



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:20 AM UTC

PDB ID : 8Y2H / pdb_00008y2h
EMDB ID : EMD-38855
Title : GK tetramer of AtP5CS1 filament with adjacent hooks, reaction state
Authors : Zhang, T.; Guo, C.J.; Liu, J.L.
Deposited on : 2024-01-26
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

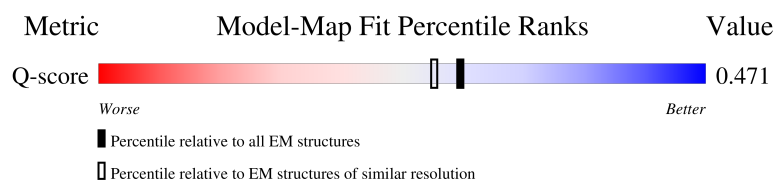
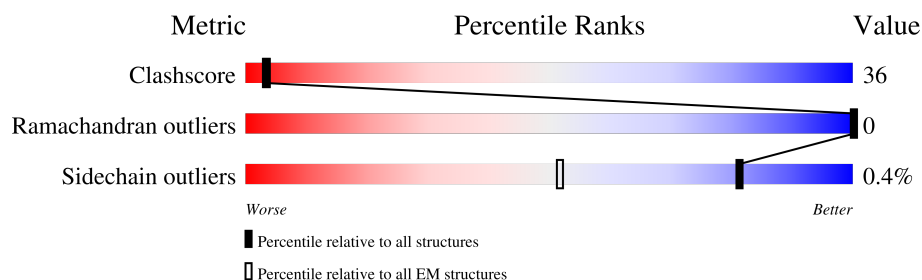
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

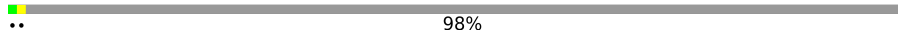
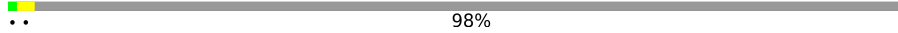
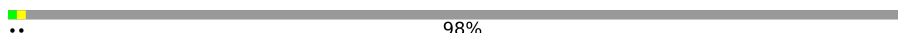
The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	 98%
1	B	727	 22% 14% 63%
1	C	727	 98%
1	D	727	 98%

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Mol	Chain	Length	Quality of chain
1	E	727	98%
1	F	727	22% 14% 63%
1	G	727	23% 14% 63%
1	H	727	22% 14% 63%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8808 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 Delta-1-pyrroline-5-carboxylate synthase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	267	Total	C	N	O	S	0	0
			2047	1289	361	391	6		
1	A	15	Total	C	N	O		0	0
			124	79	22	23			
1	F	267	Total	C	N	O	S	0	0
			2047	1289	361	391	6		
1	C	15	Total	C	N	O		0	0
			124	79	22	23			
1	G	267	Total	C	N	O	S	0	0
			2047	1289	361	391	6		
1	D	15	Total	C	N	O		0	0
			124	79	22	23			
1	H	267	Total	C	N	O	S	0	0
			2047	1289	361	391	6		
1	E	15	Total	C	N	O		0	0
			124	79	22	23			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P54887
B	-8	GLY	-	expression tag	UNP P54887
B	-7	SER	-	expression tag	UNP P54887
B	-6	SER	-	expression tag	UNP P54887
B	-5	HIS	-	expression tag	UNP P54887
B	-4	HIS	-	expression tag	UNP P54887
B	-3	HIS	-	expression tag	UNP P54887
B	-2	HIS	-	expression tag	UNP P54887
B	-1	HIS	-	expression tag	UNP P54887
B	0	HIS	-	expression tag	UNP P54887
A	-9	MET	-	initiating methionine	UNP P54887
A	-8	GLY	-	expression tag	UNP P54887
A	-7	SER	-	expression tag	UNP P54887
A	-6	SER	-	expression tag	UNP P54887

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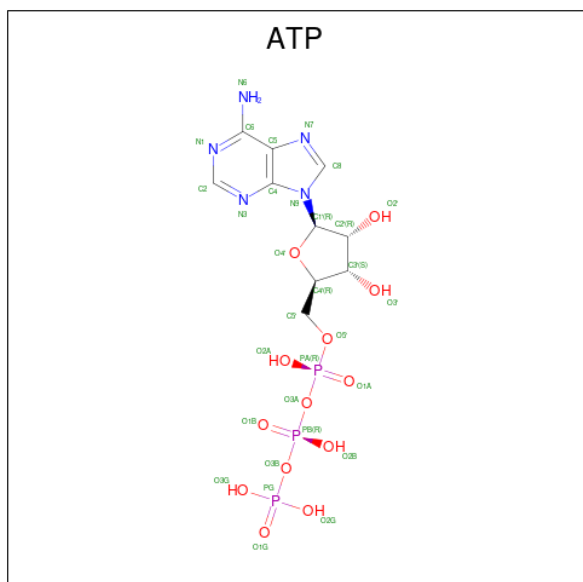
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P54887
A	-4	HIS	-	expression tag	UNP P54887
A	-3	HIS	-	expression tag	UNP P54887
A	-2	HIS	-	expression tag	UNP P54887
A	-1	HIS	-	expression tag	UNP P54887
A	0	HIS	-	expression tag	UNP P54887
F	-9	MET	-	initiating methionine	UNP P54887
F	-8	GLY	-	expression tag	UNP P54887
F	-7	SER	-	expression tag	UNP P54887
F	-6	SER	-	expression tag	UNP P54887
F	-5	HIS	-	expression tag	UNP P54887
F	-4	HIS	-	expression tag	UNP P54887
F	-3	HIS	-	expression tag	UNP P54887
F	-2	HIS	-	expression tag	UNP P54887
F	-1	HIS	-	expression tag	UNP P54887
F	0	HIS	-	expression tag	UNP P54887
C	-9	MET	-	initiating methionine	UNP P54887
C	-8	GLY	-	expression tag	UNP P54887
C	-7	SER	-	expression tag	UNP P54887
C	-6	SER	-	expression tag	UNP P54887
C	-5	HIS	-	expression tag	UNP P54887
C	-4	HIS	-	expression tag	UNP P54887
C	-3	HIS	-	expression tag	UNP P54887
C	-2	HIS	-	expression tag	UNP P54887
C	-1	HIS	-	expression tag	UNP P54887
C	0	HIS	-	expression tag	UNP P54887
G	-9	MET	-	initiating methionine	UNP P54887
G	-8	GLY	-	expression tag	UNP P54887
G	-7	SER	-	expression tag	UNP P54887
G	-6	SER	-	expression tag	UNP P54887
G	-5	HIS	-	expression tag	UNP P54887
G	-4	HIS	-	expression tag	UNP P54887
G	-3	HIS	-	expression tag	UNP P54887
G	-2	HIS	-	expression tag	UNP P54887
G	-1	HIS	-	expression tag	UNP P54887
G	0	HIS	-	expression tag	UNP P54887
D	-9	MET	-	initiating methionine	UNP P54887
D	-8	GLY	-	expression tag	UNP P54887
D	-7	SER	-	expression tag	UNP P54887
D	-6	SER	-	expression tag	UNP P54887
D	-5	HIS	-	expression tag	UNP P54887
D	-4	HIS	-	expression tag	UNP P54887

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	HIS	-	expression tag	UNP P54887
D	-2	HIS	-	expression tag	UNP P54887
D	-1	HIS	-	expression tag	UNP P54887
D	0	HIS	-	expression tag	UNP P54887
H	-9	MET	-	initiating methionine	UNP P54887
H	-8	GLY	-	expression tag	UNP P54887
H	-7	SER	-	expression tag	UNP P54887
H	-6	SER	-	expression tag	UNP P54887
H	-5	HIS	-	expression tag	UNP P54887
H	-4	HIS	-	expression tag	UNP P54887
H	-3	HIS	-	expression tag	UNP P54887
H	-2	HIS	-	expression tag	UNP P54887
H	-1	HIS	-	expression tag	UNP P54887
H	0	HIS	-	expression tag	UNP P54887
E	-9	MET	-	initiating methionine	UNP P54887
E	-8	GLY	-	expression tag	UNP P54887
E	-7	SER	-	expression tag	UNP P54887
E	-6	SER	-	expression tag	UNP P54887
E	-5	HIS	-	expression tag	UNP P54887
E	-4	HIS	-	expression tag	UNP P54887
E	-3	HIS	-	expression tag	UNP P54887
E	-2	HIS	-	expression tag	UNP P54887
E	-1	HIS	-	expression tag	UNP P54887
E	0	HIS	-	expression tag	UNP P54887

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total 31	C 10	N 5	O 13	P 3	0
2	F	1	Total 31	C 10	N 5	O 13	P 3	0
2	G	1	Total 31	C 10	N 5	O 13	P 3	0
2	H	1	Total 31	C 10	N 5	O 13	P 3	0

98%



63%

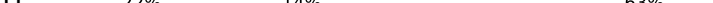






[illegible]

- Molecule 1: Delta-1-pyrroline-5-carboxylate synthase A

Chain H:  22% 14% 63%

ALA	ALA	D268	S175	K85	MET
ASN	ASN	K269	L179	P86	GLY
VAL	VAL	V270		Q87	SER
THR	THR	L271	L182	T88	SER
THR	THR	R272		E89	SER
ILE	ILE	G273	E186		HIS
LYS	LYS	L274	L187	K93	HIS
ALA	ALA	R275		A94	HIS
GLU	GLU		L191	C95	HIS
ASN	ASN	L279	L192		HIS
GLU	GLU	F280	S196	V98	MET
LEU	LEU	H281			GLU
ASP	ASP	Q282	E199	M104	GLU
VAL	VAL	D283		A105	LEU
ALA	ALA	A284		Y106	D5
SER	SER	R285	S207	Y107	R6
GLN	GLN	L286		E108	
GLU	GLU	TRP	H215	T109	F10
ALA	ALA	ALA		M110	A11
ALA	ALA	PRO	V218		R12
GLY	GLY	ILE	K219	L114	
LEU	LEU	THR	E220	Q120	T17
GLU	GLU	ASP	K221	L121	V18
GLU	GLU	SER	H222	L122	V18
SER	SER	ASN	Q223		K20
MET	MET	ALA	D224	D125	V21
VAL	VAL	ARG	E225		
ALA	ALA	ASP			K29
ARG	ARG	MET	F228	R129	
LEU	LEU	ALA	GLY	F133	R37
VAL	VAL	VAL	ASP	R134	L38
MET	MET	ALA	LYS	K135	
THR	THR	ALA	SER		L41
PRO	PRO	ARG	ARG	E139	Q42
GLY	GLY	GLU	LEU	T140	E43
LYS	LYS	SER	GLY	V141	Q44
ILE	ILE	SER	ARG	K142	L45
SER	SER	ARG	GLY	S143	A46
SER	SER	LYS			E47
LEU	LEU	LEU	G238		
ALA	ALA	GLN		D146	I56
ALA	ALA	ALA	K242	L147	L57
SER	SER	LEU	V243		V58
VAL	VAL	VAL	K244	F153	S59
ARG	ARG	SER			
LYS	LYS	GLU	V247	I159	R67
LEU	LEU	ASP		S160	Q68
ALA	ALA	ARG	Y251	T161	R69
ASP	ASP	LYS		R162	L70
MET	MET	LYS	I254	ARG	
GLU	GLU	ILE	P255	ALA	R73
ASP	ASP	LEU	V256	PRO	Q74
PRO	PRO	LEU		TYR	
ILE	ILE	ASP	S260	GLN	S78
GLY	GLY	ILE	G261	ASP	S79
ARG	ARG	ALA	Y262	S169	F80
VAL	VAL	ASP	S263		A81
LEU	LEU	LEU	A264	D175	D82
LEU	LEU	ALA	E265	N176	L83
LYS	LYS	LEU			
LYS	LYS	GLU	N266	D177	Q84



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	222855	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 ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.470	Depositor
Minimum map value	-1.623	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.097	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.87	0/126	1.10	0/169
1	B	0.43	0/2072	0.54	0/2794
1	C	0.87	0/126	1.09	0/169
1	D	0.87	0/126	1.09	0/169
1	E	0.88	0/126	1.10	0/169
1	F	0.43	0/2072	0.53	0/2794
1	G	0.44	0/2072	0.54	0/2794
1	H	0.44	0/2072	0.54	0/2794
All	All	0.47	0/8792	0.58	0/11852

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	124	0	122	20	0
1	B	2047	0	2084	147	0
1	C	124	0	122	23	0
1	D	124	0	122	22	0
1	E	124	0	122	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2047	0	2084	149	0
1	G	2047	0	2084	150	0
1	H	2047	0	2084	142	0
2	B	31	0	12	0	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
All	All	8808	0	8872	637	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 36.

