



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:21 PM UTC

PDB ID : 8YH8 / pdb_00008yh8
EMDB ID : EMD-39284
Title : F1 domain of Non-catalytic site depleted and epsilon C-terminal domain
deleted FoF1-ATPase from Bacillus PS3, under ATP saturated condition
Authors : Kobayashi, R.; Nakano, A.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2024-02-27
Resolution : 2.70 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

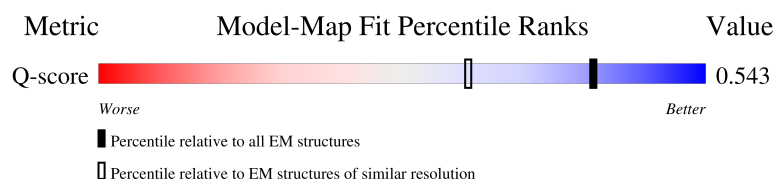
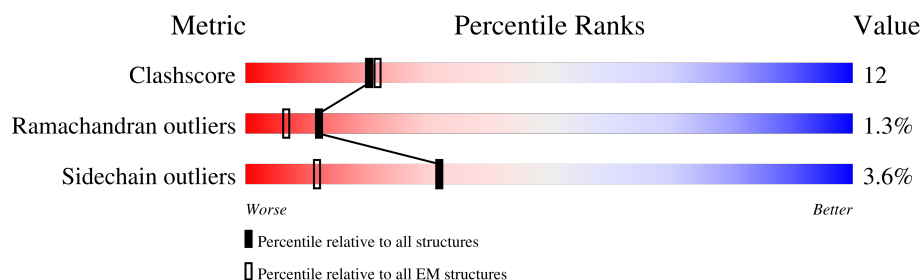
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	476	
1	B	476	
1	C	476	
2	D	471	

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Mol	Chain	Length	Quality of chain
2	E	471	
2	F	471	
3	G	282	
4	H	87	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24712 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	474	Total	C	N	O	S	0	0
			3624	2297	636	682	9		
1	B	475	Total	C	N	O	S	0	0
			3631	2302	637	683	9		
1	C	476	Total	C	N	O	S	0	0
			3637	2305	638	685	9		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	ALA	LYS	conflict	UNP A0A0M3VGF9
A	176	ALA	THR	conflict	UNP A0A0M3VGF9
A	193	SER	CYS	conflict	UNP A0A0M3VGF9
A	261	ALA	ASP	conflict	UNP A0A0M3VGF9
A	262	ALA	ASP	conflict	UNP A0A0M3VGF9
A	463	PHE	TRP	conflict	UNP A0A0M3VGF9
B	175	ALA	LYS	conflict	UNP A0A0M3VGF9
B	176	ALA	THR	conflict	UNP A0A0M3VGF9
B	193	SER	CYS	conflict	UNP A0A0M3VGF9
B	261	ALA	ASP	conflict	UNP A0A0M3VGF9
B	262	ALA	ASP	conflict	UNP A0A0M3VGF9
B	463	PHE	TRP	conflict	UNP A0A0M3VGF9
C	175	ALA	LYS	conflict	UNP A0A0M3VGF9
C	176	ALA	THR	conflict	UNP A0A0M3VGF9
C	193	SER	CYS	conflict	UNP A0A0M3VGF9
C	261	ALA	ASP	conflict	UNP A0A0M3VGF9
C	262	ALA	ASP	conflict	UNP A0A0M3VGF9
C	463	PHE	TRP	conflict	UNP A0A0M3VGF9

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	470	Total	C	N	O	S	0	0
			3622	2286	627	696	13		
2	E	470	Total	C	N	O	S	0	0
			3623	2286	627	696	14		
2	F	471	Total	C	N	O	S	0	0
			3630	2291	628	697	14		

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	282	Total	C	N	O	S	0	0
			2211	1393	388	420	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	112	CYS	SER	conflict	UNP A0A0M4TPJ7
G	215	CYS	ILE	conflict	UNP A0A0M4TPJ7

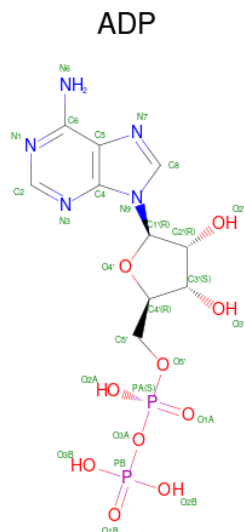
- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	87	Total	C	N	O	S	0	0
			646	411	109	124	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

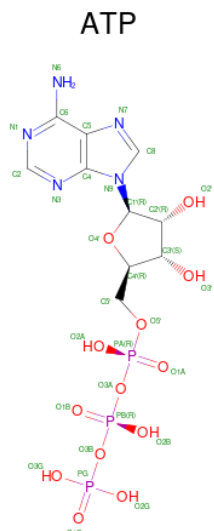
Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total 27	C 10	N 5	O 10	P 2	0
6	E	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

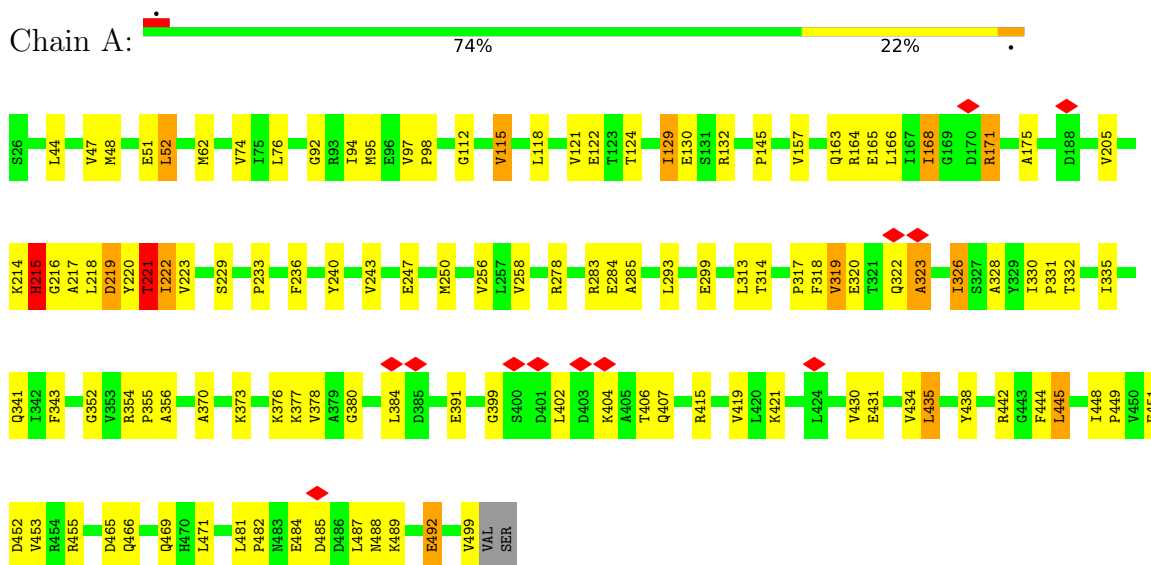


Mol	Chain	Residues	Atoms					AltConf
7	F	1	Total 31	C 10	N 5	O 13	P 3	0

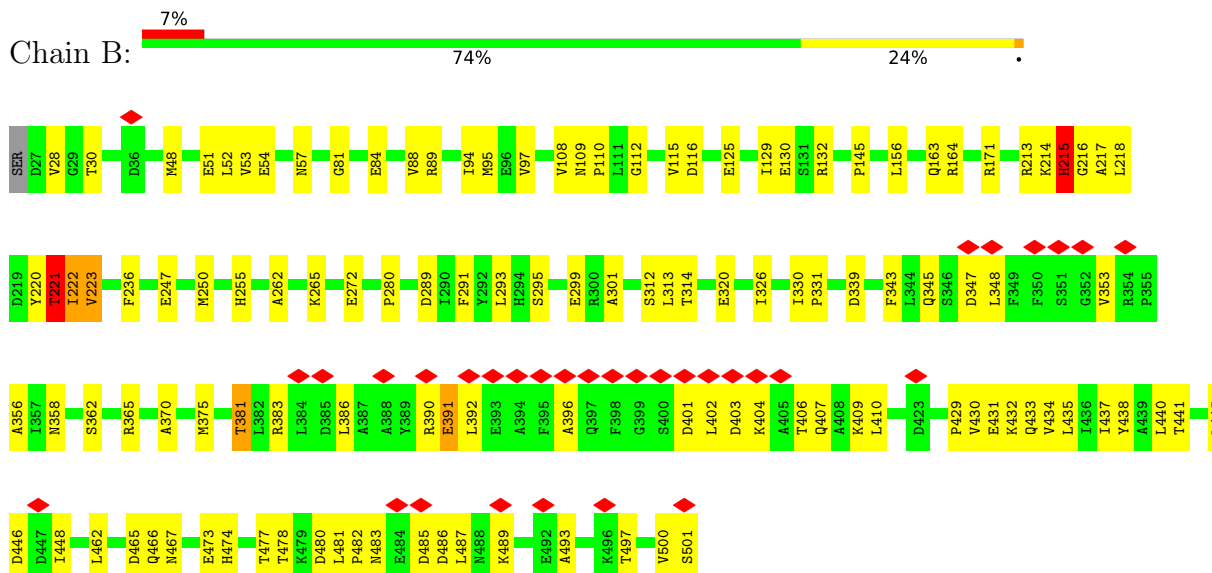
3 Residue-property plots

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

- Molecule 1: ATP synthase subunit alpha

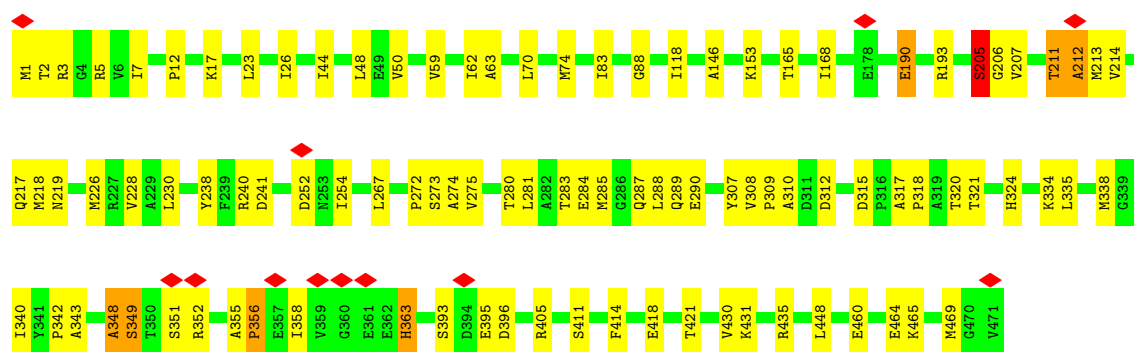


- Molecule 1: ATP synthase subunit alpha



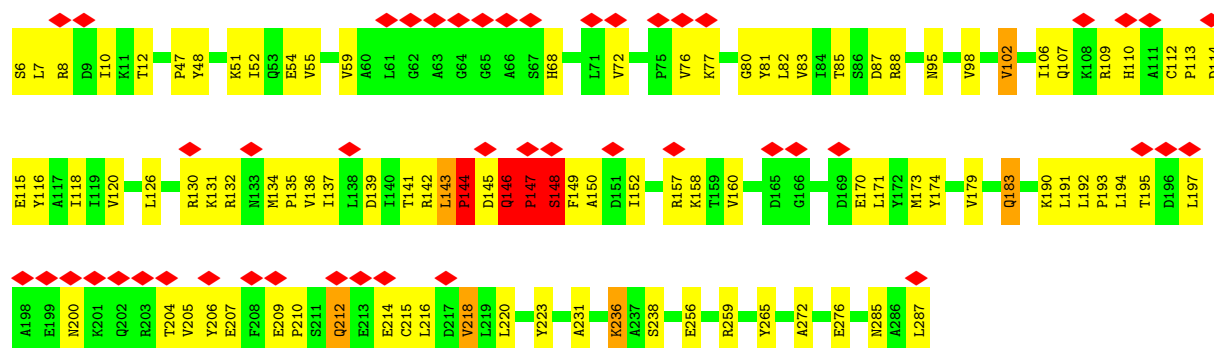
- Molecule 1: ATP synthase subunit alpha

Chain F:  79% 19%



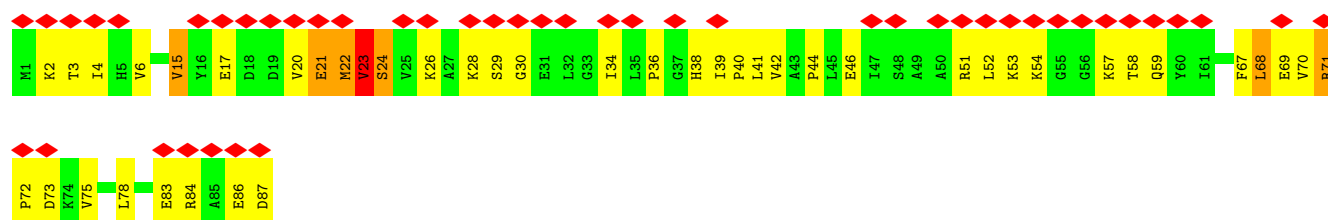
• Molecule 3: ATP synthase gamma chain

Chain G:  17% 66% 31%



• Molecule 4: ATP synthase epsilon chain

Chain H:  53% 49% 43% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00751	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ATP

