



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:24 AM UTC

PDB ID : 8IMZ / pdb_00008imz
EMDB ID : EMD-35577
Title : Cryo-EM structure of mouse Piezo1-MDFIC complex (composite map)
Authors : Zhou, Z.; Ma, X.; Lin, Y.; Cheng, D.; Bavi, N.; Li, J.V.; Sutton, D.; Yao, M.;
Harvey, N.; Corry, B.; Zhang, Y.; Cox, C.D.
Deposited on : 2023-03-07
Resolution : 3.66 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

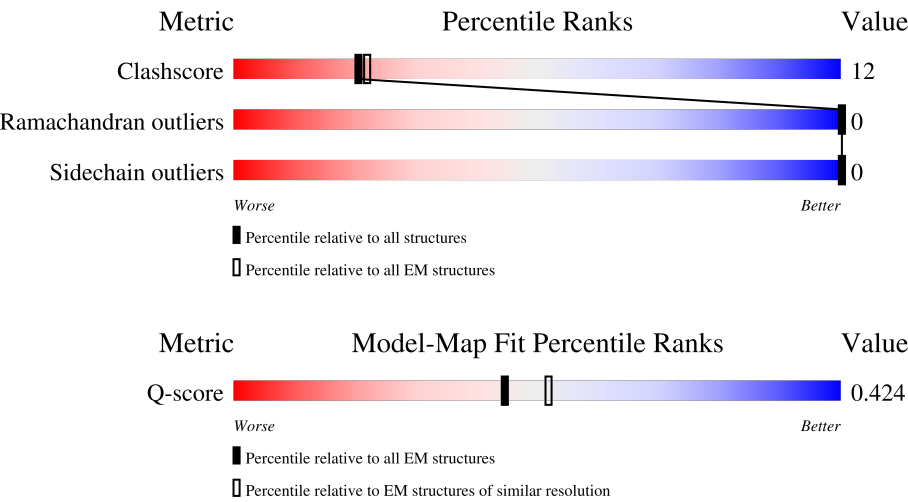
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.66 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	11491 (3.16 - 4.16)

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	2547	12% 35% 13% 52%
1	B	2547	12% 35% 13% 52%
1	C	2547	12% 34% 14% 52%
2	D	247	5% 91%

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Mol	Chain	Length	Quality of chain
2	E	247	6% • 91%
2	F	247	6% • 91%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29409 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.

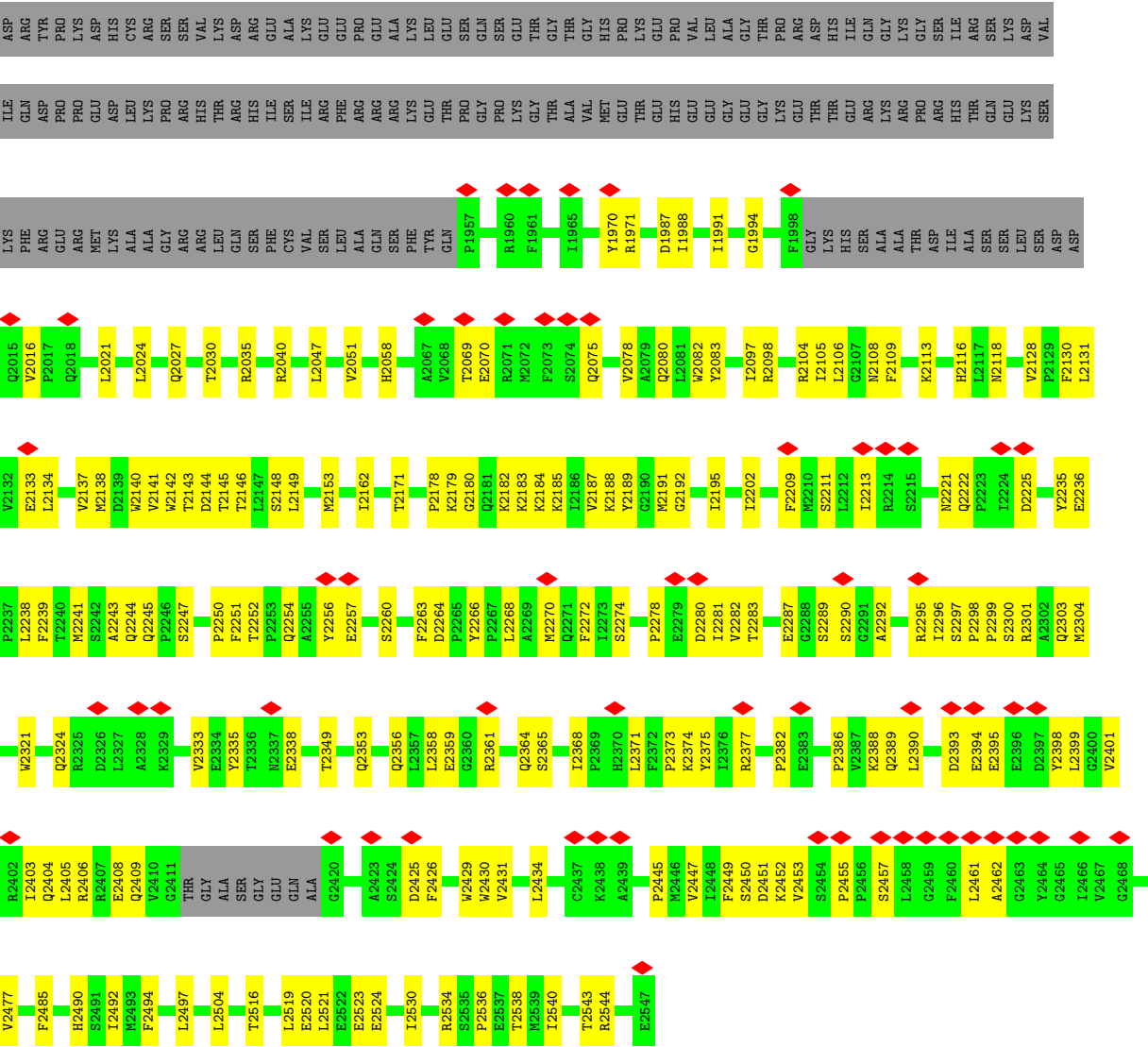
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1223	Total	C	N	O	S	0	0
			9653	6324	1626	1652	51		
1	C	1223	Total	C	N	O	S	0	0
			9653	6324	1626	1652	51		
1	B	1223	Total	C	N	O	S	0	0
			9653	6324	1626	1652	51		

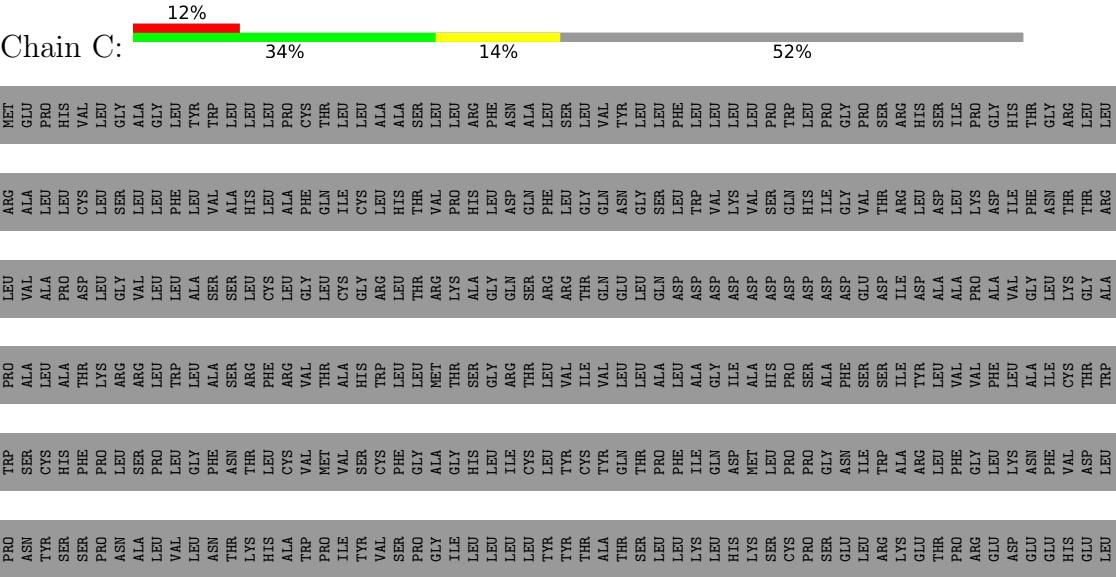
- Molecule 2 is a protein called MyoD family inhibitor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	21	Total	C	N	O	S	0	0
			150	88	21	33	8		
2	E	21	Total	C	N	O	S	0	0
			150	88	21	33	8		
2	F	21	Total	C	N	O	S	0	0
			150	88	21	33	8		