All (637) 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:H:129:ARG:NH1	1:H:129:ARG:HA	1.58	1.18
1:F:129:ARG:HA	1:F:129:ARG:NH1	1.58	1.18
1:B:129:ARG:NH1	1:B:129:ARG:HA	1.58	1.18
1:G:129:ARG:HA	1:G:129:ARG:NH1	1.58	1.17
1:B:17:ILE:HD11	1:B:271:LEU:HD21	1.19	1.13
1:B:124:ASN:ND2	1:B:126:SER:H	1.50	1.08
1:F:124:ASN:ND2	1:F:126:SER:H	1.50	1.08
1:G:124:ASN:ND2	1:G:126:SER:H	1.50	1.08
1:B:29:LYS:HA	1:B:29:LYS:CE	1.81	1.06
1:G:29:LYS:HA	1:G:29:LYS:CE	1.81	1.06
1:H:29:LYS:CE	1:H:29:LYS:HA	1.81	1.05
1:F:29:LYS:HA	1:F:29:LYS:CE	1.81	1.04
1:B:279:LEU:HD23	1:B:280:PHE:N	1.74	1.03
1:G:29:LYS:HE3	1:G:29:LYS:CA	1.86	1.03
1:G:279:LEU:HD23	1:G:280:PHE:N	1.74	1.03
1:H:29:LYS:HA	1:H:29:LYS:HE3	1.04	1.03
1:B:29:LYS:HA	1:B:29:LYS:HE3	1.04	1.02
1:B:29:LYS:HE3	1:B:29:LYS:CA	1.86	1.02
1:F:29:LYS:HA	1:F:29:LYS:HE3	1.04	1.02
1:G:29:LYS:HA	1:G:29:LYS:HE3	1.04	1.02
1:F:279:LEU:HD23	1:F:280:PHE:N	1.74	1.02
1:H:279:LEU:HD23	1:H:280:PHE:N	1.74	1.01
1:H:29:LYS:HE3	1:H:29:LYS:CA	1.86	1.00
1:G:129:ARG:HA	1:G:129:ARG:HH11	1.22	1.00
1:G:131:LYS:HZ2	1:G:134:ARG:HD2	1.27	1.00
1:F:29:LYS:HE3	1:F:29:LYS:CA	1.86	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HA	1:B:129:ARG:HH11	1.22	0.99
1:F:129:ARG:HA	1:F:129:ARG:HH11	1.22	0.99
1:H:129:ARG:HA	1:H:129:ARG:HH11	1.22	0.98
1:F:265:GLU:OE1	1:F:265:GLU:N	1.98	0.97
1:H:265:GLU:N	1:H:265:GLU:OE1	1.98	0.97
1:B:6:ARG:HD2	1:B:6:ARG:O	1.66	0.95
1:B:265:GLU:N	1:B:265:GLU:OE1	1.98	0.95
1:G:6:ARG:HD2	1:G:6:ARG:O	1.66	0.95
1:G:265:GLU:N	1:G:265:GLU:OE1	1.98	0.95
1:F:215:HIS:HB3	1:F:275:ARG:NH2	1.83	0.94
1:H:215:HIS:HB3	1:H:275:ARG:NH2	1.83	0.94
1:H:279:LEU:HD21	1:H:281:HIS:HB2	1.48	0.94
1:F:6:ARG:HD2	1:F:6:ARG:O	1.66	0.94
1:B:215:HIS:HB3	1:B:275:ARG:NH2	1.83	0.93
1:F:279:LEU:HD21	1:F:281:HIS:HB2	1.48	0.93
1:G:215:HIS:HB3	1:G:275:ARG:NH2	1.83	0.93
1:H:6:ARG:HD2	1:H:6:ARG:O	1.66	0.93
1:G:279:LEU:HD21	1:G:281:HIS:HB2	1.48	0.93
1:B:279:LEU:HD21	1:B:281:HIS:HB2	1.48	0.92
1:G:89:GLU:N	1:G:89:GLU:OE2	2.02	0.92
1:B:89:GLU:N	1:B:89:GLU:OE2	2.02	0.92
1:B:17:ILE:HD11	1:B:271:LEU:CD2	2.00	0.91
1:H:89:GLU:OE2	1:H:89:GLU:N	2.02	0.91
1:E:77:ASN:OD1	1:E:77:ASN:O	1.89	0.91
1:B:47:GLU:C	1:B:47:GLU:OE2	2.13	0.91
1:B:106:TYR:CE1	1:B:110:MET:SD	2.65	0.89
1:B:47:GLU:OE2	1:B:48:LEU:N	2.05	0.89
1:G:106:TYR:CE1	1:G:110:MET:SD	2.65	0.89
1:F:106:TYR:CE1	1:F:110:MET:SD	2.65	0.89
1:F:124:ASN:HD21	1:F:126:SER:H	1.19	0.89
1:G:67:ARG:HA	1:G:95:CYS:SG	2.13	0.89
1:B:67:ARG:HA	1:B:95:CYS:SG	2.13	0.89
1:D:77:ASN:OD1	1:D:77:ASN:O	1.90	0.89
1:C:77:ASN:OD1	1:C:77:ASN:O	1.91	0.89
1:A:77:ASN:OD1	1:A:77:ASN:O	1.90	0.89
1:H:106:TYR:CE1	1:H:110:MET:SD	2.65	0.89
1:F:67:ARG:HA	1:F:95:CYS:SG	2.13	0.88
1:H:67:ARG:HA	1:H:95:CYS:SG	2.13	0.88
1:B:17:ILE:CD1	1:B:271:LEU:HD21	2.04	0.87
1:H:106:TYR:CZ	1:H:110:MET:SD	2.69	0.85
1:G:124:ASN:HD21	1:G:126:SER:H	1.19	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:HD21	1:B:126:SER:H	1.19	0.85
1:F:17:ILE:HD11	1:F:271:LEU:HD21	1.57	0.85
1:H:17:ILE:HD11	1:H:271:LEU:HD21	1.57	0.85
1:F:37:ARG:HD2	1:F:262:TYR:HD1	1.42	0.85
1:H:37:ARG:HD2	1:H:262:TYR:HD1	1.42	0.85
1:G:131:LYS:NZ	1:G:134:ARG:HD2	1.91	0.84
1:G:17:ILE:HD11	1:G:271:LEU:HD21	1.57	0.83
1:D:73:ARG:HH11	1:D:76:VAL:HG11	1.42	0.83
1:H:223:GLN:OE1	1:H:224:ASP:N	2.10	0.83
1:F:106:TYR:CZ	1:F:110:MET:SD	2.72	0.83
1:A:73:ARG:HH11	1:A:76:VAL:HG11	1.42	0.83
1:F:124:ASN:ND2	1:F:126:SER:N	2.26	0.83
1:G:106:TYR:CZ	1:G:110:MET:SD	2.72	0.83
1:B:106:TYR:CZ	1:B:110:MET:SD	2.72	0.82
1:G:37:ARG:HD2	1:G:262:TYR:HD1	1.42	0.82
1:B:37:ARG:HD2	1:B:262:TYR:HD1	1.42	0.82
1:B:124:ASN:ND2	1:B:126:SER:N	2.26	0.82
1:G:124:ASN:ND2	1:G:126:SER:N	2.26	0.82
1:C:73:ARG:HH11	1:C:76:VAL:HG11	1.42	0.82
1:E:73:ARG:HH11	1:E:76:VAL:HG11	1.42	0.82
1:F:47:GLU:OE2	1:F:47:GLU:C	2.25	0.80
1:H:47:GLU:OE2	1:H:47:GLU:C	2.25	0.80
1:G:47:GLU:C	1:G:47:GLU:OE2	2.25	0.80
1:B:41:LEU:HD23	1:B:41:LEU:O	1.82	0.79
1:G:41:LEU:HD23	1:G:41:LEU:O	1.82	0.79
1:H:108:GLU:OE2	1:H:108:GLU:HA	1.81	0.79
1:F:108:GLU:OE2	1:F:108:GLU:HA	1.81	0.79
1:B:279:LEU:HD23	1:B:279:LEU:C	2.08	0.79
1:G:214:ILE:HD12	1:G:222:HIS:CD2	2.17	0.79
1:G:279:LEU:HD23	1:G:279:LEU:C	2.08	0.79
1:H:41:LEU:O	1:H:41:LEU:HD23	1.82	0.78
1:F:41:LEU:O	1:F:41:LEU:HD23	1.82	0.78
1:G:108:GLU:OE2	1:G:108:GLU:HA	1.81	0.78
1:B:108:GLU:HA	1:B:108:GLU:OE2	1.81	0.78
1:F:279:LEU:HD23	1:F:279:LEU:C	2.08	0.78
1:H:279:LEU:HD23	1:H:279:LEU:C	2.08	0.78
1:H:106:TYR:OH	1:H:110:MET:SD	2.42	0.76
1:G:87:GLN:CD	1:G:87:GLN:H	1.94	0.75
1:B:87:GLN:CD	1:B:87:GLN:H	1.94	0.75
1:H:87:GLN:H	1:H:87:GLN:CD	1.94	0.74
1:F:87:GLN:H	1:F:87:GLN:CD	1.94	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:TYR:OH	1:B:110:MET:SD	2.46	0.73
1:G:106:TYR:OH	1:G:110:MET:SD	2.46	0.73
1:G:199:GLU:OE2	1:G:199:GLU:HA	1.89	0.73
1:H:215:HIS:HA	1:H:275:ARG:NH1	2.04	0.73
1:F:215:HIS:HA	1:F:275:ARG:NH1	2.04	0.73
1:B:215:HIS:HA	1:B:275:ARG:NH1	2.04	0.72
1:F:41:LEU:HD23	1:F:41:LEU:C	2.14	0.72
1:G:215:HIS:HA	1:G:275:ARG:NH1	2.04	0.72
1:H:41:LEU:HD23	1:H:41:LEU:C	2.14	0.72
1:F:106:TYR:OH	1:F:110:MET:SD	2.46	0.72
1:B:41:LEU:HD23	1:B:41:LEU:C	2.14	0.72
1:G:41:LEU:HD23	1:G:41:LEU:C	2.14	0.71
1:H:223:GLN:CD	1:H:224:ASP:H	1.99	0.70
1:B:47:GLU:OE2	1:B:48:LEU:HD12	1.91	0.70
1:F:67:ARG:CA	1:F:95:CYS:SG	2.80	0.69
1:H:67:ARG:CA	1:H:95:CYS:SG	2.80	0.69
1:B:67:ARG:CA	1:B:95:CYS:SG	2.80	0.69
1:G:67:ARG:CA	1:G:95:CYS:SG	2.80	0.69
1:F:37:ARG:HD2	1:F:262:TYR:CD1	2.26	0.68
1:H:37:ARG:HD2	1:H:262:TYR:CD1	2.26	0.68
1:B:37:ARG:HD2	1:B:262:TYR:CD1	2.26	0.68
1:G:37:ARG:HD2	1:G:262:TYR:CD1	2.26	0.68
1:G:17:ILE:HD11	1:G:271:LEU:CD2	2.24	0.68
1:F:214:ILE:HD12	1:F:222:HIS:CD2	2.28	0.68
1:F:143:SER:O	1:F:147:LEU:HD13	1.94	0.68
1:H:143:SER:O	1:H:147:LEU:HD13	1.94	0.68
1:B:142:LYS:O	1:B:142:LYS:HD3	1.95	0.67
1:H:17:ILE:HD11	1:H:271:LEU:CD2	2.24	0.67
1:F:17:ILE:HD11	1:F:271:LEU:CD2	2.24	0.67
1:F:186:GLU:C	1:F:186:GLU:OE1	2.38	0.67
1:H:186:GLU:OE1	1:H:186:GLU:C	2.38	0.67
1:G:143:SER:O	1:G:147:LEU:HD13	1.94	0.66
1:B:143:SER:O	1:B:147:LEU:HD13	1.94	0.66
1:B:186:GLU:C	1:B:186:GLU:OE1	2.38	0.66
1:G:186:GLU:C	1:G:186:GLU:OE1	2.38	0.66
1:B:6:ARG:HD2	1:B:6:ARG:C	2.21	0.66
1:C:74:GLN:O	1:C:78:SER:HB2	1.96	0.66
1:G:6:ARG:HD2	1:G:6:ARG:C	2.21	0.66
1:E:74:GLN:O	1:E:78:SER:HB2	1.96	0.66
1:A:74:GLN:O	1:A:78:SER:HB2	1.96	0.66
1:D:74:GLN:O	1:D:78:SER:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HD12	1:H:122:LEU:HD12	1.77	0.66
1:F:122:LEU:HD12	1:G:122:LEU:HD12	1.77	0.66
1:F:131:LYS:HE3	1:F:131:LYS:HA	1.77	0.65
1:F:6:ARG:HD2	1:F:6:ARG:C	2.21	0.65
1:G:282:GLN:C	1:G:282:GLN:OE1	2.40	0.65
1:H:6:ARG:HD2	1:H:6:ARG:C	2.21	0.65
1:B:282:GLN:C	1:B:282:GLN:OE1	2.40	0.65
1:B:125:ASP:C	1:B:125:ASP:OD1	2.39	0.65
1:G:125:ASP:OD1	1:G:125:ASP:C	2.39	0.65
1:C:77:ASN:OD1	1:C:77:ASN:C	2.40	0.64
1:H:125:ASP:OD1	1:H:125:ASP:C	2.39	0.64
1:B:215:HIS:HA	1:B:275:ARG:CZ	2.28	0.64
1:A:77:ASN:OD1	1:A:77:ASN:C	2.40	0.64
1:G:215:HIS:HA	1:G:275:ARG:CZ	2.28	0.64
1:D:77:ASN:OD1	1:D:77:ASN:C	2.40	0.64
1:F:125:ASP:C	1:F:125:ASP:OD1	2.39	0.64
1:E:73:ARG:HD3	1:E:76:VAL:CG1	2.27	0.64
1:B:147:LEU:HD12	1:B:147:LEU:N	2.13	0.64
1:A:73:ARG:HD3	1:A:76:VAL:CG1	2.27	0.64
1:F:129:ARG:HA	1:F:129:ARG:CZ	2.28	0.64
1:C:73:ARG:HD3	1:C:76:VAL:CG1	2.27	0.64
1:G:147:LEU:HD12	1:G:147:LEU:N	2.13	0.64
1:G:199:GLU:OE2	1:G:260:SER:HB3	1.98	0.64
1:D:73:ARG:HD3	1:D:76:VAL:CG1	2.27	0.64
1:H:129:ARG:HA	1:H:129:ARG:CZ	2.28	0.64
1:H:215:HIS:HA	1:H:275:ARG:CZ	2.28	0.63
1:B:47:GLU:C	1:B:47:GLU:CD	2.66	0.63
1:F:215:HIS:HA	1:F:275:ARG:CZ	2.28	0.63
1:E:77:ASN:OD1	1:E:77:ASN:C	2.41	0.63
1:F:131:LYS:NZ	1:F:134:ARG:HD2	2.13	0.63
1:F:147:LEU:N	1:F:147:LEU:HD12	2.13	0.63
1:F:279:LEU:C	1:F:279:LEU:CD2	2.72	0.63
1:H:147:LEU:N	1:H:147:LEU:HD12	2.13	0.62
1:H:279:LEU:C	1:H:279:LEU:CD2	2.72	0.62
1:A:83:LEU:HD23	1:F:83:LEU:HD13	1.81	0.62
1:G:17:ILE:CD1	1:G:271:LEU:HD21	2.29	0.62
1:B:279:LEU:C	1:B:279:LEU:CD2	2.72	0.62
1:G:279:LEU:C	1:G:279:LEU:CD2	2.72	0.62
1:D:83:LEU:HD23	1:H:83:LEU:HD13	1.81	0.62
1:G:17:ILE:HG22	1:G:19:VAL:HG23	1.81	0.62
1:B:83:LEU:HD13	1:C:83:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:LEU:HD13	1:E:83:LEU:HD23	1.81	0.62
1:B:87:GLN:CD	1:B:87:GLN:N	2.57	0.62
1:G:87:GLN:CD	1:G:87:GLN:N	2.57	0.62
1:G:129:ARG:HA	1:G:129:ARG:CZ	2.28	0.62
1:B:129:ARG:HA	1:B:129:ARG:CZ	2.28	0.62
1:B:17:ILE:HG22	1:B:19:VAL:HG23	1.81	0.61
1:F:17:ILE:HG22	1:F:19:VAL:HG23	1.81	0.61
1:F:146:ASP:C	1:F:147:LEU:HD12	2.25	0.61
1:G:146:ASP:C	1:G:147:LEU:HD12	2.25	0.61
1:B:146:ASP:C	1:B:147:LEU:HD12	2.25	0.61
1:H:17:ILE:HG22	1:H:19:VAL:HG23	1.81	0.61
1:H:146:ASP:C	1:H:147:LEU:HD12	2.25	0.61
1:F:87:GLN:CD	1:F:87:GLN:N	2.57	0.61
1:H:87:GLN:CD	1:H:87:GLN:N	2.57	0.61
1:B:268:ASP:OD1	1:B:268:ASP:C	2.44	0.60
1:H:221:LYS:O	1:H:223:GLN:NE2	2.34	0.60
1:H:268:ASP:C	1:H:268:ASP:OD1	2.44	0.60
1:F:268:ASP:C	1:F:268:ASP:OD1	2.44	0.60
1:G:124:ASN:CG	1:G:125:ASP:N	2.60	0.60
1:B:124:ASN:CG	1:B:125:ASP:N	2.60	0.60
1:F:124:ASN:CG	1:F:125:ASP:N	2.60	0.60
1:F:17:ILE:CD1	1:F:271:LEU:HD21	2.29	0.59
1:F:215:HIS:CB	1:F:275:ARG:NH2	2.63	0.59
1:B:215:HIS:CB	1:B:275:ARG:NH2	2.63	0.59
1:G:199:GLU:OE2	1:G:260:SER:CB	2.50	0.59
1:G:215:HIS:CB	1:G:275:ARG:NH2	2.63	0.59
1:H:215:HIS:CB	1:H:275:ARG:NH2	2.63	0.59
1:H:17:ILE:CD1	1:H:271:LEU:HD21	2.29	0.59
1:F:12:ARG:NH1	1:F:272:ARG:O	2.36	0.59
1:H:12:ARG:NH1	1:H:272:ARG:O	2.36	0.59
1:B:12:ARG:NH1	1:B:272:ARG:O	2.36	0.58
1:G:12:ARG:NH1	1:G:272:ARG:O	2.36	0.58
1:F:186:GLU:C	1:F:186:GLU:CD	2.72	0.58
1:H:186:GLU:C	1:H:186:GLU:CD	2.72	0.58
1:B:186:GLU:C	1:B:186:GLU:CD	2.72	0.58
1:B:215:HIS:HB3	1:B:275:ARG:CZ	2.34	0.58
1:G:186:GLU:C	1:G:186:GLU:CD	2.72	0.58
1:B:214:ILE:HD12	1:B:222:HIS:CD2	2.38	0.58
1:G:215:HIS:HB3	1:G:275:ARG:CZ	2.34	0.58
1:G:268:ASP:OD1	1:G:268:ASP:C	2.44	0.58
1:G:131:LYS:HE3	1:G:131:LYS:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:GLU:HA	1:H:199:GLU:OE2	2.04	0.57
1:A:83:LEU:C	1:A:85:LYS:H	2.12	0.57
1:F:161:THR:O	1:F:162:ARG:C	2.48	0.57
1:D:83:LEU:C	1:D:85:LYS:H	2.12	0.57
1:B:182:LEU:O	1:B:182:LEU:HD12	2.05	0.57
1:G:182:LEU:O	1:G:182:LEU:HD12	2.05	0.57
1:H:223:GLN:OE1	1:H:224:ASP:HB2	2.05	0.57
1:H:251:TYR:O	1:H:251:TYR:CD1	2.58	0.57
1:F:251:TYR:CD1	1:F:251:TYR:O	2.58	0.57
1:B:243:VAL:O	1:B:247:VAL:HG12	2.05	0.57
1:G:108:GLU:OE2	1:G:108:GLU:CA	2.51	0.57
1:H:268:ASP:OD1	1:H:268:ASP:O	2.23	0.57
1:B:108:GLU:OE2	1:B:108:GLU:CA	2.51	0.56
1:F:268:ASP:OD1	1:F:268:ASP:O	2.23	0.56
1:G:243:VAL:O	1:G:247:VAL:HG12	2.05	0.56
1:H:6:ARG:C	1:H:6:ARG:CD	2.78	0.56
1:H:215:HIS:HB3	1:H:275:ARG:CZ	2.34	0.56
1:B:6:ARG:C	1:B:6:ARG:CD	2.78	0.56
1:F:215:HIS:HB3	1:F:275:ARG:CZ	2.34	0.56
1:G:6:ARG:C	1:G:6:ARG:CD	2.78	0.56
1:G:10:PHE:HE1	1:G:191:LEU:HD12	1.71	0.56
1:B:10:PHE:HE1	1:B:191:LEU:HD12	1.71	0.56
1:F:6:ARG:C	1:F:6:ARG:CD	2.78	0.56
1:F:124:ASN:ND2	1:F:125:ASP:N	2.54	0.56
1:F:196:SER:HB3	1:F:242:LYS:HE3	1.88	0.56
1:G:131:LYS:HE3	1:G:131:LYS:CA	2.35	0.56
1:H:196:SER:HB3	1:H:242:LYS:HE3	1.88	0.56
1:B:251:TYR:O	1:B:251:TYR:CD1	2.58	0.56
1:G:251:TYR:O	1:G:251:TYR:CD1	2.58	0.56
1:B:124:ASN:ND2	1:B:125:ASP:N	2.54	0.56
1:G:124:ASN:ND2	1:G:125:ASP:N	2.54	0.56
1:G:282:GLN:C	1:G:282:GLN:CD	2.74	0.56
1:H:223:GLN:OE1	1:H:224:ASP:CB	2.53	0.56
1:B:282:GLN:C	1:B:282:GLN:CD	2.74	0.56
1:F:41:LEU:C	1:F:41:LEU:CD2	2.79	0.56
1:F:182:LEU:HD12	1:F:182:LEU:O	2.05	0.56
1:H:41:LEU:C	1:H:41:LEU:CD2	2.79	0.56
1:H:182:LEU:HD12	1:H:182:LEU:O	2.05	0.56
1:B:196:SER:HB3	1:B:242:LYS:HE3	1.88	0.56
1:G:196:SER:HB3	1:G:242:LYS:HE3	1.88	0.56
1:C:83:LEU:C	1:C:85:LYS:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265:GLU:N	1:H:265:GLU:CD	2.64	0.56
1:F:265:GLU:N	1:F:265:GLU:CD	2.64	0.56
1:H:10:PHE:HE1	1:H:191:LEU:HD12	1.71	0.55
1:F:10:PHE:HE1	1:F:191:LEU:HD12	1.71	0.55
1:F:29:LYS:CE	1:F:29:LYS:CA	2.62	0.55
1:H:89:GLU:O	1:H:89:GLU:CD	2.50	0.55
1:H:223:GLN:CD	1:H:224:ASP:N	2.61	0.55
1:G:265:GLU:N	1:G:265:GLU:CD	2.64	0.55
1:G:268:ASP:OD1	1:G:268:ASP:O	2.23	0.55
1:H:29:LYS:CE	1:H:29:LYS:CA	2.62	0.55
1:B:265:GLU:N	1:B:265:GLU:CD	2.64	0.55
1:B:268:ASP:OD1	1:B:268:ASP:O	2.23	0.55
1:F:124:ASN:HD22	1:F:126:SER:N	2.04	0.55
1:H:243:VAL:O	1:H:247:VAL:HG12	2.05	0.55
1:B:265:GLU:CD	1:B:265:GLU:H	2.14	0.55
1:F:125:ASP:OD1	1:F:125:ASP:O	2.25	0.55
1:F:243:VAL:O	1:F:247:VAL:HG12	2.05	0.55
1:G:265:GLU:CD	1:G:265:GLU:H	2.14	0.55
1:B:257:ILE:HD13	1:B:279:LEU:HA	1.89	0.55
1:F:85:LYS:HB3	1:F:86:PRO:HD2	1.88	0.55
1:F:135:LYS:HB3	1:F:135:LYS:HZ1	1.70	0.55
1:F:265:GLU:CD	1:F:265:GLU:H	2.14	0.55
1:G:85:LYS:HB3	1:G:86:PRO:HD2	1.88	0.55
1:G:257:ILE:HD13	1:G:279:LEU:HA	1.89	0.55
1:H:85:LYS:HB3	1:H:86:PRO:HD2	1.88	0.55
1:H:125:ASP:OD1	1:H:125:ASP:O	2.25	0.55
1:H:265:GLU:CD	1:H:265:GLU:H	2.14	0.55
1:B:85:LYS:HB3	1:B:86:PRO:HD2	1.88	0.55
1:B:125:ASP:OD1	1:B:125:ASP:O	2.25	0.55
1:G:125:ASP:OD1	1:G:125:ASP:O	2.25	0.55
1:H:135:LYS:HB3	1:H:135:LYS:HZ1	1.70	0.55
1:B:89:GLU:CD	1:B:89:GLU:O	2.50	0.54
1:B:124:ASN:HD22	1:B:126:SER:N	2.04	0.54
1:F:147:LEU:N	1:F:147:LEU:CD1	2.70	0.54
1:G:89:GLU:CD	1:G:89:GLU:O	2.50	0.54
1:G:124:ASN:HD22	1:G:126:SER:N	2.04	0.54
1:H:147:LEU:N	1:H:147:LEU:CD1	2.70	0.54
1:E:73:ARG:NH1	1:E:76:VAL:HG11	2.20	0.54
1:H:161:THR:O	1:H:162:ARG:C	2.51	0.54
1:B:41:LEU:C	1:B:41:LEU:CD2	2.79	0.54
1:B:147:LEU:N	1:B:147:LEU:CD1	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:LYS:C	1:F:223:GLN:H	2.14	0.54
1:C:73:ARG:NH1	1:C:76:VAL:HG11	2.20	0.54
1:G:147:LEU:N	1:G:147:LEU:CD1	2.70	0.54
1:F:279:LEU:HD21	1:F:281:HIS:CB	2.30	0.54
1:G:41:LEU:C	1:G:41:LEU:CD2	2.79	0.54
1:H:279:LEU:HD21	1:H:281:HIS:CB	2.30	0.54
1:F:257:ILE:HD13	1:F:279:LEU:HA	1.89	0.53
1:G:135:LYS:HB3	1:G:135:LYS:HZ1	1.72	0.53
1:G:279:LEU:HD21	1:G:281:HIS:CB	2.30	0.53
1:B:199:GLU:OE2	1:B:199:GLU:HA	2.07	0.53
1:B:279:LEU:HD21	1:B:281:HIS:CB	2.30	0.53
1:E:82:ASP:C	1:E:82:ASP:OD1	2.51	0.53
1:A:73:ARG:HD3	1:A:76:VAL:HG11	1.91	0.53
1:D:73:ARG:HD3	1:D:76:VAL:HG11	1.91	0.53
1:H:108:GLU:OE2	1:H:108:GLU:CA	2.51	0.53
1:F:108:GLU:OE2	1:F:108:GLU:CA	2.51	0.52
1:C:73:ARG:HD3	1:C:76:VAL:HG11	1.91	0.52
1:E:73:ARG:HD3	1:E:76:VAL:HG11	1.91	0.52
1:E:83:LEU:C	1:E:85:LYS:H	2.17	0.52
1:B:269:LYS:HG2	1:B:274:LEU:HD12	1.92	0.52
1:F:266:ASN:O	1:F:270:VAL:HG12	2.10	0.52
1:G:269:LYS:HG2	1:G:274:LEU:HD12	1.92	0.52