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	0.49	1/3683 (0.0%)	0.87	10/4989 (0.2%)
1	B	0.42	0/3690	0.79	10/4999 (0.2%)
1	C	0.42	0/3696	0.76	7/5007 (0.1%)
2	D	0.57	2/3685 (0.1%)	0.99	13/4992 (0.3%)
2	E	0.53	0/3686	1.05	25/4992 (0.5%)
2	F	0.49	0/3693	0.94	16/5002 (0.3%)
3	G	0.44	0/2244	0.95	16/3036 (0.5%)
4	H	0.52	0/656	0.79	0/889
All	All	0.49	3/25033 (0.0%)	0.91	97/33906 (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	A	0	2
1	B	0	1
1	C	0	1
2	D	0	1
2	F	0	2
3	G	0	5
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	189	GLY	C-N	-17.25	1.16	1.33
2	D	190	GLU	C-N	5.55	1.41	1.33
1	A	222	ILE	CA-C	5.04	1.59	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	190	GLU	O-C-N	-15.77	106.26	123.13
2	D	189	GLY	O-C-N	-12.76	109.91	122.41
3	G	143	LEU	CA-C-N	9.81	132.11	119.84
3	G	143	LEU	C-N-CA	9.81	132.11	119.84
2	D	190	GLU	CA-C-N	8.71	134.75	122.72
2	D	190	GLU	C-N-CA	8.71	134.75	122.72
2	F	212	ALA	N-CA-C	8.11	128.07	110.80
3	G	144	PRO	CA-C-N	8.06	136.93	121.54
3	G	144	PRO	C-N-CA	8.06	136.93	121.54
2	F	348	ALA	CA-C-N	7.94	136.71	121.54
2	F	348	ALA	C-N-CA	7.94	136.71	121.54
3	G	147	PRO	CA-N-CD	-7.82	101.06	112.00
2	E	212	ALA	N-CA-C	7.50	126.78	110.80
1	B	222	ILE	N-CA-C	7.30	124.52	109.34
1	A	222	ILE	N-CA-C	7.18	124.27	109.34
2	F	355	ALA	CA-C-N	-7.12	110.95	119.84
2	F	355	ALA	C-N-CA	-7.12	110.95	119.84
1	A	221	THR	N-CA-C	7.09	123.15	113.37
3	G	146	GLN	CA-C-N	6.93	128.50	119.84
3	G	146	GLN	C-N-CA	6.93	128.50	119.84
1	C	219	ASP	CA-CB-CG	6.87	119.47	112.60
2	F	212	ALA	CA-C-O	-6.67	110.98	120.51
3	G	147	PRO	N-CA-CB	6.66	110.24	103.25
2	F	363	HIS	CA-CB-CG	6.59	120.39	113.80
2	E	253	ASN	CB-CA-C	6.54	123.43	110.42
2	E	211	THR	N-CA-C	6.53	120.71	112.87
2	E	355	ALA	CA-C-N	-6.53	111.68	119.84
2	E	355	ALA	C-N-CA	-6.53	111.68	119.84
1	C	222	ILE	N-CA-C	6.49	122.84	109.34
2	F	211	THR	N-CA-C	6.46	120.90	112.89
2	E	347	LEU	N-CA-C	6.45	118.31	111.28
2	F	363	HIS	CB-CG-CD2	-6.39	122.89	131.20
2	D	349	SER	CA-C-N	6.37	133.71	121.54
2	D	349	SER	C-N-CA	6.37	133.71	121.54
2	D	359	VAL	CA-C-N	6.34	127.14	120.03
2	D	359	VAL	C-N-CA	6.34	127.14	120.03
2	E	359	VAL	CB-CA-C	6.33	122.52	112.26
2	D	358	ILE	CA-C-O	6.31	128.05	121.05
2	D	383	ILE	CA-C-N	6.27	129.37	120.53
2	D	383	ILE	C-N-CA	6.27	129.37	120.53
1	A	219	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	215	HIS	O-C-N	-6.18	114.37	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	356	PRO	CA-C-N	-6.15	110.92	120.88
2	F	356	PRO	C-N-CA	-6.15	110.92	120.88
3	G	147	PRO	N-CD-CG	6.05	112.28	103.20
1	A	215	HIS	O-C-N	-6.05	114.54	122.59
2	E	356	PRO	CA-C-N	-6.05	111.08	120.88
2	E	356	PRO	C-N-CA	-6.05	111.08	120.88
3	G	47	PRO	CA-N-CD	-6.02	103.58	112.00
2	E	344	VAL	CA-C-N	5.93	127.50	122.28
2	E	344	VAL	C-N-CA	5.93	127.50	122.28
2	E	354	LEU	CA-C-N	-5.92	112.33	120.26
2	E	354	LEU	C-N-CA	-5.92	112.33	120.26
2	E	363	HIS	CB-CG-CD2	-5.87	123.56	131.20
2	D	435	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	220	TYR	N-CA-C	5.80	120.50	112.90
2	F	193	ARG	NE-CZ-NH2	5.77	124.40	119.20
2	F	435	ARG	CA-C-N	5.75	126.32	119.94
2	F	435	ARG	C-N-CA	5.75	126.32	119.94
1	A	171	ARG	NE-CZ-NH2	5.71	124.33	119.20
2	E	205	SER	O-C-N	-5.68	115.03	122.59
2	E	358	ILE	CA-C-O	5.65	127.69	120.96
1	A	326	ILE	N-CA-C	-5.60	105.95	111.77
3	G	88	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	F	358	ILE	CA-C-O	5.48	127.48	120.96
1	C	220	TYR	N-CA-C	5.47	119.12	112.23
3	G	139	ASP	CA-C-N	5.42	128.18	122.11
3	G	139	ASP	C-N-CA	5.42	128.18	122.11
1	B	116	ASP	CA-CB-CG	5.42	118.02	112.60
2	F	205	SER	O-C-N	-5.40	115.41	122.59
1	C	215	HIS	O-C-N	-5.40	115.41	122.59
1	C	221	THR	CA-C-N	5.38	131.65	121.97
1	C	221	THR	C-N-CA	5.38	131.65	121.97
1	B	221	THR	N-CA-C	5.34	122.19	110.80
2	E	213	MET	N-CA-C	5.32	122.14	110.80
2	D	363	HIS	CB-CG-CD2	-5.32	124.29	131.20
2	E	363	HIS	CA-CB-CG	5.29	119.09	113.80
1	B	221	THR	CA-C-N	5.28	131.47	121.97
1	B	221	THR	C-N-CA	5.28	131.47	121.97
1	C	221	THR	N-CA-C	5.27	122.02	110.80
1	A	222	ILE	CB-CA-C	-5.26	102.66	111.29
1	B	222	ILE	CB-CA-C	-5.22	102.73	111.29
3	G	141	THR	CA-C-N	5.21	128.94	120.60
3	G	141	THR	C-N-CA	5.21	128.94	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	THR	CA-C-N	5.17	131.28	121.97
1	A	221	THR	C-N-CA	5.17	131.28	121.97
1	B	213	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	220	TYR	N-CA-C	5.16	119.66	112.90
2	E	401	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	B	223	VAL	N-CA-C	5.12	119.99	109.34
3	G	142	ARG	N-CA-C	5.12	118.62	112.38
2	E	435	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	E	205	SER	CA-C-N	5.05	131.31	121.41
2	E	205	SER	C-N-CA	5.05	131.31	121.41
2	E	348	ALA	CA-C-N	5.04	127.54	120.28
2	E	348	ALA	C-N-CA	5.04	127.54	120.28
2	E	394	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	LYS	Mainchain
1	A	354	ARG	Sidechain
1	B	214	LYS	Mainchain
1	C	214	LYS	Mainchain
2	D	350	THR	Peptide
2	F	211	THR	Peptide
2	F	348	ALA	Mainchain
3	G	144	PRO	Peptide
3	G	146	GLN	Mainchain,Peptide
3	G	147	PRO	Peptide
3	G	148	SER	Peptide

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	3624	0	3702	99	0
1	B	3631	0	3711	90	0
1	C	3637	0	3716	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3622	0	3631	61	0
2	E	3623	0	3636	78	0
2	F	3630	0	3644	62	0
3	G	2211	0	2254	135	0
4	H	646	0	671	95	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	D	27	0	12	1	0
6	E	27	0	12	0	0
7	F	31	0	12	4	0
All	All	24712	0	25001	607	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 12.