● Molecule 1: Piezo-type mechanosensitive ion channel component 1





- Molecule 1: Piezo-type mechanosensitive ion channel component 1

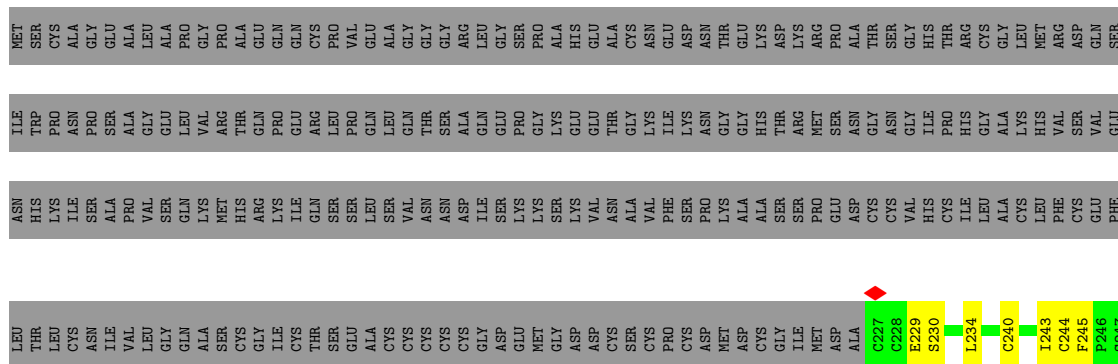






- Molecule 2: MyoD family inhibitor domain-containing protein

ASN	HIS	TRP	ILE	ASP	THR	MET
LYS	LEU	PRO	TRP	SER	SER	SER
ILE	ASN	ASN	ASN	GLY	ALA	ALA
SER	SER	PRO	SER	ALA	GLU	GLY
ALA	PRO	ALA	SER	ALA	ALA	ALA
PRO	VAL	GLY	GLY	GLY	LEU	LEU
VAL	SER	GLU	GLU	GLU	ALA	ALA
SER	GLN	LEU	LEU	PRO	PRO	PRO
LYS	LYS	VAL	VAL	ARG	GLY	GLY
MET	MET	ARG	THR	ARG	PRO	PRO
HIS	HIS	THR	THR	ALA	ALA	ALA
ARG	ARG	GLN	GLN	GLN	GLN	GLN
LYS	LYS	PRO	PRO	PRO	GLN	GLN
ILE	ILE	GLU	GLU	ARG	GLN	CYS
GLN	GLN	ARG	LEU	LEU	PRO	PRO
SER	SER	LEU	PRO	PRO	VAL	VAL
LEU	LEU	GLN	GLN	GLY	GLY	GLY
SER	SER	LEU	GLN	GLY	GLY	GLY
ASN	ASN	THR	THR	SER	GLY	GLY
ASP	ASP	ALA	ALA	ALA	ARG	ARG
ILE	ILE	GLN	GLN	LEU	GLY	GLY
SER	SER	GLY	GLY	SER	SER	SER
LYS	LYS	PRO	GLY	PRO	PRO	PRO
SER	SER	LYS	LYS	ALA	ALA	ALA
LYS	LYS	GLU	GLU	LYS	ASN	ASN
VAL	VAL	GLU	GLU	GLY	CYS	CYS
VAL	VAL	THR	THR	LYS	GLU	GLU
PHE	PHE	ILE	ILE	ASP	ASP	ASP
SER	SER	LYS	LYS	LYS	LYS	LYS
PRO	PRO	ASN	ASN	THR	THR	THR
LYS	LYS	GLY	GLY	GLY	GLY	GLY
ALA	ALA	GLY	GLY	HIS	HIS	HIS
ALA	ALA	HIS	THR	THR	ASP	ASP
SER	SER	ARG	ARG	ASP	LYS	LYS
SER	SER	ARG	ARG	ARG	ARG	ARG
PRO	PRO	MET	MET	PRO	PRO	PRO
GLU	GLU	SER	SER	ASN	ALA	ALA
ASP	ASP	ASN	ASN	GLY	THR	THR
CYS	CYS	GLY	GLY	ASN	SER	SER
VAL	VAL	GLY	GLY	VAL	GLY	GLY
HIS	HIS	ILE	ILE	THR	THR	THR
CYS	CYS	PRO	PRO	HIS	ARG	ARG
ILE	ILE	HIS	HIS	GLY	CYS	CYS
LEU	LEU	GLY	GLY	ALA	GLY	GLY
ALA	ALA	ALA	ALA	LYS	LEU	LEU
CYS	CYS	LYS	LYS	VAL	MET	MET
LEU	LEU	HIS	HIS	VAL	ARG	ARG
PHE	PHE	VAL	VAL	SER	ASP	ASP
GLU	GLU	VAL	VAL	GLY	GLN	GLN
PHE	PHE	GLY	GLY	THR	SER	SER