1:H:266:ASN:O	1:H:270:VAL:HG12	2.10	0.52
1:B:192:LEU:HD23	1:B:256:VAL:HG22	1.92	0.52
1:G:192:LEU:HD23	1:G:256:VAL:HG22	1.92	0.52
1:B:244:LYS:O	1:B:247:VAL:CG1	2.58	0.51
1:F:269:LYS:HG2	1:F:274:LEU:HD12	1.92	0.51
1:G:73:ARG:HE	1:G:73:ARG:HA	1.75	0.51
1:G:244:LYS:O	1:G:247:VAL:CG1	2.58	0.51
1:H:192:LEU:HD23	1:H:256:VAL:HG22	1.92	0.51
1:H:269:LYS:HG2	1:H:274:LEU:HD12	1.92	0.51
1:B:266:ASN:O	1:B:270:VAL:HG12	2.10	0.51
1:F:192:LEU:HD23	1:F:256:VAL:HG22	1.92	0.51
1:F:244:LYS:O	1:F:247:VAL:CG1	2.58	0.51
1:H:244:LYS:O	1:H:247:VAL:CG1	2.58	0.51
1:G:266:ASN:O	1:G:270:VAL:HG12	2.10	0.51
1:G:218:VAL:HG12	1:G:220:GLU:H	1.75	0.51
1:B:42:CYS:SG	1:B:110:MET:HE2	2.51	0.51
1:B:218:VAL:HG12	1:B:220:GLU:H	1.75	0.51
1:B:282:GLN:OE1	1:B:282:GLN:O	2.29	0.51
1:F:133:PHE:CE2	1:G:159:ILE:HG13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:CYS:SG	1:G:110:MET:HE2	2.51	0.51
1:G:282:GLN:OE1	1:G:282:GLN:O	2.29	0.51
1:B:159:ILE:HG13	1:H:133:PHE:CE2	2.46	0.51
1:F:159:ILE:HG13	1:G:133:PHE:CE2	2.46	0.51
1:D:82:ASP:OD1	1:D:82:ASP:C	2.53	0.51
1:B:161:THR:O	1:B:162:ARG:C	2.53	0.51
1:F:131:LYS:HZ1	1:F:134:ARG:HD2	1.76	0.50
1:B:47:GLU:OE2	1:B:48:LEU:CA	2.59	0.50
1:F:218:VAL:HG12	1:F:220:GLU:H	1.77	0.50
1:H:42:CYS:SG	1:H:110:MET:HE2	2.51	0.50
1:E:83:LEU:C	1:E:85:LYS:N	2.68	0.50
1:F:42:CYS:SG	1:F:110:MET:HE2	2.51	0.50
1:C:83:LEU:C	1:C:85:LYS:N	2.68	0.50
1:D:73:ARG:NH1	1:D:76:VAL:HG11	2.20	0.50
1:A:73:ARG:NH1	1:A:76:VAL:HG11	2.20	0.50
1:E:73:ARG:HD3	1:E:76:VAL:HG12	1.92	0.50
1:C:73:ARG:HD3	1:C:76:VAL:HG12	1.92	0.50
1:G:56:ILE:HD13	1:G:187:LEU:HD13	1.94	0.50
1:B:56:ILE:HD13	1:B:187:LEU:HD13	1.94	0.50
1:F:41:LEU:HD23	1:F:45:LEU:HG	1.94	0.50
1:G:135:LYS:HB3	1:G:135:LYS:NZ	2.26	0.50
1:B:44:GLN:HE22	1:B:268:ASP:HB2	1.77	0.49
1:B:133:PHE:CE2	1:H:159:ILE:HG13	2.47	0.49
1:B:135:LYS:NZ	1:B:135:LYS:HB3	2.26	0.49
1:B:135:LYS:O	1:B:139:GLU:OE2	2.30	0.49
1:F:44:GLN:HE22	1:F:268:ASP:HB2	1.77	0.49
1:G:44:GLN:HE22	1:G:268:ASP:HB2	1.77	0.49
1:G:135:LYS:O	1:G:139:GLU:OE2	2.30	0.49
1:H:44:GLN:HE22	1:H:268:ASP:HB2	1.77	0.49
1:B:124:ASN:CG	1:B:125:ASP:H	2.20	0.49
1:G:124:ASN:CG	1:G:125:ASP:H	2.20	0.49
1:H:41:LEU:HD23	1:H:45:LEU:HG	1.94	0.49
1:H:135:LYS:O	1:H:139:GLU:OE2	2.30	0.49
1:F:124:ASN:CG	1:F:125:ASP:H	2.20	0.49
1:H:218:VAL:HG12	1:H:220:GLU:H	1.77	0.49
1:C:82:ASP:C	1:C:82:ASP:OD1	2.55	0.49
1:D:83:LEU:C	1:D:85:LYS:N	2.68	0.49
1:B:80:PHE:O	1:B:81:ALA:C	2.55	0.49
1:B:244:LYS:O	1:B:247:VAL:HG13	2.13	0.49
1:F:263:SER:OG	1:F:265:GLU:OE2	2.31	0.49
1:G:221:LYS:HE2	1:G:222:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ARG:HD3	1:D:76:VAL:HG12	1.92	0.49
1:H:80:PHE:O	1:H:81:ALA:C	2.55	0.49
1:H:263:SER:OG	1:H:265:GLU:OE2	2.31	0.49
1:A:82:ASP:OD1	1:A:82:ASP:C	2.56	0.49
1:A:83:LEU:C	1:A:85:LYS:N	2.68	0.49
1:F:80:PHE:O	1:F:81:ALA:C	2.55	0.49
1:G:80:PHE:O	1:G:81:ALA:C	2.55	0.49
1:G:244:LYS:O	1:G:247:VAL:HG13	2.13	0.49
1:A:73:ARG:HD3	1:A:76:VAL:HG12	1.92	0.49
1:F:135:LYS:HB3	1:F:135:LYS:NZ	2.26	0.49
1:H:135:LYS:HB3	1:H:135:LYS:NZ	2.26	0.49
1:H:47:GLU:OE2	1:H:47:GLU:O	2.30	0.48
1:H:56:ILE:HD13	1:H:187:LEU:HD13	1.94	0.48
1:B:263:SER:OG	1:B:265:GLU:OE2	2.31	0.48
1:F:47:GLU:OE2	1:F:47:GLU:O	2.30	0.48
1:F:56:ILE:HD13	1:F:187:LEU:HD13	1.94	0.48
1:F:215:HIS:CB	1:F:275:ARG:CZ	2.92	0.48
1:G:263:SER:OG	1:G:265:GLU:OE2	2.31	0.48
1:H:215:HIS:CB	1:H:275:ARG:CZ	2.92	0.48
1:B:41:LEU:HD23	1:B:45:LEU:HG	1.94	0.48
1:B:228:PHE:CZ	1:B:243:VAL:HG21	2.47	0.48
1:H:244:LYS:O	1:H:247:VAL:HG13	2.13	0.48
1:F:244:LYS:O	1:F:247:VAL:HG13	2.13	0.48
1:G:41:LEU:HD23	1:G:45:LEU:HG	1.94	0.48
1:H:228:PHE:CZ	1:H:243:VAL:HG21	2.49	0.48
1:B:142:LYS:HD3	1:B:142:LYS:C	2.38	0.48
1:F:175:ASP:N	1:F:175:ASP:OD1	2.45	0.48
1:C:76:VAL:CG1	1:C:77:ASN:N	2.76	0.48
1:D:76:VAL:CG1	1:D:77:ASN:N	2.76	0.48
1:A:76:VAL:CG1	1:A:77:ASN:N	2.76	0.48
1:B:80:PHE:CE1	1:C:75:LEU:HB3	2.49	0.48
1:G:47:GLU:OE2	1:G:47:GLU:O	2.30	0.48
1:H:175:ASP:OD1	1:H:175:ASP:N	2.45	0.48
1:E:76:VAL:CG1	1:E:77:ASN:N	2.76	0.48
1:B:83:LEU:HD13	1:C:83:LEU:CD2	2.44	0.48
1:G:83:LEU:HD13	1:E:83:LEU:CD2	2.44	0.47
1:B:215:HIS:CB	1:B:275:ARG:CZ	2.92	0.47
1:G:215:HIS:CB	1:G:275:ARG:CZ	2.92	0.47
1:B:21:VAL:HG22	1:B:59:SER:HA	1.97	0.47
1:G:21:VAL:HG22	1:G:59:SER:HA	1.97	0.47
1:G:42:CYS:SG	1:G:110:MET:CE	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:CYS:SG	1:B:110:MET:CE	3.02	0.47
1:F:21:VAL:HG22	1:F:59:SER:HA	1.97	0.47
1:F:282:GLN:OE1	1:F:282:GLN:C	2.58	0.47
1:H:21:VAL:HG22	1:H:59:SER:HA	1.97	0.47
1:B:72:TYR:HD1	1:C:84:GLN:HE21	1.63	0.47
1:B:186:GLU:OE1	1:B:187:LEU:N	2.47	0.47
1:B:199:GLU:HA	1:B:260:SER:HB3	1.96	0.47
1:F:186:GLU:OE1	1:F:187:LEU:N	2.47	0.47
1:G:199:GLU:HA	1:G:260:SER:HB3	1.96	0.47
1:D:75:LEU:HB3	1:H:80:PHE:CE1	2.50	0.47
1:H:73:ARG:HD2	1:H:73:ARG:HA	1.67	0.47
1:F:251:TYR:CD1	1:F:251:TYR:C	2.91	0.47
1:G:186:GLU:OE1	1:G:187:LEU:N	2.47	0.47
1:H:186:GLU:OE1	1:H:187:LEU:N	2.47	0.47
1:H:251:TYR:CD1	1:H:251:TYR:C	2.91	0.47
1:B:201:LEU:HG	1:B:226:ILE:HD13	1.96	0.47
1:F:42:CYS:SG	1:F:110:MET:CE	3.02	0.47
1:H:42:CYS:SG	1:H:110:MET:CE	3.02	0.47
1:F:199:GLU:HA	1:F:260:SER:HB3	1.96	0.47
1:H:80:PHE:HB3	1:E:76:VAL:O	2.15	0.47
1:B:85:LYS:HB3	1:B:85:LYS:NZ	2.31	0.46
1:G:85:LYS:HB3	1:G:85:LYS:NZ	2.31	0.46
1:H:199:GLU:HA	1:H:260:SER:HB3	1.96	0.46
1:F:80:PHE:HB3	1:C:76:VAL:O	2.15	0.46
1:G:251:TYR:CD1	1:G:251:TYR:C	2.91	0.46
1:H:46:ALA:CB	1:H:114:LEU:HD13	2.46	0.46
1:B:35:LEU:N	1:G:43:GLU:OE1	2.48	0.46
1:B:79:SER:HA	1:A:79:SER:HA	1.97	0.46
1:B:251:TYR:CD1	1:B:251:TYR:C	2.91	0.46
1:F:46:ALA:CB	1:F:114:LEU:HD13	2.46	0.46
1:G:79:SER:HA	1:D:79:SER:HA	1.97	0.46
1:B:38:LEU:HD13	1:B:106:TYR:HE2	1.81	0.46
1:G:46:ALA:CB	1:G:114:LEU:HD13	2.46	0.46
1:G:199:GLU:OE2	1:G:199:GLU:CA	2.60	0.46
1:H:279:LEU:HD23	1:H:280:PHE:C	2.41	0.46
1:B:46:ALA:CB	1:B:114:LEU:HD13	2.46	0.46
1:B:80:PHE:HB3	1:A:76:VAL:O	2.15	0.46
1:F:279:LEU:HD23	1:F:280:PHE:C	2.41	0.46
1:G:38:LEU:HD13	1:G:106:TYR:HE2	1.81	0.46
1:G:80:PHE:HB3	1:D:76:VAL:O	2.15	0.46
1:B:175:ASP:OD1	1:B:175:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LEU:HD13	1:F:106:TYR:HE2	1.81	0.46
1:F:228:PHE:CZ	1:F:243:VAL:HG21	2.51	0.46
1:G:175:ASP:OD1	1:G:175:ASP:N	2.45	0.46
1:G:74:GLN:O	1:G:78:SER:HB2	2.15	0.46
1:D:83:LEU:CD2	1:H:83:LEU:HD13	2.44	0.46
1:B:74:GLN:O	1:B:78:SER:HB2	2.15	0.46
1:A:83:LEU:CD2	1:F:83:LEU:HD13	2.44	0.46
1:F:35:LEU:N	1:H:43:GLU:OE1	2.48	0.46
1:F:79:SER:HA	1:C:79:SER:HA	1.97	0.46
1:H:79:SER:HA	1:E:79:SER:HA	1.97	0.46
1:H:282:GLN:HG3	1:H:283:ASP:N	2.29	0.46
1:B:264:ALA:C	1:B:265:GLU:OE1	2.58	0.46
1:H:74:GLN:O	1:H:78:SER:HB2	2.15	0.46
1:B:279:LEU:HD23	1:B:280:PHE:C	2.41	0.45
1:G:264:ALA:C	1:G:265:GLU:OE1	2.58	0.45
1:G:279:LEU:HD23	1:G:280:PHE:C	2.41	0.45
1:B:159:ILE:HG13	1:H:133:PHE:HE2	1.81	0.45
1:F:74:GLN:O	1:F:78:SER:HB2	2.15	0.45
1:B:17:ILE:CG2	1:B:19:VAL:HG23	2.45	0.45
1:F:121:LEU:HD12	1:F:153:PHE:CZ	2.52	0.45
1:G:223:GLN:HG3	1:G:224:ASP:H	1.81	0.45
1:H:121:LEU:HD12	1:H:153:PHE:CZ	2.52	0.45
1:A:75:LEU:HB3	1:F:80:PHE:CE1	2.52	0.45
1:F:133:PHE:HE2	1:G:159:ILE:HG13	1.82	0.45
1:G:47:GLU:C	1:G:47:GLU:CD	2.84	0.45
1:A:83:LEU:O	1:A:85:LYS:N	2.50	0.45
1:D:83:LEU:O	1:D:85:LYS:N	2.50	0.45
1:F:70:LEU:HD21	1:F:98:VAL:HG21	1.99	0.45
1:F:159:ILE:HD11	1:G:137:LEU:HD13	1.98	0.45
1:F:47:GLU:C	1:F:47:GLU:CD	2.84	0.45
1:F:257:ILE:HD13	1:F:257:ILE:HA	1.85	0.45
1:G:80:PHE:CE1	1:E:75:LEU:HB3	2.52	0.45
1:H:47:GLU:C	1:H:47:GLU:CD	2.84	0.45
1:H:70:LEU:HD21	1:H:98:VAL:HG21	1.99	0.45
1:F:106:TYR:HE1	1:F:110:MET:SD	2.34	0.45
1:B:281:HIS:HB3	1:B:284:ALA:HB3	1.99	0.44
1:C:77:ASN:O	1:C:77:ASN:CG	2.58	0.44
1:C:83:LEU:O	1:C:85:LYS:N	2.50	0.44
1:G:281:HIS:HB3	1:G:284:ALA:HB3	1.99	0.44
1:H:85:LYS:HB3	1:H:85:LYS:NZ	2.31	0.44
1:F:281:HIS:HB3	1:F:284:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD23	1:B:70:LEU:HA	1.84	0.44
1:B:121:LEU:HD12	1:B:153:PHE:CZ	2.52	0.44
1:F:85:LYS:HB3	1:F:85:LYS:NZ	2.31	0.44
1:F:264:ALA:C	1:F:265:GLU:OE1	2.58	0.44
1:F:268:ASP:CG	1:F:272:ARG:HH21	2.26	0.44
1:H:268:ASP:CG	1:H:272:ARG:HH21	2.26	0.44
1:H:281:HIS:HB3	1:H:284:ALA:HB3	1.99	0.44
1:E:83:LEU:O	1:E:85:LYS:N	2.50	0.44
1:G:121:LEU:HD12	1:G:153:PHE:CZ	2.52	0.44
1:H:264:ALA:C	1:H:265:GLU:OE1	2.58	0.44
1:F:282:GLN:C	1:F:282:GLN:CD	2.85	0.44
1:G:279:LEU:HD23	1:G:280:PHE:CA	2.46	0.44
1:G:268:ASP:CG	1:G:272:ARG:HH21	2.26	0.44
1:B:268:ASP:CG	1:B:272:ARG:HH21	2.26	0.44
1:B:279:LEU:HD23	1:B:280:PHE:CA	2.46	0.44
1:F:45:LEU:HD11	1:F:57:LEU:HD13	2.00	0.44
1:H:45:LEU:HD11	1:H:57:LEU:HD13	2.00	0.44
1:F:221:LYS:HE2	1:F:222:HIS:CE1	2.52	0.44
1:D:73:ARG:HA	1:D:76:VAL:HG12	2.00	0.44
1:A:73:ARG:HA	1:A:76:VAL:HG12	2.00	0.43
1:H:106:TYR:HE1	1:H:110:MET:SD	2.36	0.43
1:B:45:LEU:HD11	1:B:57:LEU:HD13	2.00	0.43
1:B:70:LEU:HD21	1:B:98:VAL:HG21	1.99	0.43
1:F:104:MET:SD	1:F:120:GLN:HG3	2.58	0.43
1:G:70:LEU:HD21	1:G:98:VAL:HG21	1.99	0.43
1:H:89:GLU:OE2	1:H:89:GLU:CA	2.66	0.43
1:G:45:LEU:HD11	1:G:57:LEU:HD13	2.00	0.43
1:G:199:GLU:OE2	1:G:260:SER:OG	2.32	0.43
1:H:104:MET:SD	1:H:120:GLN:HG3	2.58	0.43
1:B:89:GLU:OE2	1:B:89:GLU:CA	2.66	0.43
1:F:82:ASP:OD1	1:F:82:ASP:C	2.62	0.43
1:F:221:LYS:C	1:F:223:GLN:N	2.76	0.43
1:G:89:GLU:OE2	1:G:89:GLU:CA	2.66	0.43
1:F:199:GLU:HA	1:F:199:GLU:OE1	2.18	0.43
1:H:82:ASP:OD1	1:H:82:ASP:C	2.62	0.43
1:B:176:ASN:HA	1:B:179:LEU:HB3	2.01	0.43
1:G:176:ASN:HA	1:G:179:LEU:HB3	2.01	0.43
1:H:38:LEU:HD13	1:H:106:TYR:HE2	1.84	0.43
1:F:282:GLN:CD	1:F:283:ASP:N	2.77	0.42
1:F:38:LEU:HD23	1:F:38:LEU:HA	1.85	0.42
1:G:214:ILE:HD12	1:G:222:HIS:NE2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LYS:HA	1:F:131:LYS:CE	2.43	0.42
1:H:38:LEU:HD23	1:H:38:LEU:HA	1.85	0.42
1:E:73:ARG:HA	1:E:76:VAL:HG12	2.00	0.42
1:C:73:ARG:HA	1:C:76:VAL:HG12	2.00	0.42
1:B:43:GLU:HA	1:B:114:LEU:HD11	2.01	0.42
1:B:74:GLN:O	1:B:78:SER:N	2.53	0.42
1:F:74:GLN:O	1:F:78:SER:N	2.53	0.42
1:G:43:GLU:HA	1:G:114:LEU:HD11	2.01	0.42
1:G:74:GLN:O	1:G:78:SER:N	2.53	0.42
1:F:44:GLN:OE1	1:F:44:GLN:HA	2.19	0.42
1:G:44:GLN:HA	1:G:44:GLN:OE1	2.19	0.42
1:H:44:GLN:OE1	1:H:44:GLN:HA	2.19	0.42
1:H:74:GLN:O	1:H:78:SER:N	2.53	0.42
1:F:43:GLU:HA	1:F:114:LEU:HD11	2.01	0.42
1:F:244:LYS:HA	1:F:247:VAL:HG12	2.01	0.42
1:H:43:GLU:HA	1:H:114:LEU:HD11	2.01	0.42
1:H:244:LYS:HA	1:H:247:VAL:HG12	2.01	0.42
1:B:44:GLN:HA	1:B:44:GLN:OE1	2.19	0.42
1:G:257:ILE:HD13	1:G:257:ILE:HA	1.85	0.42
1:D:82:ASP:O	1:D:85:LYS:HG2	2.19	0.42
1:F:108:GLU:OE1	1:G:69:ARG:NH2	2.52	0.41
1:H:222:HIS:HA	1:H:225:GLU:HB2	2.01	0.41
1:H:176:ASN:HA	1:H:179:LEU:HB3	2.01	0.41
1:B:133:PHE:HE2	1:H:159:ILE:HG13	1.82	0.41
1:B:215:HIS:CA	1:B:275:ARG:NH2	2.83	0.41
1:G:215:HIS:CA	1:G:275:ARG:NH2	2.83	0.41
1:D:77:ASN:O	1:D:77:ASN:CG	2.58	0.41
1:H:70:LEU:HD23	1:H:70:LEU:HA	1.84	0.41
1:F:176:ASN:HA	1:F:179:LEU:HB3	2.01	0.41
1:B:219:LYS:HD2	1:B:219:LYS:HA	1.96	0.41
1:B:257:ILE:HD13	1:B:257:ILE:HA	1.85	0.41
1:F:215:HIS:HA	1:F:275:ARG:HH12	1.85	0.41
1:F:244:LYS:HA	1:F:247:VAL:CG1	2.51	0.41
1:H:215:HIS:HA	1:H:275:ARG:HH12	1.85	0.41
1:H:215:HIS:CA	1:H:275:ARG:NH2	2.83	0.41
1:H:244:LYS:HA	1:H:247:VAL:CG1	2.51	0.41
1:A:77:ASN:O	1:A:77:ASN:CG	2.58	0.41
1:F:159:ILE:HG13	1:G:133:PHE:HE2	1.84	0.41
1:F:215:HIS:CA	1:F:275:ARG:NH2	2.83	0.41
1:H:219:LYS:HD2	1:H:219:LYS:HA	1.86	0.41
1:B:80:PHE:O	1:B:83:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASP:C	1:G:82:ASP:OD1	2.62	0.41
1:B:41:LEU:CD2	1:B:45:LEU:HG	2.51	0.41
1:B:244:LYS:HA	1:B:247:VAL:CG1	2.51	0.41
1:F:141:VAL:HG11	1:F:187:LEU:HD22	2.03	0.41
1:G:41:LEU:CD2	1:G:45:LEU:HG	2.51	0.41
1:G:80:PHE:O	1:G:83:LEU:N	2.54	0.41
1:G:219:LYS:HD2	1:G:219:LYS:HA	1.96	0.41
1:G:244:LYS:HA	1:G:247:VAL:CG1	2.51	0.41
1:B:244:LYS:HA	1:B:247:VAL:HG12	2.01	0.41
1:F:70:LEU:HD23	1:F:70:LEU:HA	1.84	0.41
1:F:256:VAL:HB	1:F:280:PHE:HB2	2.03	0.41
1:G:221:LYS:HE2	1:G:222:HIS:HE1	1.86	0.41
1:H:141:VAL:HG11	1:H:187:LEU:HD22	2.03	0.41
1:H:256:VAL:HB	1:H:280:PHE:HB2	2.03	0.41
1:B:82:ASP:OD1	1:B:82:ASP:C	2.62	0.40
1:D:73:ARG:HD3	1:D:73:ARG:HA	1.82	0.40
1:B:121:LEU:HD11	1:B:144:MET:HE1	2.04	0.40
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.89	0.40
1:B:256:VAL:HB	1:B:280:PHE:HB2	2.03	0.40
1:F:41:LEU:CD2	1:F:45:LEU:HG	2.51	0.40
1:F:93:LYS:HB2	1:F:93:LYS:HE3	1.90	0.40
1:C:76:VAL:HG13	1:C:77:ASN:N	2.36	0.40
1:G:121:LEU:HD11	1:G:144:MET:HE1	2.04	0.40
1:G:244:LYS:HA	1:G:247:VAL:HG12	2.01	0.40
1:H:41:LEU:CD2	1:H:45:LEU:HG	2.51	0.40
1:B:108:GLU:OE1	1:H:69:ARG:NH2	2.52	0.40
1:F:80:PHE:O	1:F:83:LEU:N	2.54	0.40
1:G:256:VAL:HB	1:G:280:PHE:HB2	2.03	0.40
1:H:80:PHE:O	1:H:83:LEU:N	2.54	0.40
1:E:76:VAL:HG13	1:E:77:ASN:N	2.36	0.40
1:B:214:ILE:HD12	1:B:222:HIS:NE2	2.36	0.40
1:F:279:LEU:HD23	1:F:280:PHE:CA	2.46	0.40
1:H:279:LEU:HD23	1:H:280:PHE:CA	2.46	0.40
1:F:214:ILE:HD12	1:F:222:HIS:NE2	2.37	0.40
1:C:73:ARG:HD3	1:C:73:ARG:HA	1.82	0.40
1:H:93:LYS:HB2	1:H:93:LYS:HE3	1.90	0.40
1:H:254:ILE:HD13	1:H:254:ILE:HA	1.83	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	13/727 (2%)	11 (85%)	2 (15%)	0	100	100
1	B	261/727 (36%)	251 (96%)	10 (4%)	0	100	100
1	C	13/727 (2%)	11 (85%)	2 (15%)	0	100	100
1	D	13/727 (2%)	11 (85%)	2 (15%)	0	100	100
1	E	13/727 (2%)	11 (85%)	2 (15%)	0	100	100
1	F	261/727 (36%)	250 (96%)	11 (4%)	0	100	100
1	G	261/727 (36%)	250 (96%)	11 (4%)	0	100	100
1	H	261/727 (36%)	251 (96%)	10 (4%)	0	100	100
All	All	1096/5816 (19%)	1046 (95%)	50 (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	14/597 (2%)	14 (100%)	0	100	100
1	B	220/597 (37%)	219 (100%)	1 (0%)	81	83
1	C	14/597 (2%)	14 (100%)	0	100	100
1	D	14/597 (2%)	14 (100%)	0	100	100
1	E	14/597 (2%)	14 (100%)	0	100	100
1	F	220/597 (37%)	218 (99%)	2 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	220/597 (37%)	219 (100%)	1 (0%)	81	83
1	H	220/597 (37%)	220 (100%)	0	100	100
All	All	936/4776 (20%)	932 (100%)	4 (0%)	81	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	ARG
1	F	159	ILE
1	F	177	ASP
1	G	159	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	ASN
1	F	124	ASN
1	G	124	ASN
1	G	222	HIS
1	H	282	GLN
1	E	84	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	H	801	-	32,33,33	0.30	0	48,52,52	0.41	0
2	ATP	F	801	-	32,33,33	0.30	0	48,52,52	0.41	0
2	ATP	B	801	-	32,33,33	0.30	0	48,52,52	0.41	0
2	ATP	G	801	-	32,33,33	0.30	0	48,52,52	0.41	0