All (607) 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)
3:G:48:TYR:CD2	4:H:78:LEU:HD23	1.63	1.32
3:G:209:GLU:CB	4:H:28:LYS:HE3	1.37	1.32
3:G:204:THR:CG2	4:H:70:VAL:O	1.77	1.31
3:G:204:THR:HG21	4:H:70:VAL:O	1.17	1.27
3:G:48:TYR:CD2	4:H:78:LEU:CD2	2.20	1.23
3:G:204:THR:OG1	4:H:71:ARG:HA	1.43	1.17
3:G:204:THR:HB	4:H:71:ARG:HD3	1.23	1.14
3:G:204:THR:HG1	4:H:71:ARG:HA	1.03	1.11
3:G:106:ILE:HD11	3:G:134:MET:HE1	1.29	1.10
1:A:52:LEU:HD21	1:A:95:MET:HE2	1.37	1.07
3:G:209:GLU:HB2	4:H:28:LYS:HE3	1.35	1.06
3:G:209:GLU:CB	4:H:28:LYS:CE	2.33	1.04
2:D:190:GLU:OE2	2:D:253:ASN:ND2	1.89	1.03
3:G:206:TYR:HA	4:H:41:LEU:HA	1.41	1.02
1:A:168:ILE:HD13	1:A:326:ILE:HD11	1.43	1.01
3:G:209:GLU:HB3	4:H:28:LYS:HE3	1.44	0.99
3:G:204:THR:HB	4:H:71:ARG:CD	1.93	0.97
3:G:48:TYR:HD2	4:H:78:LEU:HD23	1.24	0.97
3:G:206:TYR:CA	4:H:41:LEU:HA	1.95	0.96
1:C:95:MET:HG3	1:C:129:ILE:HG12	1.49	0.93
2:F:44:ILE:HD13	2:F:70:LEU:HD23	1.54	0.89
3:G:207:GLU:N	4:H:41:LEU:HA	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLU:HG2	2:F:219:ASN:HB3	1.54	0.89
3:G:194:LEU:HB3	3:G:197:LEU:HD21	1.52	0.88
3:G:209:GLU:CA	4:H:29:SER:HB3	2.00	0.88
1:C:482:PRO:HG2	1:C:487:LEU:HD12	1.54	0.88
3:G:206:TYR:HA	4:H:41:LEU:CA	2.03	0.87
3:G:106:ILE:HD11	3:G:134:MET:CE	2.06	0.86
3:G:218:VAL:HG11	4:H:44:PRO:HB3	1.58	0.85
1:A:482:PRO:HG2	1:A:487:LEU:HG	1.58	0.85
3:G:210:PRO:HB2	3:G:214:GLU:HB2	1.57	0.85
3:G:204:THR:HG23	4:H:70:VAL:O	1.74	0.84
3:G:206:TYR:C	4:H:41:LEU:HA	2.02	0.84
3:G:272:ALA:O	3:G:276:GLU:HG2	1.76	0.84
3:G:112:CYS:O	3:G:115:GLU:HG3	1.78	0.84
1:A:229:SER:HB2	2:D:290:GLU:HG3	1.60	0.83
3:G:48:TYR:CE2	4:H:78:LEU:HD22	2.14	0.82
3:G:205:VAL:CG1	4:H:39:ILE:HB	2.09	0.82
2:E:295:THR:HG22	2:E:296:ALA:H	1.43	0.82
3:G:48:TYR:CE2	4:H:78:LEU:CD2	2.62	0.81
2:E:465:LYS:O	2:E:469:MET:HG2	1.81	0.81
1:C:474:HIS:O	1:C:478:THR:HG22	1.80	0.80
3:G:205:VAL:CG1	4:H:39:ILE:CB	2.45	0.80
2:F:334:LYS:HD3	2:F:334:LYS:N	1.98	0.79
7:F:500:ATP:H5'1	7:F:500:ATP:H8	1.48	0.79
3:G:204:THR:HG21	4:H:70:VAL:C	2.07	0.78
3:G:112:CYS:SG	3:G:113:PRO:HD2	2.23	0.78
1:A:481:LEU:HD22	1:A:482:PRO:HD2	1.66	0.77
2:E:238:TYR:CE1	2:E:242:GLU:HG3	2.19	0.77
1:B:403:ASP:O	1:B:407:GLN:HG3	1.84	0.77
3:G:48:TYR:CD2	4:H:78:LEU:HD22	2.13	0.76
3:G:204:THR:CG2	4:H:40:PRO:HB3	2.17	0.75
1:C:494:PHE:O	1:C:497:THR:HG22	1.86	0.75
1:A:62:MET:HE3	1:A:95:MET:HG3	1.69	0.74
2:E:118:ILE:HD12	2:E:231:THR:HA	1.68	0.74
1:B:403:ASP:OD1	1:B:404:LYS:N	2.21	0.74
3:G:204:THR:HB	4:H:71:ARG:CG	2.18	0.74
1:C:365:ARG:NH2	6:D:502:ADP:O1A	2.21	0.73
2:F:12:PRO:HD2	2:F:267:LEU:HD13	1.70	0.73
1:A:471:LEU:HD13	1:A:487:LEU:HD23	1.70	0.72
2:E:160:ALA:H	2:E:333:ARG:HH11	1.34	0.72
1:A:168:ILE:HD13	1:A:326:ILE:CD1	2.19	0.72
1:B:396:ALA:HA	1:B:402:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:209:GLU:HB2	4:H:28:LYS:CE	2.08	0.71
2:D:275:VAL:HG12	2:D:275:VAL:O	1.88	0.71
1:A:452:ASP:OD1	1:A:455:ARG:NH2	2.23	0.71
2:E:124:LYS:HB2	2:E:127:GLU:HG3	1.73	0.71
1:A:415:ARG:NH1	1:A:448:ILE:O	2.21	0.71
1:C:438:TYR:CE1	1:C:487:LEU:HD22	2.25	0.71
1:B:375:MET:HE1	1:B:437:ILE:CD1	2.21	0.70
2:E:295:THR:HG22	2:E:296:ALA:N	2.05	0.70
1:C:127:ARG:NH1	1:C:247:GLU:OE2	2.20	0.70
2:F:460:GLU:O	2:F:464:GLU:HG2	1.92	0.69
1:A:431:GLU:O	1:A:434:VAL:HG22	1.93	0.69
1:B:89:ARG:HH21	1:B:89:ARG:HG3	1.56	0.69
4:H:57:LYS:HE2	4:H:57:LYS:HA	1.73	0.69
2:D:8:GLN:OE1	2:D:10:MET:HE1	1.92	0.69
1:C:109:ASN:ND2	1:C:110:PRO:HD2	2.07	0.69
1:B:365:ARG:HG2	7:F:500:ATP:O3'	1.93	0.68
1:C:175:ALA:HB1	1:C:318:PHE:HE1	1.58	0.68
3:G:216:LEU:HD22	3:G:220:LEU:HD21	1.74	0.68
1:A:404:LYS:NZ	1:A:407:GLN:OE1	2.27	0.68
1:B:438:TYR:CE1	1:B:487:LEU:HD23	2.29	0.68
4:H:46:GLU:OE1	4:H:46:GLU:N	2.27	0.68
4:H:23:VAL:HG13	4:H:34:ILE:HB	1.77	0.67
3:G:204:THR:HG23	4:H:40:PRO:HB3	1.75	0.67
3:G:51:LYS:HG3	3:G:52:ILE:N	2.08	0.67
1:C:229:SER:HB2	2:F:290:GLU:HG3	1.76	0.67
2:F:465:LYS:O	2:F:469:MET:HG3	1.93	0.67
1:A:74:VAL:CG1	1:A:233:PRO:HG3	2.24	0.67
1:B:440:LEU:HD13	1:B:445:LEU:HD23	1.77	0.67
2:F:334:LYS:HD3	2:F:334:LYS:H	1.58	0.67
2:F:1:MET:HB3	2:F:3:ARG:HD2	1.77	0.67
1:C:52:LEU:HG	1:C:95:MET:HE2	1.75	0.67
1:A:402:LEU:HB3	1:A:406:THR:OG1	1.94	0.67
1:A:430:VAL:O	1:A:434:VAL:HG13	1.94	0.67
2:D:317:ALA:HB3	2:D:318:PRO:HD3	1.77	0.67
3:G:216:LEU:O	3:G:220:LEU:HD23	1.94	0.67
1:B:485:ASP:O	1:B:489:LYS:HG2	1.94	0.67
3:G:204:THR:CB	4:H:71:ARG:HG2	2.25	0.67
1:A:62:MET:CE	1:A:95:MET:HG3	2.25	0.66
1:C:415:ARG:NH1	1:C:448:ILE:O	2.27	0.66
3:G:218:VAL:HG11	4:H:44:PRO:CB	2.25	0.66
2:F:280:THR:O	2:F:284:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:170:GLU:OE2	3:G:190:LYS:HD2	1.95	0.66
1:B:289:ASP:OD1	1:B:289:ASP:O	2.12	0.66
1:C:217:ALA:O	1:C:221:THR:HG23	1.96	0.66
1:A:466:GLN:OE1	1:A:466:GLN:HA	1.96	0.66
1:C:95:MET:HE2	1:C:95:MET:HA	1.76	0.66
1:B:348:LEU:HB3	1:B:356:ALA:HB1	1.78	0.65
2:F:190:GLU:OE1	2:F:252:ASP:HB3	1.95	0.65
1:C:52:LEU:HG	1:C:95:MET:CE	2.26	0.65
2:E:342:PRO:HG3	2:E:414:PHE:CZ	2.32	0.65
2:D:283:THR:O	2:D:287:GLN:HG2	1.97	0.65
1:A:484:GLU:H	1:A:484:GLU:CD	2.03	0.65
1:A:484:GLU:OE1	1:A:484:GLU:N	2.18	0.65
2:D:50:VAL:HG13	2:D:59:VAL:CG1	2.27	0.65
2:E:332:GLU:OE1	2:E:332:GLU:HA	1.96	0.65
2:E:1:MET:SD	2:E:3:ARG:HG2	2.37	0.65
1:C:74:VAL:CG1	1:C:233:PRO:HB3	2.27	0.64
3:G:204:THR:OG1	4:H:71:ARG:CA	2.35	0.64
3:G:83:VAL:HG13	3:G:120:VAL:HG23	1.77	0.64
1:B:54:GLU:OE2	1:B:89:ARG:NH1	2.31	0.64
2:E:189:GLY:O	2:E:218:MET:HE3	1.97	0.64
1:C:344:LEU:HA	1:C:356:ALA:O	1.98	0.64
2:D:19:GLU:HA	2:D:19:GLU:OE1	1.97	0.64
1:B:164:ARG:NH1	1:B:339:ASP:OD1	2.27	0.63
2:F:317:ALA:HB3	2:F:318:PRO:HD3	1.79	0.63
1:B:391:GLU:N	1:B:391:GLU:OE1	2.30	0.63
1:A:236:PHE:HE1	1:A:293:LEU:HD11	1.62	0.63
1:B:429:PRO:O	1:B:433:GLN:HG3	1.99	0.63
1:C:262:ALA:HB1	1:C:265:LYS:HD2	1.81	0.63
1:A:168:ILE:HG23	1:A:319:VAL:HG13	1.81	0.63
3:G:192:LEU:HD23	3:G:194:LEU:CD2	2.29	0.63
1:B:435:LEU:CD2	1:B:487:LEU:HD11	2.29	0.62
1:B:435:LEU:HD22	1:B:487:LEU:HD11	1.80	0.62
3:G:204:THR:HB	4:H:71:ARG:HG2	1.80	0.62
3:G:68:HIS:O	3:G:72:VAL:HG23	1.99	0.62
2:F:273:SER:OG	2:F:274:ALA:N	2.32	0.62
3:G:256:GLU:OE2	3:G:259:ARG:NH2	2.33	0.62
2:D:88:GLY:HA2	2:D:238:TYR:CE2	2.35	0.61
3:G:85:THR:HG22	3:G:98:VAL:HG11	1.82	0.61
2:F:307:TYR:CE2	2:F:309:PRO:HA	2.36	0.61
3:G:206:TYR:CZ	4:H:42:VAL:HG11	2.35	0.61
2:E:333:ARG:O	2:E:337:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:318:PRO:O	2:F:321:THR:HG22	2.00	0.61
3:G:212:GLN:HE21	3:G:216:LEU:HD11	1.66	0.61
1:B:483:ASN:OD1	1:B:486:ASP:HB2	2.01	0.61
1:A:278:ARG:HH22	3:G:287:LEU:CD2	2.14	0.60
1:A:415:ARG:O	1:A:419:VAL:HG13	2.01	0.60
1:C:169:GLY:O	1:C:321:THR:OG1	2.13	0.60
2:D:238:TYR:CE1	2:D:242:GLU:HG3	2.37	0.60
1:C:102:ALA:HB1	1:C:121:VAL:O	2.01	0.60
1:C:485:ASP:O	1:C:489:LYS:HD3	2.01	0.60
3:G:204:THR:OG1	4:H:72:PRO:HD3	2.01	0.60
1:A:175:ALA:HB1	1:A:318:PHE:CE1	2.37	0.60
1:C:95:MET:CG	1:C:129:ILE:HG12	2.28	0.60
2:F:281:LEU:HD21	2:F:320:THR:HG21	1.83	0.60
1:B:132:ARG:HD2	1:B:132:ARG:N	2.16	0.60
1:C:74:VAL:HG13	1:C:233:PRO:CG	2.32	0.60
3:G:118:ILE:HB	3:G:136:VAL:HA	1.84	0.60
1:B:345:GLN:HG3	1:B:358:ASN:HB2	1.84	0.60
1:B:375:MET:HE1	1:B:437:ILE:HD12	1.83	0.60
2:F:88:GLY:HA2	2:F:238:TYR:CE1	2.37	0.60
2:F:190:GLU:CD	2:F:252:ASP:HB3	2.27	0.60
3:G:82:LEU:HD22	3:G:173:MET:HG2	1.84	0.60
1:A:449:PRO:HB2	1:A:451:GLU:OE1	2.02	0.59
2:F:340:ILE:HG23	2:F:411:SER:HB3	1.82	0.59
1:A:299:GLU:HG3	2:E:219:ASN:HB3	1.83	0.59
1:B:381:THR:HG23	1:B:441:THR:HG21	1.83	0.59
1:C:375:MET:HG2	1:C:434:VAL:HG12	1.84	0.59
7:F:500:ATP:H5'1	7:F:500:ATP:C8	2.35	0.59
3:G:205:VAL:HG21	4:H:39:ILE:N	1.80	0.59
1:B:406:THR:O	1:B:410:LEU:HG	2.02	0.59
2:D:238:TYR:CD1	2:D:242:GLU:HG3	2.37	0.59
1:A:166:LEU:HD11	1:A:319:VAL:HG12	1.83	0.59
1:B:295:SER:HB3	2:F:218:MET:HB2	1.85	0.59
1:B:396:ALA:CB	1:B:410:LEU:HD11	2.32	0.59
3:G:80:GLY:O	3:G:171:LEU:HD12	2.02	0.59
1:A:243:VAL:O	1:A:247:GLU:HG3	2.02	0.59
1:B:272:GLU:OE2	2:E:280:THR:HG22	2.02	0.59
2:D:50:VAL:HG13	2:D:59:VAL:HG11	1.85	0.59
3:G:204:THR:HG21	4:H:71:ARG:HG2	1.85	0.59
1:A:250:MET:HE2	1:A:313:LEU:HB3	1.85	0.59
3:G:212:GLN:NE2	3:G:216:LEU:HD11	2.17	0.59
1:A:258:VAL:HG23	1:A:313:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:HH22	3:G:287:LEU:HD21	1.68	0.58
2:D:108:ASP:OD1	2:D:109:ILE:N	2.36	0.58
1:C:174:GLY:O	1:C:178:VAL:HG23	2.04	0.58
2:E:1:MET:SD	2:E:2:THR:N	2.77	0.58
2:E:99:LEU:HB2	2:E:101:GLU:OE1	2.03	0.58
2:E:456:VAL:HG12	2:E:457:GLY:N	2.17	0.58
2:E:32:ILE:HG21	2:E:44:ILE:HD11	1.84	0.58
1:C:132:ARG:HD2	1:C:132:ARG:N	2.18	0.58
3:G:81:TYR:OH	3:G:110:HIS:NE2	2.04	0.58
1:A:175:ALA:HB1	1:A:318:PHE:HE1	1.68	0.57
1:C:347:ASP:OD1	1:C:347:ASP:N	2.32	0.57
2:F:3:ARG:H	2:F:3:ARG:HD3	1.69	0.57
2:E:1:MET:HE3	2:E:1:MET:C	2.29	0.57
2:E:178:GLU:HG2	2:E:427:TYR:CZ	2.40	0.57
1:B:215:HIS:C	1:B:217:ALA:H	2.13	0.57
2:E:271:MET:HE2	3:G:285:ASN:HD21	1.69	0.57
4:H:22:MET:HB2	4:H:53:LYS:HB2	1.87	0.57
1:A:215:HIS:C	1:A:217:ALA:H	2.12	0.57
2:F:342:PRO:HG3	2:F:414:PHE:CZ	2.39	0.57
1:A:448:ILE:HG22	1:A:452:ASP:HB2	1.86	0.57
1:C:215:HIS:C	1:C:217:ALA:H	2.12	0.57
2:E:220:GLU:O	2:E:225:ARG:NH2	2.37	0.57
3:G:204:THR:CG2	4:H:71:ARG:HG2	2.35	0.57
1:A:44:LEU:O	1:A:47:VAL:HG12	2.04	0.57
1:A:168:ILE:HG21	1:A:326:ILE:HD12	1.87	0.57
1:A:258:VAL:CG2	1:A:313:LEU:HD11	2.35	0.57
1:C:52:LEU:CD2	1:C:95:MET:HE1	2.35	0.57
1:B:95:MET:HG2	1:B:129:ILE:HG12	1.86	0.56
1:C:328:ALA:HB3	1:C:331:PRO:HG2	1.87	0.56
2:E:118:ILE:CD1	2:E:231:THR:HA	2.35	0.56
2:E:317:ALA:HB3	2:E:318:PRO:HD3	1.85	0.56
2:E:342:PRO:O	2:E:343:ALA:HB3	2.05	0.56
1:A:52:LEU:HD21	1:A:95:MET:CE	2.23	0.56
1:B:431:GLU:O	1:B:434:VAL:HG22	2.05	0.56
2:E:295:THR:CG2	2:E:296:ALA:H	2.17	0.56
2:F:118:ILE:HG23	2:F:230:LEU:HB3	1.87	0.56
2:D:2:THR:HG23	2:D:3:ARG:N	2.21	0.56
2:D:254:ILE:HD11	2:D:288:LEU:HD21	1.88	0.56
1:A:168:ILE:HD12	1:A:343:PHE:CZ	2.41	0.56
2:E:271:MET:HE2	3:G:285:ASN:ND2	2.20	0.56
1:A:121:VAL:O	1:A:122:GLU:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:ILE:HG23	2:E:26:ILE:O	2.04	0.55
1:B:218:LEU:HA	1:B:221:THR:HG22	1.87	0.55
1:C:403:ASP:OD1	1:C:403:ASP:N	2.37	0.55
2:D:429:PRO:HG2	2:D:432:GLU:HG2	1.87	0.55
2:E:233:LEU:HD21	2:E:291:ARG:HB2	1.87	0.55
1:B:438:TYR:CZ	1:B:487:LEU:HD23	2.42	0.55
2:E:1:MET:HE3	2:E:1:MET:O	2.06	0.55
3:G:204:THR:CB	4:H:71:ARG:CG	2.83	0.55
3:G:157:ARG:HG3	3:G:158:LYS:N	2.18	0.55
3:G:206:TYR:CZ	4:H:42:VAL:CG1	2.89	0.55
2:E:340:ILE:HG23	2:E:411:SER:HB3	1.89	0.55
1:A:482:PRO:CG	1:A:487:LEU:HG	2.34	0.55
2:D:248:LEU:HD23	2:D:301:THR:HB	1.89	0.55
2:F:310:ALA:O	2:F:312:ASP:N	2.40	0.55
2:D:294:SER:CB	2:D:299:SER:HA	2.36	0.54
1:B:448:ILE:N	1:B:448:ILE:HD12	2.21	0.54
3:G:205:VAL:HG21	4:H:38:HIS:C	2.28	0.54
1:B:375:MET:HE1	1:B:437:ILE:HD13	1.88	0.54
1:C:381:THR:HG22	1:C:381:THR:O	2.07	0.54
2:D:275:VAL:O	2:D:275:VAL:CG1	2.54	0.54
2:F:205:SER:C	2:F:207:VAL:H	2.16	0.54
3:G:109:ARG:O	3:G:110:HIS:ND1	2.40	0.54
3:G:207:GLU:N	3:G:207:GLU:OE1	2.41	0.54
1:A:168:ILE:HG21	1:A:326:ILE:CD1	2.38	0.54
2:E:160:ALA:N	2:E:333:ARG:HH11	2.04	0.54
3:G:206:TYR:CD1	4:H:42:VAL:HG13	2.42	0.54
1:A:52:LEU:HD23	1:A:95:MET:HG2	1.90	0.54
1:C:175:ALA:CB	1:C:318:PHE:HE1	2.20	0.54
4:H:26:LYS:HZ3	4:H:30:GLY:HA2	1.73	0.54
1:A:163:GLN:NE2	1:A:165:GLU:OE1	2.41	0.54
1:C:132:ARG:N	1:C:132:ARG:CD	2.71	0.54
1:C:326:ILE:HG12	1:C:343:PHE:CZ	2.43	0.54
2:E:244:GLY:HA2	2:E:297:LYS:O	2.08	0.54
1:B:347:ASP:OD1	1:B:348:LEU:N	2.41	0.53
3:G:209:GLU:C	4:H:29:SER:HB3	2.33	0.53
4:H:2:LYS:HD3	4:H:36:PRO:HB2	1.91	0.53
1:A:52:LEU:CD2	1:A:95:MET:HG2	2.39	0.53
1:B:482:PRO:HG2	1:B:487:LEU:HD13	1.90	0.53
1:C:169:GLY:HA3	1:C:175:ALA:HB2	1.91	0.53
1:A:74:VAL:HG13	1:A:233:PRO:HG3	1.90	0.53
3:G:204:THR:HG23	4:H:40:PRO:CA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:209:GLU:HB3	4:H:29:SER:N	2.24	0.53
1:B:262:ALA:CB	1:B:265:LYS:HG3	2.38	0.53
2:E:454:ARG:O	2:E:456:VAL:HG23	2.09	0.53
2:F:5:ARG:HA	2:F:74:MET:O	2.09	0.53
2:F:44:ILE:CD1	2:F:70:LEU:HD23	2.34	0.53
2:F:393:SER:OG	2:F:396:ASP:HB2	2.08	0.53
1:B:392:LEU:HG	1:B:410:LEU:HD21	1.91	0.53
2:D:342:PRO:O	2:D:343:ALA:HB3	2.07	0.53
1:A:76:LEU:HD23	1:A:233:PRO:HB2	1.91	0.53
1:A:283:ARG:HD3	1:A:284:GLU:HG3	1.91	0.53
1:B:132:ARG:N	1:B:132:ARG:CD	2.72	0.53
1:C:431:GLU:O	1:C:434:VAL:HG22	2.09	0.53
1:C:483:ASN:HB3	1:C:486:ASP:OD2	2.09	0.53
3:G:206:TYR:CA	4:H:41:LEU:CA	2.75	0.53
1:A:74:VAL:CG1	1:A:233:PRO:CG	2.86	0.53
2:E:88:GLY:HA2	2:E:238:TYR:CE2	2.44	0.53
2:F:308:VAL:HG23	2:F:310:ALA:O	2.08	0.53
4:H:3:THR:HG22	4:H:21:GLU:OE1	2.09	0.53
1:B:89:ARG:HG3	1:B:89:ARG:NH2	2.21	0.52
1:B:280:PRO:HB3	2:F:272:PRO:HG3	1.92	0.52
1:B:353:VAL:O	1:B:356:ALA:HB2	2.09	0.52
2:E:384:ILE:HA	2:E:388:GLY:HA3	1.90	0.52
3:G:48:TYR:CE2	4:H:78:LEU:HD23	2.28	0.52
1:C:345:GLN:CD	1:C:358:ASN:HD22	2.17	0.52
3:G:192:LEU:HD23	3:G:194:LEU:HD22	1.91	0.52
3:G:118:ILE:HB	3:G:136:VAL:HG22	1.91	0.52
3:G:116:TYR:HE1	3:G:135:PRO:HD2	1.73	0.52
1:A:471:LEU:HD13	1:A:487:LEU:CD2	2.39	0.52
2:E:464:GLU:N	2:E:464:GLU:OE1	2.43	0.52
1:C:330:ILE:HB	1:C:331:PRO:HD3	1.91	0.52
2:F:50:VAL:HG13	2:F:59:VAL:CG2	2.40	0.52
1:B:164:ARG:HH11	1:B:339:ASP:CG	2.17	0.52
2:D:11:GLY:O	2:D:67:THR:HG21	2.10	0.52
2:F:342:PRO:O	2:F:343:ALA:HB3	2.10	0.52
2:F:146:ALA:HB2	2:F:349:SER:HB3	1.90	0.52
1:A:47:VAL:HG23	1:A:51:GLU:OE1	2.10	0.51
1:A:145:PRO:HB3	1:A:370:ALA:O	2.10	0.51
1:C:478:THR:HG23	1:C:480:ASP:H	1.75	0.51
2:E:275:VAL:O	2:E:275:VAL:HG12	2.08	0.51
1:A:166:LEU:O	1:A:341:GLN:HA	2.09	0.51