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102644	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 ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.164	Depositor
Minimum map value	-4.718	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.168	Depositor
Recommended contour level	1.3	Depositor
Map size (Å)	421.99997, 421.99997, 421.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/9877	0.45	1/13401 (0.0%)
1	B	0.29	0/9877	0.45	1/13401 (0.0%)
1	C	0.29	0/9877	0.45	1/13401 (0.0%)
2	D	0.24	0/151	0.45	0/200
2	E	0.24	0/151	0.45	0/200
2	F	0.24	0/151	0.45	0/200
All	All	0.29	0/30084	0.45	3/40803 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1180	PHE	N-CA-C	-6.65	107.04	114.62
1	B	1180	PHE	N-CA-C	-6.60	107.10	114.62
1	A	1180	PHE	N-CA-C	-6.59	107.11	114.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9653	0	9495	247	0
1	B	9653	0	9495	255	0
1	C	9653	0	9495	254	0
2	D	150	0	132	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	150	0	132	7	0
2	F	150	0	132	5	0
All	All	29409	0	28881	706	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 (706) 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:A:2295:ARG:HD2	1:C:2295:ARG:HH12	1.18	1.05
1:A:2295:ARG:HH12	1:B:2295:ARG:HD2	1.19	1.04
1:C:2295:ARG:HD2	1:B:2295:ARG:HH12	1.19	1.03
1:C:1971:ARG:NE	1:C:2098:ARG:O	2.02	0.92
1:A:1971:ARG:NE	1:A:2098:ARG:O	2.02	0.91
1:B:1971:ARG:NE	1:B:2098:ARG:O	2.02	0.91
1:C:1724:ARG:HH22	1:C:1805:LEU:H	1.20	0.89
1:A:1724:ARG:HH22	1:A:1805:LEU:H	1.20	0.87
1:A:2295:ARG:HH22	1:B:2295:ARG:HB2	1.40	0.85
1:B:1724:ARG:HH22	1:B:1805:LEU:H	1.20	0.85
1:C:2295:ARG:HB2	1:B:2295:ARG:HH22	1.42	0.84
1:C:2292:ALA:HB1	1:B:2295:ARG:HG2	1.60	0.84
1:A:2295:ARG:HB2	1:C:2295:ARG:HH22	1.41	0.83
1:A:2292:ALA:HB1	1:C:2295:ARG:HG2	1.61	0.82
1:A:2295:ARG:HG2	1:B:2292:ALA:HB1	1.63	0.81
1:B:2225:ASP:HB3	1:B:2324:GLN:HB3	1.68	0.76
1:A:2225:ASP:HB3	1:A:2324:GLN:HB3	1.68	0.76
1:C:2225:ASP:HB3	1:C:2324:GLN:HB3	1.68	0.76
1:B:1118:GLU:HB3	1:B:1120:GLN:HG3	1.67	0.76
1:A:2179:LYS:NZ	1:B:1402:ASP:OD1	2.17	0.75
1:C:1118:GLU:HB3	1:C:1120:GLN:HG3	1.67	0.75
1:C:1402:ASP:OD1	1:B:2179:LYS:NZ	2.20	0.74
1:A:1118:GLU:HB3	1:A:1120:GLN:HG3	1.67	0.74
1:A:1402:ASP:OD1	1:C:2179:LYS:NZ	2.19	0.74
1:A:1971:ARG:CD	1:A:2098:ARG:O	2.35	0.74
1:C:1971:ARG:CD	1:C:2098:ARG:O	2.35	0.74
1:C:1702:THR:HB	1:C:1784:LYS:HD2	1.70	0.73
1:B:1971:ARG:CD	1:B:2098:ARG:O	2.35	0.73
1:B:1702:THR:HB	1:B:1784:LYS:HD2	1.70	0.73
1:A:1702:THR:HB	1:A:1784:LYS:HD2	1.70	0.72
1:A:2113:LYS:O	1:A:2118:ASN:ND2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2202:ILE:HG21	1:B:2477:VAL:HG11	1.72	0.72
1:B:2252:THR:OG1	1:B:2254:GLN:NE2	2.23	0.71
1:A:2252:THR:OG1	1:A:2254:GLN:NE2	2.23	0.71
1:B:2035:ARG:HH12	1:B:2109:PHE:HZ	1.37	0.71
1:A:2035:ARG:HH12	1:A:2109:PHE:HZ	1.36	0.71
1:C:2252:THR:OG1	1:C:2254:GLN:NE2	2.23	0.71
1:C:2270:MET:O	1:C:2274:SER:OG	2.07	0.71
1:B:2113:LYS:O	1:B:2118:ASN:ND2	2.23	0.71
1:C:2202:ILE:HG21	1:C:2477:VAL:HG11	1.72	0.71
1:A:2202:ILE:HG21	1:A:2477:VAL:HG11	1.72	0.70
1:C:2113:LYS:O	1:C:2118:ASN:ND2	2.23	0.70
1:C:2035:ARG:HH12	1:C:2109:PHE:HZ	1.36	0.70
1:B:2069:THR:HG22	1:B:2070:GLU:H	1.57	0.70
1:A:2356:GLN:O	1:A:2359:GLU:HG2	1.92	0.70
1:C:2356:GLN:O	1:C:2359:GLU:HG2	1.92	0.70
1:A:2069:THR:HG22	1:A:2070:GLU:H	1.57	0.70
1:A:2270:MET:O	1:A:2274:SER:OG	2.07	0.70
1:B:2356:GLN:O	1:B:2359:GLU:HG2	1.92	0.70
1:A:2295:ARG:NH1	1:B:2295:ARG:HH11	1.90	0.70
1:C:2069:THR:HG22	1:C:2070:GLU:H	1.57	0.70
1:C:1708:LEU:HD11	1:C:2058:HIS:HB3	1.73	0.69
1:B:1708:LEU:HD11	1:B:2058:HIS:HB3	1.73	0.69
1:B:1010:VAL:HG13	1:B:1225:ASN:HD21	1.58	0.69
1:A:1708:LEU:HD11	1:A:2058:HIS:HB3	1.73	0.69
1:A:1344:GLN:OE1	1:A:1347:ARG:NH2	2.26	0.69
1:A:2295:ARG:HD2	1:C:2295:ARG:NH1	2.02	0.68
1:C:2295:ARG:HH11	1:B:2295:ARG:NH1	1.91	0.68
1:C:1344:GLN:OE1	1:C:1347:ARG:NH2	2.26	0.68
1:B:1344:GLN:OE1	1:B:1347:ARG:NH2	2.26	0.68
1:A:1010:VAL:HG13	1:A:1225:ASN:HD21	1.58	0.68
1:B:2404:GLN:OE1	1:B:2406:ARG:NH2	2.25	0.68
1:A:1994:GLY:HA3	1:A:2078:VAL:HG11	1.76	0.68
1:B:2270:MET:O	1:B:2274:SER:OG	2.07	0.68
1:A:1141:PRO:HB2	1:A:1304:HIS:HB2	1.76	0.68
1:C:1994:GLY:HA3	1:C:2078:VAL:HG11	1.76	0.68
1:C:1010:VAL:HG13	1:C:1225:ASN:HD21	1.58	0.67
1:A:2295:ARG:HH11	1:C:2295:ARG:NH1	1.91	0.67
1:B:2040:ARG:NH2	1:B:2142:TRP:O	2.28	0.67
1:A:1687:SER:OG	1:A:1796:HIS:ND1	2.27	0.67
1:C:1800:LEU:HD22	1:C:1806:TRP:HE3	1.60	0.67
1:C:2040:ARG:NH2	1:C:2142:TRP:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:PRO:HB2	1:B:1304:HIS:HB2	1.76	0.67
1:A:1800:LEU:HD22	1:A:1806:TRP:HE3	1.59	0.66
1:A:1201:LYS:O	1:A:1206:GLN:NE2	2.29	0.66
1:C:2388:LYS:HE3	1:C:2394:GLU:HB2	1.78	0.66
1:A:2295:ARG:NH1	1:B:2295:ARG:HD2	2.03	0.66
1:C:1141:PRO:HB2	1:C:1304:HIS:HB2	1.77	0.66
1:C:1201:LYS:O	1:C:1206:GLN:NE2	2.29	0.66
1:B:1800:LEU:HD22	1:B:1806:TRP:HE3	1.59	0.66
1:A:2040:ARG:NH2	1:A:2142:TRP:O	2.28	0.66
1:A:1671:ARG:HG3	1:A:1672:THR:HG23	1.78	0.66
1:A:2404:GLN:OE1	1:A:2406:ARG:NH2	2.25	0.66
1:B:1994:GLY:HA3	1:B:2078:VAL:HG11	1.76	0.66
1:B:1201:LYS:O	1:B:1206:GLN:NE2	2.29	0.65
1:B:1671:ARG:HG3	1:B:1672:THR:HG23	1.78	0.65
1:C:1671:ARG:HG3	1:C:1672:THR:HG23	1.78	0.65
1:B:1191:LEU:O	1:B:1195:GLY:N	2.29	0.65
1:A:1191:LEU:O	1:A:1195:GLY:N	2.29	0.65
1:A:2388:LYS:HE3	1:A:2394:GLU:HB2	1.78	0.65
1:B:1051:CYS:HG	1:B:1091:SER:HG	1.44	0.65
1:C:1191:LEU:O	1:C:1195:GLY:N	2.29	0.65
1:B:2388:LYS:HE3	1:B:2394:GLU:HB2	1.78	0.65
1:C:2016:VAL:HB	1:C:2069:THR:HG21	1.80	0.64
1:B:2338:GLU:OE2	1:B:2386:PRO:HD3	1.98	0.64
1:A:1699:HIS:ND1	1:A:1707:SER:O	2.31	0.64
1:B:2016:VAL:HB	1:B:2069:THR:HG21	1.80	0.63
1:C:1699:HIS:ND1	1:C:1707:SER:O	2.31	0.63
1:C:2338:GLU:OE2	1:C:2386:PRO:HD3	1.98	0.63
1:B:1699:HIS:ND1	1:B:1707:SER:O	2.31	0.63
1:A:2243:ALA:HB1	1:A:2247:SER:HB3	1.81	0.63
1:C:1118:GLU:OE1	1:C:1120:GLN:NE2	2.30	0.63
1:C:2404:GLN:OE1	1:C:2406:ARG:NH2	2.25	0.63
1:A:2016:VAL:HB	1:A:2069:THR:HG21	1.80	0.62
1:A:2221:ASN:HB2	1:A:2453:VAL:HB	1.81	0.62
1:C:1687:SER:OG	1:C:1796:HIS:ND1	2.27	0.62
1:A:2338:GLU:OE2	1:A:2386:PRO:HD3	1.98	0.62
1:B:2221:ASN:HB2	1:B:2453:VAL:HB	1.81	0.62
1:B:2243:ALA:HB1	1:B:2247:SER:HB3	1.81	0.62
1:A:1988:ILE:HG23	1:A:2024:LEU:HD11	1.82	0.62
1:B:1988:ILE:HG23	1:B:2024:LEU:HD11	1.82	0.62
1:A:1118:GLU:OE1	1:A:1120:GLN:NE2	2.30	0.62
1:A:998:ALA:O	1:A:1002:ILE:HG12	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1232:CYS:SG	1:B:1233:VAL:N	2.73	0.62
1:B:998:ALA:O	1:B:1002:ILE:HG12	2.00	0.61
1:C:2221:ASN:HB2	1:C:2453:VAL:HB	1.81	0.61
1:C:998:ALA:O	1:C:1002:ILE:HG12	2.00	0.61
1:C:2494:PHE:HD2	1:B:2490:HIS:HD1	1.48	0.61
1:A:1051:CYS:HG	1:A:1091:SER:HG	1.46	0.61
1:A:1232:CYS:SG	1:A:1233:VAL:N	2.73	0.61
1:C:1232:CYS:SG	1:C:1233:VAL:N	2.73	0.61
2:E:240:CYS:HA	1:B:2191:MET:HE1	1.83	0.61
1:C:1988:ILE:HG23	1:C:2024:LEU:HD11	1.82	0.61
1:A:2494:PHE:HD2	1:C:2490:HIS:HD1	1.49	0.61
1:B:1748:GLN:NE2	1:B:1779:THR:O	2.34	0.61
1:C:1748:GLN:NE2	1:C:1779:THR:O	2.34	0.60
1:C:2243:ALA:HB1	1:C:2247:SER:HB3	1.81	0.60
1:C:2497:LEU:HD23	1:C:2543:THR:HG21	1.83	0.60
1:B:1165:VAL:HG22	1:B:1289:PHE:HB3	1.83	0.60
1:A:2497:LEU:HD23	1:A:2543:THR:HG21	1.83	0.60
1:B:1687:SER:OG	1:B:1796:HIS:ND1	2.27	0.60
1:A:1246:ILE:HG13	1:A:1251:LEU:HB2	1.84	0.60
1:B:1118:GLU:OE1	1:B:1120:GLN:NE2	2.30	0.60
1:B:2268:LEU:HD12	1:B:2268:LEU:H	1.67	0.60
1:A:1748:GLN:NE2	1:A:1779:THR:O	2.34	0.60
1:A:2184:LYS:HB2	1:A:2187:VAL:HG12	1.84	0.59
1:A:2268:LEU:HD12	1:A:2268:LEU:H	1.67	0.59
1:B:2184:LYS:HB2	1:B:2187:VAL:HG12	1.84	0.59
1:A:1165:VAL:HG22	1:A:1289:PHE:HB3	1.83	0.59
1:C:1165:VAL:HG22	1:C:1289:PHE:HB3	1.83	0.59
1:A:2408:GLU:OE2	1:A:2409:GLN:N	2.35	0.59
1:B:1246:ILE:HG13	1:B:1251:LEU:HB2	1.84	0.59
1:C:1345:LEU:HD12	1:C:2104:ARG:HH11	1.67	0.59
1:C:2268:LEU:H	1:C:2268:LEU:HD12	1.67	0.59
1:C:2408:GLU:OE2	1:C:2409:GLN:N	2.35	0.59
1:B:2408:GLU:OE2	1:B:2409:GLN:N	2.35	0.59
1:B:2497:LEU:HD23	1:B:2543:THR:HG21	1.83	0.59
1:A:2134:LEU:HB3	1:A:2138:MET:HE2	1.85	0.59
1:A:2182:LYS:HE2	1:B:2144:ASP:HB2	1.85	0.58
1:A:2377:ARG:HA	1:A:2449:PHE:HB2	1.84	0.58
1:C:2377:ARG:HA	1:C:2449:PHE:HB2	1.84	0.58
1:A:2490:HIS:HD1	1:B:2494:PHE:HD2	1.51	0.58
1:C:2184:LYS:HB2	1:C:2187:VAL:HG12	1.84	0.58
1:A:2185:LYS:HD2	1:A:2189:TYR:HE2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2434:LEU:HD11	1:A:2445:PRO:HD2	1.86	0.58
1:B:2058:HIS:NE2	1:B:2083:TYR:OH	2.33	0.58
1:C:2434:LEU:HD11	1:C:2445:PRO:HD2	1.86	0.58
1:B:1345:LEU:HD12	1:B:2104:ARG:HH11	1.67	0.58
1:A:2021:LEU:HD11	1:C:2211:SER:HB3	1.85	0.58
1:B:2185:LYS:HD2	1:B:2189:TYR:HE2	1.69	0.58
1:A:1345:LEU:HD12	1:A:2104:ARG:HH11	1.68	0.58
1:A:2144:ASP:HB2	1:C:2182:LYS:HE2	1.85	0.58