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
2	ATP	H	801	-	-	7/22/38/38	0/3/3/3
2	ATP	F	801	-	-	7/22/38/38	0/3/3/3
2	ATP	B	801	-	-	7/22/38/38	0/3/3/3
2	ATP	G	801	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ATP	C5'-O5'-PA-O1A
2	B	801	ATP	C5'-O5'-PA-O2A
2	B	801	ATP	C5'-O5'-PA-O3A
2	F	801	ATP	C5'-O5'-PA-O1A
2	F	801	ATP	C5'-O5'-PA-O2A
2	F	801	ATP	C5'-O5'-PA-O3A
2	G	801	ATP	C5'-O5'-PA-O1A
2	G	801	ATP	C5'-O5'-PA-O2A
2	G	801	ATP	C5'-O5'-PA-O3A
2	H	801	ATP	C5'-O5'-PA-O1A

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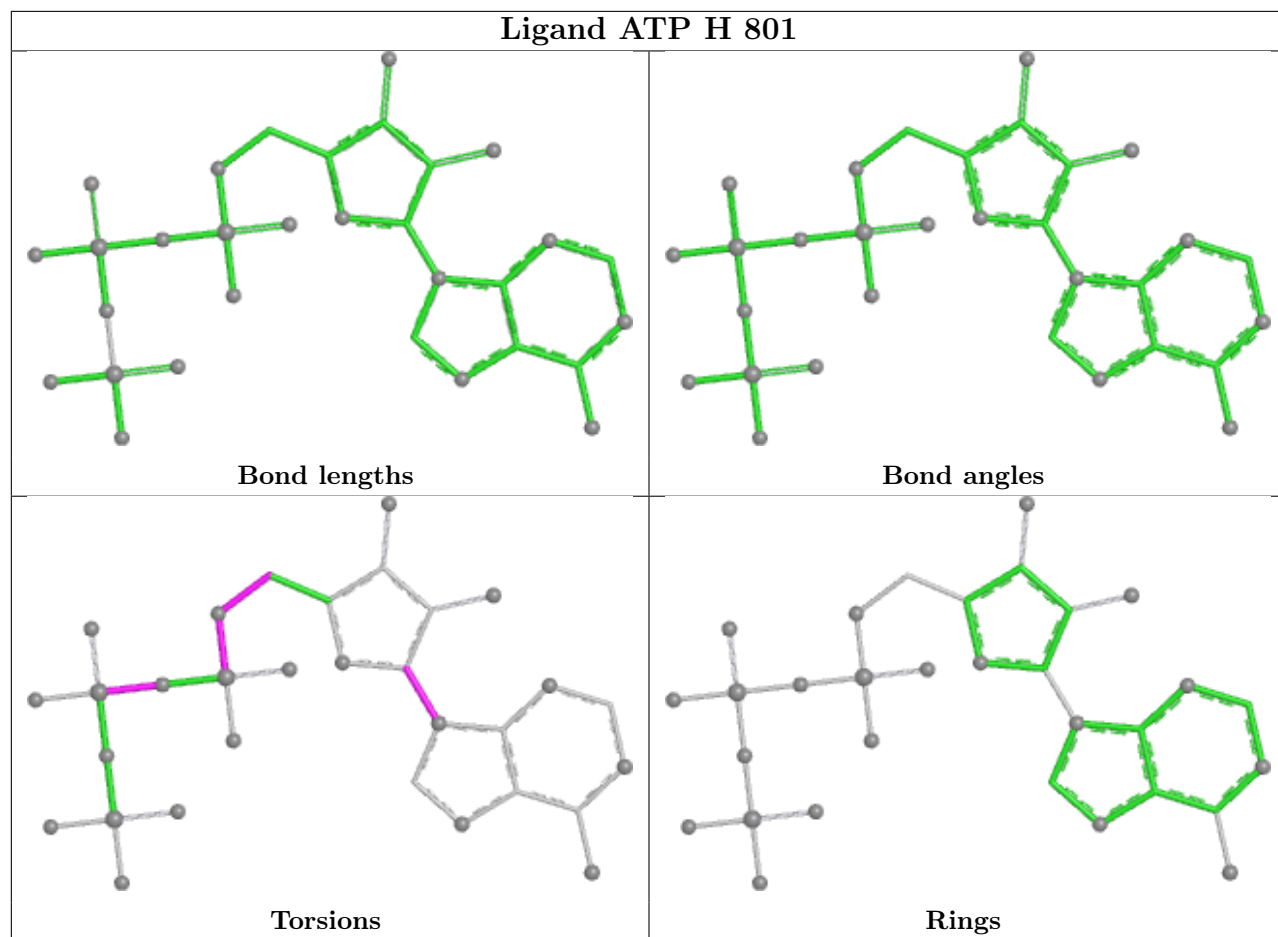
Continued from previous page...