1:A:284:GLU:O	1:A:285:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:456:VAL:CG1	2:E:461:GLU:HB2	2.39	0.51
1:B:48:MET:HE3	1:B:94:ILE:HG12	1.91	0.51
1:A:124:THR:HG22	1:A:124:THR:O	2.11	0.51
1:B:326:ILE:HD11	1:B:343:PHE:CE2	2.46	0.51
1:C:397:GLN:HA	1:C:397:GLN:OE1	2.11	0.51
2:D:287:GLN:HA	2:D:287:GLN:OE1	2.11	0.51
1:A:355:PRO:O	1:A:356:ALA:HB3	2.09	0.51
1:B:330:ILE:HB	1:B:331:PRO:HD3	1.92	0.51
1:A:94:ILE:HG22	1:A:95:MET:N	2.26	0.51
1:A:326:ILE:HG12	1:A:335:ILE:HD11	1.93	0.51
1:A:328:ALA:O	1:A:332:THR:HG23	2.10	0.51
2:E:228:VAL:O	2:E:231:THR:HG23	2.11	0.51
1:A:485:ASP:O	1:A:489:LYS:HG3	2.11	0.51
2:F:165:THR:OG1	7:F:500:ATP:O2B	2.28	0.51
4:H:23:VAL:HA	4:H:51:ARG:O	2.10	0.51
2:D:243:GLN:HB3	2:D:245:GLN:HG3	1.93	0.50
2:E:120:ARG:HG2	2:E:121:PRO:O	2.12	0.50
2:E:151:GLY:HA2	2:E:300:ILE:O	2.12	0.50
3:G:204:THR:HG23	4:H:40:PRO:HA	1.93	0.50
4:H:22:MET:HE1	4:H:34:ILE:H	1.76	0.50
1:A:341:GLN:HG3	1:A:343:PHE:CE2	2.46	0.50
1:B:171:ARG:HB3	1:B:171:ARG:CZ	2.40	0.50
1:A:229:SER:HB2	2:D:290:GLU:CG	2.38	0.50
3:G:82:LEU:O	3:G:173:MET:HA	2.12	0.50
3:G:118:ILE:CG2	3:G:136:VAL:HG22	2.41	0.50
3:G:173:MET:HE1	3:G:231:ALA:HB2	1.93	0.50
3:G:206:TYR:CE2	4:H:42:VAL:HG11	2.46	0.50
1:B:84:GLU:OE2	2:E:55:GLY:HA2	2.12	0.50
1:B:430:VAL:O	1:B:434:VAL:HG13	2.12	0.50
1:C:110:PRO:HD3	1:C:225:THR:O	2.12	0.50
3:G:194:LEU:CD1	3:G:223:TYR:HE2	2.24	0.50
1:A:97:VAL:HG23	1:A:129:ILE:HG13	1.92	0.50
1:A:499:VAL:HG13	1:A:499:VAL:O	2.12	0.50
1:C:288:GLY:O	2:D:263:GLU:HG2	2.11	0.50
1:A:380:GLY:O	1:A:384:LEU:HD23	2.12	0.50
1:A:444:PHE:HZ	1:A:488:ASN:OD1	1.94	0.50
1:A:484:GLU:CD	1:A:484:GLU:N	2.68	0.50
1:B:57:ASN:HD21	1:B:81:GLY:HA3	1.76	0.50
1:B:262:ALA:HB1	1:B:265:LYS:HG3	1.93	0.50
1:C:378:VAL:CG1	1:C:437:ILE:HG22	2.41	0.50
1:C:469:GLN:OE1	1:C:469:GLN:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:8:ARG:O	3:G:12:THR:HG23	2.12	0.49
3:G:207:GLU:H	4:H:41:LEU:HA	1.72	0.49
3:G:209:GLU:HA	4:H:29:SER:HB3	1.90	0.49
1:A:326:ILE:HG12	1:A:335:ILE:CD1	2.43	0.49
2:F:3:ARG:HD3	2:F:3:ARG:O	2.11	0.49
3:G:204:THR:HG23	4:H:40:PRO:CB	2.37	0.49
3:G:210:PRO:HB2	3:G:214:GLU:CB	2.37	0.49
1:C:31:VAL:HG11	1:C:34:VAL:CG2	2.42	0.49
1:B:109:ASN:HB3	1:B:112:GLY:O	2.11	0.49
1:B:163:GLN:HG2	1:B:164:ARG:N	2.28	0.49
1:A:98:PRO:HG2	1:A:112:GLY:HA3	1.95	0.49
2:F:50:VAL:HG13	2:F:59:VAL:HG22	1.95	0.49
3:G:207:GLU:H	4:H:42:VAL:H	1.61	0.49
2:F:285:MET:SD	2:F:289:GLN:HG3	2.53	0.49
1:B:326:ILE:HD11	1:B:343:PHE:HE2	1.77	0.49
1:B:473:GLU:OE1	1:B:477:THR:HG23	2.12	0.49
2:E:295:THR:CG2	2:E:296:ALA:N	2.74	0.49
4:H:20:VAL:HA	4:H:54:LYS:HE3	1.95	0.48
1:A:444:PHE:CZ	1:A:488:ASN:OD1	2.67	0.48
3:G:114:ASP:OD1	3:G:114:ASP:N	2.46	0.48
3:G:192:LEU:HA	3:G:193:PRO:C	2.38	0.48
1:B:483:ASN:OD1	1:B:483:ASN:C	2.56	0.48
1:B:381:THR:HG23	1:B:441:THR:CG2	2.43	0.48
2:E:315:ASP:OD1	2:E:316:PRO:HD2	2.13	0.48
1:B:386:LEU:O	1:B:390:ARG:HG2	2.13	0.48
3:G:206:TYR:CE1	4:H:42:VAL:HG13	2.49	0.48
1:C:163:GLN:NE2	1:C:165:GLU:OE1	2.47	0.48
2:D:153:LYS:HD2	2:D:324:HIS:O	2.14	0.48
4:H:20:VAL:HB	4:H:53:LYS:O	2.14	0.48
1:C:31:VAL:HG11	1:C:34:VAL:HG22	1.95	0.48
2:E:227:ARG:HD2	2:E:230:LEU:HD12	1.94	0.48
2:F:317:ALA:O	2:F:320:THR:HG22	2.14	0.48
3:G:220:LEU:N	3:G:220:LEU:HD22	2.28	0.48
3:G:191:LEU:O	3:G:192:LEU:HG	2.14	0.47
1:A:438:TYR:CZ	1:A:442:ARG:HG3	2.49	0.47
2:E:122:ALA:HB1	2:E:123:PRO:HD2	1.95	0.47
2:E:188:VAL:HG22	2:E:228:VAL:HG13	1.96	0.47
2:F:334:LYS:H	2:F:334:LYS:CD	2.26	0.47
3:G:205:VAL:HG11	4:H:39:ILE:CB	1.93	0.47
3:G:216:LEU:CD2	3:G:220:LEU:HD21	2.44	0.47
1:A:132:ARG:HD2	1:A:132:ARG:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HA	1:A:221:THR:HG22	1.95	0.47
1:C:480:ASP:OD1	1:C:481:LEU:N	2.46	0.47
2:E:44:ILE:CD1	2:E:70:LEU:HD23	2.44	0.47
2:F:431:LYS:HB3	2:F:431:LYS:HE3	1.63	0.47
2:D:3:ARG:HE	2:D:77:ILE:HD11	1.78	0.47
1:A:240:TYR:O	1:A:243:VAL:HG12	2.14	0.47
1:A:444:PHE:HE1	1:A:492:GLU:OE2	1.98	0.47
1:B:291:PHE:HZ	2:F:218:MET:HE2	1.79	0.47
3:G:209:GLU:HB3	4:H:29:SER:H	1.79	0.47
1:B:247:GLU:HA	1:B:250:MET:HB3	1.95	0.47
1:B:343:PHE:H	1:B:362:SER:HB3	1.80	0.47
2:D:85:VAL:HG11	2:D:231:THR:HG23	1.96	0.47
2:D:230:LEU:HD23	2:D:288:LEU:HD13	1.96	0.47
2:E:292:ILE:O	2:E:293:THR:HG23	2.15	0.47
2:F:190:GLU:HG2	2:F:217:GLN:HE22	1.79	0.47
2:F:281:LEU:CD2	2:F:320:THR:HG21	2.45	0.47
3:G:81:TYR:HD2	3:G:174:TYR:CE1	2.33	0.47
1:C:54:GLU:O	1:C:54:GLU:HG3	2.15	0.47
4:H:22:MET:HE3	4:H:23:VAL:H	1.80	0.47
1:B:431:GLU:HG2	1:B:432:LYS:N	2.30	0.47
1:B:500:VAL:O	1:B:501:SER:OG	2.27	0.47
2:E:44:ILE:HD11	2:E:74:MET:SD	2.55	0.47
4:H:84:ARG:NH2	4:H:86:GLU:OE2	2.35	0.46
2:D:456:VAL:HG21	2:D:462:VAL:CG2	2.45	0.46
3:G:95:ASN:O	3:G:98:VAL:HG12	2.16	0.46
2:D:243:GLN:HB3	2:D:245:GLN:CG	2.46	0.46
1:A:168:ILE:HG23	1:A:319:VAL:CG1	2.44	0.46
1:B:483:ASN:OD1	1:B:483:ASN:O	2.33	0.46
2:F:334:LYS:N	2:F:334:LYS:CD	2.76	0.46
3:G:102:VAL:O	3:G:106:ILE:HG23	2.16	0.46
3:G:126:LEU:O	3:G:130:ARG:HG3	2.16	0.46
3:G:148:SER:C	3:G:150:ALA:H	2.23	0.46
3:G:206:TYR:HA	4:H:41:LEU:N	2.29	0.46
1:B:109:ASN:OD1	1:B:110:PRO:N	2.49	0.46
1:C:188:ASP:OD1	1:C:188:ASP:N	2.44	0.46
2:F:7:ILE:HG13	2:F:17:LYS:HB2	1.96	0.46
4:H:24:SER:O	4:H:51:ARG:NH2	2.48	0.46
1:B:129:ILE:CD1	1:B:130:GLU:HG2	2.46	0.46
2:F:405:ARG:NH1	2:F:448:LEU:O	2.39	0.46
1:C:33:GLN:O	1:C:39:ALA:HA	2.16	0.45
2:D:207:VAL:HG13	2:D:210:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:83:ILE:O	2:F:118:ILE:HG12	2.15	0.45
2:E:249:LEU:O	2:E:302:SER:HA	2.16	0.45
2:E:456:VAL:CG1	2:E:457:GLY:N	2.79	0.45
1:A:482:PRO:HG2	1:A:487:LEU:CG	2.38	0.45
2:D:452:ALA:HA	2:D:465:LYS:HE2	1.99	0.45
2:E:205:SER:C	2:E:207:VAL:H	2.25	0.45
1:A:132:ARG:N	1:A:132:ARG:CD	2.80	0.45
2:D:271:MET:HG2	3:G:287:LEU:CD2	2.47	0.45
3:G:204:THR:CB	4:H:71:ARG:HD3	2.17	0.45
1:A:435:LEU:HA	1:A:435:LEU:HD12	1.74	0.45
1:B:462:LEU:HD23	1:B:462:LEU:HA	1.71	0.45
2:E:439:GLU:HA	2:E:439:GLU:OE1	2.17	0.45
2:F:240:ARG:NH1	2:F:241:ASP:OD2	2.36	0.45
4:H:20:VAL:HG12	4:H:54:LYS:HB2	1.98	0.45
1:B:236:PHE:CE1	1:B:293:LEU:HD11	2.52	0.45
1:A:322:GLN:O	1:A:323:ALA:HB2	2.15	0.45
2:E:127:GLU:O	2:E:295:THR:HG23	2.15	0.45
4:H:83:GLU:OE1	4:H:83:GLU:N	2.49	0.45
1:A:373:LYS:HG2	1:A:377:LYS:HE2	1.98	0.45
1:B:115:VAL:O	1:B:115:VAL:CG1	2.65	0.45
2:E:1:MET:SD	2:E:1:MET:C	3.00	0.45
2:E:233:LEU:HD21	2:E:291:ARG:CB	2.47	0.45
2:E:247:VAL:HG12	2:E:248:LEU:N	2.32	0.45
2:E:354:LEU:O	2:E:355:ALA:C	2.60	0.45
4:H:22:MET:HB3	4:H:53:LYS:HG2	1.99	0.45
4:H:52:LEU:O	4:H:59:GLN:N	2.49	0.44
1:C:233:PRO:HG3	1:C:273:LEU:HD21	2.00	0.44
1:C:345:GLN:HB3	1:C:347:ASP:OD1	2.17	0.44
2:E:141:VAL:HG13	2:E:142:VAL:N	2.32	0.44
3:G:48:TYR:CG	4:H:78:LEU:CD2	2.90	0.44
4:H:68:LEU:HD11	4:H:75:VAL:HG13	1.99	0.44
2:D:109:ILE:HG23	2:D:110:PRO:HD2	1.99	0.44
2:E:228:VAL:O	2:E:231:THR:CG2	2.65	0.44
3:G:81:TYR:CE2	3:G:106:ILE:HG22	2.51	0.44
1:B:392:LEU:HD23	1:B:409:LYS:HB3	2.00	0.44
3:G:77:LYS:HB2	3:G:77:LYS:HE2	1.71	0.44
3:G:206:TYR:CE1	4:H:42:VAL:CG1	3.00	0.44
1:B:396:ALA:HB1	1:B:410:LEU:HD11	1.99	0.44
2:D:203:LYS:HE2	2:D:203:LYS:HB3	1.80	0.44
2:F:62:ILE:HD13	2:F:226:MET:HE1	1.98	0.44
1:C:429:PRO:O	1:C:433:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:205:VAL:HB	4:H:39:ILE:HB	1.55	0.44
1:A:52:LEU:HD22	1:A:52:LEU:HA	1.77	0.44
2:D:280:THR:OG1	2:D:284:GLU:OE2	2.16	0.44
2:E:228:VAL:HA	2:E:231:THR:HG22	1.99	0.44
1:A:51:GLU:OE2	1:A:92:GLY:HA2	2.18	0.43
1:C:326:ILE:H	1:C:326:ILE:HD12	1.83	0.43
2:F:309:PRO:HG2	2:F:315:ASP:CG	2.43	0.43
4:H:68:LEU:HD12	4:H:69:GLU:N	2.33	0.43
3:G:116:TYR:CE1	3:G:135:PRO:HD2	2.52	0.43
3:G:131:LYS:O	3:G:132:ARG:HB2	2.18	0.43
3:G:215:CYS:SG	4:H:67:PHE:HZ	2.40	0.43
3:G:236:LYS:HA	3:G:236:LYS:HE2	2.00	0.43
1:A:164:ARG:HH12	2:E:191:ARG:HD3	1.83	0.43
1:A:326:ILE:CD1	1:A:335:ILE:HD11	2.47	0.43
1:A:445:LEU:HD23	1:A:448:ILE:HG13	2.00	0.43
1:B:51:GLU:HG2	1:B:52:LEU:N	2.32	0.43
1:B:301:ALA:HB1	1:B:313:LEU:O	2.18	0.43
1:A:48:MET:HB3	2:E:71:ILE:HG12	2.00	0.43
1:C:150:ILE:HD12	1:C:153:ILE:HD12	2.00	0.43
1:C:363:VAL:HG12	1:C:383:ARG:NH1	2.33	0.43
4:H:17:GLU:OE1	4:H:17:GLU:HA	2.18	0.43
2:D:127:GLU:H	2:D:127:GLU:HG2	1.73	0.43
2:D:198:LEU:HD11	2:D:202:MET:HE2	1.99	0.43
2:F:418:GLU:O	2:F:421:THR:O	2.37	0.43
4:H:42:VAL:HB	4:H:67:PHE:HE2	1.83	0.43
1:B:115:VAL:O	1:B:115:VAL:HG12	2.18	0.43
4:H:73:ASP:N	4:H:73:ASP:OD1	2.51	0.43
1:A:129:ILE:HG23	1:A:240:TYR:HB3	2.01	0.43
1:C:430:VAL:O	1:C:434:VAL:HG13	2.18	0.43
2:F:418:GLU:HA	2:F:421:THR:O	2.19	0.43
2:D:354:LEU:O	2:D:355:ALA:C	2.62	0.43
2:F:3:ARG:HD3	2:F:3:ARG:N	2.28	0.43
1:A:115:VAL:O	1:A:115:VAL:CG1	2.66	0.43
1:A:330:ILE:HB	1:A:331:PRO:HD3	2.01	0.43
1:B:381:THR:HG21	1:B:441:THR:HB	1.99	0.43
1:B:493:ALA:O	1:B:497:THR:HG23	2.18	0.43
1:C:52:LEU:HG	1:C:95:MET:HE1	2.00	0.43
2:D:85:VAL:HG13	2:D:118:ILE:HD11	2.00	0.43
2:E:342:PRO:O	2:E:343:ALA:CB	2.67	0.43
3:G:54:GLU:OE2	3:G:200:ASN:ND2	2.30	0.43
4:H:3:THR:HG22	4:H:21:GLU:CD	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ASP:O	1:A:469:GLN:NE2	2.50	0.42
1:C:375:MET:HG2	1:C:434:VAL:CG1	2.48	0.42
2:F:254:ILE:HD12	2:F:254:ILE:HA	1.90	0.42
3:G:81:TYR:HD2	3:G:174:TYR:HE1	1.67	0.42
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.81	0.42
2:D:233:LEU:HD13	2:D:292:ILE:HG12	2.00	0.42
2:D:410:LEU:HD23	2:D:437:PHE:CZ	2.54	0.42
2:E:450:GLU:HG3	2:E:451:ASP:N	2.34	0.42
4:H:2:LYS:HB2	4:H:36:PRO:HG2	2.00	0.42
1:B:474:HIS:O	1:B:478:THR:OG1	2.35	0.42
1:C:189:GLN:O	1:C:190:ASN:HB2	2.20	0.42
2:E:84:SER:HA	2:E:116:ASP:O	2.19	0.42
3:G:85:THR:HB	3:G:95:ASN:OD1	2.19	0.42
2:D:141:VAL:HG23	2:D:410:LEU:HD22	2.01	0.42
2:E:178:GLU:HG2	2:E:427:TYR:CE1	2.54	0.42
2:E:451:ASP:OD1	2:E:451:ASP:O	2.37	0.42
2:F:48:LEU:HD23	2:F:63:ALA:HA	2.01	0.42
2:F:283:THR:O	2:F:287:GLN:HG3	2.20	0.42
2:F:335:LEU:HD23	2:F:338:MET:HE2	2.00	0.42
3:G:7:LEU:HG	3:G:265:TYR:CE2	2.53	0.42
1:C:95:MET:HG3	1:C:129:ILE:CG1	2.34	0.42
2:D:256:ARG:NH2	2:D:259:GLN:OE1	2.46	0.42
2:D:294:SER:HB2	2:D:299:SER:HA	2.02	0.42
2:D:360:GLY:HA2	2:D:364:TYR:HB2	2.01	0.42
2:F:118:ILE:CG2	2:F:230:LEU:HB3	2.48	0.42
3:G:6:SER:O	3:G:10:ILE:HG13	2.19	0.42
3:G:193:PRO:HB2	3:G:195:THR:HG23	2.02	0.42
1:A:438:TYR:CE1	1:A:442:ARG:HG3	2.54	0.42
3:G:48:TYR:HA	4:H:78:LEU:HD21	2.02	0.42
1:B:345:GLN:CD	1:B:358:ASN:HD22	2.28	0.42
1:C:397:GLN:OE1	1:C:397:GLN:CA	2.68	0.42
2:D:333:ARG:HG2	2:D:337:GLU:OE2	2.19	0.42
1:A:399:GLY:HA2	1:A:402:LEU:HD23	2.02	0.42
2:D:3:ARG:HG2	2:D:75:GLU:CD	2.44	0.42
2:D:458:ARG:O	2:D:461:GLU:HB2	2.20	0.42
2:F:44:ILE:HD12	2:F:74:MET:HE1	2.01	0.42
1:C:74:VAL:HG11	1:C:233:PRO:HB3	2.00	0.42
2:E:228:VAL:HA	2:E:231:THR:CG2	2.49	0.42
2:F:2:THR:O	2:F:2:THR:HG23	2.20	0.42
1:B:401:ASP:OD2	3:G:183:GLN:HG2	2.19	0.42
3:G:52:ILE:HA	3:G:55:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:179:VAL:HB	3:G:183:GLN:O	2.20	0.42
1:C:378:VAL:HG12	1:C:437:ILE:HG22	2.02	0.41
2:D:251:ILE:HG21	2:D:254:ILE:HD13	2.01	0.41
2:D:294:SER:HB3	2:D:299:SER:HA	2.02	0.41
2:E:337:GLU:OE1	2:E:337:GLU:HA	2.19	0.41
1:A:165:GLU:O	1:A:317:PRO:HD2	2.20	0.41
2:D:43:ASP:N	2:D:43:ASP:OD1	2.53	0.41
3:G:59:VAL:HG12	3:G:216:LEU:HD21	2.02	0.41
1:A:166:LEU:HG	1:A:168:ILE:HG12	2.01	0.41
1:B:435:LEU:HD23	1:B:435:LEU:HA	1.92	0.41
1:C:109:ASN:HD22	1:C:110:PRO:HD2	1.85	0.41
2:D:181:GLY:C	2:D:182:ILE:HD12	2.45	0.41
2:D:349:SER:C	2:D:351:SER:N	2.79	0.41
3:G:146:GLN:C	3:G:148:SER:N	2.78	0.41
1:B:53:VAL:CG1	1:B:88:VAL:CG2	2.99	0.41
1:B:156:LEU:HB3	1:B:383:ARG:NH1	2.35	0.41
1:B:255:HIS:ND1	1:B:312:SER:HB3	2.35	0.41
2:D:315:ASP:O	2:D:318:PRO:HD2	2.21	0.41
4:H:53:LYS:HE2	4:H:58:THR:OG1	2.21	0.41
4:H:84:ARG:HB2	4:H:87:ASP:OD2	2.20	0.41
1:B:348:LEU:HA	1:B:348:LEU:HD23	1.80	0.41
3:G:107:GLN:OE1	3:G:107:GLN:HA	2.21	0.41
2:E:332:GLU:HG3	2:E:334:LYS:HB2	2.03	0.41
3:G:116:TYR:CD1	3:G:116:TYR:C	2.99	0.41
1:A:376:LYS:HB2	1:A:376:LYS:HE2	1.72	0.41
2:D:35:LYS:HE2	2:D:35:LYS:HB2	1.88	0.41
3:G:210:PRO:HG3	4:H:28:LYS:HG2	1.73	0.41
1:B:466:GLN:HB3	1:B:467:ASN:OD1	2.21	0.41
1:C:496:LYS:HB2	1:C:496:LYS:HE2	1.87	0.41
2:D:188:VAL:HG22	2:D:228:VAL:HG13	2.02	0.41
2:D:350:THR:C	2:D:352:ARG:N	2.78	0.41
2:E:2:THR:O	2:E:2:THR:HG23	2.20	0.41
2:E:31:LYS:HD3	2:E:31:LYS:HA	1.89	0.41
1:A:352:GLY:O	1:A:421:LYS:HE3	2.20	0.41
1:B:448:ILE:N	1:B:448:ILE:CD1	2.84	0.40
1:B:109:ASN:OD1	1:B:110:PRO:HD2	2.21	0.40
2:E:238:TYR:CD1	2:E:242:GLU:HG3	2.54	0.40
3:G:205:VAL:HG11	4:H:39:ILE:HA	0.73	0.40
4:H:68:LEU:HD12	4:H:69:GLU:H	1.87	0.40
1:B:236:PHE:HE1	1:B:293:LEU:CD1	2.35	0.40
1:C:474:HIS:CE1	1:C:478:THR:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:ALA:HB3	2:E:333:ARG:NH1	2.36	0.40
2:F:23:LEU:HD23	2:F:23:LEU:HA	1.77	0.40
2:F:153:LYS:HD2	2:F:324:HIS:O	2.22	0.40
1:A:419:VAL:HG12	1:A:453:VAL:CG1	2.52	0.40
1:B:145:PRO:HB3	1:B:370:ALA:O	2.21	0.40
1:C:163:GLN:OE1	1:C:366:VAL:HG11	2.21	0.40
2:D:85:VAL:CG1	2:D:118:ILE:HD11	2.52	0.40
1:B:480:ASP:CG	1:B:481:LEU:H	2.28	0.40
2:D:451:ASP:O	2:D:451:ASP:OD1	2.38	0.40
2:E:44:ILE:HD12	2:E:70:LEU:HD23	2.04	0.40
3:G:194:LEU:HD11	3:G:223:TYR:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	472/476 (99%)	452 (96%)	14 (3%)	6 (1%)	9	25
1	B	473/476 (99%)	452 (96%)	17 (4%)	4 (1%)	16	37
1	C	474/476 (100%)	449 (95%)	21 (4%)	4 (1%)	16	37
2	D	468/471 (99%)	444 (95%)	21 (4%)	3 (1%)	21	44
2	E	468/471 (99%)	444 (95%)	16 (3%)	8 (2%)	7	19
2	F	469/471 (100%)	439 (94%)	23 (5%)	7 (2%)	8	22
3	G	280/282 (99%)	263 (94%)	11 (4%)	6 (2%)	5	15
4	H	85/87 (98%)	77 (91%)	6 (7%)	2 (2%)	4	12
All	All	3189/3210 (99%)	3020 (95%)	129 (4%)	40 (1%)	12	25