1:C:2021:LEU:HD11	1:B:2211:SER:HB3	1.84	0.58
1:B:2377:ARG:HA	1:B:2449:PHE:HB2	1.84	0.58
1:B:2434:LEU:HD11	1:B:2445:PRO:HD2	1.86	0.58
1:C:2144:ASP:HB2	1:B:2182:LYS:HE2	1.85	0.58
1:C:1213:LEU:HG	1:C:1290:LEU:HD21	1.86	0.57
1:C:1246:ILE:HG13	1:C:1251:LEU:HB2	1.84	0.57
1:B:1705:ALA:HA	1:B:1708:LEU:HB3	1.86	0.57
1:B:2373:PRO:HB3	1:B:2398:TYR:CE1	2.39	0.57
1:A:1213:LEU:HG	1:A:1290:LEU:HD21	1.86	0.57
1:B:1213:LEU:HG	1:B:1290:LEU:HD21	1.86	0.57
1:A:1359:TYR:OH	1:A:1418:ASP:OD2	2.17	0.57
1:A:2058:HIS:NE2	1:A:2083:TYR:OH	2.33	0.57
1:C:2361:ARG:HB3	1:C:2364:GLN:HE21	1.70	0.57
1:A:2361:ARG:HB3	1:A:2364:GLN:HE21	1.70	0.57
1:B:2361:ARG:HB3	1:B:2364:GLN:HE21	1.70	0.57
1:A:1724:ARG:HH22	1:A:1805:LEU:N	1.99	0.57
1:A:2128:VAL:HG11	1:A:2131:LEU:HD12	1.86	0.57
1:B:1184:TYR:OH	1:B:1283:ASP:OD1	2.20	0.57
1:B:2134:LEU:HB3	1:B:2138:MET:HE2	1.85	0.57
1:C:2134:LEU:HB3	1:C:2138:MET:HE2	1.85	0.57
1:B:1541:LEU:HD13	1:B:1555:VAL:HG11	1.87	0.57
1:C:2185:LYS:HD2	1:C:2189:TYR:HE2	1.69	0.57
1:A:1005:ARG:HE	1:A:1007:ASN:ND2	2.03	0.57
1:B:2280:ASP:OD2	1:B:2452:LYS:NZ	2.34	0.56
1:A:2373:PRO:HB3	1:A:2398:TYR:CE1	2.39	0.56
1:C:2058:HIS:NE2	1:C:2083:TYR:OH	2.33	0.56
1:A:1541:LEU:HD13	1:A:1555:VAL:HG11	1.87	0.56
1:A:2211:SER:HB3	1:B:2021:LEU:HD11	1.86	0.56
1:A:2295:ARG:HH11	1:C:2295:ARG:HH12	1.52	0.56
1:C:1705:ALA:HA	1:C:1708:LEU:HB3	1.86	0.56
1:C:2295:ARG:HH11	1:B:2295:ARG:HH12	1.52	0.56
1:B:1005:ARG:HE	1:B:1007:ASN:ND2	2.03	0.56
1:B:2128:VAL:HG11	1:B:2131:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2257:GLU:O	1:A:2260:SER:OG	2.17	0.56
1:C:2295:ARG:HD2	1:B:2295:ARG:NH1	2.04	0.56
1:A:1705:ALA:HA	1:A:1708:LEU:HB3	1.86	0.56
1:C:1005:ARG:HE	1:C:1007:ASN:ND2	2.03	0.56
1:B:2361:ARG:HB3	1:B:2364:GLN:NE2	2.21	0.56
1:C:2373:PRO:HB3	1:C:2398:TYR:CE1	2.40	0.56
1:C:2128:VAL:HG11	1:C:2131:LEU:HD12	1.86	0.55
1:B:2257:GLU:O	1:B:2260:SER:OG	2.17	0.55
1:C:1541:LEU:HD13	1:C:1555:VAL:HG11	1.87	0.55
1:C:2361:ARG:HB3	1:C:2364:GLN:NE2	2.21	0.55
1:A:2108:ASN:OD1	1:A:2109:PHE:N	2.40	0.55
1:A:2425:ASP:HB3	1:A:2426:PHE:HD1	1.72	0.55
1:C:2108:ASN:OD1	1:C:2109:PHE:N	2.40	0.55
1:C:2280:ASP:O	1:C:2450:SER:OG	2.24	0.55
1:A:2280:ASP:O	1:A:2450:SER:OG	2.24	0.55
1:A:2295:ARG:HH12	1:B:2295:ARG:HH11	1.51	0.55
1:C:2368:ILE:HD12	1:C:2403:ILE:HD12	1.89	0.55
1:C:2425:ASP:HB3	1:C:2426:PHE:HD1	1.72	0.55
1:A:2530:ILE:HD12	1:C:2492:ILE:HD11	1.89	0.55
1:C:2104:ARG:HG2	1:C:2104:ARG:HH21	1.72	0.55
1:A:1117:GLU:HG2	1:A:1118:GLU:HG2	1.89	0.55
1:A:1971:ARG:HD2	1:A:2098:ARG:O	2.08	0.55
1:B:1117:GLU:HG2	1:B:1118:GLU:HG2	1.89	0.55
1:B:2368:ILE:HD12	1:B:2403:ILE:HD12	1.89	0.54
1:A:1670:GLY:HA2	1:A:1674:ARG:HG3	1.89	0.54
1:A:2368:ILE:HD12	1:A:2403:ILE:HD12	1.89	0.54
1:C:2530:ILE:HD12	1:B:2492:ILE:HD11	1.89	0.54
1:B:1296:ILE:O	1:B:1299:SER:OG	2.24	0.54
1:B:2104:ARG:HG2	1:B:2104:ARG:HH21	1.71	0.54
1:B:1971:ARG:HD2	1:B:2098:ARG:O	2.07	0.54
1:A:2361:ARG:HB3	1:A:2364:GLN:NE2	2.21	0.54
1:A:2377:ARG:NH1	1:A:2451:ASP:OD2	2.41	0.54
1:C:1670:GLY:HA2	1:C:1674:ARG:HG3	1.89	0.54
1:C:2298:PRO:HG2	1:C:2299:PRO:HD3	1.89	0.54
1:B:2108:ASN:OD1	1:B:2109:PHE:N	2.40	0.54
1:B:2280:ASP:O	1:B:2450:SER:OG	2.24	0.54
1:B:1670:GLY:HA2	1:B:1674:ARG:HG3	1.89	0.54
1:A:1152:MET:HE3	1:A:1665:PHE:HE2	1.72	0.54
1:C:1117:GLU:HG2	1:C:1118:GLU:HG2	1.89	0.54
1:C:1971:ARG:HD2	1:C:2098:ARG:O	2.07	0.54
1:B:1152:MET:HE3	1:B:1665:PHE:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2104:ARG:HG2	1:A:2104:ARG:HH21	1.71	0.54
1:B:2298:PRO:HG2	1:B:2299:PRO:HD3	1.89	0.54
1:A:2298:PRO:HG2	1:A:2299:PRO:HD3	1.89	0.53
1:B:2425:ASP:HB3	1:B:2426:PHE:HD1	1.72	0.53
1:C:1774:LEU:HG	1:C:1776:LEU:HD13	1.91	0.53
1:C:2377:ARG:NH1	1:C:2451:ASP:OD2	2.41	0.53
1:B:2377:ARG:NH1	1:B:2451:ASP:OD2	2.41	0.53
1:C:1152:MET:HE3	1:C:1665:PHE:HE2	1.72	0.53
1:A:1783:ILE:O	1:A:1783:ILE:HG13	2.09	0.53
1:C:1783:ILE:HG13	1:C:1783:ILE:O	2.09	0.53
1:A:1650:LEU:O	1:A:1652:ARG:NH2	2.35	0.53
1:C:2296:ILE:HD11	1:C:2300:SER:OG	2.09	0.53
1:A:1184:TYR:OH	1:A:1283:ASP:OD1	2.20	0.52
1:B:1724:ARG:HH22	1:B:1805:LEU:N	1.99	0.52
1:A:1774:LEU:HG	1:A:1776:LEU:HD13	1.91	0.52
1:C:1217:ASN:HD21	1:C:1287:PHE:HB2	1.74	0.52
1:B:1774:LEU:HG	1:B:1776:LEU:HD13	1.91	0.52
1:A:2116:HIS:CE1	2:D:234:LEU:HD11	2.44	0.52
1:C:2250:PRO:HA	1:C:2282:VAL:HA	1.92	0.52
1:B:1217:ASN:HD21	1:B:1287:PHE:HB2	1.74	0.52
1:C:2272:PHE:HD2	1:C:2389:GLN:OE1	1.92	0.52
1:B:1783:ILE:HG13	1:B:1783:ILE:O	2.09	0.52
1:B:2272:PHE:HD2	1:B:2389:GLN:OE1	1.92	0.52
1:A:2105:ILE:HG13	1:A:2106:LEU:HD12	1.92	0.52
1:C:1002:ILE:HG23	1:C:1225:ASN:HD22	1.75	0.52
1:B:1002:ILE:HG23	1:B:1225:ASN:HD22	1.75	0.52
1:B:2296:ILE:HD11	1:B:2300:SER:OG	2.09	0.52
1:C:2105:ILE:HG13	1:C:2106:LEU:HD12	1.92	0.52
1:A:1002:ILE:HG23	1:A:1225:ASN:HD22	1.75	0.52
1:C:2257:GLU:O	1:C:2260:SER:OG	2.17	0.52
1:B:2105:ILE:HG13	1:B:2106:LEU:HD12	1.92	0.52
1:A:2492:ILE:HD11	1:B:2530:ILE:HD12	1.91	0.52
1:C:1650:LEU:O	1:C:1652:ARG:NH2	2.35	0.52
1:C:2153:MET:HE3	1:B:2485:PHE:CZ	2.45	0.52
1:A:2333:VAL:HG21	1:A:2382:PRO:HD3	1.92	0.52
1:C:1724:ARG:HH22	1:C:1805:LEU:N	1.99	0.52
1:A:1217:ASN:HD21	1:A:1287:PHE:HB2	1.74	0.51
1:A:2153:MET:HE3	1:C:2485:PHE:CE1	2.45	0.51
1:A:2544:ARG:NH1	1:B:1411:ASP:OD1	2.42	0.51
1:C:2272:PHE:HZ	1:C:2377:ARG:HD2	1.76	0.51
1:B:2333:VAL:HG21	1:B:2382:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2333:VAL:HG21	1:C:2382:PRO:HD3	1.93	0.51
1:A:2250:PRO:HA	1:A:2282:VAL:HA	1.92	0.51
1:B:2250:PRO:HA	1:B:2282:VAL:HA	1.92	0.51
1:B:2272:PHE:HZ	1:B:2377:ARG:HD2	1.75	0.51
1:A:2272:PHE:HZ	1:A:2377:ARG:HD2	1.75	0.51
1:A:2290:SER:O	1:A:2290:SER:OG	2.26	0.51
1:C:1411:ASP:OD1	1:B:2544:ARG:NH1	2.43	0.51
1:C:2287:GLU:HG3	1:C:2290:SER:HB3	1.92	0.51
1:B:2287:GLU:HG3	1:B:2290:SER:HB3	1.92	0.51
1:B:2290:SER:O	1:B:2290:SER:OG	2.26	0.51
1:B:2324:GLN:HB2	1:B:2335:TYR:HE1	1.76	0.51
1:A:2153:MET:HE3	1:C:2485:PHE:CZ	2.45	0.50
1:A:2272:PHE:HD2	1:A:2389:GLN:OE1	1.92	0.50
1:C:2405:LEU:HD12	1:C:2430:TRP:CH2	2.47	0.50
1:A:2146:THR:HG23	1:A:2519:LEU:HD22	1.93	0.50
1:A:2296:ILE:HD11	1:A:2300:SER:OG	2.09	0.50
1:A:2406:ARG:HB3	1:A:2429:TRP:CE2	2.46	0.50
1:C:2146:THR:HG23	1:C:2519:LEU:HD22	1.93	0.50
1:C:2153:MET:HE3	1:B:2485:PHE:CE1	2.45	0.50
1:B:1178:SER:HB3	1:B:1250:SER:HB3	1.93	0.50
1:B:2405:LEU:HD12	1:B:2430:TRP:CH2	2.47	0.50
1:A:1411:ASP:OD1	1:C:2544:ARG:NH1	2.43	0.50
1:A:2405:LEU:HD12	1:A:2430:TRP:CH2	2.47	0.50
1:A:2485:PHE:CE1	1:B:2153:MET:HE3	2.46	0.50
1:B:2406:ARG:HB3	1:B:2429:TRP:CE2	2.46	0.50
1:A:1139:PRO:HD2	1:A:1301:TYR:HE1	1.77	0.50
1:A:2324:GLN:HB2	1:A:2335:TYR:HE1	1.77	0.50
1:C:2324:GLN:HB2	1:C:2335:TYR:HE1	1.77	0.50
1:B:2146:THR:HG23	1:B:2519:LEU:HD22	1.94	0.50
1:A:2287:GLU:HG3	1:A:2290:SER:HB3	1.92	0.50
1:C:2290:SER:O	1:C:2290:SER:OG	2.26	0.50
1:A:2485:PHE:CZ	1:B:2153:MET:HE3	2.47	0.50
1:C:1716:LEU:HD21	1:C:2051:VAL:HA	1.94	0.50
1:C:1724:ARG:HH12	1:C:1804:GLY:HA3	1.77	0.50
1:C:2280:ASP:OD2	1:C:2452:LYS:NZ	2.34	0.50
1:A:1178:SER:HB3	1:A:1250:SER:HB3	1.93	0.49
1:C:2406:ARG:HB3	1:C:2429:TRP:CE2	2.46	0.49
1:B:1650:LEU:O	1:B:1652:ARG:NH2	2.35	0.49
2:D:243:ILE:HD11	1:B:2149:LEU:HD23	1.95	0.49
1:C:1178:SER:HB3	1:C:1250:SER:HB3	1.93	0.49
1:A:2280:ASP:OD2	1:A:2452:LYS:NZ	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1139:PRO:HD2	1:C:1301:TYR:HE1	1.77	0.49
1:A:1716:LEU:HD21	1:A:2051:VAL:HA	1.94	0.49
1:B:2183:LYS:HB3	1:B:2188:LYS:HD2	1.95	0.49
1:B:1326:ALA:HA	1:B:1649:LEU:HD21	1.94	0.49
1:B:2345:ALA:O	1:B:2348:SER:OG	2.22	0.49
1:A:1308:ASP:OD1	1:A:1538:ARG:NH1	2.46	0.49
2:D:229:GLU:HG3	2:D:230:SER:H	1.78	0.49
1:B:1359:TYR:OH	1:B:1418:ASP:OD2	2.17	0.49
1:A:1311:ALA:HB2	1:A:1542:THR:HB	1.95	0.49
1:A:1698:ASN:ND2	1:A:1789:GLN:OE1	2.41	0.49
1:A:1724:ARG:HH12	1:A:1804:GLY:HA3	1.77	0.49
2:F:229:GLU:HG3	2:F:230:SER:H	1.78	0.49
2:E:229:GLU:HG3	2:E:230:SER:H	1.78	0.49
1:C:1326:ALA:HA	1:C:1649:LEU:HD21	1.94	0.49
1:B:1139:PRO:HD2	1:B:1301:TYR:HE1	1.77	0.49
1:B:1716:LEU:HD21	1:B:2051:VAL:HA	1.94	0.49
1:A:1326:ALA:HA	1:A:1649:LEU:HD21	1.94	0.48
2:E:243:ILE:HD11	1:C:2149:LEU:HD23	1.95	0.48
1:C:1710:LEU:HB3	1:C:1711:PRO:HD3	1.95	0.48
1:B:2236:GLU:HG2	1:B:2295:ARG:O	2.13	0.48
1:A:1710:LEU:HB3	1:A:1711:PRO:HD3	1.95	0.48
1:A:2236:GLU:HG2	1:A:2295:ARG:O	2.13	0.48
1:B:1311:ALA:HB2	1:B:1542:THR:HB	1.95	0.48
1:A:2371:LEU:HD22	1:A:2401:VAL:HG11	1.96	0.48
1:C:1698:ASN:ND2	1:C:1789:GLN:OE1	2.41	0.48
1:C:2236:GLU:HG2	1:C:2295:ARG:O	2.13	0.48
1:B:1218:VAL:HA	1:B:1221:ILE:HG22	1.96	0.48
1:A:2283:THR:HG22	1:A:2447:VAL:HG22	1.96	0.48
1:C:2283:THR:HG22	1:C:2447:VAL:HG22	1.96	0.48
1:B:1308:ASP:OD1	1:B:1538:ARG:NH1	2.46	0.48
1:C:2183:LYS:HB3	1:C:2188:LYS:HD2	1.95	0.48