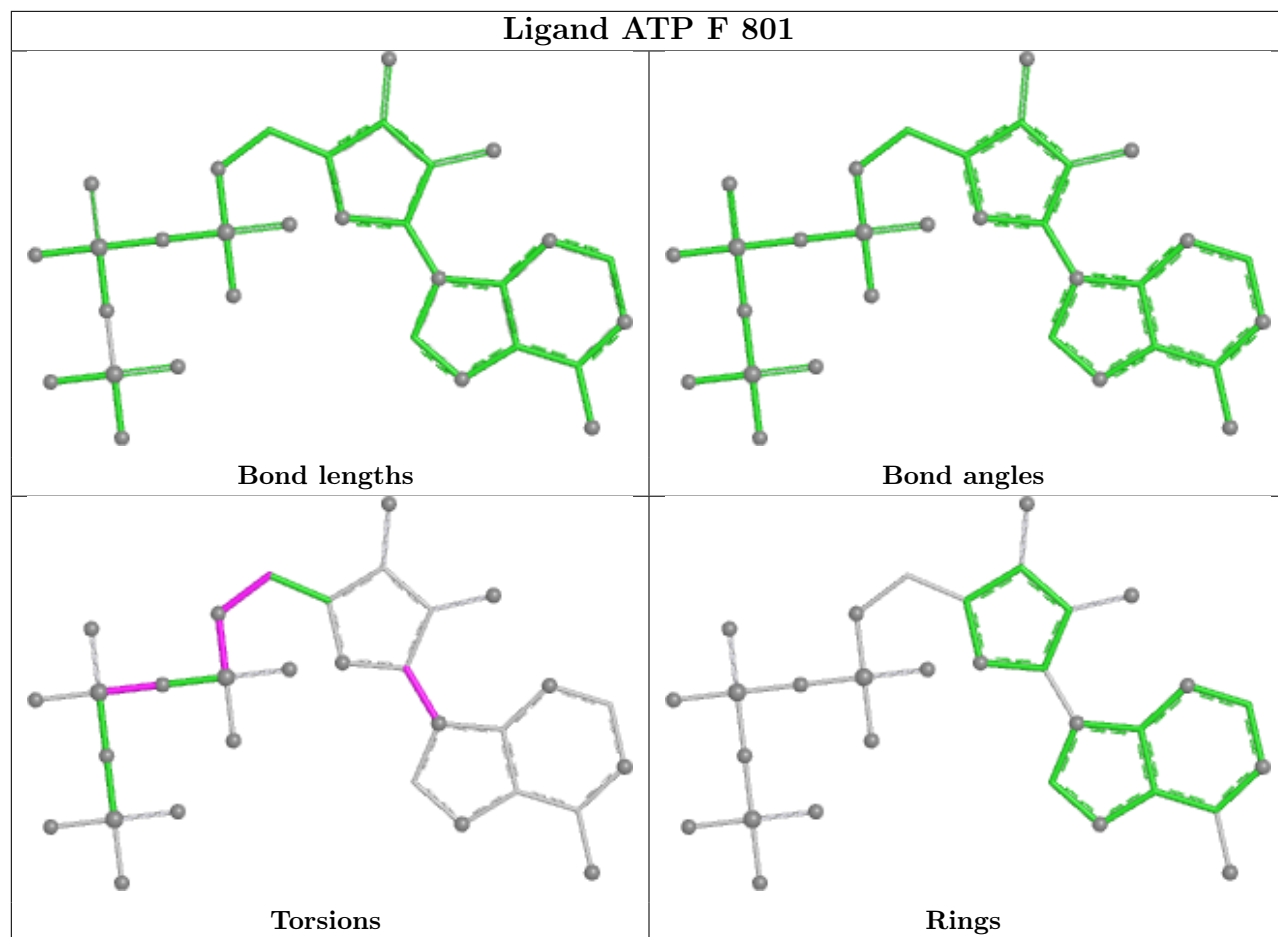
Mol	Chain	Res	Type	Atoms
2	H	801	ATP	C5'-O5'-PA-O2A
2	H	801	ATP	C5'-O5'-PA-O3A
2	B	801	ATP	C4'-C5'-O5'-PA
2	F	801	ATP	C4'-C5'-O5'-PA
2	G	801	ATP	C4'-C5'-O5'-PA
2	H	801	ATP	C4'-C5'-O5'-PA
2	B	801	ATP	PA-O3A-PB-O3B
2	F	801	ATP	PA-O3A-PB-O3B
2	G	801	ATP	PA-O3A-PB-O3B
2	H	801	ATP	PA-O3A-PB-O3B
2	B	801	ATP	O4'-C1'-N9-C8
2	F	801	ATP	O4'-C1'-N9-C8
2	G	801	ATP	O4'-C1'-N9-C8
2	H	801	ATP	O4'-C1'-N9-C8
2	B	801	ATP	PA-O3A-PB-O1B
2	F	801	ATP	PA-O3A-PB-O1B
2	G	801	ATP	PA-O3A-PB-O1B
2	H	801	ATP	PA-O3A-PB-O1B