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	GLY
1	A	222	ILE
1	A	323	ALA
1	B	216	GLY
1	B	222	ILE
1	C	216	GLY
1	C	222	ILE
2	D	350	THR
2	D	351	SER
2	E	206	GLY
2	E	212	ALA
2	F	206	GLY
2	F	349	SER
3	G	143	LEU
3	G	144	PRO
3	G	145	ASP
3	G	147	PRO
3	G	148	SER
3	G	149	PHE
1	C	215	HIS
2	D	349	SER
4	H	23	VAL
1	A	215	HIS
1	B	215	HIS
1	B	223	VAL
2	E	205	SER
2	E	213	MET
2	E	253	ASN
2	E	346	PRO
2	F	212	ALA
2	F	351	SER
1	A	223	VAL
2	F	205	SER
1	A	118	LEU
1	C	223	VAL
2	E	356	PRO
2	F	275	VAL
2	F	356	PRO
4	H	15	VAL
2	E	275	VAL

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	382/384 (100%)	363 (95%)	19 (5%)	22	48
1	B	383/384 (100%)	371 (97%)	12 (3%)	35	65
1	C	384/384 (100%)	368 (96%)	16 (4%)	26	55
2	D	386/387 (100%)	380 (98%)	6 (2%)	55	80
2	E	386/387 (100%)	375 (97%)	11 (3%)	38	68
2	F	387/387 (100%)	376 (97%)	11 (3%)	38	68
3	G	238/238 (100%)	227 (95%)	11 (5%)	24	51
4	H	70/70 (100%)	61 (87%)	9 (13%)	4	10
All	All	2616/2621 (100%)	2521 (96%)	95 (4%)	32	60

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	115	VAL
1	A	129	ILE
1	A	130	GLU
1	A	157	VAL
1	A	168	ILE
1	A	171	ARG
1	A	205	VAL
1	A	219	ASP
1	A	221	THR
1	A	256	VAL
1	A	314	THR
1	A	319	VAL
1	A	320	GLU
1	A	378	VAL
1	A	391	GLU
1	A	435	LEU
1	A	445	LEU
1	A	492	GLU

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Mol	Chain	Res	Type
1	B	28	VAL
1	B	30	THR
1	B	97	VAL
1	B	108	VAL
1	B	125	GLU
1	B	221	THR
1	B	314	THR
1	B	320	GLU
1	B	381	THR
1	B	391	GLU
1	B	446	ASP
1	B	465	ASP
1	C	64	LEU
1	C	74	VAL
1	C	97	VAL
1	C	108	VAL
1	C	109	ASN
1	C	141	SER
1	C	186	GLN
1	C	219	ASP
1	C	243	VAL
1	C	274	SER
1	C	326	ILE
1	C	347	ASP
1	C	467	ASN
1	C	484	GLU
1	C	487	LEU
1	C	500	VAL
2	D	33	GLN
2	D	48	LEU
2	D	126	GLU
2	D	168	ILE
2	D	202	MET
2	D	384	ILE
2	E	26	ILE
2	E	120	ARG
2	E	211	THR
2	E	231	THR
2	E	328	THR
2	E	329	THR
2	E	346	PRO
2	E	354	LEU

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Mol	Chain	Res	Type
2	E	363	HIS
2	E	448	LEU
2	E	464	GLU
2	F	26	ILE
2	F	168	ILE
2	F	190	GLU
2	F	213	MET
2	F	214	VAL
2	F	228	VAL
2	F	288	LEU
2	F	352	ARG
2	F	363	HIS
2	F	395	GLU
2	F	430	VAL
3	G	76	VAL
3	G	87	ASP
3	G	102	VAL
3	G	137	ILE
3	G	152	ILE
3	G	160	VAL
3	G	183	GLN
3	G	212	GLN
3	G	218	VAL
3	G	236	LYS
3	G	238	SER
4	H	4	ILE
4	H	6	VAL
4	H	15	VAL
4	H	21	GLU
4	H	22	MET
4	H	23	VAL
4	H	24	SER
4	H	68	LEU
4	H	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	345	GLN
1	A	358	ASN
1	A	488	ASN

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Mol	Chain	Res	Type
1	B	70	ASN
1	B	474	HIS
1	C	172	GLN
1	C	185	ASN
1	C	186	GLN
1	C	200	GLN
1	C	358	ASN
1	C	474	HIS
2	D	173	HIS
2	D	375	GLN
2	E	40	ASN
2	E	253	ASN
2	E	324	HIS
2	E	447	HIS
2	F	217	GLN
2	F	381	GLN
3	G	176	ASN
3	G	184	GLN
3	G	212	GLN
3	G	240	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ATP	F	500	5	32,33,33	1.04	2 (6%)	48,52,52	0.54	1 (2%)
6	ADP	D	502	5	28,29,29	1.36	4 (14%)	43,45,45	1.91	11 (25%)
6	ADP	E	501	5	28,29,29	1.13	2 (7%)	43,45,45	1.30	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	F	500	5	-	3/22/38/38	0/3/3/3
6	ADP	D	502	5	-	2/16/32/32	0/3/3/3
6	ADP	E	501	5	-	2/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	500	ATP	PB-O3B	-4.81	1.54	1.59
6	D	502	ADP	C5-C4	4.05	1.46	1.39
6	E	501	ADP	PA-O3A	-2.69	1.56	1.59
6	D	502	ADP	C5-N7	-2.66	1.34	1.39
6	D	502	ADP	C5-C6	2.43	1.47	1.41
6	D	502	ADP	C4-N9	-2.23	1.33	1.37
7	F	500	ATP	PA-O3A	-2.12	1.57	1.59
6	E	501	ADP	C5-C4	-2.09	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	502	ADP	C5-C4-N3	-5.76	118.79	126.72
6	D	502	ADP	N3-C4-N9	4.68	135.12	127.17
6	D	502	ADP	C2-N3-C4	3.86	121.27	111.83
6	D	502	ADP	N3-C2-N1	-3.84	122.78	128.58
6	D	502	ADP	C4-C5-N7	-3.58	106.49	110.58
6	D	502	ADP	C4-N9-C8	3.28	109.18	105.74
6	E	501	ADP	C4-C5-N7	2.98	113.99	110.58
6	E	501	ADP	O2B-PB-O3A	2.96	114.57	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	502	ADP	C5-N7-C8	2.88	107.98	103.45
6	E	501	ADP	O2A-PA-O3A	2.82	114.89	107.27
6	E	501	ADP	C5-C4-N3	-2.74	122.94	126.72
6	D	502	ADP	N9-C8-N7	-2.58	110.27	113.94
6	E	501	ADP	O3B-PB-O1B	-2.47	101.21	110.83
6	D	502	ADP	C2-N1-C6	2.31	122.52	118.73
6	D	502	ADP	C6-C5-N7	2.18	136.29	132.09
6	D	502	ADP	C2'-C1'-N9	-2.13	108.02	113.30
6	E	501	ADP	C5-C6-N1	2.11	122.86	117.51
6	E	501	ADP	N3-C4-N9	2.06	130.67	127.17
7	F	500	ATP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	502	ADP	C5'-O5'-PA-O1A
6	E	501	ADP	PA-O3A-PB-O3B
7	F	500	ATP	PA-O3A-PB-O1B
6	E	501	ADP	O4'-C4'-C5'-O5'
6	D	502	ADP	C5'-O5'-PA-O3A
7	F	500	ATP	PA-O3A-PB-O2B
7	F	500	ATP	O4'-C4'-C5'-O5'

