:A:130:LYS:NZ	1:A:256:HIS:CE1	2.05	1.24
1:F:379:LYS:CD	1:F:412:PHE:HZ	1.48	1.21
2:c:73:HIS:CG	2:c:74:PRO:HD2	1.75	1.21
2:c:73:HIS:ND1	2:c:74:PRO:HD2	1.54	1.20
1:C:85:GLN:OE1	2:c:10:CYS:SG	2.02	1.16
1:F:21:MET:HB3	1:F:41:GLN:NE2	1.59	1.16
2:b:30:LEU:HD23	2:b:67:LYS:O	1.52	1.09
2:b:30:LEU:CD2	2:b:67:LYS:O	2.02	1.08
1:A:130:LYS:HZ3	1:A:256:HIS:CE1	1.70	1.07
2:d:31:LYS:HG3	2:d:69:THR:OG1	1.50	1.06
2:b:31:LYS:CA	2:b:69:THR:OG1	2.03	1.06
1:C:85:GLN:CD	2:c:10:CYS:SG	2.39	1.05
1:C:143:SER:O	1:C:371:LEU:HD23	1.56	1.05
1:D:47:GLU:OE1	1:D:100:LYS:HD2	1.58	1.03
1:F:21:MET:CB	1:F:41:GLN:HE22	1.69	1.03
2:b:73:HIS:CG	2:b:74:PRO:HD2	1.96	1.00
1:B:406:THR:OG1	1:B:411:ASP:OD1	1.81	0.98
1:F:393:ILE:HG22	1:F:397:GLU:OE1	1.64	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:28:LEU:HB2	2:b:70:SER:O	1.64	0.97
2:b:30:LEU:O	2:b:69:THR:OG1	1.83	0.97
2:d:28:LEU:HD23	2:d:28:LEU:H	1.31	0.95
1:F:393:ILE:O	1:F:397:GLU:HG3	1.66	0.95
1:B:160:ARG:HE	1:B:409:ASN:HD21	1.13	0.94
2:d:31:LYS:HB2	2:d:67:LYS:O	1.67	0.94
1:E:128:ARG:HG3	1:E:128:ARG:HH11	1.33	0.93
1:D:128:ARG:HE	1:E:25:ASN:ND2	1.67	0.92
1:C:143:SER:O	1:C:371:LEU:CD2	2.15	0.92
1:A:130:LYS:HZ2	1:A:256:HIS:CE1	1.83	0.92
2:b:25:MET:SD	2:b:25:MET:N	2.34	0.92
1:F:21:MET:HB3	1:F:41:GLN:HE22	0.77	0.91
1:E:143:SER:O	1:E:371:LEU:HD21	1.71	0.91
2:c:25:MET:SD	2:c:25:MET:N	2.43	0.91
2:d:5:TYR:CG	2:d:5:TYR:O	2.24	0.91
2:b:61:ARG:HG2	2:b:61:ARG:HH11	1.35	0.90
2:b:30:LEU:C	2:b:69:THR:OG1	2.15	0.90
2:b:28:LEU:CB	2:b:70:SER:O	2.20	0.88
1:B:144:ARG:NH2	1:B:167:PRO:HB3	1.88	0.88
1:B:156:ASP:O	1:B:160:ARG:HG3	1.74	0.88
1:E:294:LEU:O	1:E:298:LYS:HG3	1.74	0.88
2:c:73:HIS:CG	2:c:74:PRO:CD	2.57	0.86
1:F:379:LYS:CG	1:F:412:PHE:CZ	2.58	0.86
2:c:61:ARG:HG2	2:c:61:ARG:HH11	1.40	0.84
2:b:36:LEU:O	2:b:36:LEU:HD23	1.79	0.83
1:D:47:GLU:O	1:D:47:GLU:HG3	1.78	0.82
1:F:2:ASN:OD1	1:F:50:PHE:HB2	1.80	0.82
1:F:21:MET:HE3	1:F:41:GLN:OE1	1.78	0.81
2:b:31:LYS:HG2	2:b:68:ILE:O	1.81	0.81
1:F:379:LYS:CD	1:F:412:PHE:CE2	2.50	0.81
2:d:5:TYR:O	2:d:5:TYR:CD2	2.34	0.81
1:F:184:LYS:HD2	1:F:318:THR:HG21	1.64	0.80
2:b:25:MET:HB3	2:b:39:LYS:HD3	1.62	0.80
1:B:160:ARG:HE	1:B:409:ASN:ND2	1.82	0.78
1:E:143:SER:O	1:E:371:LEU:CD2	2.32	0.78
1:F:21:MET:O	1:F:41:GLN:NE2	2.14	0.78
2:b:62:GLU:OE2	2:b:62:GLU:HA	1.84	0.78
2:d:23:HIS:HB3	2:d:39:LYS:HE3	1.64	0.78
2:b:46:ARG:CZ	2:b:46:ARG:HB3	2.11	0.78
1:F:393:ILE:CG2	1:F:397:GLU:OE1	2.31	0.78
1:D:128:ARG:HE	1:E:25:ASN:HD21	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:43:LEU:HD12	2:d:43:LEU:O	1.85	0.77
1:C:144:ARG:NH2	1:C:163:ASP:OD1	2.18	0.77
2:c:73:HIS:CE1	2:c:74:PRO:HD2	2.20	0.76
2:b:64:ARG:HD3	2:b:66:ASP:HB3	1.66	0.76
1:D:407:LYS:HZ3	1:D:407:LYS:HB2	1.49	0.76
2:b:5:TYR:CG	2:b:5:TYR:O	2.39	0.76
1:D:47:GLU:CD	1:D:100:LYS:NZ	2.44	0.76
1:B:160:ARG:NE	1:B:409:ASN:ND2	2.36	0.74
1:F:356:PRO:HG2	1:F:400:ILE:HD11	1.69	0.74
1:C:85:GLN:CD	2:c:10:CYS:HG	1.92	0.74
1:F:21:MET:CE	1:F:41:GLN:OE1	2.36	0.74
2:d:40:ALA:HA	2:d:54:VAL:HG12	1.69	0.74
1:F:21:MET:CB	1:F:41:GLN:NE2	2.40	0.73
1:D:407:LYS:HB2	1:D:407:LYS:NZ	2.02	0.73
1:A:141:ALA:CB	1:A:172:GLN:HE21	2.01	0.73
2:d:26:LEU:HD23	2:d:71:PHE:HB2	1.71	0.72
1:A:130:LYS:NZ	1:A:256:HIS:HE1	1.82	0.72
1:B:160:ARG:NE	1:B:409:ASN:HD21	1.87	0.71
1:C:1:MET:HE2	1:C:1:MET:HA	1.72	0.71
2:c:31:LYS:HG3	2:c:31:LYS:O	1.91	0.71
1:E:145:LEU:HD11	1:E:170:ARG:HE	1.56	0.71
2:b:31:LYS:N	2:b:69:THR:OG1	2.24	0.71
2:d:25:MET:HE2	2:d:39:LYS:HB2	1.73	0.71
2:b:73:HIS:CD2	2:b:74:PRO:CD	2.62	0.70
2:b:31:LYS:HB3	2:b:69:THR:HA	1.71	0.70
2:b:46:ARG:HB3	2:b:46:ARG:NH1	2.07	0.70
1:B:2:ASN:HB3	1:B:5:GLU:HG2	1.73	0.70
2:d:70:SER:HA	2:d:79:VAL:HG12	1.74	0.69
2:d:59:GLU:OE2	2:d:59:GLU:HA	1.90	0.69
1:F:83:PRO:HA	1:F:86:ILE:HD12	1.74	0.69
2:c:32:ASP:OD1	2:c:32:ASP:N	2.22	0.69
2:b:61:ARG:HG2	2:b:61:ARG:NH1	2.08	0.69
1:D:265:ASP:O	1:D:318:THR:HB	1.93	0.68
1:E:373:THR:HG23	1:E:376:GLU:HB2	1.76	0.67
2:d:31:LYS:HG3	2:d:69:THR:HG1	1.58	0.67
1:B:88:ARG:HD2	2:b:13:TYR:CE1	2.29	0.67
1:E:128:ARG:HG3	1:E:128:ARG:NH1	1.98	0.67
1:F:379:LYS:HG2	1:F:412:PHE:CZ	2.29	0.67
1:F:148:GLU:OE1	1:F:408:THR:HG22	1.95	0.67
1:D:23:LEU:HD21	1:D:41:GLN:HG3	1.76	0.67
1:A:71:SER:O	1:A:238:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:GLU:HA	1:E:128:ARG:HD2	1.77	0.66
2:f:40:ALA:HA	2:f:54:VAL:HG12	1.76	0.66
1:B:417:LYS:HE3	1:B:417:LYS:C	2.19	0.66
1:F:379:LYS:HD3	1:F:412:PHE:HZ	0.95	0.66
1:D:233:ASP:OD1	1:D:233:ASP:N	2.29	0.65
1:A:141:ALA:HB2	1:A:172:GLN:HE21	1.60	0.65
2:d:26:LEU:HD12	2:d:26:LEU:N	2.10	0.65
2:d:16:LEU:HD23	2:d:16:LEU:O	1.96	0.65
1:C:85:GLN:CG	2:c:10:CYS:SG	2.85	0.65
1:F:66:ARG:NH1	1:F:78:ASP:OD2	2.30	0.65
1:A:394:ASP:OD1	1:A:395:ALA:N	2.30	0.64
1:A:129:ASN:HA	1:B:27:ALA:CB	2.26	0.64
1:B:144:ARG:HG3	1:B:144:ARG:O	1.97	0.64
1:E:413:PHE:O	1:E:416:MET:HG3	1.97	0.64
1:F:212:ARG:NH2	1:F:215:GLU:OE1	2.31	0.64
2:c:5:TYR:CG	2:c:5:TYR:O	2.49	0.64
2:b:25:MET:H	2:b:25:MET:CE	2.10	0.64
1:F:160:ARG:HH22	1:F:407:LYS:HA	1.63	0.63
1:E:157:LEU:HD13	1:E:403:LEU:HD23	1.81	0.63
1:D:224:LYS:O	1:D:224:LYS:HG3	1.99	0.63
2:b:5:TYR:O	2:b:5:TYR:CD1	2.50	0.63
1:F:49:ILE:HG22	1:F:101:ILE:HG13	1.81	0.63
1:C:411:ASP:OD1	1:C:411:ASP:N	2.32	0.62
2:c:41:SER:HB3	2:c:53:VAL:HG23	1.81	0.62
1:C:415:MET:O	1:C:415:MET:HG2	1.99	0.62
2:b:76:ILE:HG22	2:b:78:THR:HG22	1.82	0.61
1:F:157:LEU:HA	1:F:160:ARG:HD3	1.82	0.61
1:C:85:GLN:HG3	2:c:10:CYS:SG	2.40	0.61
2:b:15:ASN:OD1	2:b:15:ASN:N	2.33	0.61
2:e:5:TYR:CE1	2:e:66:ASP:HB2	2.36	0.61
2:b:64:ARG:HH11	2:b:64:ARG:CG	2.13	0.61
1:D:275:ASN:HD21	1:D:290:ASP:H	1.49	0.61
2:b:36:LEU:HD23	2:b:36:LEU:C	2.26	0.60
2:c:5:TYR:O	2:c:5:TYR:CD2	2.54	0.60
1:A:160:ARG:NH1	1:A:406:THR:O	2.34	0.60
1:E:399:LEU:O	1:E:403:LEU:HB2	2.01	0.60
1:A:127:ALA:O	1:B:28:ARG:NH2	2.34	0.60
2:b:28:LEU:CD2	2:b:70:SER:O	2.47	0.60
2:b:46:ARG:HH11	2:b:46:ARG:HG2	1.66	0.60
1:B:132:LEU:HD22	1:B:251:LYS:HD3	1.84	0.60
1:E:66:ARG:NH1	1:E:78:ASP:OD2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5:TYR:CD1	2:b:5:TYR:C	2.80	0.59
2:a:13:TYR:HA	2:a:16:LEU:HB2	1.84	0.59
2:d:31:LYS:CG	2:d:69:THR:OG1	2.40	0.59
2:b:81:VAL:HG12	2:b:81:VAL:O	2.02	0.59
1:B:144:ARG:O	1:B:144:ARG:CG	2.50	0.59
2:b:43:LEU:HD23	2:b:43:LEU:N	2.18	0.59
2:b:46:ARG:HH11	2:b:46:ARG:CG	2.14	0.59
2:d:22:HIS:HB2	2:d:24:LEU:HD21	1.85	0.59
1:A:123:LYS:HG2	1:A:126:ASN:H	1.67	0.59
1:E:128:ARG:NH1	1:F:25:ASN:OD1	2.35	0.59
2:c:79:VAL:HG12	2:c:79:VAL:O	2.01	0.59
1:D:66:ARG:NH1	1:D:78:ASP:OD2	2.35	0.59
2:d:64:ARG:HH21	2:d:66:ASP:HB3	1.68	0.59
1:E:402:LYS:HA	1:E:405:MET:SD	2.42	0.58
2:d:24:LEU:N	2:d:24:LEU:HD23	2.18	0.58
2:b:64:ARG:NH1	2:b:64:ARG:HG3	2.18	0.58
1:D:47:GLU:CD	1:D:100:LYS:HZ1	2.09	0.58
1:E:12:SER:O	1:E:16:THR:HG23	2.04	0.58
1:D:47:GLU:OE2	1:D:100:LYS:CE	2.51	0.58
2:a:29:GLU:HG3	2:a:36:LEU:HG	1.85	0.58
1:D:128:ARG:NE	1:E:25:ASN:ND2	2.48	0.58
1:F:3:LEU:HD11	1:F:39:LEU:HD11	1.84	0.58
2:c:61:ARG:HG2	2:c:61:ARG:NH1	2.16	0.58
2:e:5:TYR:HE1	2:e:66:ASP:HB2	1.67	0.58
1:A:325:SER:OG	1:A:328:ASP:OD2	2.21	0.58
1:C:95:ASP:OD1	1:C:120:ASN:ND2	2.36	0.58
2:a:50:GLU:HB2	2:a:65:LEU:HD11	1.86	0.58
2:d:28:LEU:H	2:d:28:LEU:CD2	1.94	0.58
1:A:375:GLU:OE2	1:A:375:GLU:N	2.33	0.57
2:e:25:MET:HE1	2:e:27:THR:HG23	1.84	0.57
1:A:379:LYS:HD3	1:A:412:PHE:HB2	1.85	0.57
1:D:276:THR:HG22	1:D:276:THR:O	2.04	0.57
1:A:162:LEU:HD13	1:A:343:LEU:HD21	1.86	0.57
1:D:184:LYS:HD2	1:D:318:THR:HG21	1.86	0.57
2:d:28:LEU:HD23	2:d:28:LEU:N	2.12	0.57
2:d:28:LEU:HD12	2:d:63:LEU:HD13	1.87	0.57
1:F:292:ASN:HA	1:F:295:HIS:CE1	2.39	0.57
2:e:8:ILE:HD12	2:e:12:ASP:OD1	2.04	0.56
2:b:73:HIS:CG	2:b:74:PRO:CD	2.80	0.56
1:B:417:LYS:HD2	1:B:417:LYS:O	2.04	0.56
1:A:160:ARG:NH1	1:A:403:LEU:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:GLU:OE2	1:D:211:GLU:HA	2.05	0.56
2:b:71:PHE:CD1	2:b:71:PHE:N	2.73	0.56