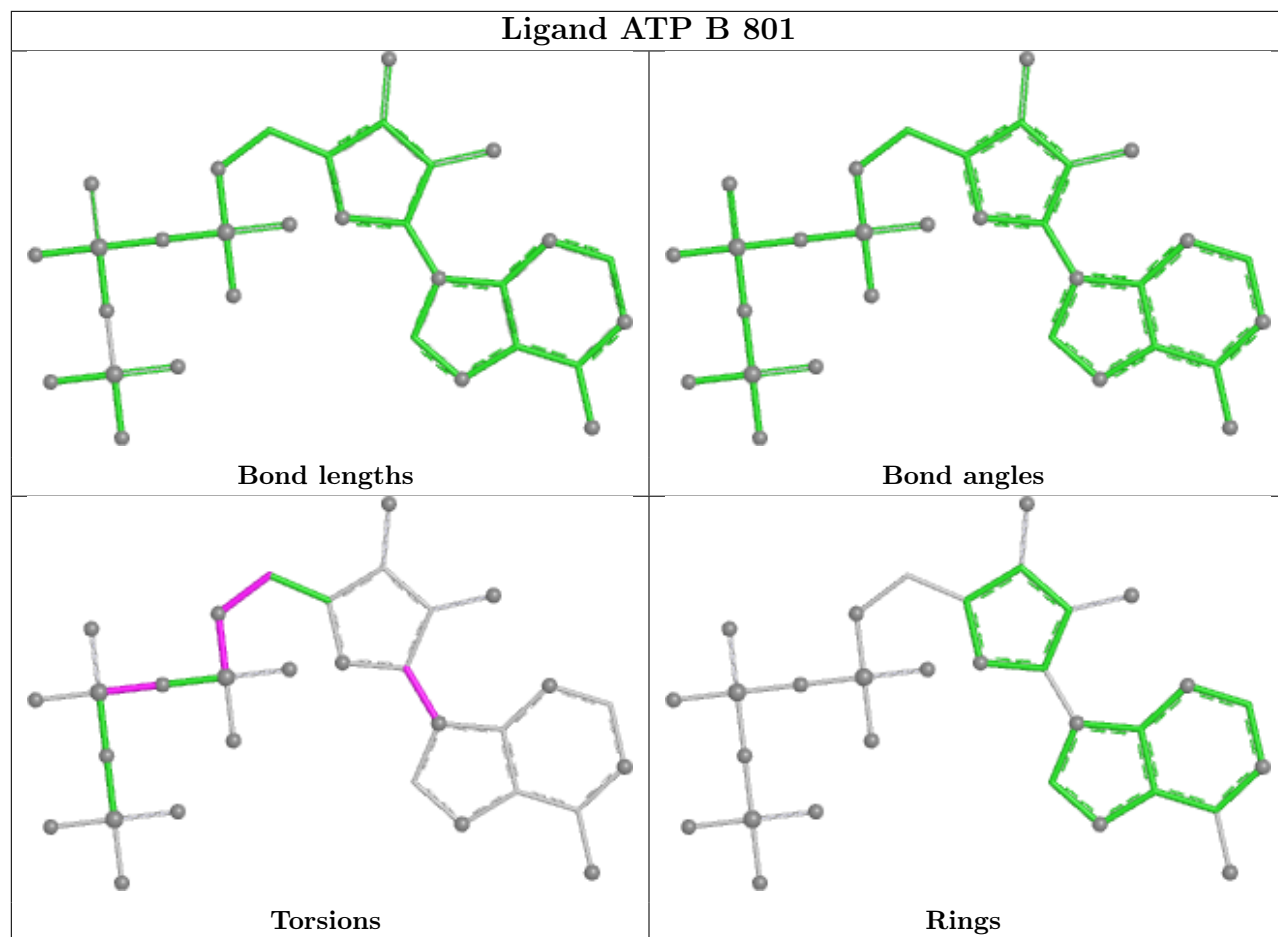
There are no ring outliers.

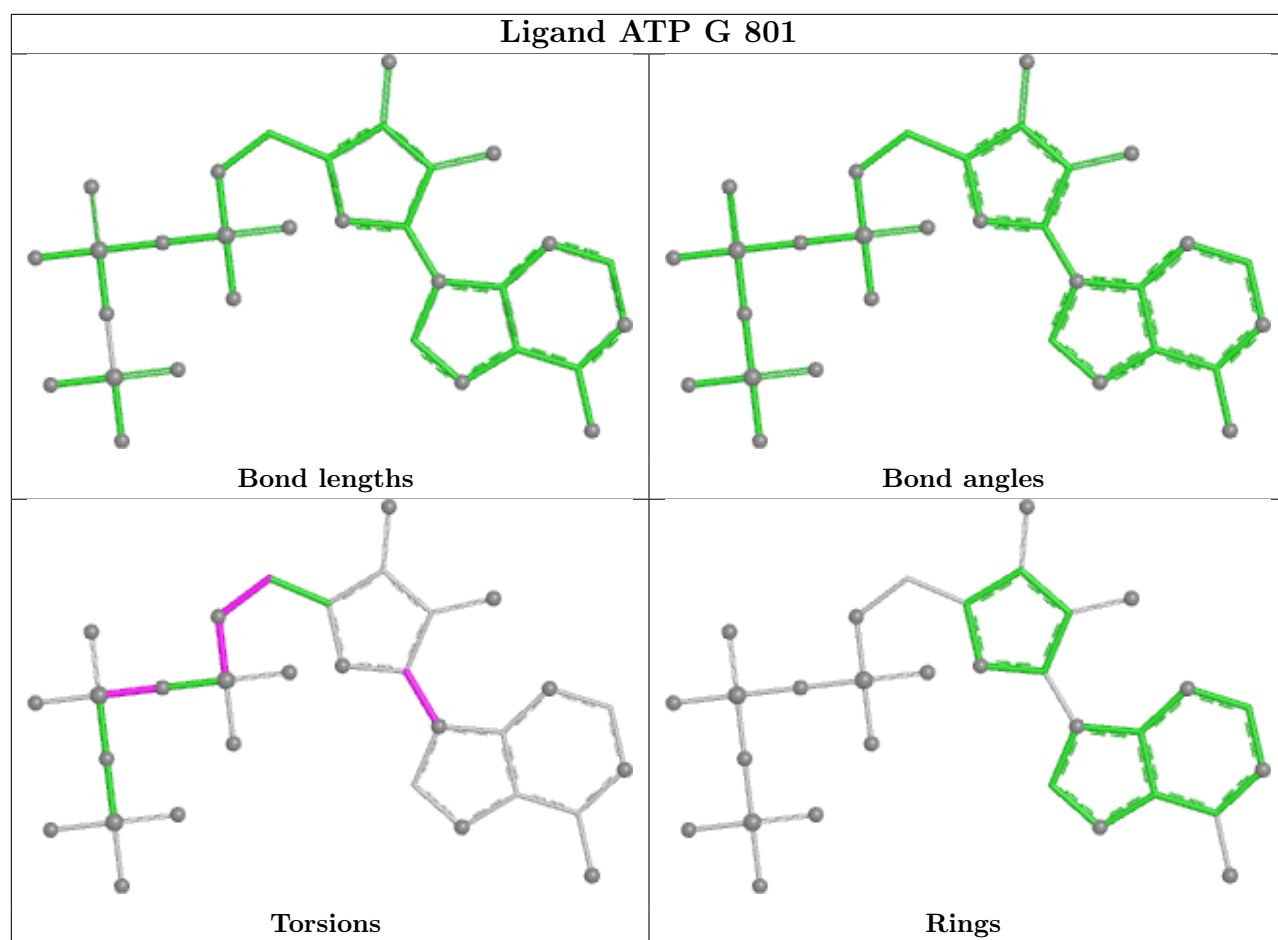
No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

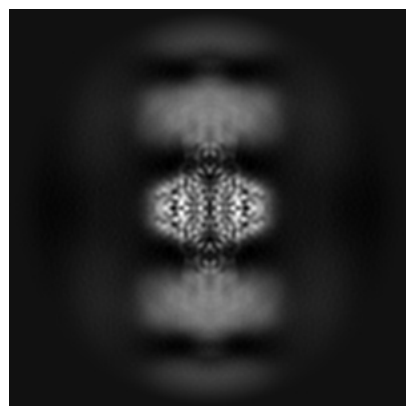
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38855. These allow visual inspection of the internal detail of the map and identification of artifacts.

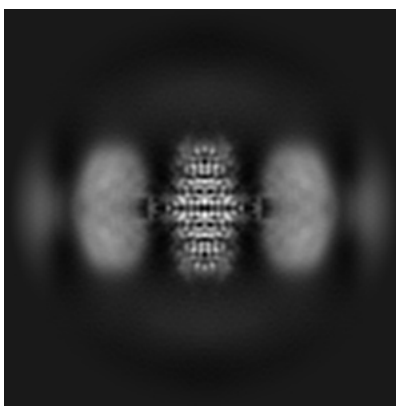
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

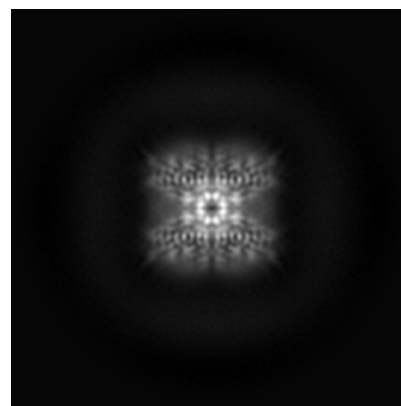
6.1.1 Primary map



X

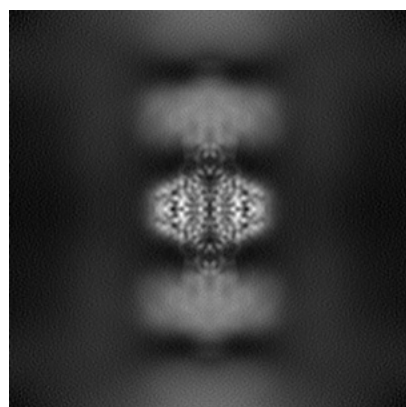


Y

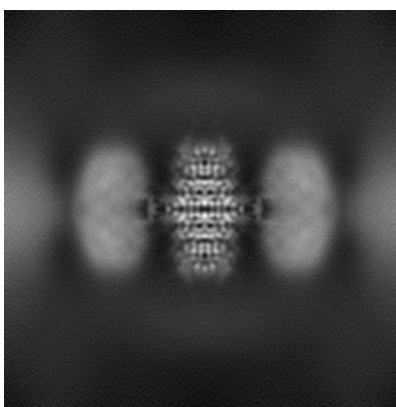


Z

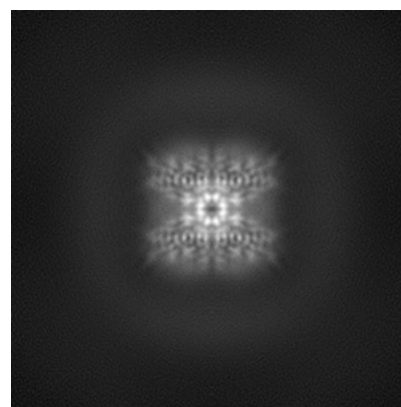
6.1.2 Raw map



X



Y

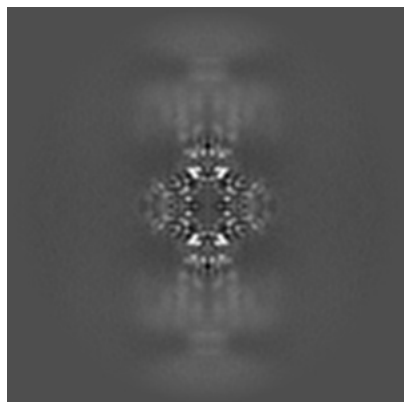


Z

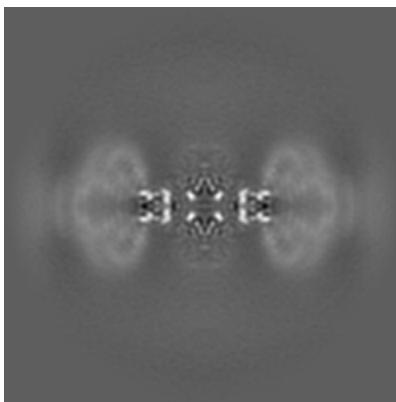
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

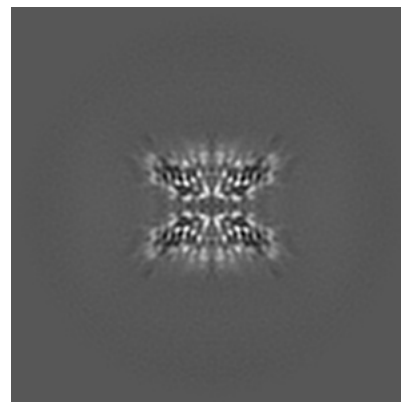
6.2.1 Primary map



X Index: 120

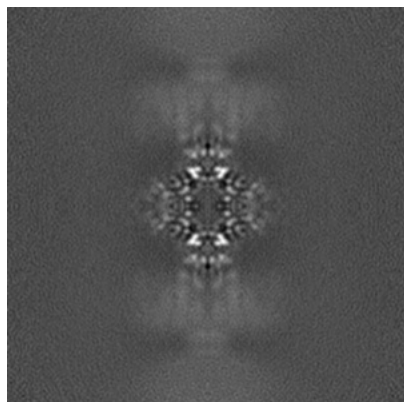


Y Index: 120

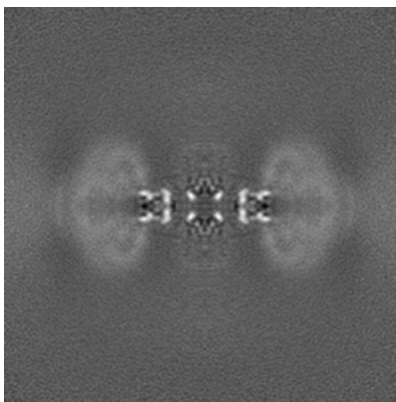


Z Index: 120

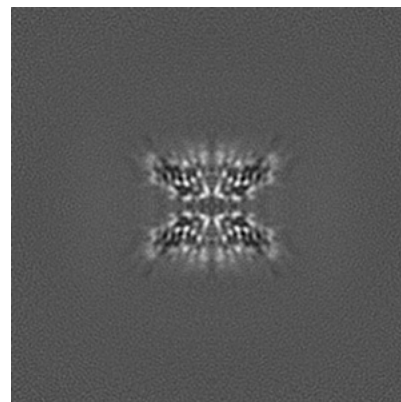
6.2.2 Raw map



X Index: 120



Y Index: 120

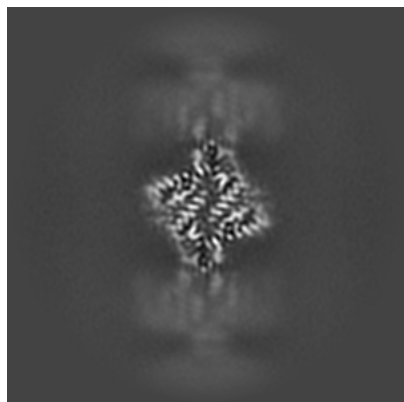


Z Index: 120

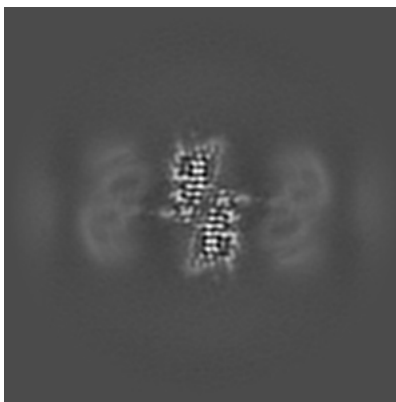
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