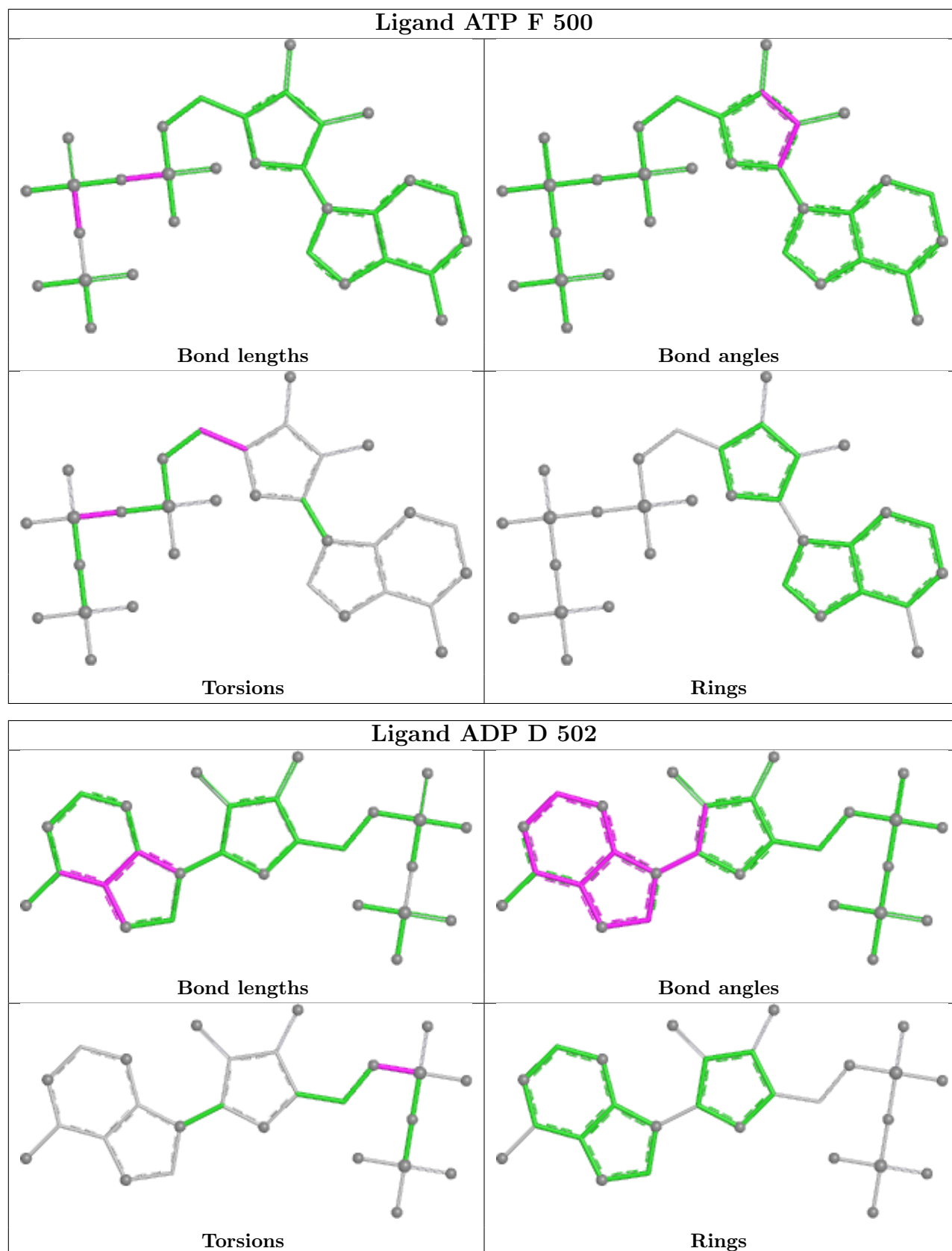
There are no ring outliers.

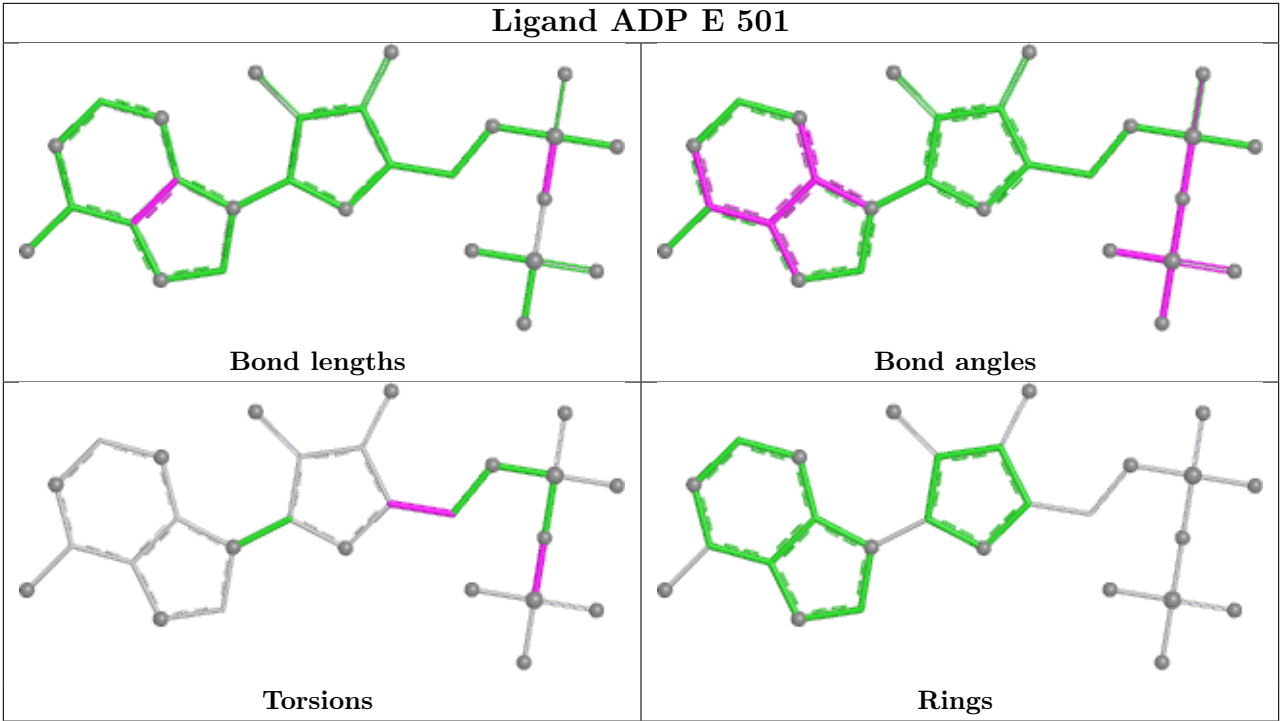
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	500	ATP	4	0
6	D	502	ADP	1	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	189:GLY	C	190:GLU	N	1.16

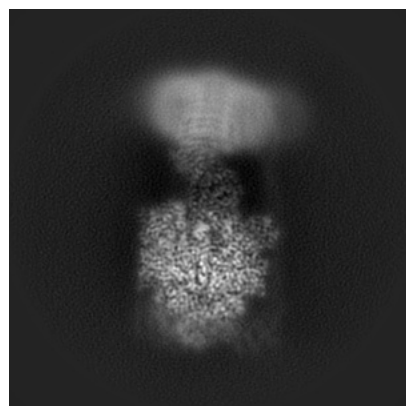
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39284. These allow visual inspection of the internal detail of the map and identification of artifacts.

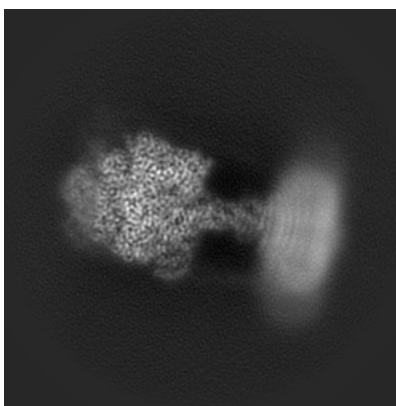
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

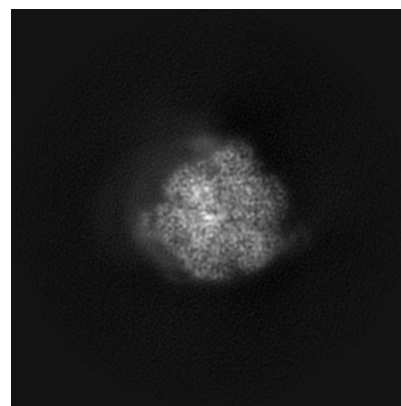
6.1.1 Primary map



X

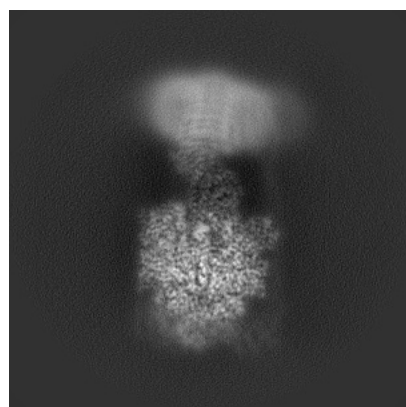


Y

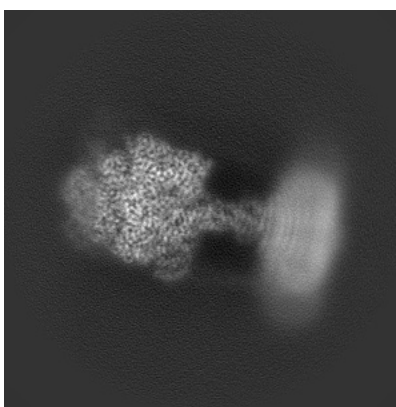


Z

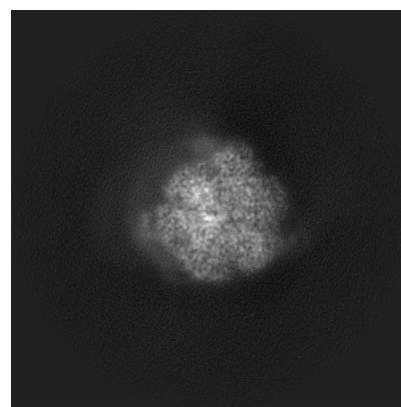
6.1.2 Raw map



X



Y

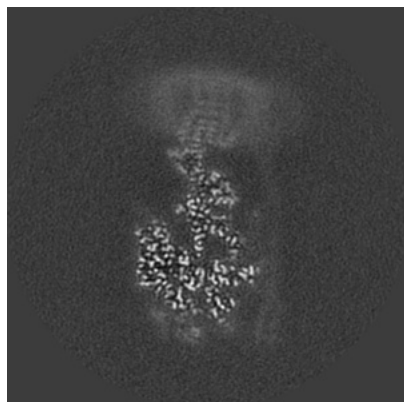


Z

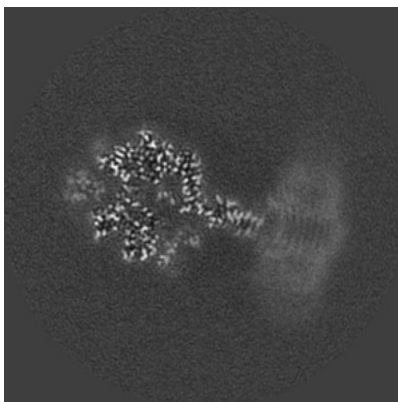
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

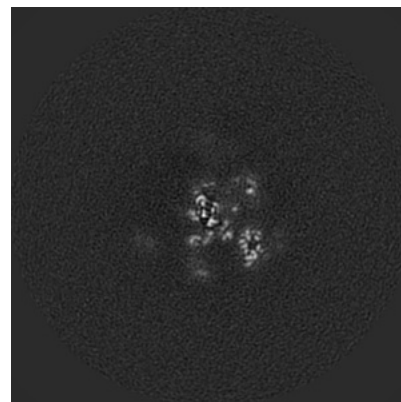
6.2.1 Primary map



X Index: 180

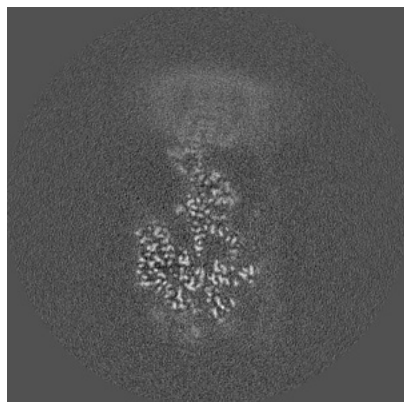


Y Index: 180

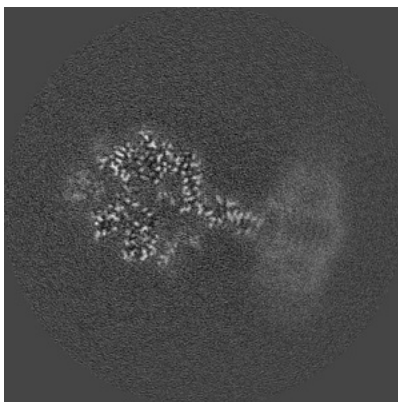


Z Index: 180

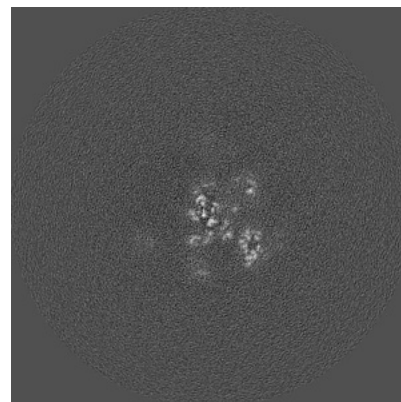
6.2.2 Raw map



X Index: 180



Y Index: 180

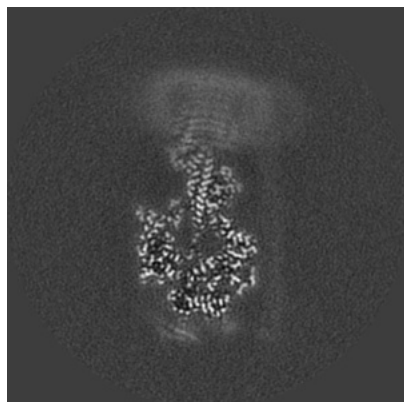


Z Index: 180

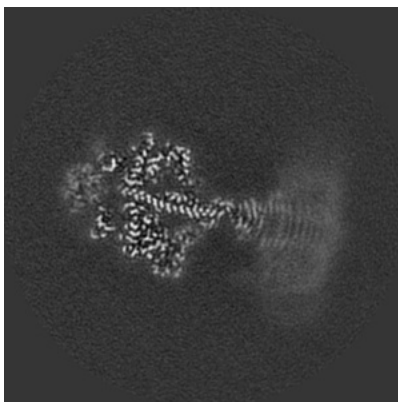
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