2:b:30:LEU:HD21	2:b:67:LYS:O	2.02	0.56
1:A:256:HIS:O	1:A:258:LYS:NZ	2.36	0.56
1:E:286:THR:O	1:E:286:THR:OG1	2.17	0.56
2:c:37:GLN:OE1	2:c:37:GLN:HA	2.05	0.56
2:b:23:HIS:O	2:b:23:HIS:CD2	2.59	0.56
1:D:47:GLU:CD	1:D:100:LYS:HD2	2.29	0.56
1:E:184:LYS:HD2	1:E:318:THR:HG21	1.87	0.56
1:E:348:LYS:NZ	1:E:392:GLU:OE1	2.36	0.56
1:F:65:LEU:HB2	1:F:79:ILE:HB	1.87	0.56
1:A:356:PRO:HG2	1:A:396:MET:HE2	1.88	0.55
1:F:379:LYS:CG	1:F:412:PHE:HZ	2.04	0.55
2:b:31:LYS:CG	2:b:68:ILE:O	2.53	0.55
1:F:14:LEU:HD11	1:F:35:ILE:HD11	1.88	0.55
1:B:43:ALA:HB1	1:B:103:PRO:HG3	1.88	0.55
1:D:47:GLU:OE2	1:D:100:LYS:HE3	2.06	0.55
2:c:77:GLY:O	2:c:78:THR:CG2	2.55	0.55
1:A:180:PRO:O	1:A:347:ARG:NH1	2.40	0.55
1:E:414:GLU:O	1:E:417:LYS:HG3	2.07	0.55
1:B:32:GLN:OE1	1:B:32:GLN:N	2.40	0.55
1:C:147:MET:O	1:C:194:SER:OG	2.25	0.55
1:D:47:GLU:OE1	1:D:100:LYS:CD	2.46	0.55
1:F:272:ARG:O	1:F:276:THR:HG23	2.07	0.55
2:f:6:GLN:HG2	2:f:7:PRO:HD2	1.90	0.54
1:C:257:LYS:NZ	1:C:309:GLU:O	2.39	0.54
1:B:406:THR:HG21	1:B:412:PHE:HB2	1.89	0.54
1:A:402:LYS:HG2	1:A:415:MET:HE3	1.89	0.54
1:B:144:ARG:NH2	1:B:167:PRO:CB	2.66	0.54
1:F:31:LYS:NZ	3:F:501:HOH:O	2.40	0.54
2:b:5:TYR:CD2	2:b:49:VAL:HA	2.43	0.54
2:b:28:LEU:HD22	2:b:70:SER:O	1.82	0.54
1:A:102:ARG:HB2	1:A:114:LEU:HD13	1.90	0.54
1:C:184:LYS:HD2	1:C:318:THR:HG21	1.89	0.54
1:F:407:LYS:HD3	1:F:407:LYS:N	2.21	0.53
1:B:181:LYS:O	1:B:347:ARG:NH1	2.41	0.53
1:D:249:LYS:O	1:D:249:LYS:HG3	2.06	0.53
1:E:134:GLU:O	1:E:134:GLU:HG3	2.07	0.53
1:A:240:VAL:O	1:A:244:GLU:HG2	2.07	0.53
2:e:53:VAL:HG22	2:e:62:GLU:HG3	1.90	0.53
1:F:85:GLN:OE1	2:f:10:CYS:SG	2.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:GLN:HG2	1:F:219:MET:HE1	1.91	0.53
2:e:5:TYR:CD2	2:e:49:VAL:HG22	2.43	0.53
1:B:375:GLU:O	1:B:379:LYS:HG3	2.09	0.53
1:D:415:MET:O	1:D:415:MET:HG2	2.08	0.53
1:B:144:ARG:HH21	1:B:167:PRO:HB3	1.71	0.53
1:F:88:ARG:HD2	2:f:13:TYR:CE2	2.44	0.52
2:e:32:ASP:OD1	2:e:32:ASP:N	2.43	0.52
1:C:113:LEU:HD21	1:C:116:VAL:HG22	1.92	0.52
1:F:298:LYS:O	1:F:302:GLY:N	2.42	0.52
1:D:25:ASN:O	1:D:25:ASN:ND2	2.35	0.52
1:F:148:GLU:OE1	1:F:408:THR:CG2	2.58	0.52
1:A:54:VAL:HG22	1:A:96:THR:HG22	1.92	0.52
1:A:355:PHE:CG	1:A:356:PRO:HD3	2.45	0.52
1:A:129:ASN:HA	1:B:27:ALA:HB2	1.92	0.52
2:c:68:ILE:CG2	2:c:80:VAL:HG21	2.40	0.52
1:E:341:MET:HG3	1:E:365:THR:HG22	1.93	0.51
1:F:360:TYR:HD2	1:F:387:ILE:HG21	1.75	0.51
2:c:77:GLY:O	2:c:78:THR:HG22	2.09	0.51
2:a:12:ASP:OD1	2:a:13:TYR:N	2.42	0.51
2:a:10:CYS:HA	2:a:13:TYR:CE1	2.45	0.51
1:A:390:MET:HE2	1:A:395:ALA:HA	1.92	0.51
1:D:47:GLU:OE2	1:D:100:LYS:NZ	2.44	0.51
1:A:254:VAL:HG21	1:A:313:LEU:HB2	1.91	0.51
2:c:61:ARG:HH11	2:c:61:ARG:CG	2.13	0.51
1:E:6:LEU:HD22	1:E:14:LEU:HD21	1.93	0.51
1:E:414:GLU:O	1:E:417:LYS:N	2.44	0.51
1:F:374:GLN:OE1	1:F:374:GLN:N	2.43	0.51
1:A:148:GLU:HG3	1:A:150:GLY:H	1.76	0.51
1:D:341:MET:HG2	1:D:365:THR:HG22	1.91	0.51
2:c:5:TYR:CD1	2:c:66:ASP:HB2	2.46	0.51
2:b:64:ARG:CG	2:b:64:ARG:NH1	2.73	0.51
1:B:71:SER:O	1:B:238:ARG:NH2	2.42	0.50
2:a:40:ALA:HA	2:a:54:VAL:HA	1.92	0.50
2:d:71:PHE:O	2:d:72:SER:C	2.53	0.50
1:E:352:LYS:HD2	1:E:393:ILE:HG21	1.93	0.50
1:A:129:ASN:HD22	1:A:129:ASN:H	1.59	0.50
1:E:381:TRP:CG	1:F:353:ARG:HH21	2.29	0.50
2:e:26:LEU:HG	2:e:40:ALA:HB2	1.94	0.50
1:A:26:LEU:HD12	1:A:34:ILE:HG23	1.94	0.50
1:C:125:GLU:CD	1:C:125:GLU:H	2.20	0.50
2:b:46:ARG:NH1	2:b:46:ARG:CB	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:64:ARG:HH11	2:b:64:ARG:HG3	1.73	0.50
2:d:29:GLU:HG3	2:d:36:LEU:HG	1.94	0.50
1:C:236:ALA:HA	1:C:239:HIS:CD2	2.47	0.50
1:D:375:GLU:O	1:D:379:LYS:HG3	2.12	0.50
1:F:356:PRO:HG2	1:F:400:ILE:CD1	2.41	0.50
2:f:25:MET:HE1	2:f:39:LYS:HG3	1.93	0.50
2:d:71:PHE:CD1	2:d:77:GLY:O	2.64	0.50
1:C:240:VAL:O	1:C:244:GLU:HG3	2.12	0.49
1:A:161:VAL:HG21	1:A:396:MET:HE1	1.93	0.49
1:F:236:ALA:HA	1:F:239:HIS:CD2	2.47	0.49
2:b:37:GLN:O	2:b:37:GLN:NE2	2.44	0.49
2:a:5:TYR:H	2:a:64:ARG:HH22	1.59	0.49
1:D:342:GLU:O	1:D:342:GLU:HG2	2.11	0.49
1:A:117:ASN:O	1:A:124:PRO:HD3	2.11	0.49
1:F:1:MET:HG2	1:F:48:ASP:OD2	2.13	0.49
1:F:387:ILE:HD11	1:F:398:PHE:CD2	2.47	0.49
2:c:71:PHE:CD1	2:c:71:PHE:C	2.91	0.49
1:B:417:LYS:C	1:B:417:LYS:CE	2.86	0.49
1:C:169:GLY:H	1:C:172:GLN:HG3	1.78	0.49
1:D:65:LEU:HB2	1:D:79:ILE:HB	1.95	0.49
1:E:236:ALA:HA	1:E:239:HIS:CD2	2.48	0.49
1:F:26:LEU:HB3	1:F:29:MET:HE2	1.95	0.49
2:d:4:THR:HG23	2:d:4:THR:O	2.13	0.49
1:F:156:ASP:OD1	1:F:156:ASP:N	2.39	0.49
1:C:349:ILE:HG22	1:C:354:VAL:HB	1.95	0.48
1:D:47:GLU:CD	1:D:100:LYS:CE	2.85	0.48
1:A:354:VAL:HG12	1:A:356:PRO:HD2	1.95	0.48
2:e:70:SER:OG	2:e:71:PHE:N	2.45	0.48
1:A:100:LYS:HD2	1:A:115:LYS:HD2	1.95	0.48
1:B:406:THR:CG2	1:B:412:PHE:HB2	2.43	0.48
1:B:109:ARG:HG3	1:B:109:ARG:HH11	1.78	0.48
1:B:240:VAL:O	1:B:244:GLU:HG3	2.14	0.48
1:D:3:LEU:HD21	1:D:39:LEU:HD11	1.94	0.48
1:A:15:ILE:O	1:A:19:GLU:HG3	2.13	0.48
2:b:5:TYR:HD1	2:b:66:ASP:HB2	1.77	0.48
1:A:166:SER:O	1:A:166:SER:OG	2.31	0.48
1:A:387:ILE:HG23	1:A:395:ALA:HB1	1.95	0.48
1:C:77:ASP:OD1	1:C:77:ASP:N	2.39	0.48
1:F:92:ARG:HH21	1:F:128:ARG:HH21	1.61	0.48
1:A:353:ARG:CZ	1:A:353:ARG:HA	2.44	0.48
1:A:31:LYS:O	1:A:35:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:72:SER:HA	2:d:77:GLY:HA2	1.96	0.48
1:B:415:MET:HE3	1:B:415:MET:HB3	1.71	0.48
1:D:128:ARG:NE	1:E:25:ASN:HD21	2.03	0.48
1:E:375:GLU:N	1:E:375:GLU:OE2	2.47	0.48
2:c:5:TYR:HD1	2:c:66:ASP:HB2	1.79	0.48
1:C:42:HIS:O	1:C:42:HIS:ND1	2.47	0.47
1:E:257:LYS:HE2	1:E:309:GLU:HB3	1.95	0.47
1:F:379:LYS:HD3	1:F:412:PHE:HE2	1.58	0.47
2:d:21:GLN:HA	2:d:21:GLN:OE1	2.13	0.47
1:E:407:LYS:HB3	1:E:407:LYS:HE3	1.42	0.47
2:e:73:HIS:CG	2:e:74:PRO:HD2	2.49	0.47
1:E:102:ARG:HB3	1:E:114:LEU:HD13	1.96	0.47
2:d:32:ASP:OD1	2:d:32:ASP:N	2.47	0.47
1:A:141:ALA:CB	1:A:172:GLN:NE2	2.76	0.47
1:D:333:GLU:O	1:D:333:GLU:HG2	2.14	0.47
2:b:43:LEU:HD23	2:b:43:LEU:H	1.77	0.47
1:D:307:VAL:HG12	1:D:309:GLU:H	1.78	0.47
2:b:28:LEU:CG	2:b:70:SER:O	2.62	0.47
1:C:65:LEU:HB2	1:C:79:ILE:HB	1.97	0.47
1:C:393:ILE:HD12	1:C:393:ILE:H	1.79	0.47
1:F:134:GLU:O	1:F:134:GLU:HG2	2.15	0.47
2:b:37:GLN:NE2	2:b:37:GLN:C	2.73	0.47
2:b:46:ARG:NH1	2:b:46:ARG:CG	2.73	0.47
2:b:61:ARG:NH1	2:b:61:ARG:CG	2.73	0.47
2:d:29:GLU:HG3	2:d:36:LEU:H	1.79	0.47
2:d:47:LYS:HA	2:d:47:LYS:HD2	1.70	0.47
1:A:248:GLU:O	1:A:252:ARG:HG2	2.15	0.47
2:d:25:MET:CE	2:d:39:LYS:HB2	2.43	0.47
1:A:129:ASN:HD22	1:A:129:ASN:N	2.12	0.47
2:f:54:VAL:HG23	2:f:61:ARG:HB2	1.95	0.47
1:A:101:ILE:HG22	1:A:113:LEU:HA	1.98	0.46
1:A:129:ASN:N	1:A:129:ASN:ND2	2.63	0.46
2:c:43:LEU:C	2:c:43:LEU:HD12	2.40	0.46
1:F:1:MET:HE2	1:F:48:ASP:OD1	2.14	0.46
1:F:399:LEU:HD22	1:F:403:LEU:CD1	2.45	0.46
1:A:186:MET:HE2	1:A:186:MET:HA	1.97	0.46
1:F:47:GLU:OE1	1:F:47:GLU:HA	2.15	0.46
1:B:250:ALA:O	1:B:254:VAL:HG23	2.16	0.46
2:b:25:MET:N	2:b:25:MET:CE	2.75	0.46
2:d:26:LEU:HB2	2:d:28:LEU:CD2	2.45	0.46
1:E:126:ASN:ND2	1:E:126:ASN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:LEU:CD1	1:F:39:LEU:HD11	2.44	0.46
1:B:144:ARG:HA	1:B:169:GLY:HA2	1.96	0.46
1:F:122:ASP:OD1	1:F:123:LYS:N	2.49	0.46
1:F:326:LYS:O	1:F:329:GLU:HG2	2.15	0.46
1:B:321:ILE:HG13	1:B:322:ASP:N	2.31	0.46
1:A:92:ARG:NH1	1:B:28:ARG:HB3	2.31	0.46
1:A:128:ARG:HG2	1:A:129:ASN:ND2	2.31	0.46
1:C:406:THR:HB	1:C:411:ASP:HB2	1.98	0.45
2:c:43:LEU:HG	2:c:43:LEU:O	2.17	0.45
2:a:67:LYS:HE2	2:a:67:LYS:HB3	1.77	0.45
1:A:1:MET:N	3:A:502:HOH:O	2.39	0.45
1:C:355:PHE:HB2	1:C:356:PRO:HD3	1.97	0.45
1:F:407:LYS:N	1:F:407:LYS:CD	2.80	0.45
1:A:32:GLN:O	1:A:36:PHE:HD1	1.99	0.45
2:b:16:LEU:HD22	2:b:16:LEU:HA	1.80	0.45
1:F:106:GLU:CD	1:F:106:GLU:H	2.25	0.45
2:c:23:HIS:CE1	2:c:40:ALA:O	2.69	0.45
2:d:5:TYR:CD1	2:d:66:ASP:HB2	2.52	0.45
1:A:21:MET:SD	1:A:21:MET:N	2.90	0.45
2:e:64:ARG:HD3	2:e:66:ASP:HB3	1.97	0.45
1:A:207:LEU:HD23	1:A:264:LEU:HG	1.98	0.45
1:B:409:ASN:HA	1:B:412:PHE:HB3	1.98	0.45
2:b:35:LYS:HE3	2:b:35:LYS:HB2	1.41	0.45