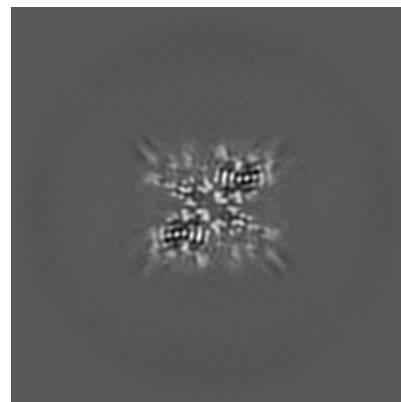
6.3.1 Primary map



X Index: 117

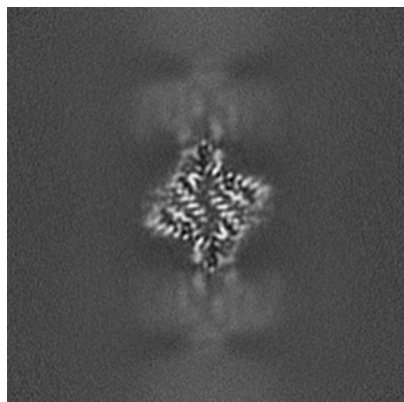


Y Index: 103

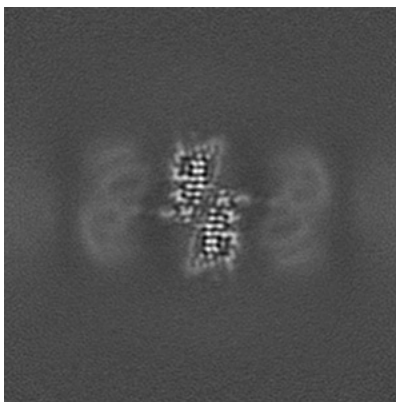


Z Index: 124

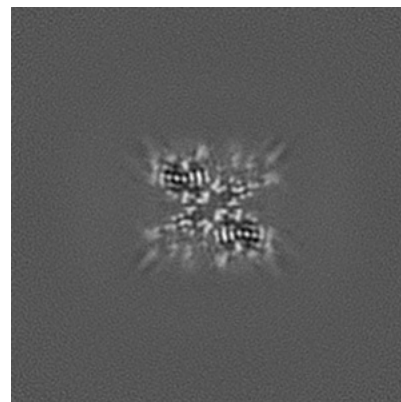
6.3.2 Raw map



X Index: 123



Y Index: 103

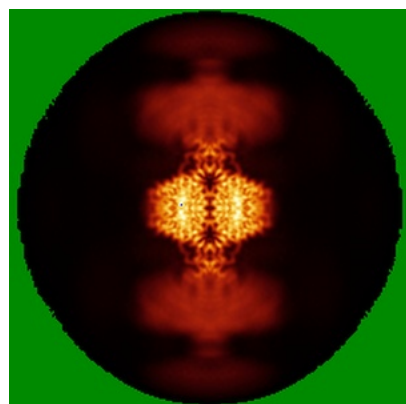


Z Index: 116

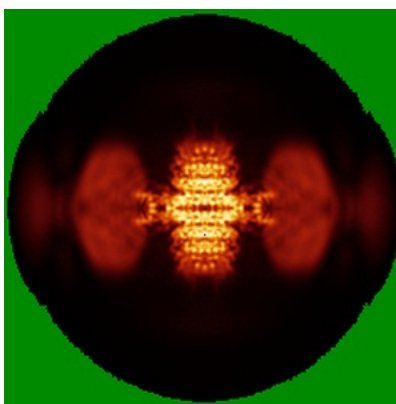
The images above show the largest variance slices of the map in three orthogonal directions.

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

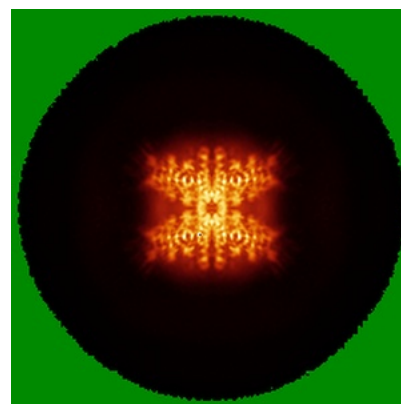
6.4.1 Primary map



X

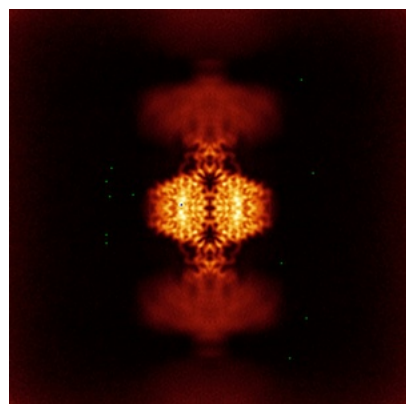


Y

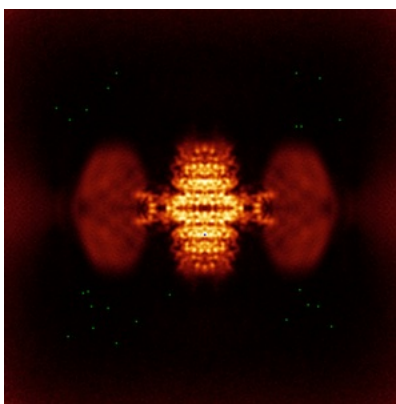


Z

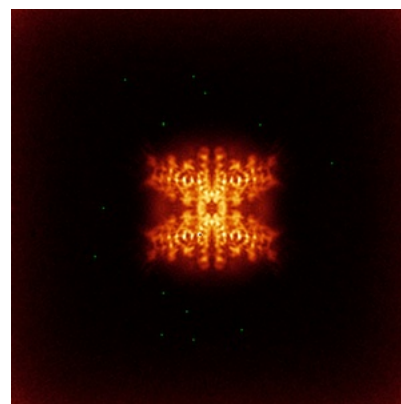
6.4.2 Raw map



X



Y



Z

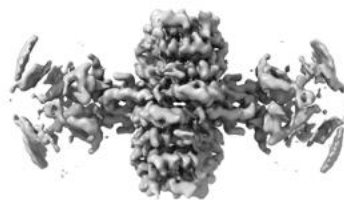
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

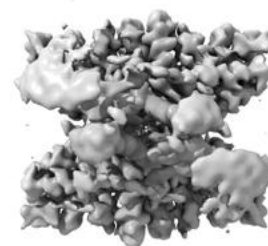
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

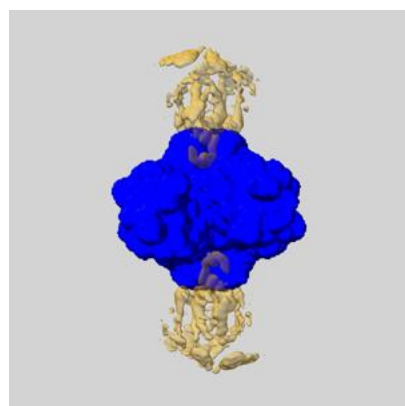
6.6 Mask visualisation [i](#)

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

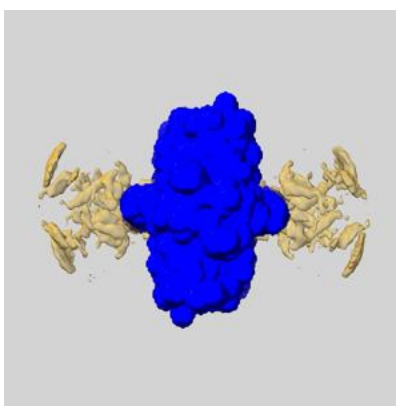
A mask typically either:

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

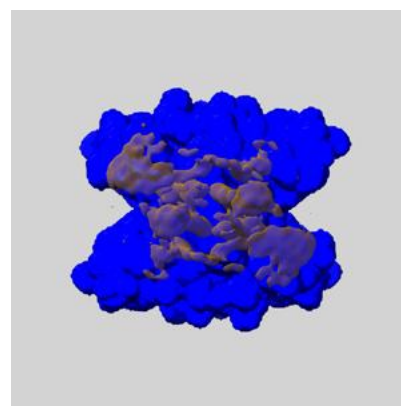
6.6.1 emd_38855_msk_1.map [i](#)



X



Y

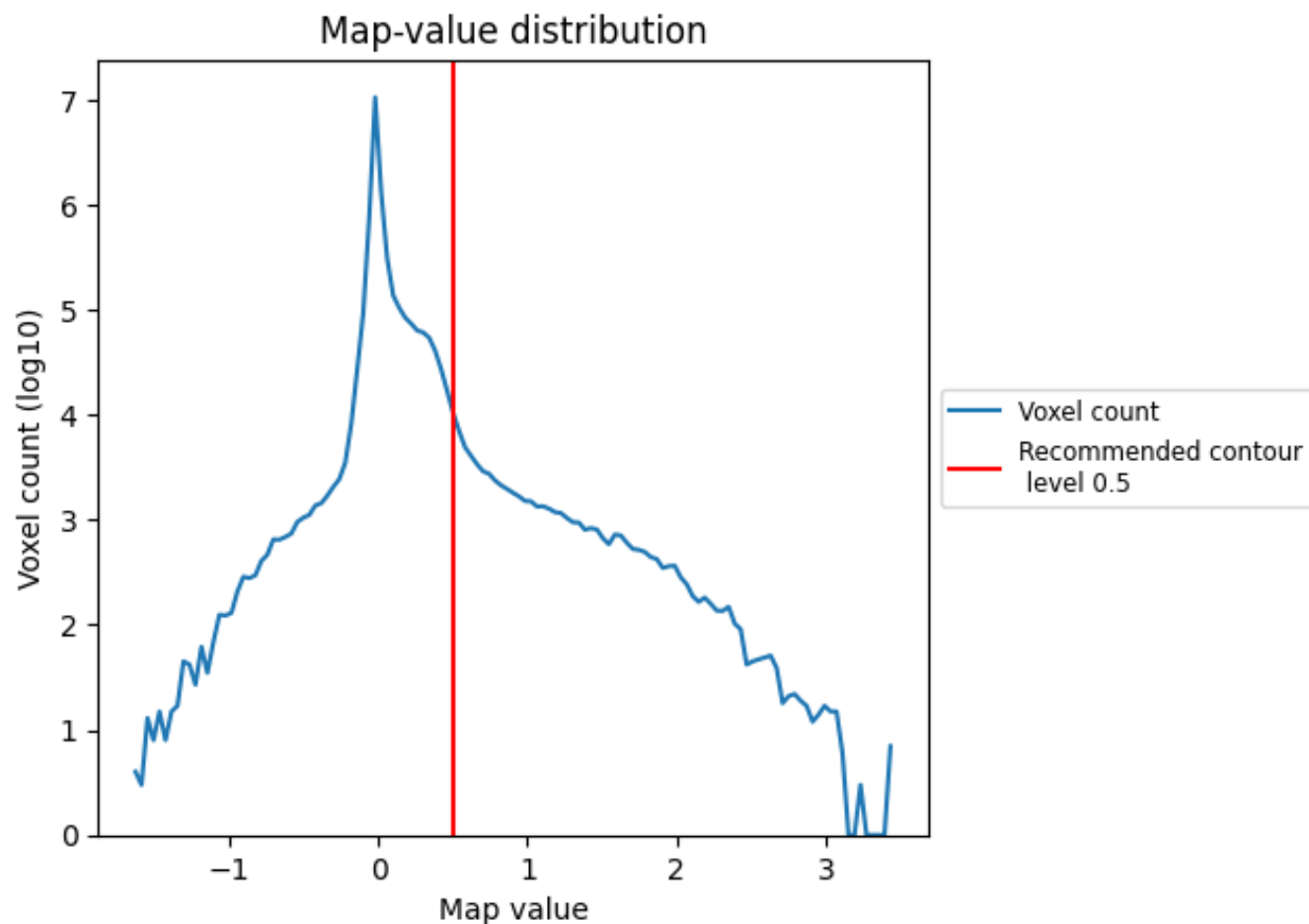


Z

7 Map analysis [i](#)

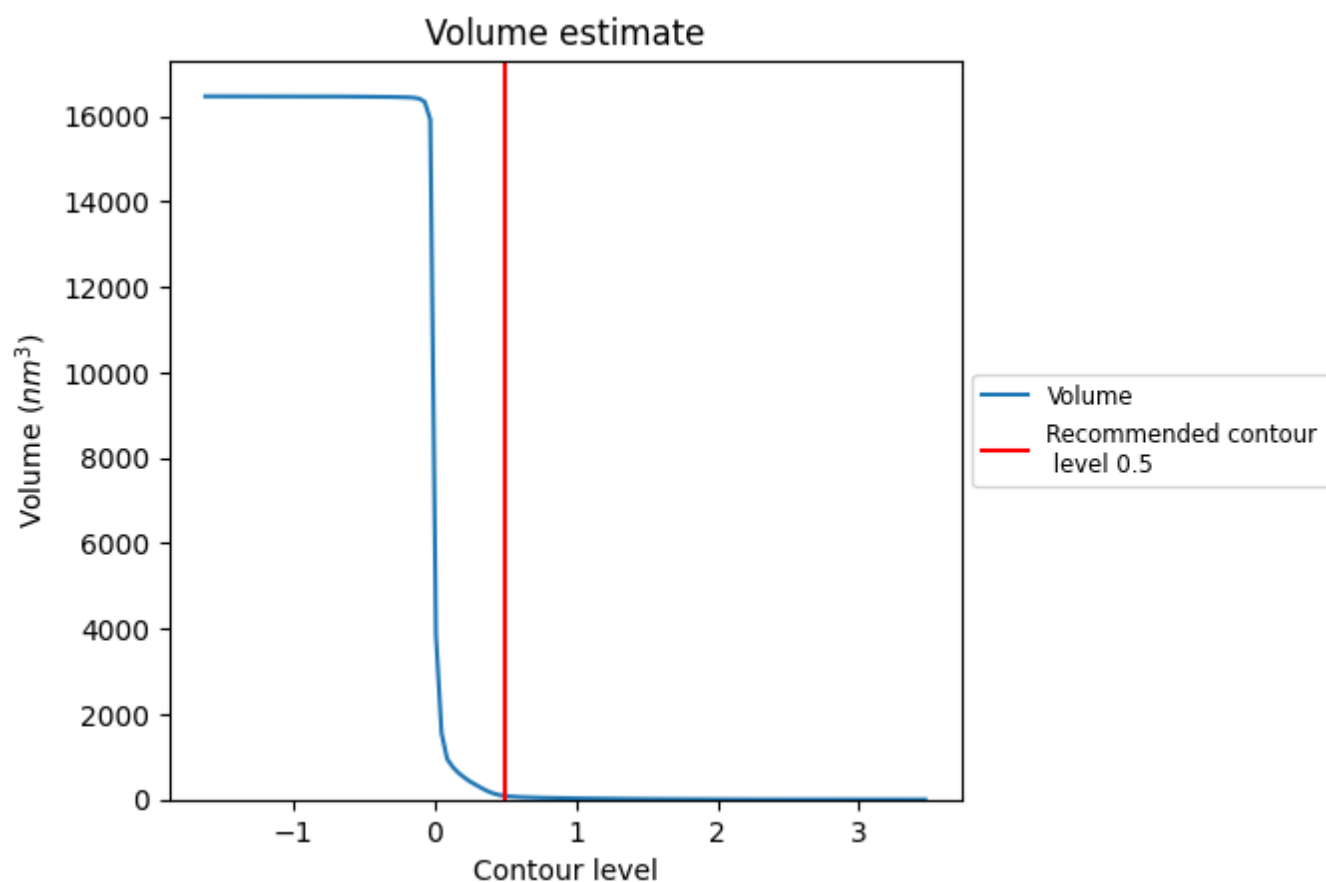
This section contains the results of statistical analysis of the map.

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.