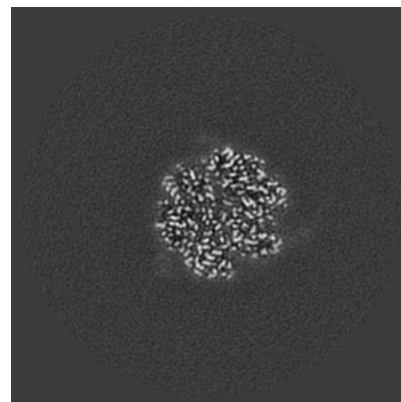
6.3.1 Primary map



X Index: 173

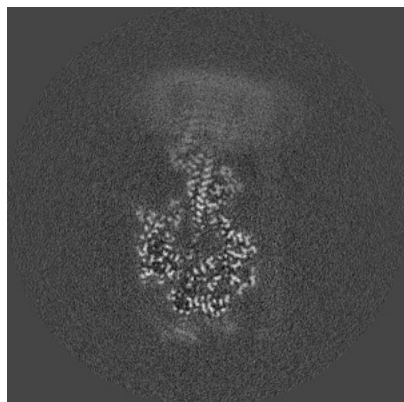


Y Index: 173

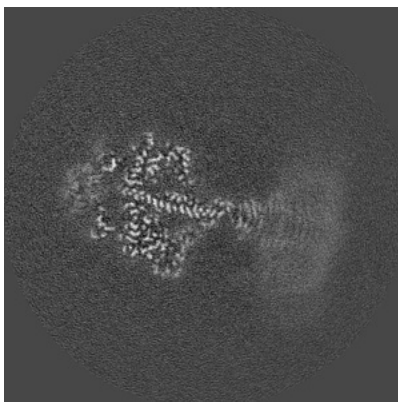


Z Index: 122

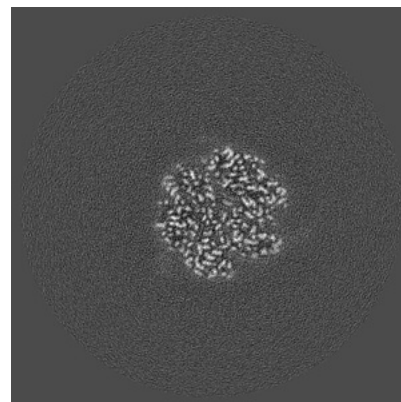
6.3.2 Raw map



X Index: 173



Y Index: 173

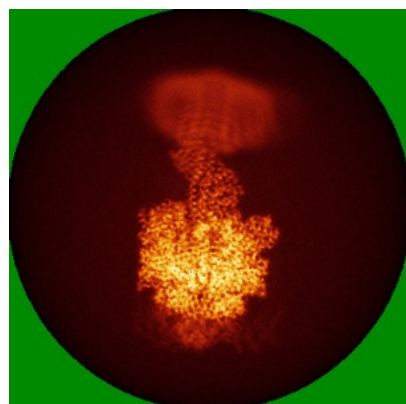


Z Index: 122

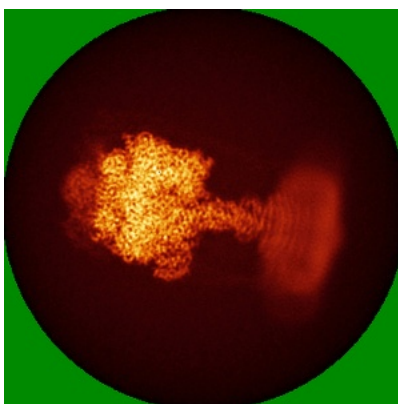
The images above show the largest variance slices of the map in three orthogonal directions.

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

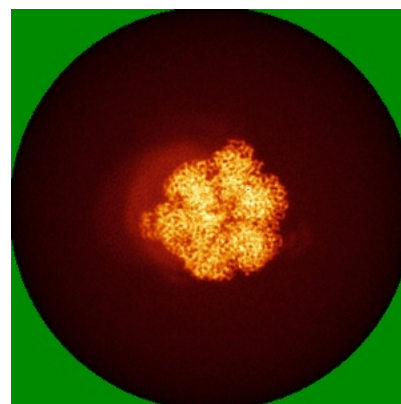
6.4.1 Primary map



X

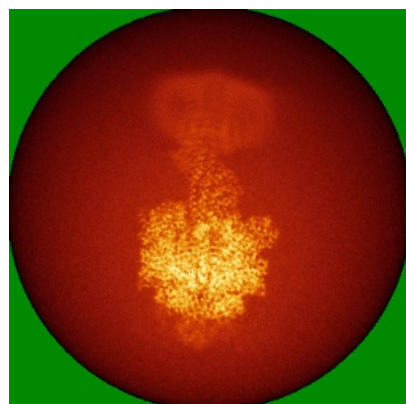


Y

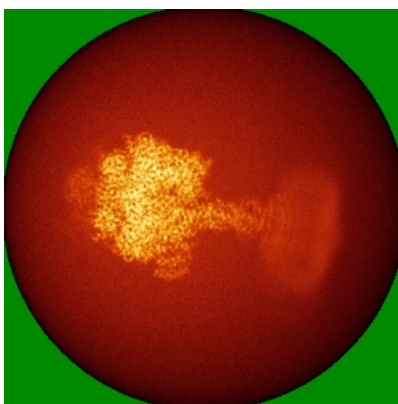


Z

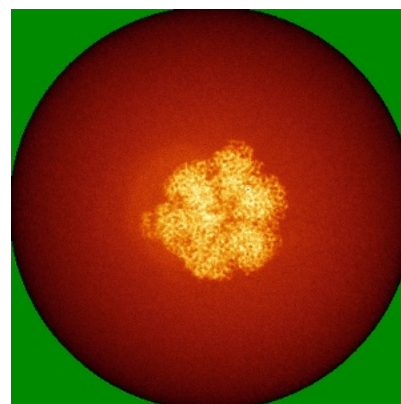
6.4.2 Raw map



X



Y



Z

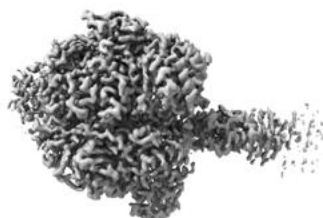
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



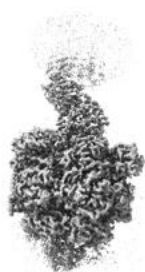
Y



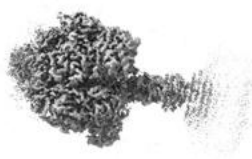
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00751. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

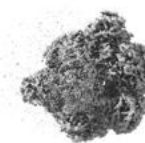
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

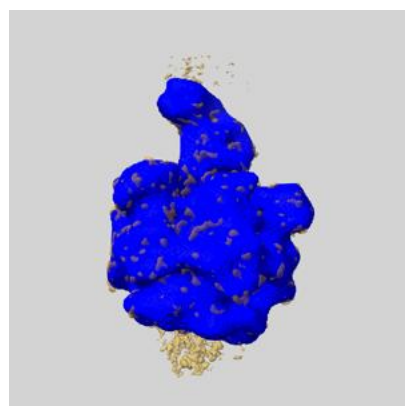
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

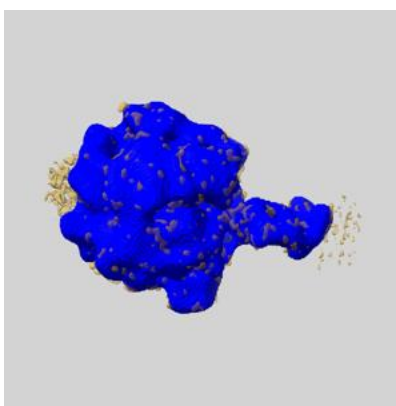
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

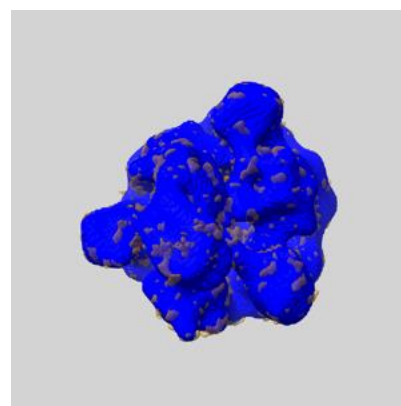
6.6.1 emd_39284_msk_1.map [i](#)



X



Y

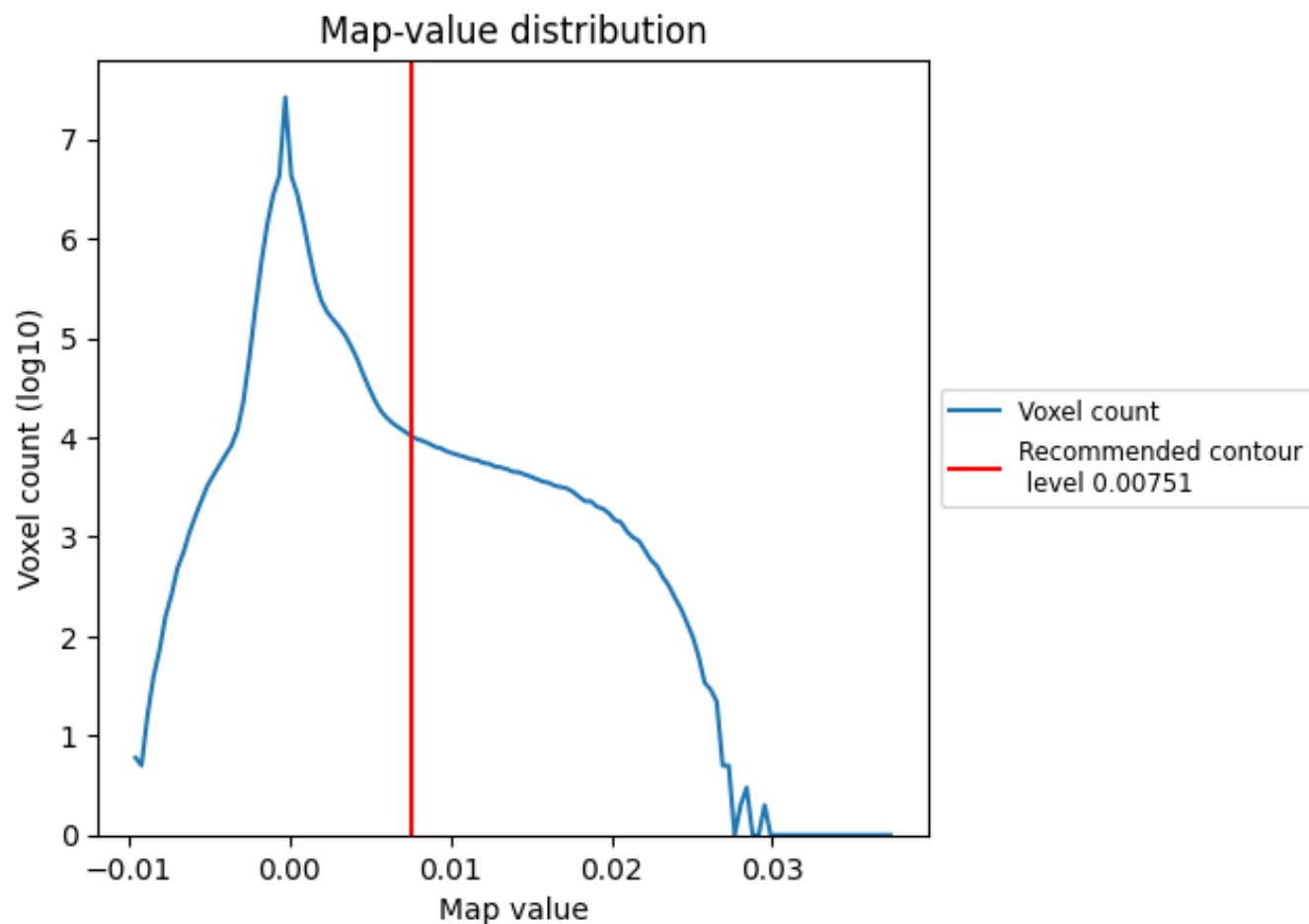


Z

7 Map analysis [i](#)

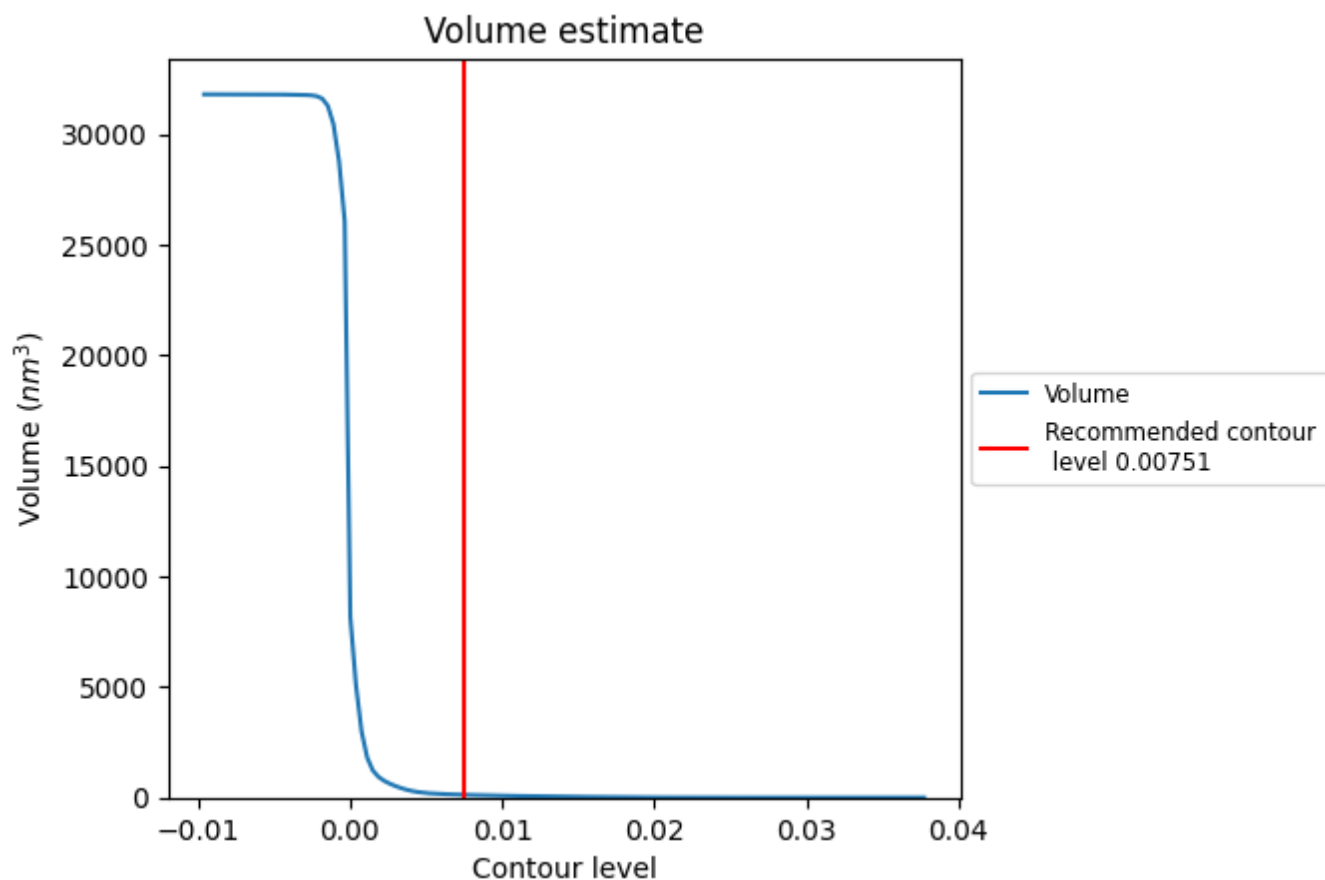
This section contains the results of statistical analysis of the map.

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.