2:b:37:GLN:O	2:b:37:GLN:HG3	2.16	0.45
1:E:405:MET:H	1:E:405:MET:HG3	1.66	0.45
1:F:297:PRO:HB2	1:F:335:PHE:HZ	1.82	0.45
2:d:29:GLU:HB3	2:d:30:LEU:H	1.71	0.45
2:d:29:GLU:CB	2:d:35:LYS:HA	2.47	0.45
1:A:226:GLU:OE1	1:A:226:GLU:N	2.46	0.45
2:c:68:ILE:HA	2:c:68:ILE:HD12	1.78	0.45
1:F:376:GLU:HB3	1:F:380:MET:HE3	1.98	0.44
1:A:263:LEU:HD22	1:A:316:ILE:HB	1.98	0.44
1:A:144:ARG:NH2	1:A:376:GLU:OE1	2.50	0.44
1:A:413:PHE:HA	1:A:416:MET:HG2	1.99	0.44
1:A:144:ARG:HD2	1:A:146:ARG:HG2	2.00	0.44
1:D:26:LEU:HD12	1:D:26:LEU:O	2.18	0.44
1:D:265:ASP:O	1:D:318:THR:CB	2.64	0.44
1:F:42:HIS:CD2	1:F:42:HIS:O	2.70	0.44
1:A:82:SER:OG	1:A:85:GLN:NE2	2.39	0.44
1:A:102:ARG:N	1:A:112:ALA:O	2.45	0.44
1:A:133:PHE:CG	1:A:133:PHE:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LEU:O	1:D:7:LYS:HG3	2.18	0.44
1:D:414:GLU:O	1:D:414:GLU:HG2	2.18	0.44
1:A:374:GLN:O	1:A:378:GLN:HG2	2.17	0.44
1:A:34:ILE:H	1:A:34:ILE:HG13	1.63	0.44
1:C:143:SER:O	1:C:371:LEU:HD22	2.14	0.44
1:A:164:LEU:HA	1:A:380:MET:HE1	2.00	0.43
1:A:335:PHE:O	1:A:338:THR:OG1	2.36	0.43
1:B:348:LYS:HB2	1:B:348:LYS:HE2	1.68	0.43
1:D:178:ALA:HB2	1:D:345:LEU:HD12	1.99	0.43
1:D:252:ARG:HA	1:D:252:ARG:HD3	1.67	0.43
2:b:13:TYR:O	2:b:13:TYR:CD1	2.70	0.43
1:A:71:SER:O	1:A:71:SER:OG	2.24	0.43
1:B:92:ARG:HG3	1:C:28:ARG:HH11	1.82	0.43
2:b:37:GLN:C	2:b:37:GLN:CD	2.85	0.43
1:B:376:GLU:O	1:B:380:MET:HG3	2.18	0.43
1:C:408:THR:O	1:C:408:THR:HG22	2.19	0.43
2:d:76:ILE:H	2:d:76:ILE:HG13	1.39	0.43
1:B:3:LEU:HD21	1:B:39:LEU:HD11	2.00	0.43
1:F:326:LYS:O	1:F:330:VAL:HG12	2.19	0.43
1:D:207:LEU:HD23	1:D:264:LEU:HD13	2.01	0.43
1:D:387:ILE:HA	1:D:390:MET:HE3	2.01	0.43
1:E:171:GLY:H	1:E:314:THR:HB	1.82	0.43
1:F:42:HIS:O	1:F:42:HIS:CG	2.71	0.43
2:c:13:TYR:CD1	2:c:13:TYR:O	2.70	0.43
1:C:102:ARG:HB3	1:C:114:LEU:HD22	2.00	0.43
1:D:160:ARG:NH2	1:D:403:LEU:O	2.51	0.43
1:D:272:ARG:NH2	1:D:328:ASP:OD1	2.43	0.43
2:a:39:LYS:HB2	2:a:55:GLU:O	2.18	0.43
1:A:161:VAL:HG13	1:A:358:ILE:HD12	1.99	0.43
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.88	0.43
1:E:321:ILE:HD11	1:E:332:TYR:CD2	2.54	0.43
1:F:89:PHE:CE1	1:F:124:PRO:HB2	2.54	0.43
2:a:56:ALA:O	2:a:59:GLU:HB2	2.18	0.43
2:f:11:ASP:OD1	2:f:12:ASP:N	2.52	0.43
1:B:275:ASN:HA	1:B:293:ALA:HB1	2.01	0.43
1:C:208:LEU:HB3	1:C:211:GLU:HG3	2.01	0.43
1:F:185:THR:O	1:F:189:GLN:HG3	2.19	0.43
2:a:10:CYS:HA	2:a:13:TYR:CD1	2.54	0.43
2:a:16:LEU:HD23	2:a:16:LEU:HA	1.87	0.43
2:d:31:LYS:CG	2:d:31:LYS:O	2.62	0.43
1:C:30:ARG:NH2	1:C:32:GLN:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LYS:C	1:B:417:LYS:CD	2.92	0.42
1:F:123:LYS:HE3	1:F:123:LYS:HA	2.01	0.42
1:A:123:LYS:HG3	1:A:125:GLU:H	1.84	0.42
1:A:141:ALA:HB2	1:A:172:GLN:NE2	2.32	0.42
1:A:169:GLY:H	1:A:172:GLN:HG3	1.84	0.42
1:A:393:ILE:H	1:A:393:ILE:HG13	1.67	0.42
1:B:399:LEU:O	1:B:403:LEU:HD22	2.18	0.42
1:B:43:ALA:HB2	1:B:49:ILE:HD11	2.02	0.42
1:E:378:GLN:H	1:E:378:GLN:HG2	1.71	0.42
1:F:39:LEU:HD22	1:F:39:LEU:HA	1.83	0.42
1:F:48:ASP:HB3	1:F:49:ILE:H	1.64	0.42
1:F:379:LYS:NZ	1:F:412:PHE:HE2	2.17	0.42
2:c:61:ARG:NH1	2:c:61:ARG:CG	2.73	0.42
1:B:185:THR:O	1:B:189:GLN:HG3	2.19	0.42
1:A:125:GLU:CD	1:A:125:GLU:C	2.87	0.42
1:A:130:LYS:HA	1:A:130:LYS:HD2	1.92	0.42
1:B:54:VAL:HG22	1:B:96:THR:HG22	2.02	0.42
1:E:414:GLU:H	1:E:414:GLU:HG3	1.68	0.42
1:C:323:THR:OG1	1:C:328:ASP:OD2	2.31	0.42
1:D:358:ILE:O	1:D:358:ILE:HG22	2.18	0.42
1:E:296:ARG:HB2	1:E:297:PRO:HD3	2.02	0.42
1:F:88:ARG:HD2	2:f:13:TYR:HE2	1.84	0.42
1:F:137:THR:O	1:F:137:THR:OG1	2.37	0.42
2:b:36:LEU:C	2:b:36:LEU:CD2	2.91	0.42
2:f:27:THR:HG22	2:f:35:LYS:HB3	2.02	0.42
2:f:64:ARG:HE	2:f:66:ASP:HB3	1.83	0.42
2:a:32:ASP:OD1	2:a:32:ASP:N	2.51	0.42
1:A:30:ARG:HG2	1:A:33:ASP:OD2	2.20	0.41
1:B:24:GLU:HG2	1:B:25:ASN:OD1	2.19	0.41
1:C:3:LEU:HD13	1:C:39:LEU:HD11	2.02	0.41
1:C:132:LEU:HD23	1:C:132:LEU:HA	1.80	0.41
1:C:209:ILE:HD13	1:C:209:ILE:HA	1.88	0.41
2:b:63:LEU:HD12	2:b:63:LEU:HA	1.82	0.41
1:B:26:LEU:HB3	1:B:34:ILE:HG12	2.03	0.41
1:C:266:SER:OG	1:C:269:ARG:HG3	2.20	0.41
1:D:23:LEU:HD23	1:D:23:LEU:HA	1.93	0.41
1:D:321:ILE:HD12	1:D:321:ILE:HA	1.68	0.41
1:F:87:ARG:HH22	2:f:17:GLU:CD	2.29	0.41
1:F:92:ARG:HE	1:F:128:ARG:NH2	2.18	0.41
1:F:168:ILE:HD13	1:F:341:MET:SD	2.60	0.41
1:A:133:PHE:HE1	1:A:254:VAL:HG11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLN:OE1	1:C:59:GLN:N	2.33	0.41
1:D:30:ARG:O	1:D:34:ILE:HG13	2.20	0.41
1:F:356:PRO:CG	1:F:400:ILE:HD11	2.44	0.41
1:F:379:LYS:HA	1:F:382:ILE:HD12	2.01	0.41
1:A:133:PHE:CE1	1:A:254:VAL:HG11	2.55	0.41
1:E:188:LEU:HD23	1:E:188:LEU:HA	1.86	0.41
1:F:144:ARG:HA	1:F:169:GLY:HA2	2.03	0.41
2:b:16:LEU:HD21	2:b:71:PHE:HE2	1.86	0.41
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.91	0.41
1:E:44:LYS:HA	1:E:45:SER:HA	1.86	0.41
2:f:16:LEU:HD23	2:f:16:LEU:HA	1.89	0.41
1:A:212:ARG:HB3	1:A:215:GLU:OE1	2.19	0.41
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.85	0.41
1:B:415:MET:O	1:B:415:MET:SD	2.79	0.41
1:D:347:ARG:O	1:D:347:ARG:HG3	2.21	0.41
1:E:88:ARG:HD3	2:e:13:TYR:CZ	2.55	0.41
1:A:224:LYS:HA	1:A:224:LYS:HD2	1.81	0.41
1:B:169:GLY:H	1:B:172:GLN:HG3	1.86	0.41
1:F:360:TYR:CD2	1:F:387:ILE:HG21	2.55	0.41
1:A:31:LYS:HA	1:A:34:ILE:HD12	2.03	0.41
1:A:100:LYS:HD3	1:A:114:LEU:HD23	2.02	0.41
1:B:247:ILE:HD12	1:B:247:ILE:HA	1.88	0.41
1:F:138:PRO:HD2	1:F:306:ASN:O	2.20	0.41
2:d:71:PHE:CE1	2:d:77:GLY:O	2.74	0.41
1:A:189:GLN:O	1:A:193:GLN:HG3	2.21	0.41
1:A:252:ARG:NH1	1:A:255:GLU:OE2	2.54	0.41
1:B:236:ALA:HA	1:B:239:HIS:CD2	2.55	0.41
2:c:31:LYS:HD2	2:c:69:THR:CG2	2.51	0.41
2:a:5:TYR:H	2:a:64:ARG:NH2	2.18	0.41
2:d:53:VAL:O	2:d:53:VAL:HG23	2.20	0.41
1:B:11:VAL:O	1:B:15:ILE:HG13	2.21	0.41
2:b:46:ARG:CZ	2:b:46:ARG:CB	2.86	0.41
1:A:214:GLU:HG2	1:A:215:GLU:OE1	2.21	0.40
1:B:213:PRO:O	1:B:217:THR:HG23	2.21	0.40
1:C:133:PHE:CD2	1:C:251:LYS:HD3	2.56	0.40
1:F:24:GLU:H	1:F:24:GLU:HG3	1.75	0.40
2:f:64:ARG:NH2	2:f:66:ASP:OD2	2.54	0.40
1:E:143:SER:O	1:E:371:LEU:HD23	2.18	0.40
1:E:280:ALA:HB1	1:E:283:LYS:HD2	2.02	0.40
1:F:57:ILE:HD13	1:F:63:GLY:HA3	2.03	0.40
2:b:64:ARG:HH11	2:b:64:ARG:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:52:LEU:HB2	2:f:65:LEU:HD11	2.02	0.40
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.89	0.40
1:C:358:ILE:O	1:C:396:MET:HE3	2.21	0.40
1:A:191:ILE:O	1:A:195:ILE:HG12	2.21	0.40
1:B:212:ARG:NH2	1:B:215:GLU:OE2	2.42	0.40
1:E:95:ASP:OD1	1:E:120:ASN:ND2	2.46	0.40
1:A:307:VAL:HG12	1:A:309:GLU:H	1.86	0.40
2:e:64:ARG:HG2	2:e:66:ASP:H	1.86	0.40
2:b:31:LYS:C	2:b:31:LYS:HE2	2.46	0.40
2:d:29:GLU:HG3	2:d:36:LEU:N	2.35	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	410/419 (98%)	400 (98%)	10 (2%)	0	100	100
1	B	406/419 (97%)	400 (98%)	6 (2%)	0	100	100
1	C	410/419 (98%)	398 (97%)	12 (3%)	0	100	100
1	D	410/419 (98%)	398 (97%)	12 (3%)	0	100	100
1	E	415/419 (99%)	401 (97%)	14 (3%)	0	100	100
1	F	406/419 (97%)	388 (96%)	18 (4%)	0	100	100
2	a	68/84 (81%)	61 (90%)	7 (10%)	0	100	100
2	b	68/84 (81%)	55 (81%)	13 (19%)	0	100	100
2	c	70/84 (83%)	57 (81%)	13 (19%)	0	100	100
2	d	77/84 (92%)	57 (74%)	20 (26%)	0	100	100
2	e	73/84 (87%)	69 (94%)	4 (6%)	0	100	100
2	f	68/84 (81%)	63 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2881/3018 (96%)	2747 (95%)	134 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	355/359 (99%)	346 (98%)	9 (2%)	42	76
1	B	353/359 (98%)	339 (96%)	14 (4%)	28	63
1	C	355/359 (99%)	343 (97%)	12 (3%)	32	68
1	D	355/359 (99%)	312 (88%)	43 (12%)	5	16
1	E	357/359 (99%)	326 (91%)	31 (9%)	9	30
1	F	350/359 (98%)	338 (97%)	12 (3%)	32	68
2	a	63/76 (83%)	63 (100%)	0	100	100
2	b	67/76 (88%)	38 (57%)	29 (43%)	0	0
2	c	67/76 (88%)	51 (76%)	16 (24%)	1	3
2	d	71/76 (93%)	43 (61%)	28 (39%)	0	0
2	e	67/76 (88%)	66 (98%)	1 (2%)	57	84
2	f	63/76 (83%)	63 (100%)	0	100	100
All	All	2523/2610 (97%)	2328 (92%)	195 (8%)	14	36