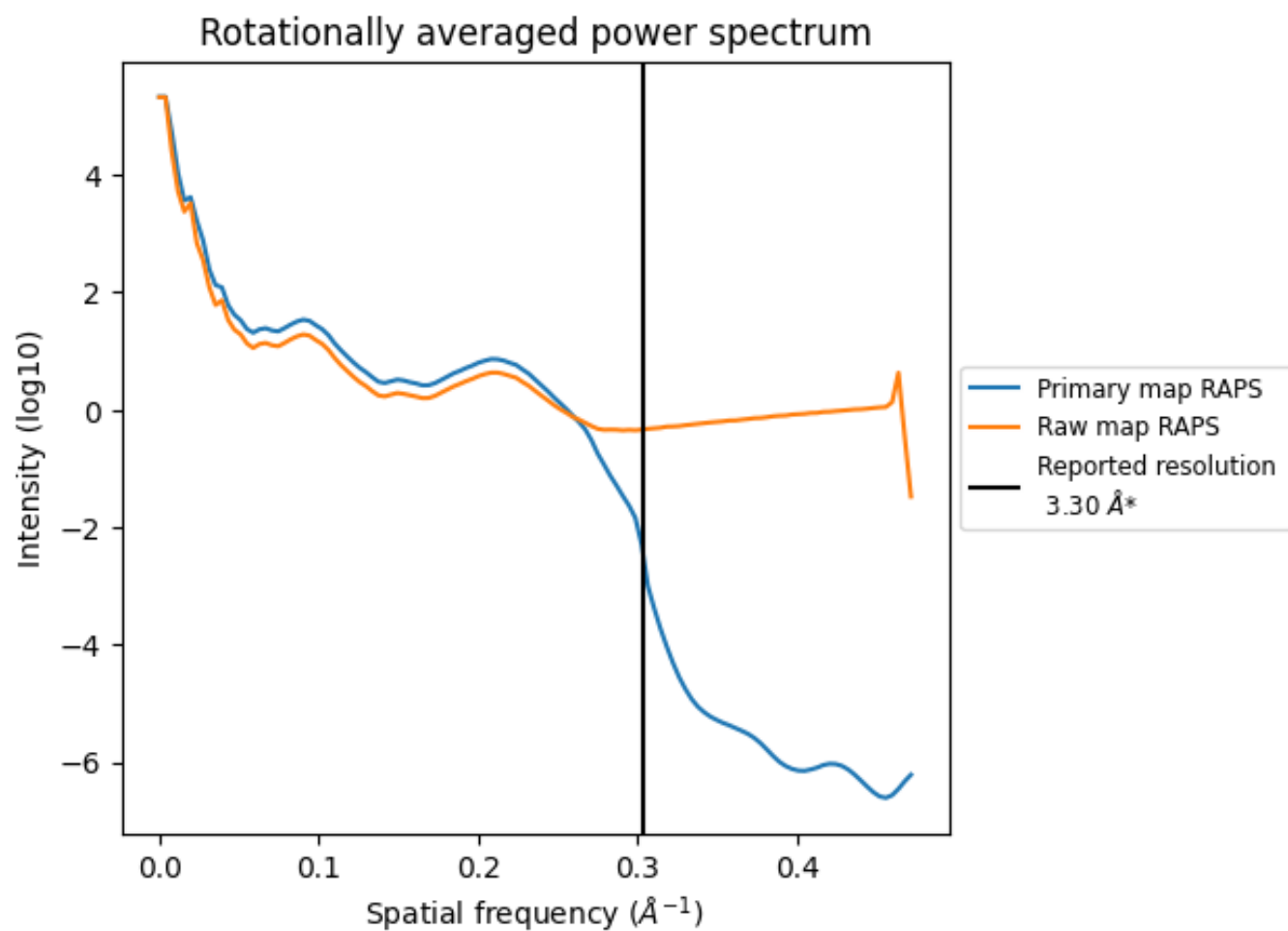
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

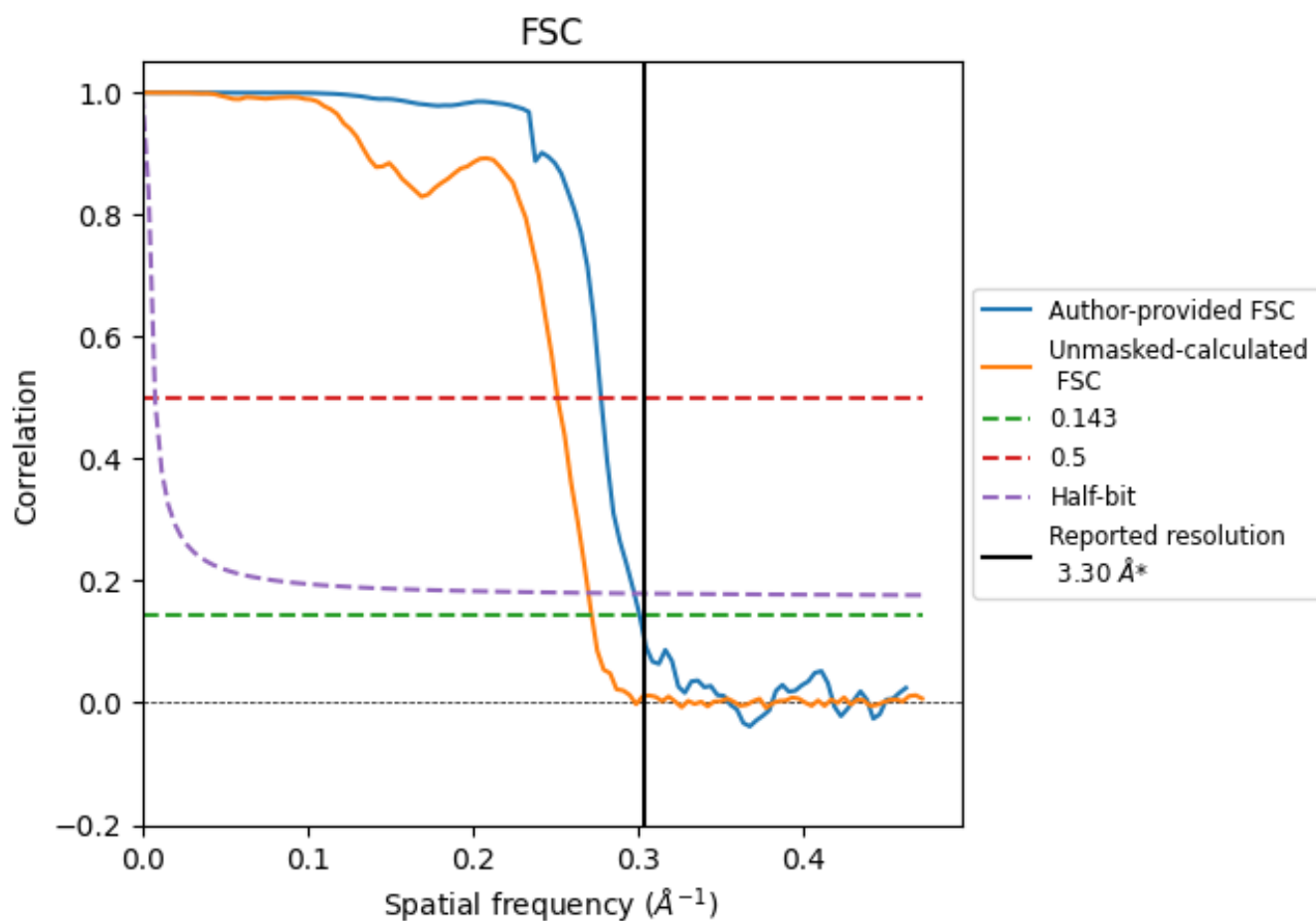


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.60	3.36
Unmasked-calculated*	3.68	3.98	3.71

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

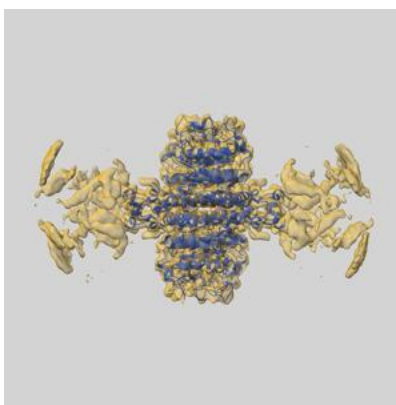
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38855 and PDB model 8Y2H. Per-residue inclusion information can be found in section [3](#) on page [8](#).

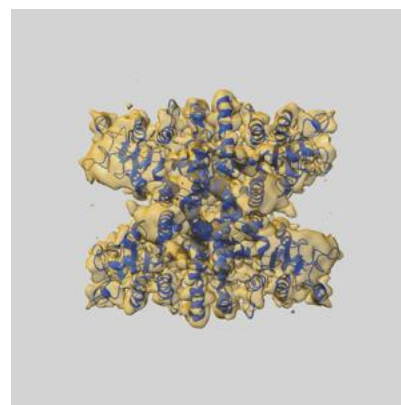
9.1 Map-model overlay [i](#)



X



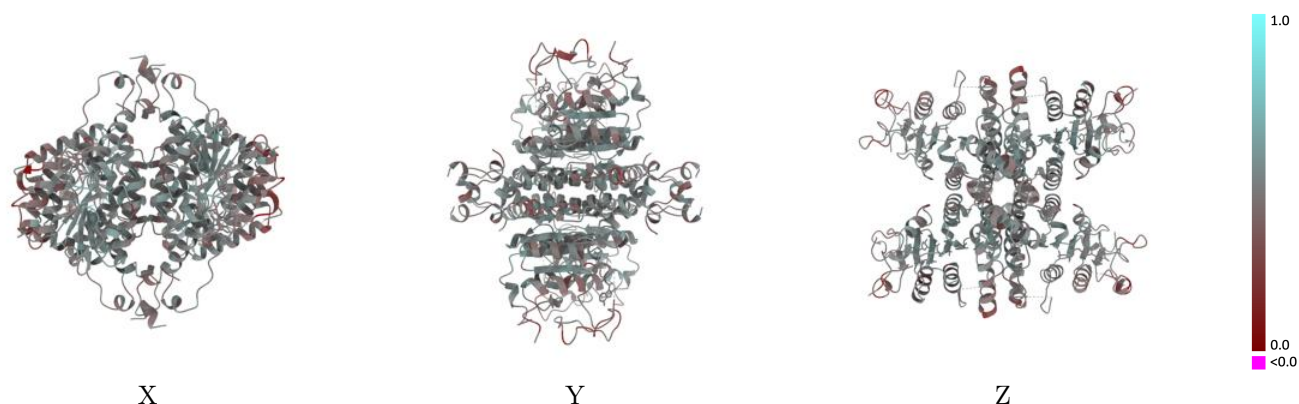
Y



Z

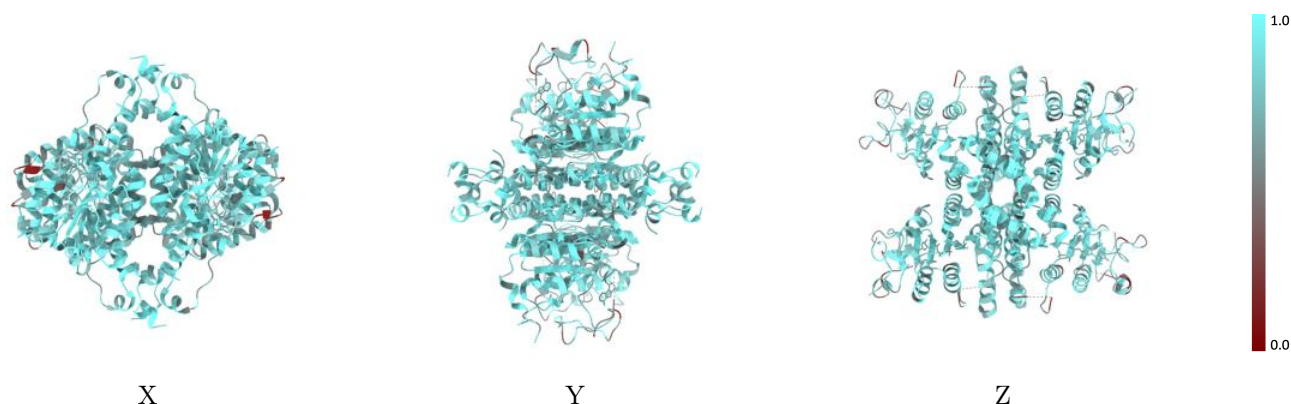
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



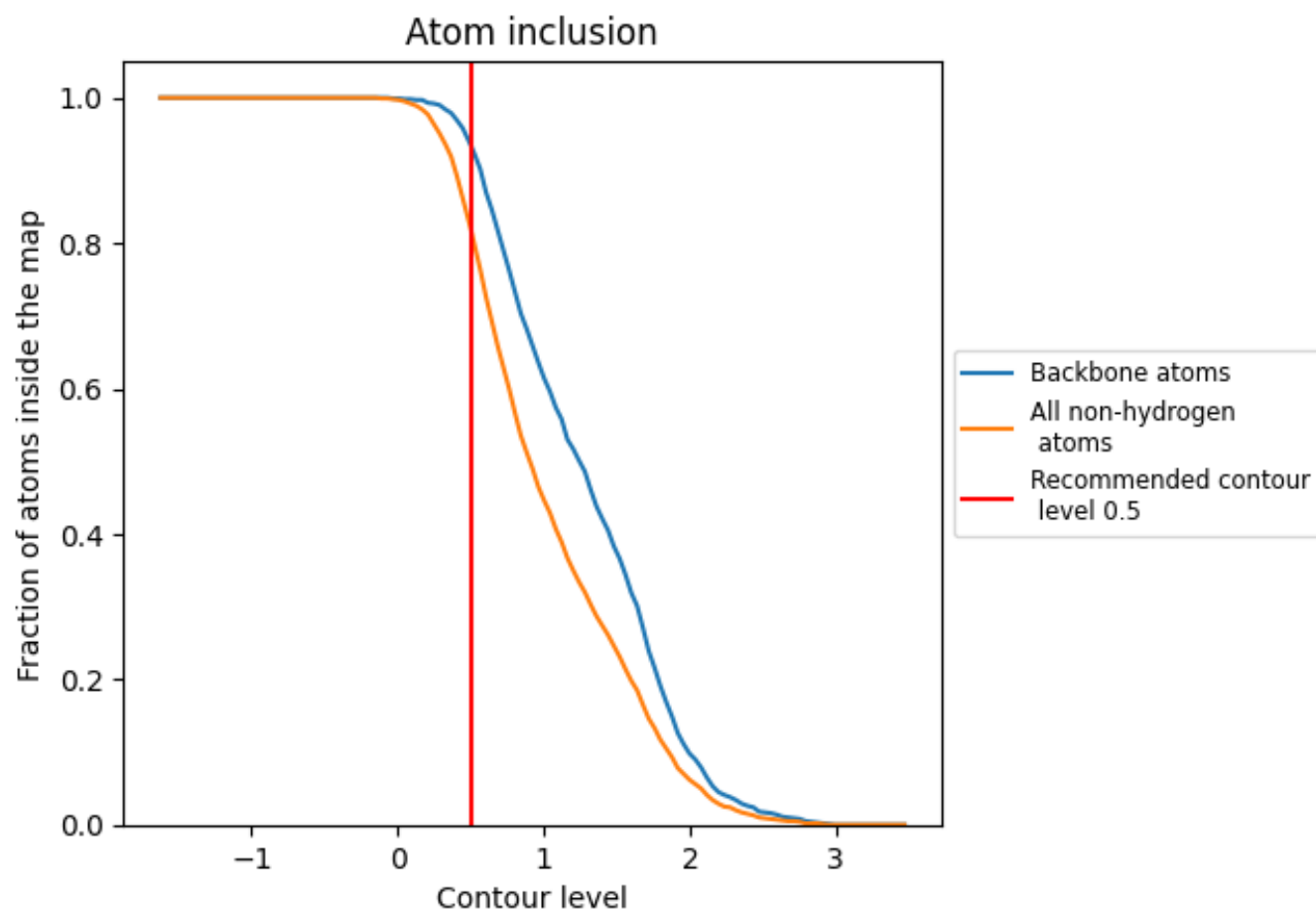
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.4710
A	0.8760	0.4410
B	0.8160	0.4730
C	0.8680	0.4420
D	0.8680	0.4440
E	0.8680	0.4410
F	0.8190	0.4740
G	0.8150	0.4710
H	0.8170	0.4740