1:A:2143:THR:O	1:C:2188:LYS:NZ	2.42	0.48
1:A:2183:LYS:HB3	1:A:2188:LYS:HD2	1.95	0.48
1:C:1559:LEU:HD23	1:C:1559:LEU:H	1.79	0.48
1:A:2162:ILE:HG22	1:A:2504:LEU:HD13	1.96	0.48
1:C:2162:ILE:HG22	1:C:2504:LEU:HD13	1.96	0.48
1:B:1724:ARG:HH12	1:B:1804:GLY:HA3	1.77	0.47
1:C:2137:VAL:O	1:C:2141:VAL:HG23	2.14	0.47
1:A:998:ALA:O	1:A:1001:VAL:HG12	2.14	0.47
1:B:1710:LEU:HB3	1:B:1711:PRO:HD3	1.95	0.47
1:A:1780:ASP:OD1	1:A:1781:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1308:ASP:OD1	1:C:1538:ARG:NH1	2.46	0.47
1:C:1311:ALA:HB2	1:C:1542:THR:HB	1.95	0.47
1:B:998:ALA:O	1:B:1001:VAL:HG12	2.14	0.47
1:C:1334:HIS:HA	1:C:1337:ILE:HG22	1.97	0.47
1:B:2371:LEU:HD22	1:B:2401:VAL:HG11	1.95	0.47
1:A:2264:ASP:O	1:A:2266:TYR:N	2.48	0.47
1:C:1359:TYR:OH	1:C:1418:ASP:OD2	2.17	0.47
1:C:1780:ASP:OD1	1:C:1781:SER:N	2.48	0.47
1:B:1514:ASP:OD1	1:B:1674:ARG:NH2	2.43	0.47
1:B:2162:ILE:HG22	1:B:2504:LEU:HD13	1.96	0.47
1:B:2264:ASP:O	1:B:2266:TYR:N	2.48	0.47
1:A:1218:VAL:HA	1:A:1221:ILE:HG22	1.96	0.47
1:A:1553:ARG:HH11	1:A:1556:LEU:HD11	1.80	0.47
1:C:1044:LEU:HD21	1:C:1098:PHE:CE1	2.50	0.47
1:C:1218:VAL:HA	1:C:1221:ILE:HG22	1.96	0.47
1:B:2137:VAL:O	1:B:2141:VAL:HG23	2.14	0.47
1:A:1334:HIS:HA	1:A:1337:ILE:HG22	1.97	0.47
1:A:1554:GLY:O	1:A:1558:GLN:HB2	2.15	0.47
1:A:2140:TRP:CD1	1:A:2145:THR:HG21	2.50	0.47
1:C:2345:ALA:O	1:C:2348:SER:OG	2.22	0.47
1:C:2371:LEU:HD22	1:C:2401:VAL:HG11	1.95	0.47
1:A:2256:TYR:HB2	1:A:2278:PRO:HB3	1.97	0.47
1:C:2140:TRP:CD1	1:C:2145:THR:HG21	2.50	0.47
1:C:2143:THR:O	1:B:2188:LYS:NZ	2.42	0.47
1:B:2365:SER:OG	1:B:2404:GLN:HG3	2.15	0.47
1:A:2321:TRP:HE1	1:A:2338:GLU:HG2	1.80	0.46
1:C:1184:TYR:OH	1:C:1283:ASP:OD1	2.20	0.46
1:C:2070:GLU:OE1	1:C:2075:GLN:HB2	2.15	0.46
1:B:2283:THR:HG22	1:B:2447:VAL:HG22	1.96	0.46
1:A:2149:LEU:HD23	2:F:243:ILE:HD11	1.96	0.46
1:C:998:ALA:O	1:C:1001:VAL:HG12	2.14	0.46
1:C:2264:ASP:O	1:C:2266:TYR:N	2.48	0.46
1:A:2137:VAL:O	1:A:2141:VAL:HG23	2.14	0.46
1:B:2244:GLN:HG2	1:B:2245:GLN:H	1.80	0.46
1:B:2256:TYR:HB2	1:B:2278:PRO:HB3	1.97	0.46
1:B:1559:LEU:HD23	1:B:1559:LEU:H	1.79	0.46
1:B:2321:TRP:HE1	1:B:2338:GLU:HG2	1.80	0.46
1:A:1044:LEU:HD21	1:A:1098:PHE:CE1	2.50	0.46
1:C:1514:ASP:OD1	1:C:1674:ARG:NH2	2.43	0.46
1:C:1551:VAL:HG22	1:C:1553:ARG:H	1.81	0.46
1:C:2321:TRP:HE1	1:C:2338:GLU:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1780:ASP:OD1	1:B:1781:SER:N	2.48	0.46
1:B:2140:TRP:CD1	1:B:2145:THR:HG21	2.50	0.46
1:A:1179:ILE:HG23	1:A:1179:ILE:O	2.15	0.46
1:A:2070:GLU:OE1	1:A:2075:GLN:HB2	2.15	0.46
1:C:1296:ILE:O	1:C:1299:SER:OG	2.24	0.46
1:C:1553:ARG:HH11	1:C:1556:LEU:HD11	1.80	0.46
1:C:2235:TYR:CD2	1:C:2304:MET:HG3	2.51	0.46
1:C:2289:SER:HA	1:C:2431:VAL:HG22	1.97	0.46
1:B:1334:HIS:HA	1:B:1337:ILE:HG22	1.97	0.46
1:A:2104:ARG:HG2	1:A:2104:ARG:NH2	2.31	0.46
1:A:2365:SER:OG	1:A:2404:GLN:HG3	2.15	0.46
1:C:1554:GLY:O	1:C:1558:GLN:HB2	2.15	0.46
1:C:2365:SER:OG	1:C:2404:GLN:HG3	2.15	0.46
1:B:1179:ILE:HG23	1:B:1179:ILE:O	2.15	0.46
1:B:1353:ARG:HG2	1:B:2521:LEU:HD21	1.98	0.46
1:B:1554:GLY:O	1:B:1558:GLN:HB2	2.15	0.46
1:B:2131:LEU:HD23	1:B:2131:LEU:HA	1.78	0.46
1:B:1553:ARG:HH11	1:B:1556:LEU:HD11	1.80	0.46
1:A:1559:LEU:HD23	1:A:1559:LEU:H	1.79	0.46
1:C:2104:ARG:HG2	1:C:2104:ARG:NH2	2.31	0.46
1:C:2244:GLN:HG2	1:C:2245:GLN:H	1.80	0.46
1:B:2070:GLU:OE1	1:B:2075:GLN:HB2	2.15	0.46
1:A:1170:PHE:CE1	1:A:1787:LEU:HB2	2.51	0.46
1:A:1551:VAL:HG22	1:A:1553:ARG:H	1.81	0.46
1:A:2301:ARG:NH2	1:A:2358:LEU:O	2.33	0.46
1:C:2256:TYR:HB2	1:C:2278:PRO:HB3	1.97	0.46
1:B:2301:ARG:NH2	1:B:2358:LEU:O	2.33	0.46
1:A:2149:LEU:O	1:A:2153:MET:HG2	2.16	0.45
1:C:1179:ILE:O	1:C:1179:ILE:HG23	2.15	0.45
1:B:1044:LEU:HD21	1:B:1098:PHE:CE1	2.50	0.45
1:A:1412:TYR:HD1	1:A:2538:THR:HG21	1.82	0.45
1:A:2406:ARG:HD3	1:A:2406:ARG:HA	1.87	0.45
1:C:2149:LEU:O	1:C:2153:MET:HG2	2.16	0.45
1:B:1170:PHE:CE1	1:B:1787:LEU:HB2	2.51	0.45
1:B:1182:LEU:HB2	1:B:1745:TYR:HE2	1.81	0.45
1:A:2140:TRP:CE3	1:A:2149:LEU:HD13	2.52	0.45
1:A:2188:LYS:NZ	1:B:2143:THR:O	2.43	0.45
1:A:2461:LEU:HD23	1:A:2462:ALA:N	2.32	0.45
1:C:1170:PHE:CE1	1:C:1787:LEU:HB2	2.51	0.45
1:C:1716:LEU:HD22	1:C:2051:VAL:HG22	1.99	0.45
1:B:1412:TYR:HD1	1:B:2538:THR:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2140:TRP:CE3	1:B:2149:LEU:HD13	2.52	0.45
1:B:2149:LEU:O	1:B:2153:MET:HG2	2.16	0.45
1:B:2235:TYR:CD2	1:B:2304:MET:HG3	2.51	0.45
1:A:1716:LEU:HD23	1:A:1716:LEU:HA	1.74	0.45
1:C:1716:LEU:HD23	1:C:1716:LEU:HA	1.74	0.45
1:C:2141:VAL:HG21	1:B:2192:GLY:HA3	1.99	0.45
1:B:2289:SER:HA	1:B:2431:VAL:HG22	1.97	0.45
1:A:2235:TYR:CD2	1:A:2304:MET:HG3	2.51	0.45
1:A:2289:SER:HA	1:A:2431:VAL:HG22	1.97	0.45
1:C:1353:ARG:HG2	1:C:2521:LEU:HD21	1.98	0.45
1:C:2140:TRP:CE3	1:C:2149:LEU:HD13	2.52	0.45
1:B:1150:LEU:O	1:B:1154:LYS:HG2	2.17	0.45
1:A:1514:ASP:OD1	1:A:1674:ARG:NH2	2.43	0.45
1:B:2516:THR:O	1:B:2516:THR:HG22	2.17	0.45
1:A:1007:ASN:HB2	1:A:1079:TRP:O	2.17	0.45
1:A:1411:ASP:HB2	1:A:1413:PHE:CD2	2.52	0.45
1:A:2244:GLN:HG2	1:A:2245:GLN:H	1.80	0.45
1:C:1007:ASN:HB2	1:C:1079:TRP:O	2.17	0.45
1:B:2104:ARG:HG2	1:B:2104:ARG:NH2	2.31	0.45
1:A:1090:ASN:OD1	1:A:1091:SER:N	2.50	0.45
1:A:1150:LEU:O	1:A:1154:LYS:HG2	2.17	0.45
1:A:2141:VAL:HG21	1:C:2192:GLY:HA3	1.99	0.45
1:A:2523:GLU:OE2	1:C:2180:GLY:HA2	2.17	0.45
1:C:1411:ASP:HB2	1:C:1413:PHE:CD2	2.52	0.45
1:C:1412:TYR:HD1	1:C:2538:THR:HG21	1.82	0.45
1:B:2461:LEU:HD23	1:B:2462:ALA:N	2.32	0.45
1:A:1182:LEU:HB2	1:A:1745:TYR:HE2	1.81	0.45
1:A:2349:THR:O	1:A:2353:GLN:HG2	2.17	0.45
1:B:2251:PHE:HE2	1:B:2281:ILE:HG22	1.82	0.45
1:B:2455:PRO:C	1:B:2457:SER:H	2.25	0.45
1:A:1177:ILE:O	1:A:1177:ILE:HG22	2.17	0.44
1:A:2180:GLY:HA2	1:B:2523:GLU:OE2	2.16	0.44
1:A:2516:THR:HG22	1:A:2516:THR:O	2.17	0.44
1:C:1090:ASN:OD1	1:C:1091:SER:N	2.50	0.44
1:C:1182:LEU:HB2	1:C:1745:TYR:HE2	1.81	0.44
1:C:1991:ILE:HD11	1:C:2082:TRP:HE1	1.82	0.44
1:B:1036:TYR:CE2	1:B:1040:LEU:HD11	2.52	0.44
1:A:1353:ARG:HG2	1:A:2521:LEU:HD21	1.98	0.44
1:A:1724:ARG:NH2	1:A:1805:LEU:O	2.50	0.44
1:C:2349:THR:O	1:C:2353:GLN:HG2	2.17	0.44
1:B:2297:SER:O	1:B:2300:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2349:THR:O	1:B:2353:GLN:HG2	2.17	0.44
1:A:2297:SER:O	1:A:2300:SER:N	2.51	0.44
1:C:1036:TYR:CE2	1:C:1040:LEU:HD11	2.53	0.44
1:C:2182:LYS:HB2	1:C:2182:LYS:HE3	1.80	0.44
1:C:2251:PHE:HE2	1:C:2281:ILE:HG22	1.82	0.44
1:B:1698:ASN:ND2	1:B:1789:GLN:OE1	2.41	0.44
1:B:1722:ILE:HG23	1:B:1723:PRO:HD2	2.00	0.44
1:A:2455:PRO:C	1:A:2457:SER:H	2.25	0.44
2:E:243:ILE:HD11	1:B:2195:ILE:HD11	2.00	0.44
1:C:1170:PHE:HB2	1:C:1188:CYS:SG	2.58	0.44
1:C:1177:ILE:HG22	1:C:1177:ILE:O	2.17	0.44
2:E:234:LEU:HD11	1:B:2116:HIS:CE1	2.51	0.44
1:C:2516:THR:HG22	1:C:2516:THR:O	2.17	0.44
1:C:2523:GLU:OE2	1:B:2180:GLY:HA2	2.17	0.44
1:A:2295:ARG:HB2	1:C:2295:ARG:NH2	2.21	0.44
1:C:1150:LEU:O	1:C:1154:LYS:HG2	2.17	0.44
1:C:2301:ARG:NH2	1:C:2358:LEU:O	2.33	0.44
1:B:1090:ASN:OD1	1:B:1091:SER:N	2.50	0.44
1:B:1411:ASP:HB2	1:B:1413:PHE:CD2	2.52	0.44
1:B:1987:ASP:OD1	1:B:2082:TRP:NE1	2.51	0.44
1:C:2461:LEU:HD23	1:C:2462:ALA:N	2.32	0.44
1:B:1551:VAL:HG22	1:B:1553:ARG:H	1.81	0.44
1:B:1716:LEU:HA	1:B:1716:LEU:HD23	1.74	0.44
1:B:2250:PRO:HB3	1:B:2282:VAL:HG12	2.00	0.44
1:A:1036:TYR:CE2	1:A:1040:LEU:HD11	2.52	0.44
1:B:1007:ASN:HB2	1:B:1079:TRP:O	2.17	0.44
1:A:2235:TYR:OH	1:A:2303:GLN:HG2	2.18	0.44
1:B:1716:LEU:HD22	1:B:2051:VAL:HG22	1.99	0.44
1:B:2239:PHE:CE1	1:B:2241:MET:HB2	2.53	0.44
1:A:2250:PRO:HB3	1:A:2282:VAL:HG12	2.00	0.43
1:A:2251:PHE:HE2	1:A:2281:ILE:HG22	1.82	0.43
1:A:2536:PRO:O	1:A:2540:ILE:HG13	2.18	0.43
1:C:1724:ARG:NH2	1:C:1805:LEU:O	2.50	0.43
1:C:2239:PHE:CE1	1:C:2241:MET:HB2	2.53	0.43
1:A:1716:LEU:HD22	1:A:2051:VAL:HG22	1.99	0.43
1:A:2239:PHE:CE1	1:A:2241:MET:HB2	2.53	0.43
1:C:2235:TYR:OH	1:C:2303:GLN:HG2	2.18	0.43
1:C:2297:SER:O	1:C:2300:SER:N	2.51	0.43
1:B:1033:TRP:HD1	1:B:1108:TRP:CD1	2.36	0.43
1:B:1991:ILE:HD11	1:B:2082:TRP:HE1	1.82	0.43
1:B:2235:TYR:OH	1:B:2303:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:TRP:HD1	1:A:1108:TRP:CD1	2.36	0.43
1:A:1170:PHE:HB2	1:A:1188:CYS:SG	2.58	0.43
1:B:1170:PHE:HB2	1:B:1188:CYS:SG	2.57	0.43
1:B:1724:ARG:NH2	1:B:1805:LEU:O	2.50	0.43
1:C:1012:LEU:HD21	1:C:1043:PHE:CE2	2.53	0.43
1:B:1012:LEU:HD21	1:B:1043:PHE:CE2	2.54	0.43
1:B:2148:SER:OG	1:B:2149:LEU:N	2.52	0.43
1:B:2519:LEU:HD23	1:B:2519:LEU:HA	1.88	0.43
1:B:2536:PRO:O	1:B:2540:ILE:HG13	2.18	0.43
1:A:1987:ASP:OD1	1:A:2082:TRP:NE1	2.51	0.43
1:C:1033:TRP:HD1	1:C:1108:TRP:CD1	2.36	0.43
1:C:1713:LEU:HD23	1:C:1713:LEU:HA	1.82	0.43
1:A:1141:PRO:HB2	1:A:1304:HIS:CB	2.47	0.43