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	128	ARG
1	A	129	ASN
1	A	130	LYS
1	A	131	ILE
1	A	134	GLU

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Mol	Chain	Res	Type
1	A	137	THR
1	A	144	ARG
1	A	390	MET
1	B	115	LYS
1	B	137	THR
1	B	142	ASN
1	B	149	ARG
1	B	155	GLU
1	B	158	THR
1	B	193	GLN
1	B	403	LEU
1	B	405	MET
1	B	411	ASP
1	B	414	GLU
1	B	415	MET
1	B	416	MET
1	B	417	LYS
1	C	125	GLU
1	C	131	ILE
1	C	132	LEU
1	C	134	GLU
1	C	137	THR
1	C	210	ASP
1	C	407	LYS
1	C	409	ASN
1	C	411	ASP
1	C	412	PHE
1	C	416	MET
1	C	417	LYS
1	D	25	ASN
1	D	41	GLN
1	D	44	LYS
1	D	115	LYS
1	D	125	GLU
1	D	128	ARG
1	D	134	GLU
1	D	137	THR
1	D	139	LEU
1	D	143	SER
1	D	184	LYS
1	D	190	ASN
1	D	210	ASP

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Mol	Chain	Res	Type
1	D	211	GLU
1	D	217	THR
1	D	218	GLU
1	D	220	GLN
1	D	222	LEU
1	D	233	ASP
1	D	242	VAL
1	D	249	LYS
1	D	252	ARG
1	D	277	VAL
1	D	285	LEU
1	D	289	VAL
1	D	294	LEU
1	D	296	ARG
1	D	305	ARG
1	D	312	SER
1	D	314	THR
1	D	321	ILE
1	D	326	LYS
1	D	336	LYS
1	D	342	GLU
1	D	346	SER
1	D	347	ARG
1	D	352	LYS
1	D	405	MET
1	D	406	THR
1	D	407	LYS
1	D	412	PHE
1	D	414	GLU
1	D	415	MET
1	E	19	GLU
1	E	24	GLU
1	E	123	LYS
1	E	125	GLU
1	E	128	ARG
1	E	131	ILE
1	E	136	LEU
1	E	142	ASN
1	E	143	SER
1	E	145	LEU
1	E	147	MET
1	E	148	GLU