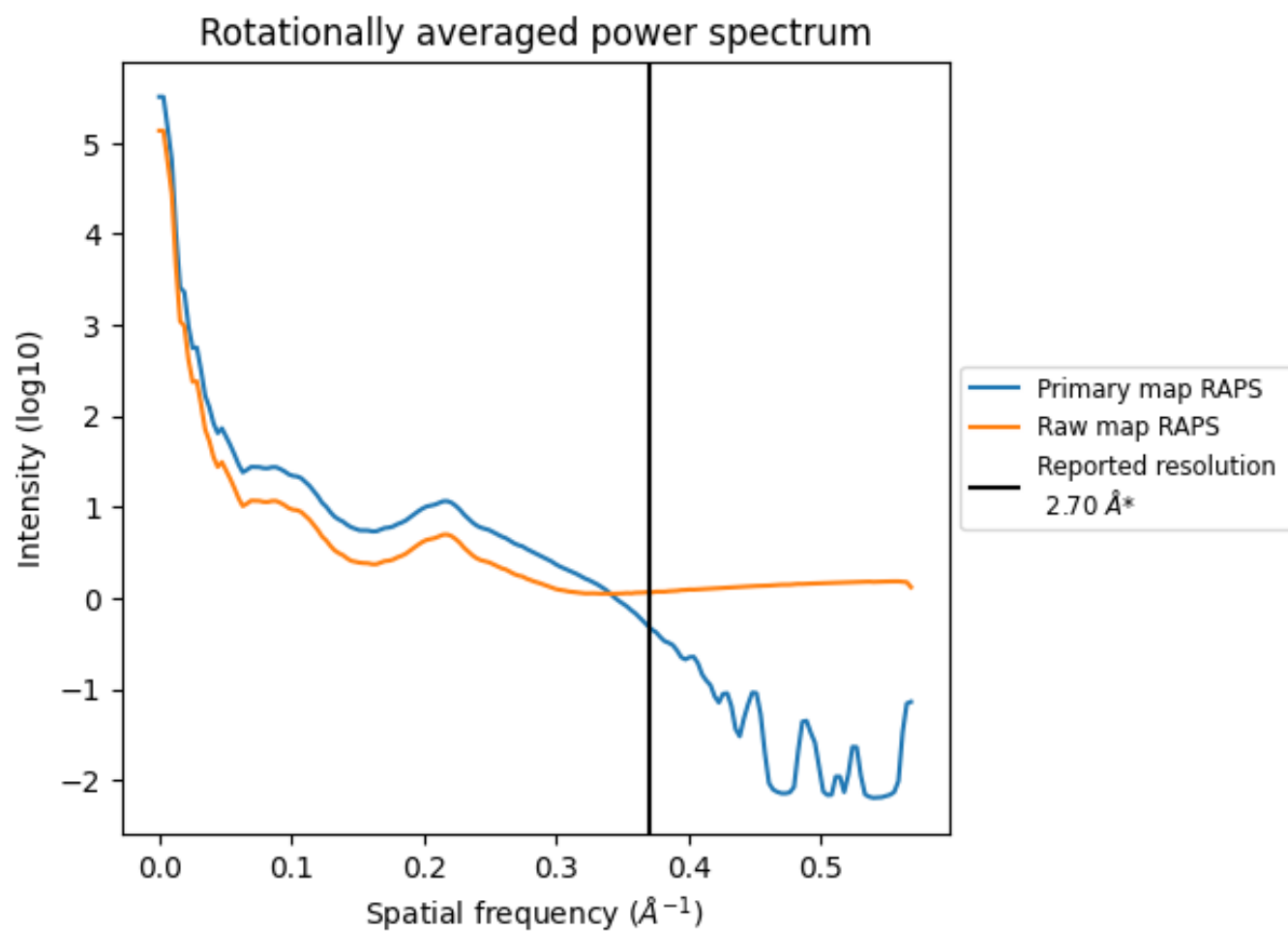
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm^3 ; this corresponds to an approximate mass of 112 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 ⓘ

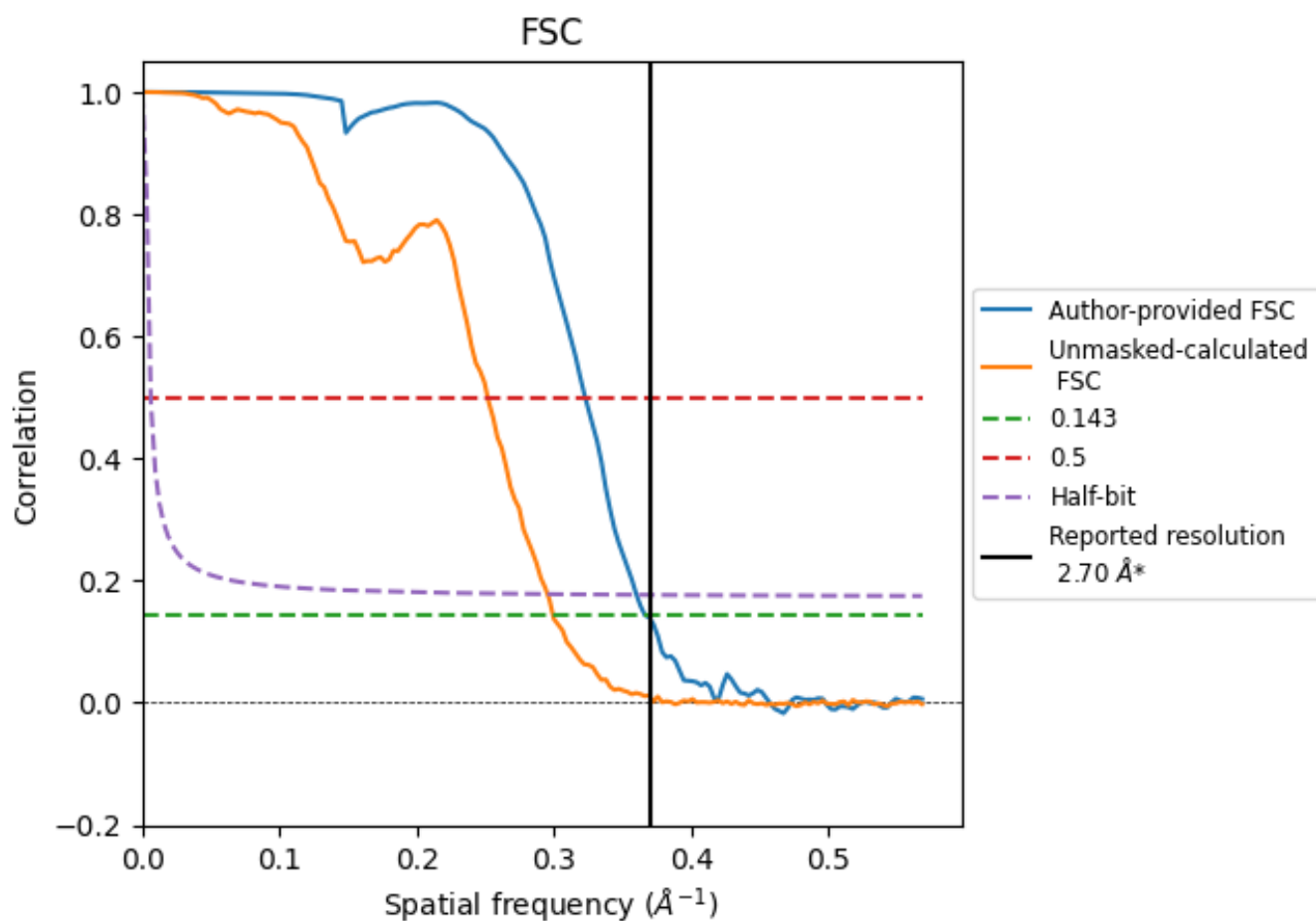


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

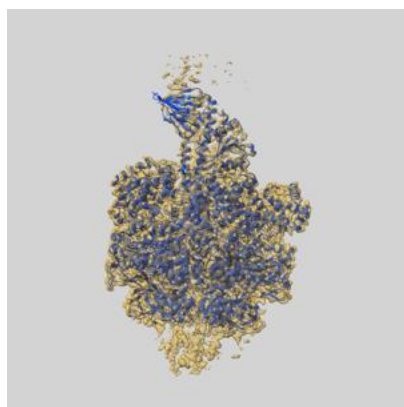
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.10	2.78
Unmasked-calculated*	3.34	3.97	3.39

*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 3.34 differs from the reported value 2.7 by more than 10 %

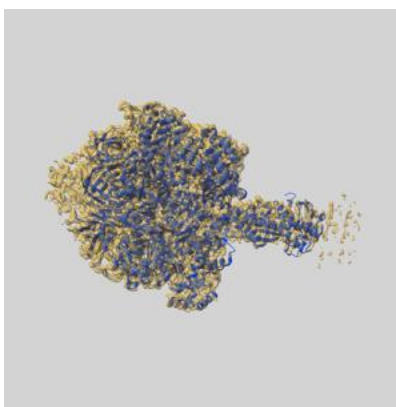
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39284 and PDB model 8YH8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

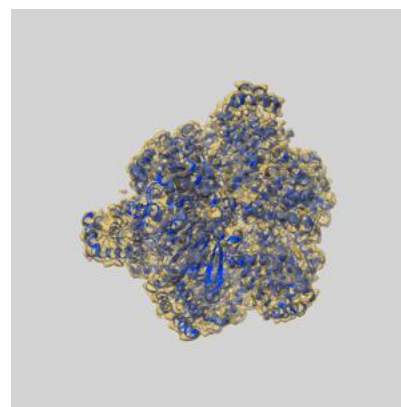
9.1 Map-model overlay [i](#)



X



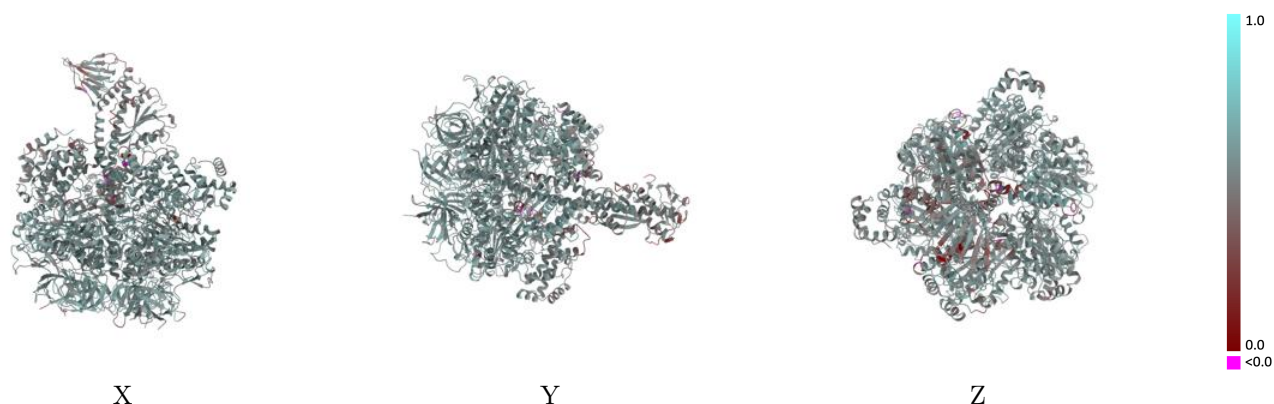
Y



Z

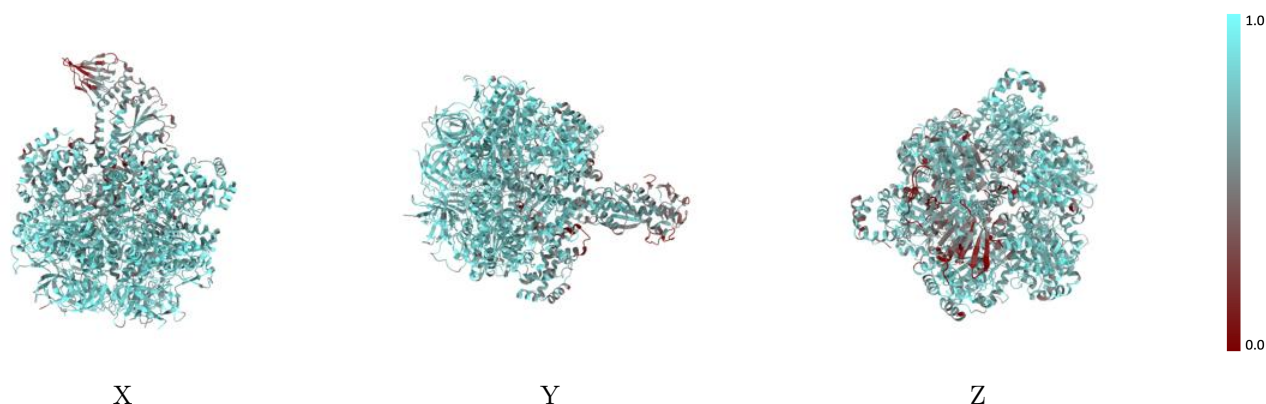
The images above show the 3D surface view of the map at the recommended contour level 0.00751 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



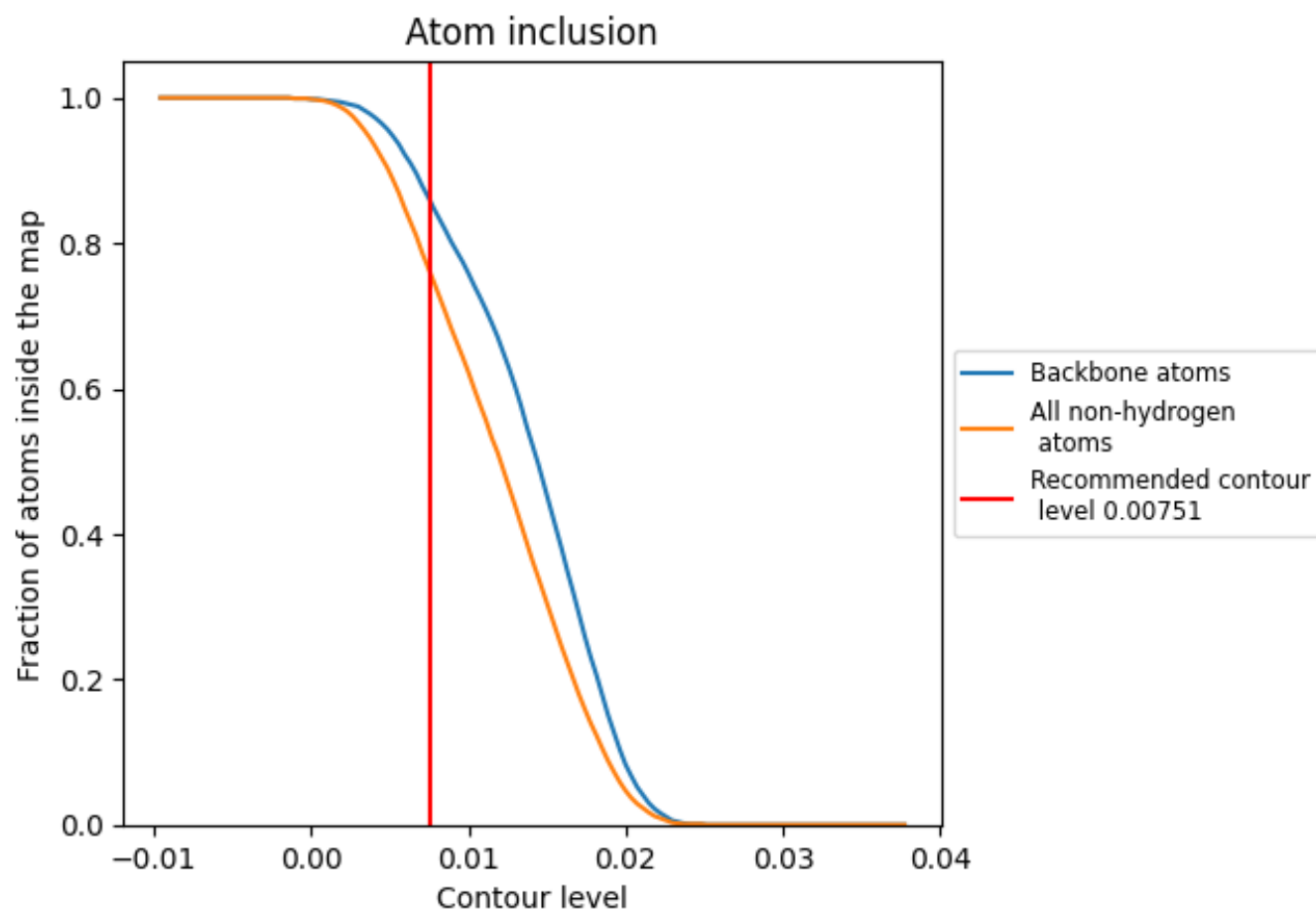
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00751).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.00751) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7620	0.5430
A	0.7860	0.5480
B	0.7710	0.5510
C	0.8010	0.5600
D	0.7920	0.5460
E	0.7680	0.5400
F	0.8060	0.5600
G	0.6280	0.4910
H	0.3640	0.4580

1.0

0.0

<0.0