1:A:1991:ILE:HD11	1:A:2082:TRP:HE1	1.82	0.43
1:A:2148:SER:OG	1:A:2149:LEU:N	2.52	0.43
1:A:2520:GLU:O	1:A:2524:GLU:HG3	2.19	0.43
1:C:1722:ILE:HG23	1:C:1723:PRO:HD2	2.00	0.43
1:C:2455:PRO:C	1:C:2457:SER:H	2.25	0.43
1:B:1177:ILE:HG22	1:B:1177:ILE:O	2.17	0.43
1:A:1012:LEU:HD21	1:A:1043:PHE:CE2	2.53	0.43
1:A:1233:VAL:HG13	1:A:1233:VAL:O	2.19	0.43
1:A:2192:GLY:HA3	1:B:2141:VAL:HG21	2.01	0.43
1:C:2534:ARG:HG2	1:C:2534:ARG:O	2.19	0.43
1:A:1154:LYS:HA	1:A:1154:LYS:HD2	1.83	0.43
1:A:1248:LEU:HD12	1:A:1751:PHE:CD2	2.54	0.43
1:A:2047:LEU:HA	1:A:2097:ILE:HD13	2.01	0.43
1:C:1166:LEU:HD23	1:C:1166:LEU:HA	1.81	0.43
1:C:2250:PRO:HB3	1:C:2282:VAL:HG12	2.00	0.43
1:C:2116:HIS:CE1	2:F:234:LEU:HD11	2.53	0.43
1:C:2536:PRO:O	1:C:2540:ILE:HG13	2.18	0.43
1:B:2182:LYS:HE3	1:B:2182:LYS:HB2	1.80	0.43
1:B:2520:GLU:O	1:B:2524:GLU:HG3	2.19	0.43
1:A:1722:ILE:HG23	1:A:1723:PRO:HD2	2.00	0.43
1:C:1684:ALA:O	1:C:1799:GLN:NE2	2.52	0.43
1:C:2520:GLU:O	1:C:2524:GLU:HG3	2.19	0.43
1:A:1530:MET:SD	1:A:1803:TYR:CZ	3.12	0.42
1:C:1530:MET:SD	1:C:1803:TYR:CZ	3.12	0.42
1:C:1717:TRP:O	1:C:1721:THR:HG23	2.19	0.42
1:C:1987:ASP:OD1	1:C:2082:TRP:NE1	2.51	0.42
1:C:2525:LEU:HD23	1:C:2525:LEU:HA	1.84	0.42
1:B:2393:ASP:C	1:B:2395:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1530:MET:SD	1:B:1803:TYR:CZ	3.12	0.42
2:E:240:CYS:HA	1:B:2191:MET:CE	2.49	0.42
1:C:1028:ALA:O	1:C:1031:ARG:HG3	2.20	0.42
1:C:1233:VAL:HG13	1:C:1233:VAL:O	2.19	0.42
1:C:2027:GLN:HA	1:C:2030:THR:HG22	2.01	0.42
1:C:2191:MET:HE3	1:C:2195:ILE:HD11	2.01	0.42
1:C:2504:LEU:HD12	1:C:2504:LEU:HA	1.84	0.42
1:B:1700:MET:HE3	1:B:2080:GLN:HB3	2.01	0.42
1:B:2534:ARG:O	1:B:2534:ARG:HG2	2.19	0.42
1:A:1010:VAL:O	1:A:1013:HIS:HB2	2.20	0.42
1:A:1028:ALA:O	1:A:1031:ARG:HG3	2.19	0.42
1:A:1670:GLY:CA	1:A:1674:ARG:HE	2.33	0.42
1:A:2504:LEU:HD12	1:A:2504:LEU:HA	1.84	0.42
1:B:1248:LEU:HD12	1:B:1751:PHE:CD2	2.54	0.42
1:A:1530:MET:SD	1:A:1803:TYR:OH	2.70	0.42
1:A:1717:TRP:O	1:A:1721:THR:HG23	2.19	0.42
1:A:2130:PHE:HA	1:A:2133:GLU:HG3	2.02	0.42
1:C:1010:VAL:O	1:C:1013:HIS:HB2	2.20	0.42
1:C:1178:SER:O	1:C:1745:TYR:OH	2.38	0.42
1:C:1700:MET:HE3	1:C:2080:GLN:HB3	2.01	0.42
1:C:2130:PHE:HA	1:C:2133:GLU:HG3	2.02	0.42
1:B:1010:VAL:O	1:B:1013:HIS:HB2	2.19	0.42
1:B:1670:GLY:CA	1:B:1674:ARG:HE	2.33	0.42
1:B:1684:ALA:O	1:B:1799:GLN:NE2	2.52	0.42
1:B:2092:LEU:HD23	1:B:2092:LEU:HA	1.86	0.42
1:A:1178:SER:O	1:A:1745:TYR:OH	2.38	0.42
1:A:2027:GLN:HA	1:A:2030:THR:HG22	2.01	0.42
1:B:1335:ARG:HH21	1:B:1970:TYR:HB2	1.84	0.42
2:F:244:CYS:HB2	2:F:245:PHE:CD1	2.55	0.42
1:A:2116:HIS:HE1	2:D:234:LEU:HD11	1.84	0.42
1:A:2182:LYS:HB2	1:A:2182:LYS:HE3	1.80	0.42
1:A:2534:ARG:O	1:A:2534:ARG:HG2	2.19	0.42
1:C:1138:ASN:HA	1:C:1139:PRO:HD3	1.89	0.42
1:C:2047:LEU:HA	1:C:2097:ILE:HD13	2.01	0.42
1:C:2295:ARG:HB2	1:B:2295:ARG:NH2	2.23	0.42
1:C:2374:LYS:HE3	1:C:2399:LEU:HD21	2.01	0.42
1:C:2393:ASP:C	1:C:2395:GLU:H	2.27	0.42
1:B:1028:ALA:O	1:B:1031:ARG:HG3	2.19	0.42
1:B:1154:LYS:HA	1:B:1154:LYS:HD2	1.83	0.42
1:B:2027:GLN:HA	1:B:2030:THR:HG22	2.01	0.42
1:B:2191:MET:HE3	1:B:2195:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1183:GLY:HA3	1:A:1216:TYR:OH	2.20	0.42
1:A:2131:LEU:HA	1:A:2131:LEU:HD23	1.78	0.42
1:A:2191:MET:HE3	1:A:2195:ILE:HD11	2.01	0.42
1:C:1782:TYR:CE2	1:C:1783:ILE:HG23	2.55	0.42
1:B:1020:ILE:HG23	1:B:1029:ILE:HD12	2.02	0.42
1:B:1717:TRP:O	1:B:1721:THR:HG23	2.19	0.42
1:A:2171:THR:HG21	2:D:238:MET:HE1	2.01	0.42
1:A:2263:PHE:CZ	1:A:2390:LEU:HD23	2.55	0.42
1:C:974:LEU:HG	1:C:975:LEU:HD12	2.02	0.42
1:B:2121:LEU:HD23	1:B:2121:LEU:HA	1.85	0.42
1:B:2130:PHE:HA	1:B:2133:GLU:HG3	2.02	0.42
1:B:2374:LYS:HE3	1:B:2399:LEU:HD21	2.01	0.42
1:A:1020:ILE:HG23	1:A:1029:ILE:HD12	2.02	0.41
1:A:2272:PHE:CZ	1:A:2377:ARG:HD2	2.54	0.41
1:C:1248:LEU:HD12	1:C:1751:PHE:CD2	2.54	0.41
1:C:2209:PHE:O	1:C:2213:ILE:HG12	2.20	0.41
1:B:1183:GLY:HA3	1:B:1216:TYR:OH	2.20	0.41
1:B:2047:LEU:HA	1:B:2097:ILE:HD13	2.01	0.41
1:A:1335:ARG:HD3	1:A:1335:ARG:HA	1.90	0.41
1:A:2209:PHE:O	1:A:2213:ILE:HG12	2.20	0.41
1:A:2353:GLN:OE1	1:A:2353:GLN:HA	2.20	0.41
1:C:2131:LEU:HA	1:C:2131:LEU:HD23	1.78	0.41
1:C:2148:SER:OG	1:C:2149:LEU:N	2.52	0.41
1:C:2238:LEU:HD23	1:C:2430:TRP:CD2	2.55	0.41
1:C:2519:LEU:HA	1:C:2519:LEU:HD23	1.88	0.41
1:B:974:LEU:HG	1:B:975:LEU:HD12	2.02	0.41
1:B:1233:VAL:HG13	1:B:1233:VAL:O	2.19	0.41
1:B:1782:TYR:CE2	1:B:1783:ILE:HG23	2.55	0.41
1:B:2144:ASP:OD1	1:B:2144:ASP:N	2.54	0.41
2:D:244:CYS:HB2	2:D:245:PHE:CD1	2.55	0.41
1:C:1727:LYS:HG3	1:C:1806:TRP:CZ2	2.56	0.41
1:C:2345:ALA:HB3	1:C:2348:SER:HB3	2.02	0.41
1:A:1335:ARG:HH21	1:A:1970:TYR:HB2	1.85	0.41
1:A:1700:MET:HE3	1:A:2080:GLN:HB3	2.01	0.41
1:B:2033:ILE:HD13	1:B:2033:ILE:HA	1.88	0.41
1:B:2209:PHE:O	1:B:2213:ILE:HG12	2.20	0.41
1:B:2264:ASP:C	1:B:2266:TYR:H	2.29	0.41
1:B:2353:GLN:OE1	1:B:2353:GLN:HA	2.20	0.41
2:E:244:CYS:HB2	2:E:245:PHE:CD1	2.55	0.41
1:B:2263:PHE:CZ	1:B:2390:LEU:HD23	2.55	0.41
1:A:1138:ASN:HA	1:A:1139:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1684:ALA:O	1:A:1799:GLN:NE2	2.52	0.41
1:A:2393:ASP:C	1:A:2395:GLU:H	2.27	0.41
1:C:1670:GLY:CA	1:C:1674:ARG:HE	2.33	0.41
1:C:2264:ASP:C	1:C:2266:TYR:H	2.29	0.41
1:C:2353:GLN:HA	1:C:2353:GLN:OE1	2.20	0.41
1:B:2238:LEU:HD23	1:B:2430:TRP:CD2	2.55	0.41
1:B:2345:ALA:HB3	1:B:2348:SER:HB3	2.02	0.41
1:A:2178:PRO:O	1:B:1403:HIS:HB2	2.20	0.41
1:C:993:ILE:O	1:C:997:MET:HG2	2.21	0.41
1:A:1782:TYR:CE2	1:A:1783:ILE:HG23	2.55	0.41
1:C:1072:MET:HG3	1:C:1072:MET:O	2.21	0.41
1:C:1717:TRP:CD1	1:C:1717:TRP:C	2.99	0.41
1:B:1036:TYR:O	1:B:1040:LEU:HG	2.21	0.41
1:B:1717:TRP:CD1	1:B:1717:TRP:C	2.99	0.41
1:A:974:LEU:HG	1:A:975:LEU:HD12	2.02	0.41
1:A:1727:LYS:HG3	1:A:1806:TRP:CZ2	2.56	0.41
1:A:2187:VAL:HG11	2:D:235:GLU:OE1	2.21	0.41
1:A:2222:GLN:NE2	1:A:2282:VAL:HG11	2.36	0.41
1:C:1020:ILE:HG23	1:C:1029:ILE:HD12	2.02	0.41
1:C:2263:PHE:CZ	1:C:2390:LEU:HD23	2.55	0.41
1:B:1072:MET:O	1:B:1072:MET:HG3	2.21	0.41
1:B:1178:SER:O	1:B:1745:TYR:OH	2.38	0.41
1:B:1727:LYS:HG3	1:B:1806:TRP:CZ2	2.56	0.41
1:B:2061:MET:HE1	1:B:2079:ALA:HB1	2.03	0.41
1:C:1183:GLY:HA3	1:C:1216:TYR:OH	2.20	0.41
1:C:2033:ILE:HD13	1:C:2033:ILE:HA	1.88	0.41
1:B:2296:ILE:HD12	1:B:2296:ILE:HA	1.97	0.41
1:A:2238:LEU:HD23	1:A:2430:TRP:CD2	2.56	0.40
1:C:1032:LEU:HD12	1:C:1032:LEU:HA	1.91	0.40
1:C:2061:MET:HE1	1:C:2079:ALA:HB1	2.04	0.40
1:B:1016:TRP:HD1	1:B:1036:TYR:CD1	2.40	0.40
1:A:2264:ASP:C	1:A:2266:TYR:H	2.29	0.40
1:C:2368:ILE:HA	1:C:2369:PRO:HD3	1.93	0.40
1:B:1079:TRP:HE3	1:B:1080:LEU:HD12	1.86	0.40
1:B:1143:PHE:HZ	1:B:1301:TYR:CG	2.39	0.40
1:A:1072:MET:O	1:A:1072:MET:HG3	2.21	0.40
1:A:1548:VAL:HG23	1:A:1549:GLY:N	2.36	0.40
1:A:2374:LYS:HE3	1:A:2399:LEU:HD21	2.01	0.40
1:A:2375:TYR:HA	1:A:2447:VAL:O	2.22	0.40
1:C:1143:PHE:HZ	1:C:1301:TYR:CG	2.39	0.40
1:C:1331:ILE:HD13	1:C:1331:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1335:ARG:HH21	1:C:1970:TYR:HB2	1.85	0.40
1:C:2281:ILE:HD13	1:C:2449:PHE:CE1	2.56	0.40
1:A:993:ILE:O	1:A:997:MET:HG2	2.21	0.40
1:A:2187:VAL:HG23	2:D:236:ILE:CG1	2.52	0.40
1:C:1202:ASP:OD1	1:C:1202:ASP:N	2.55	0.40
1:C:1403:HIS:HB2	1:B:2178:PRO:O	2.22	0.40
1:C:1719:MET:HB3	1:C:2094:ALA:HB1	2.04	0.40
1:C:2166:LYS:NZ	1:C:2501:ASP:OD1	2.41	0.40
1:C:2191:MET:HE1	2:F:240:CYS:HA	2.04	0.40
1:B:1141:PRO:HB2	1:B:1304:HIS:CB	2.47	0.40
1:B:1548:VAL:HG23	1:B:1549:GLY:N	2.37	0.40
1:B:2281:ILE:HD13	1:B:2449:PHE:CE1	2.56	0.40
1:A:1403:HIS:HB2	1:C:2178:PRO:O	2.22	0.40
1:A:1717:TRP:CD1	1:A:1717:TRP:C	2.99	0.40
1:C:1152:MET:HE3	1:C:1665:PHE:CE2	2.54	0.40
1:C:1694:ILE:HG21	1:C:1789:GLN:HA	2.04	0.40
1:B:993:ILE:O	1:B:997:MET:HG2	2.21	0.40
1:B:2162:ILE:HD13	1:B:2162:ILE:HA	1.83	0.40
1:B:2525:LEU:HD23	1:B:2525:LEU:HA	1.84	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	1193/2547 (47%)	1107 (93%)	86 (7%)	0	100	100
1	B	1193/2547 (47%)	1108 (93%)	85 (7%)	0	100	100
1	C	1193/2547 (47%)	1107 (93%)	86 (7%)	0	100	100
2	D	19/247 (8%)	18 (95%)	1 (5%)	0	100	100
2	E	19/247 (8%)	18 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	19/247 (8%)	18 (95%)	1 (5%)	0	100	100
All	All	3636/8382 (43%)	3376 (93%)	260 (7%)	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	983/2246 (44%)	983 (100%)	0	100	100
1	B	983/2246 (44%)	983 (100%)	0	100	100
1	C	983/2246 (44%)	983 (100%)	0	100	100
2	D	20/206 (10%)	20 (100%)	0	100	100
2	E	20/206 (10%)	20 (100%)	0	100	100
2	F	20/206 (10%)	20 (100%)	0	100	100
All	All	3009/7356 (41%)	3009 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1200	GLN
1	A	1217	ASN
1	A	1225	ASN
1	A	1403	HIS
1	A	1408	HIS
1	A	1681	GLN
1	A	2116	HIS
1	A	2254	GLN
1	A	2364	GLN
1	C	1200	GLN
1	C	1217	ASN