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Mol	Chain	Res	Type
1	E	278	VAL
1	E	283	LYS
1	E	286	THR
1	E	289	VAL
1	E	323	THR
1	E	367	LYS
1	E	368	GLU
1	E	370	LEU
1	E	371	LEU
1	E	373	THR
1	E	374	GLN
1	E	402	LYS
1	E	403	LEU
1	E	405	MET
1	E	407	LYS
1	E	408	THR
1	E	414	GLU
1	E	415	MET
1	E	416	MET
1	F	1	MET
1	F	25	ASN
1	F	39	LEU
1	F	40	LYS
1	F	44	LYS
1	F	48	ASP
1	F	49	ILE
1	F	405	MET
1	F	407	LYS
1	F	408	THR
1	F	409	ASN
1	F	410	ASP
2	c	6	GLN
2	c	10	CYS
2	c	16	LEU
2	c	18	LEU
2	c	24	LEU
2	c	25	MET
2	c	32	ASP
2	c	37	GLN
2	c	43	LEU
2	c	53	VAL
2	c	61	ARG

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Mol	Chain	Res	Type
2	c	68	ILE
2	c	71	PHE
2	c	79	VAL
2	c	80	VAL
2	c	81	VAL
2	e	9	ASN
2	b	8	ILE
2	b	15	ASN
2	b	16	LEU
2	b	17	GLU
2	b	18	LEU
2	b	21	GLN
2	b	25	MET
2	b	26	LEU
2	b	27	THR
2	b	28	LEU
2	b	31	LYS
2	b	32	ASP
2	b	35	LYS
2	b	36	LEU
2	b	37	GLN
2	b	39	LYS
2	b	43	LEU
2	b	46	ARG
2	b	53	VAL
2	b	61	ARG
2	b	62	GLU
2	b	63	LEU
2	b	64	ARG
2	b	67	LYS
2	b	71	PHE
2	b	72	SER
2	b	75	GLU
2	b	76	ILE
2	b	78	THR
2	d	3	ASP
2	d	4	THR
2	d	20	CYS
2	d	23	HIS
2	d	24	LEU
2	d	25	MET
2	d	26	LEU

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Mol	Chain	Res	Type
2	d	28	LEU
2	d	29	GLU
2	d	30	LEU
2	d	32	ASP
2	d	34	GLU
2	d	35	LYS
2	d	36	LEU
2	d	43	LEU
2	d	45	SER
2	d	46	ARG
2	d	47	LYS
2	d	50	GLU
2	d	59	GLU
2	d	60	THR
2	d	68	ILE
2	d	71	PHE
2	d	72	SER
2	d	76	ILE
2	d	78	THR
2	d	80	VAL
2	d	81	VAL

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

Mol	Chain	Res	Type
1	A	129	ASN
1	A	172	GLN
1	A	256	HIS
1	B	151	ASN
1	B	189	GLN
1	B	306	ASN
1	B	361	ASN
1	B	409	ASN
1	C	340	ASN
1	C	361	ASN
1	C	409	ASN
1	D	20	ASN
1	D	140	HIS
1	D	190	ASN
1	D	193	GLN
1	D	198	ASN
1	D	275	ASN

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Mol	Chain	Res	Type
1	D	344	HIS
1	E	25	ASN
1	E	142	ASN
1	E	151	ASN
1	E	172	GLN
1	E	199	HIS
1	E	256	HIS
1	F	42	HIS
2	e	9	ASN
2	b	23	HIS
2	b	73	HIS
2	a	21	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](#)

There are no chain breaks in this entry.

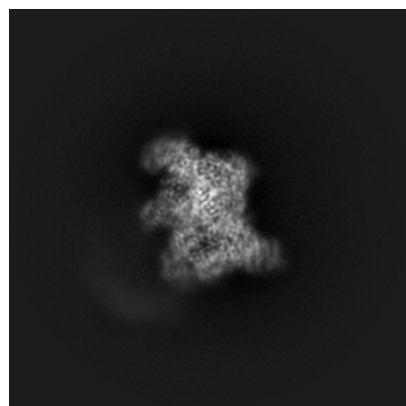
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37342. These allow visual inspection of the internal detail of the map and identification of artifacts.

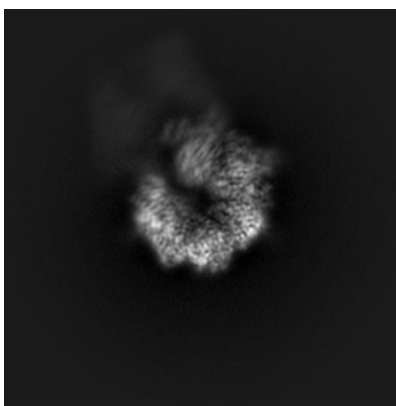
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

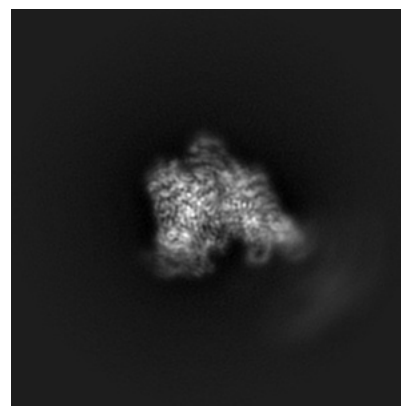
6.1.1 Primary map



X

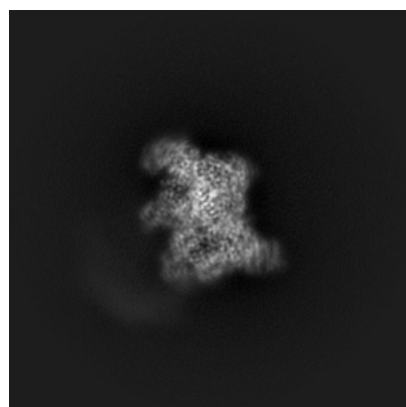


Y

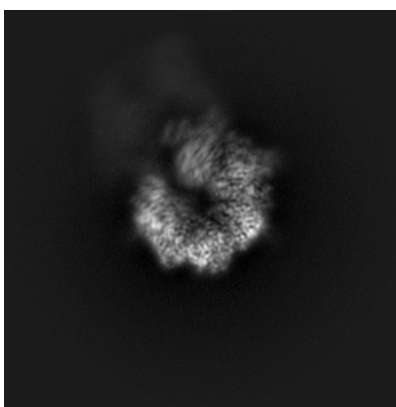


Z

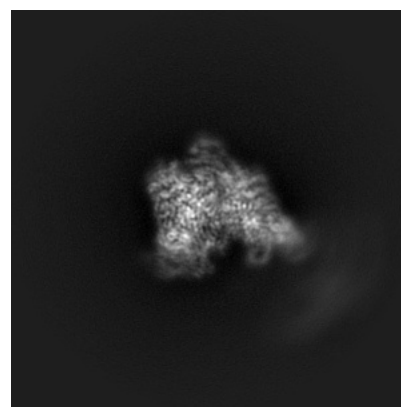
6.1.2 Raw map



X



Y

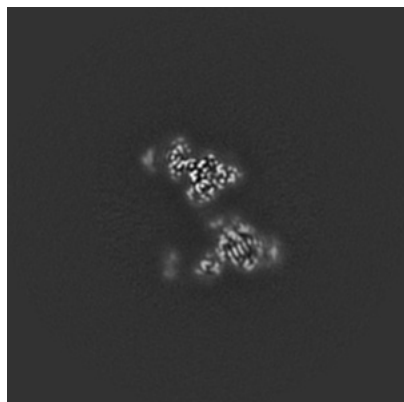


Z

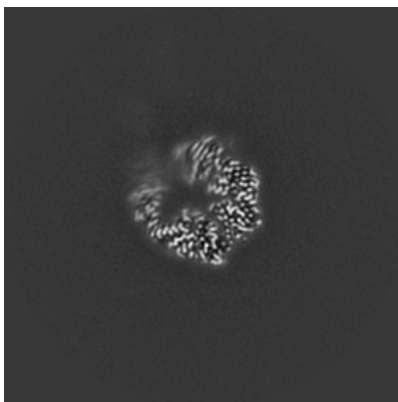
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