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Mol	Chain	Res	Type
1	C	1225	ASN
1	C	1403	HIS
1	C	1408	HIS
1	C	1681	GLN
1	C	2027	GLN
1	C	2116	HIS
1	C	2254	GLN
1	C	2364	GLN
1	B	1200	GLN
1	B	1217	ASN
1	B	1225	ASN
1	B	1403	HIS
1	B	1408	HIS
1	B	1681	GLN
1	B	2116	HIS
1	B	2254	GLN
1	B	2364	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

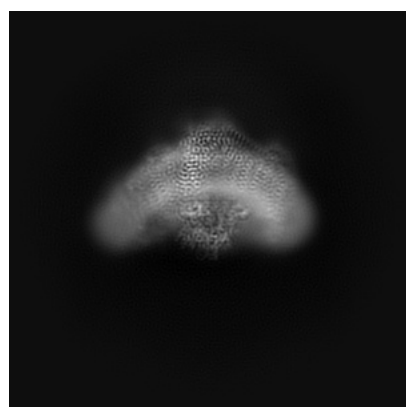
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35577. These allow visual inspection of the internal detail of the map and identification of artifacts.

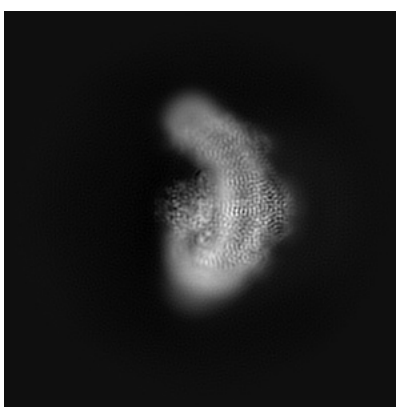
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