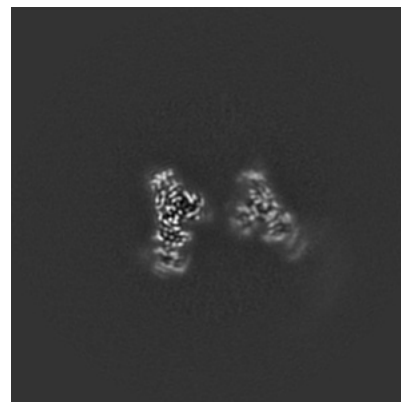
6.2.1 Primary map



X Index: 150

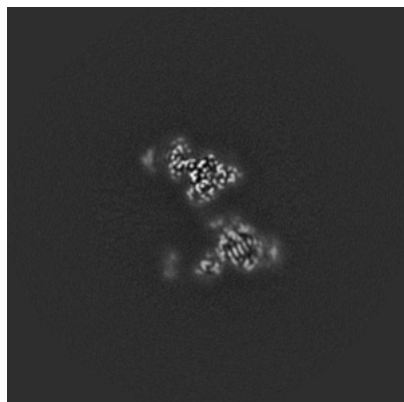


Y Index: 150

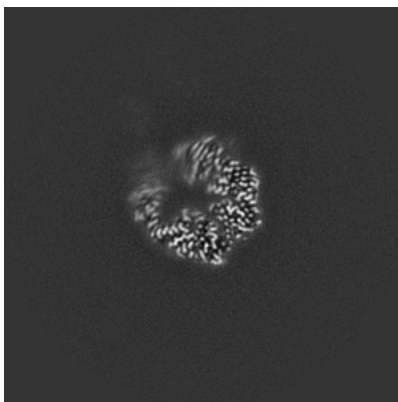


Z Index: 150

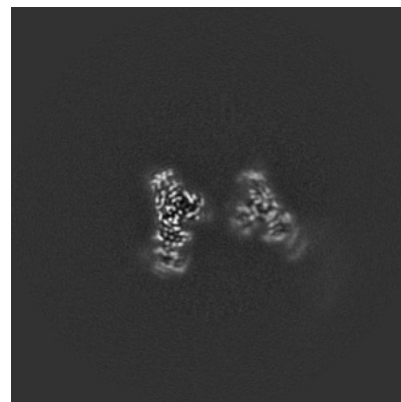
6.2.2 Raw map



X Index: 150



Y Index: 150

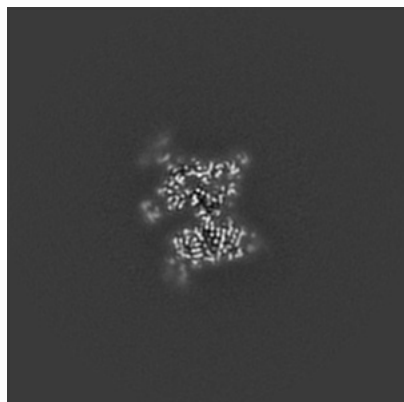


Z Index: 150

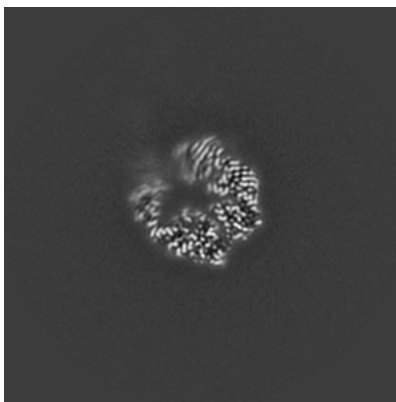
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

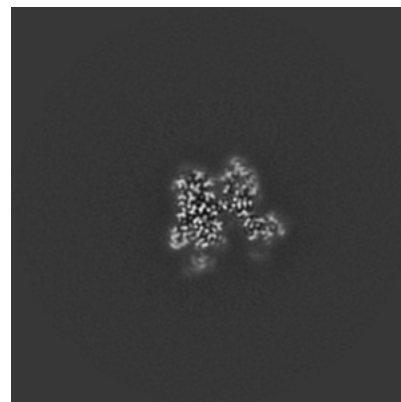
6.3.1 Primary map



X Index: 128

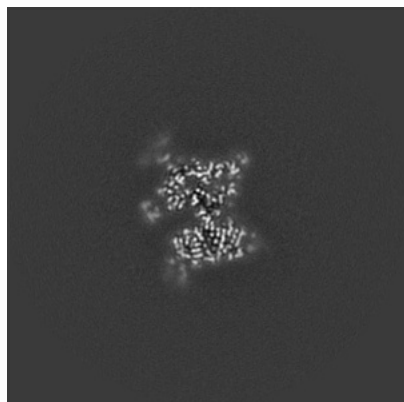


Y Index: 151

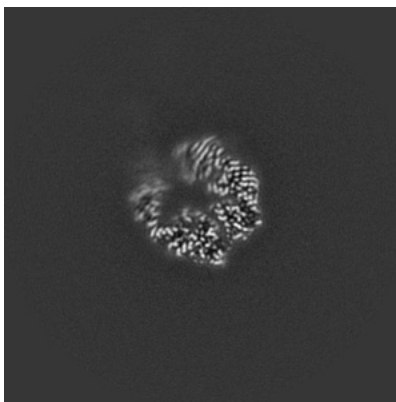


Z Index: 179

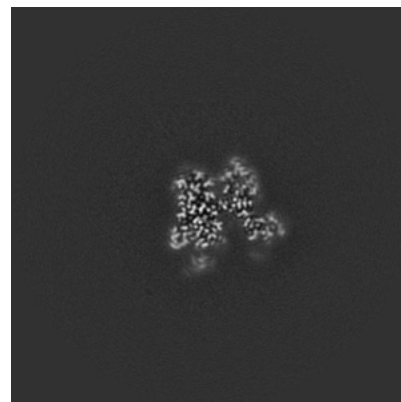
6.3.2 Raw map



X Index: 128



Y Index: 151

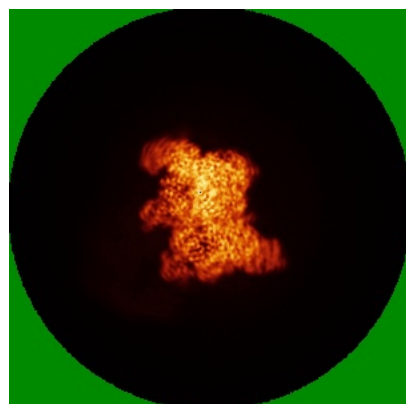


Z Index: 179

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

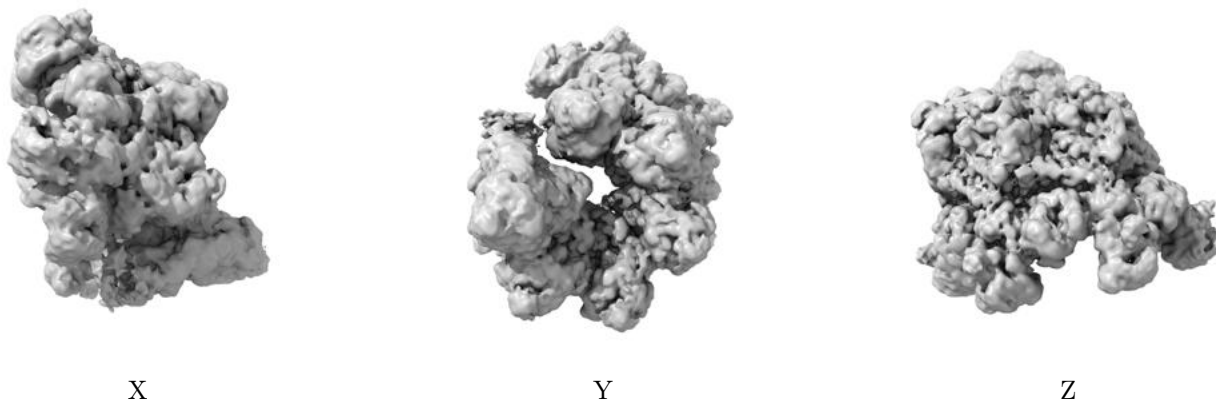


Z

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.

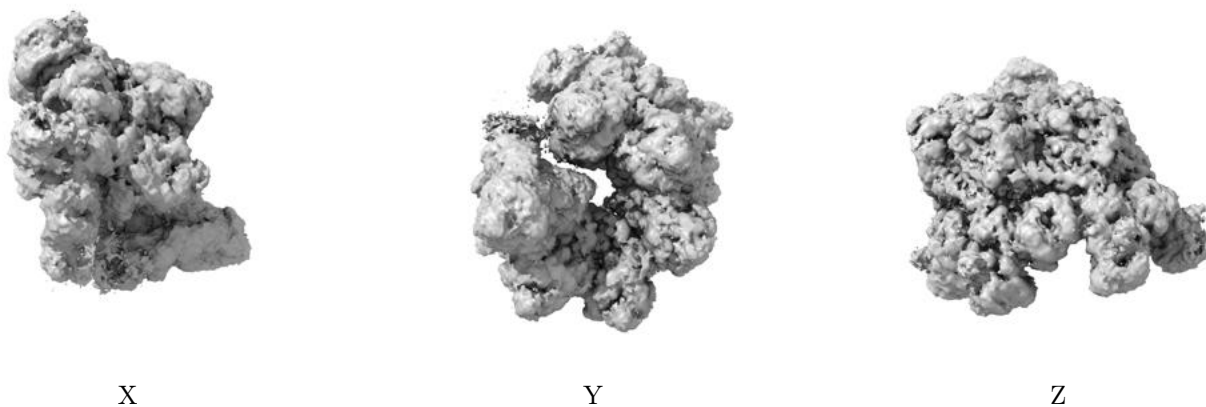
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00451. 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.

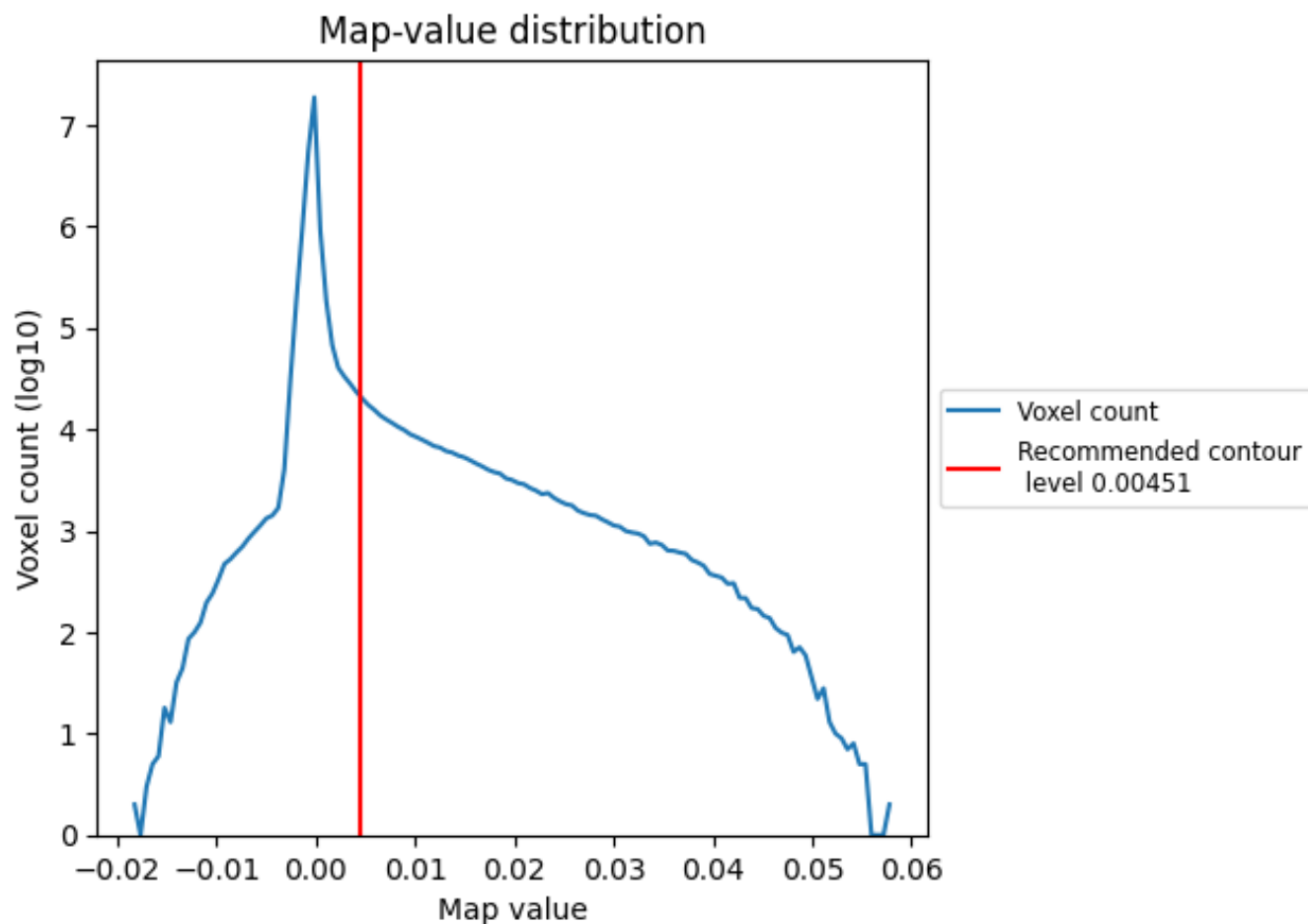
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

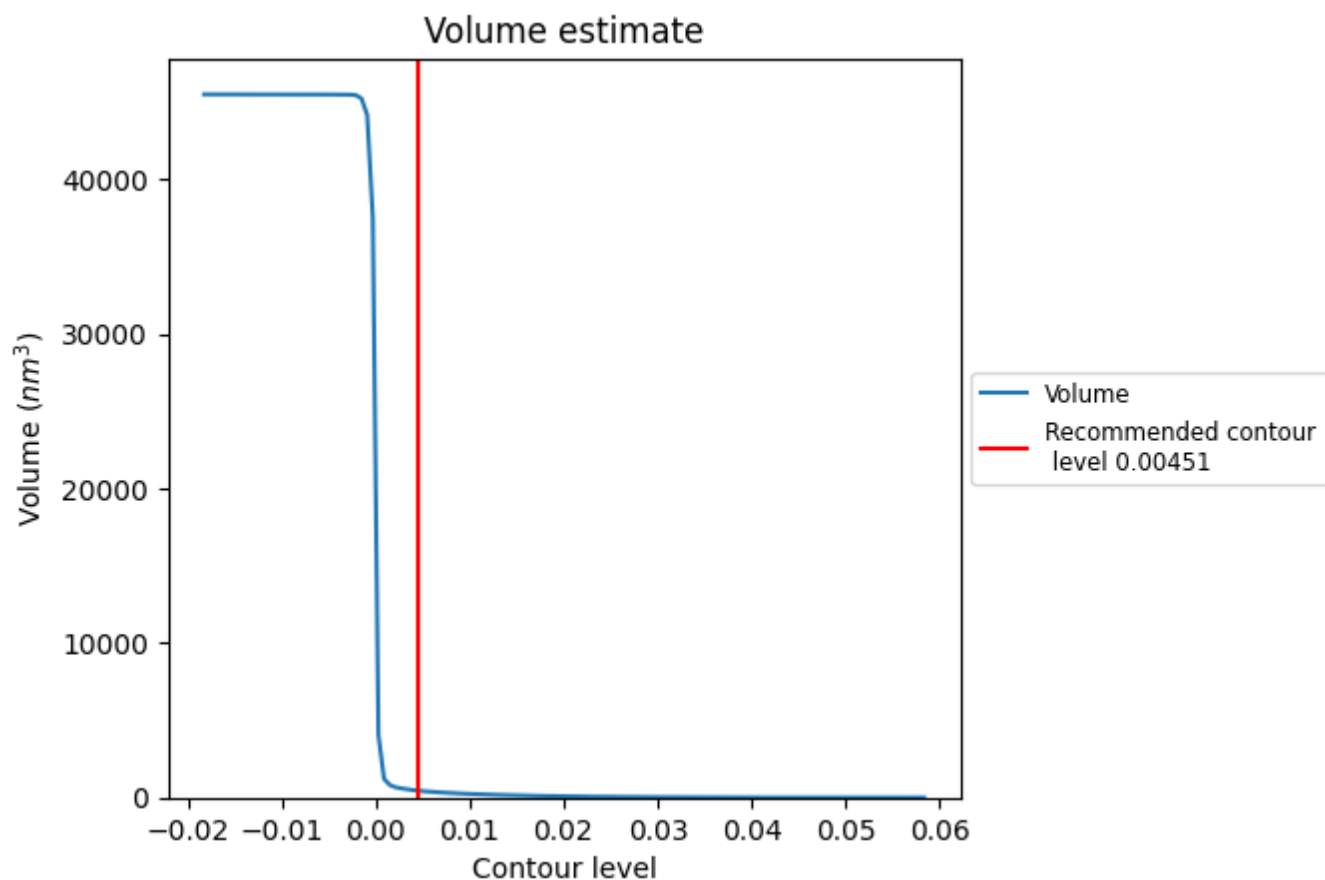
This section contains the results of statistical analysis of the map.

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.

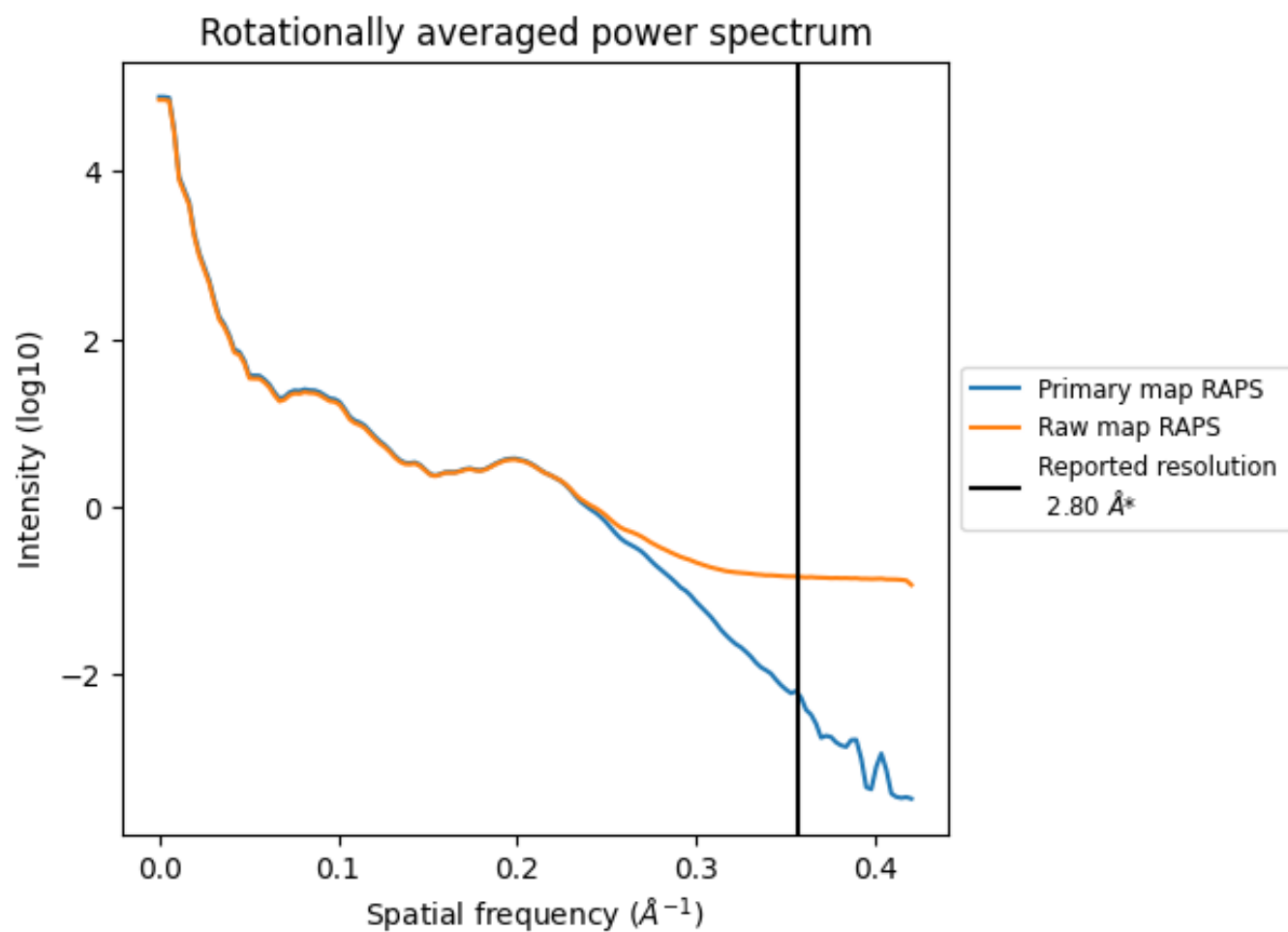
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm³; this corresponds to an approximate mass of 404 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 ⓘ

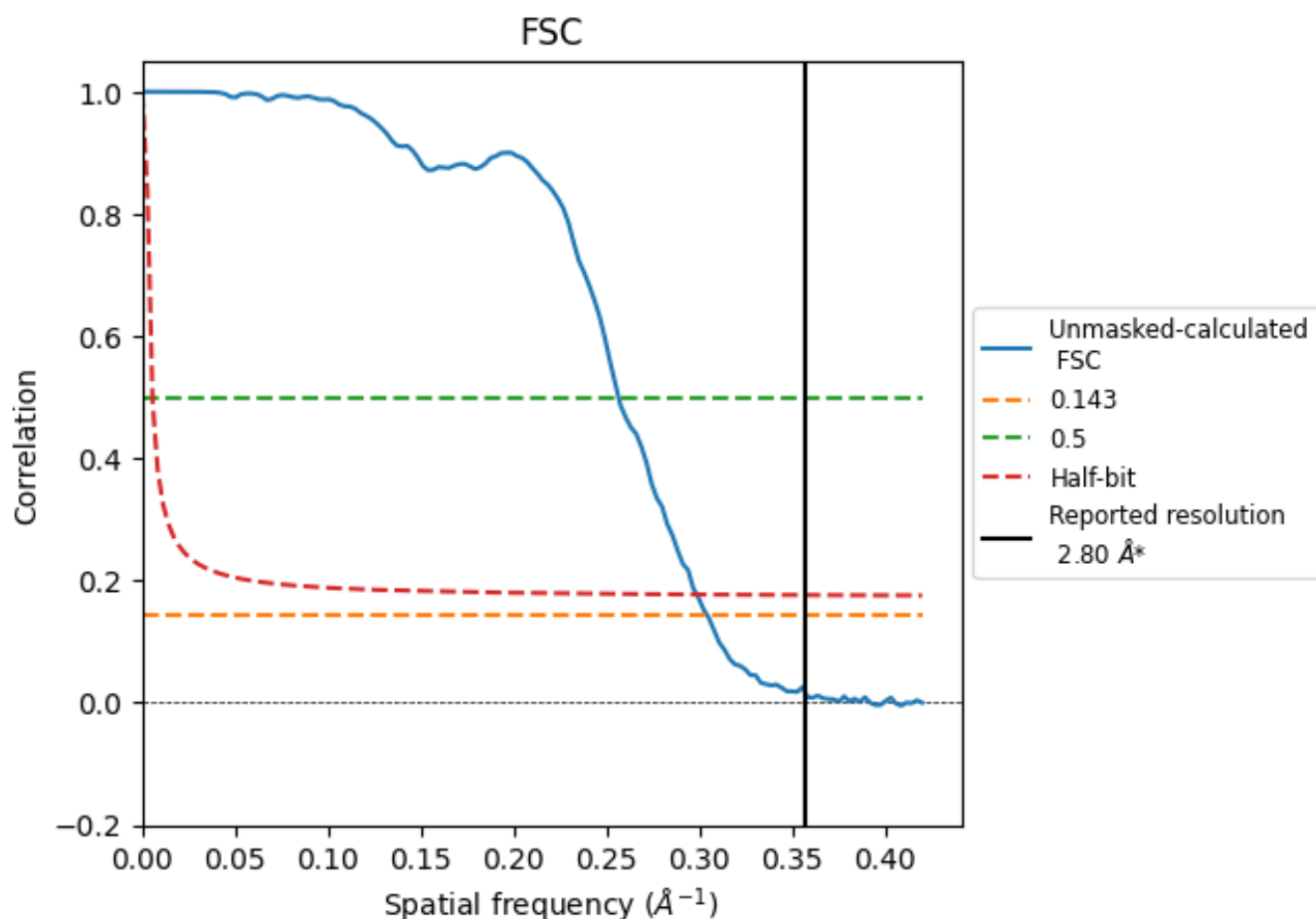


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

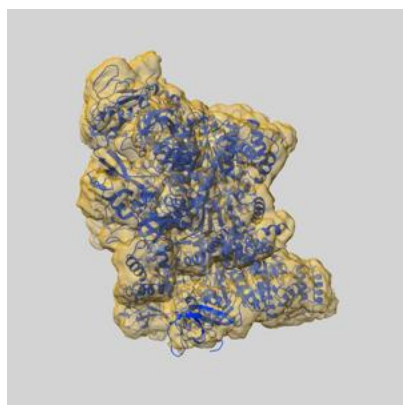
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.29	3.90	3.35

*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 3.29 differs from the reported value 2.8 by more than 10 %

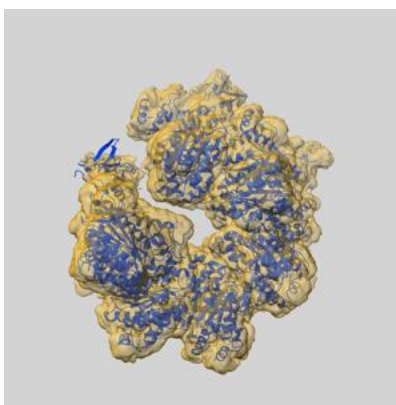
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37342 and PDB model 8W8D. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

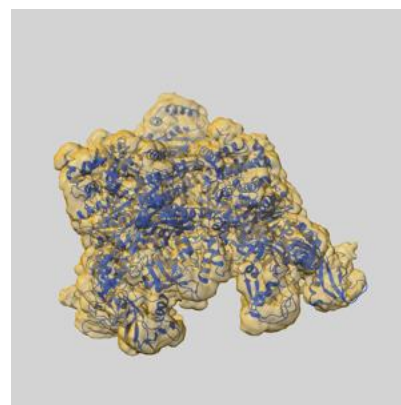
9.1 Map-model overlay [i](#)



X



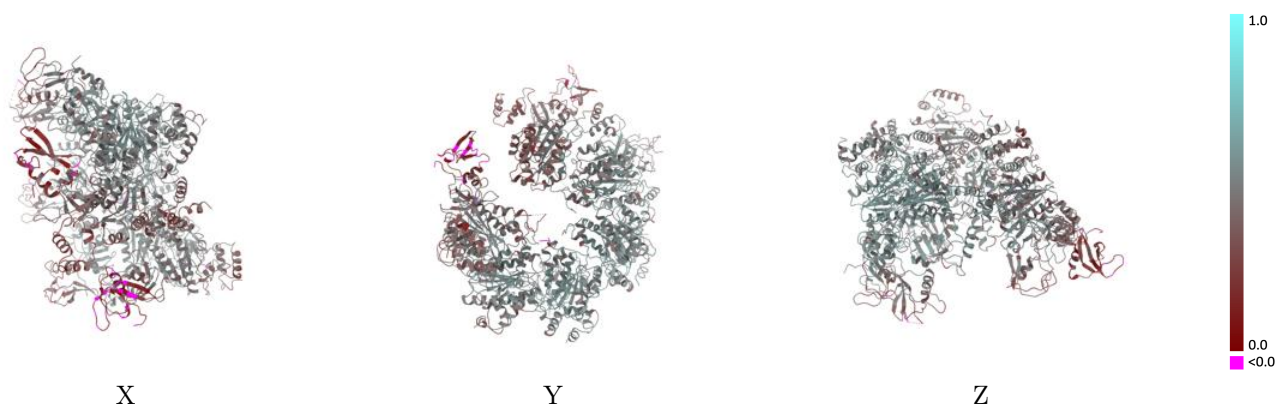
Y



Z

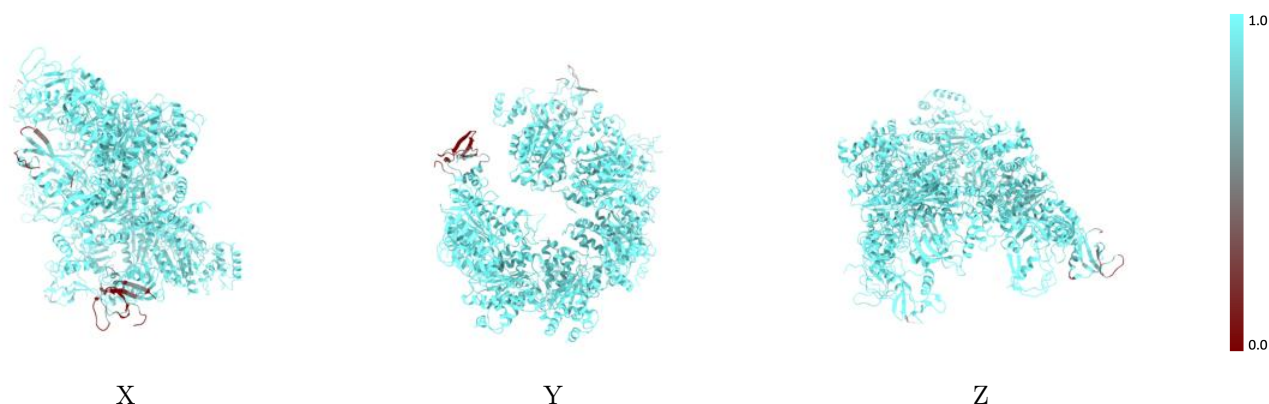
The images above show the 3D surface view of the map at the recommended contour level 0.00451 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



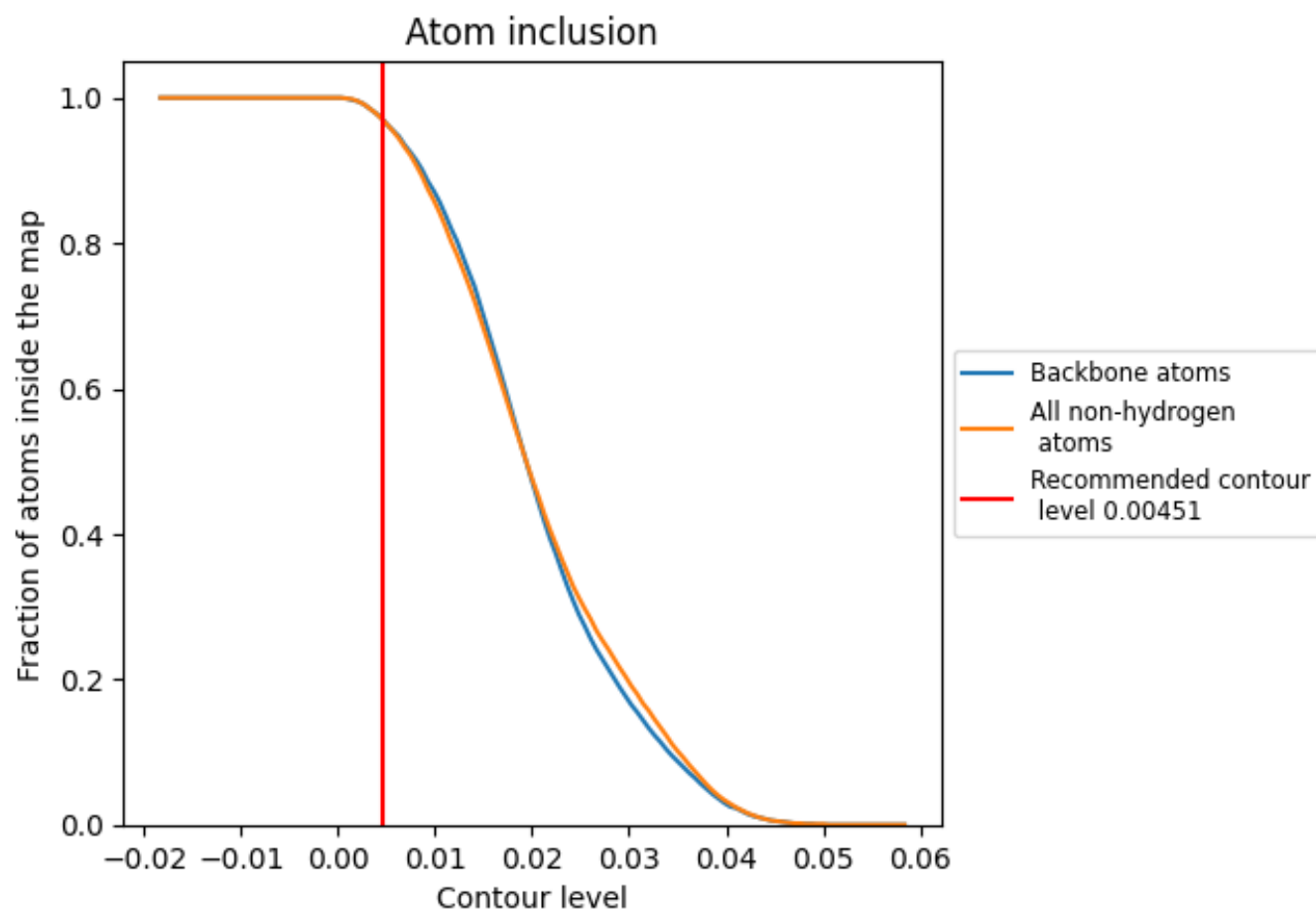
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00451).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.00451) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9710	0.4520
A	0.9930	0.3890
B	0.9930	0.4990
C	0.9920	0.5250
D	0.9950	0.5320
E	0.9930	0.5010
F	0.9930	0.4200
a	0.7600	0.2050
b	0.9930	0.3850
c	0.9780	0.4050
d	0.9740	0.3980
e	0.9540	0.3320
f	0.4330	0.1050

1.0

0.0

<0.0