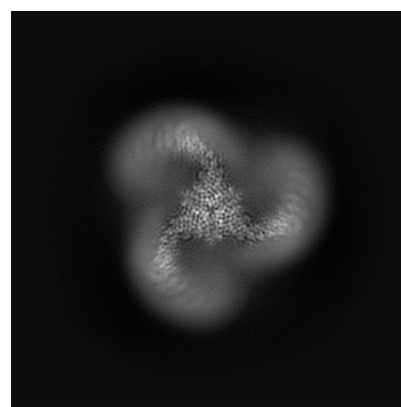
6.1.1 Primary map



X



Y

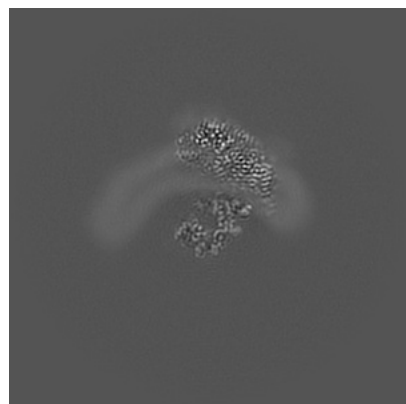


Z

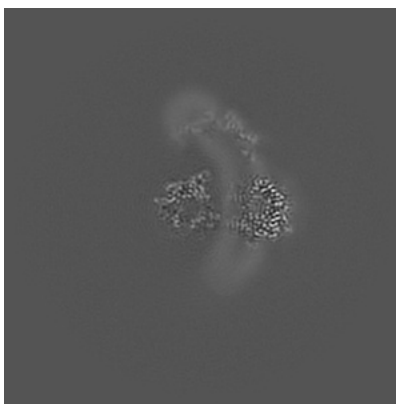
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

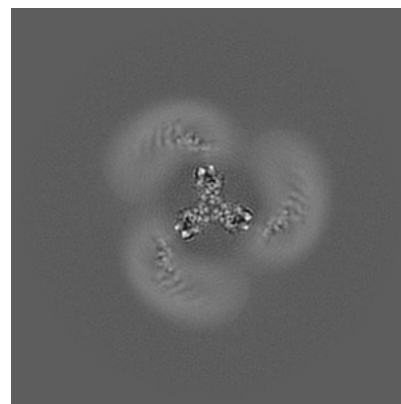
6.2.1 Primary map



X Index: 200



Y Index: 200

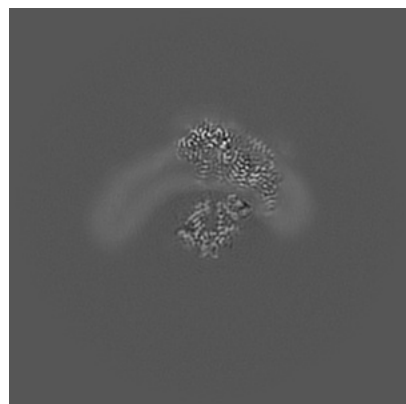


Z Index: 200

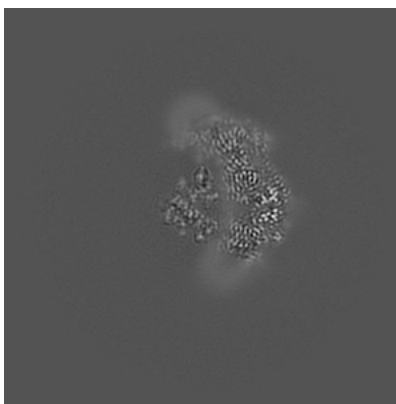
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

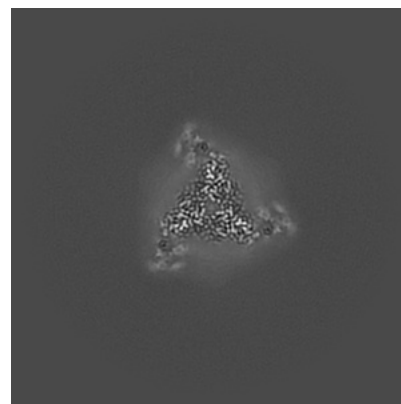
6.3.1 Primary map



X Index: 195



Y Index: 185

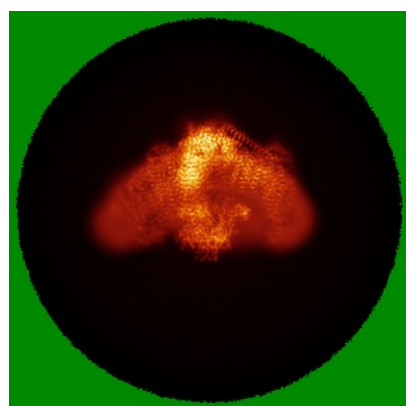


Z Index: 250

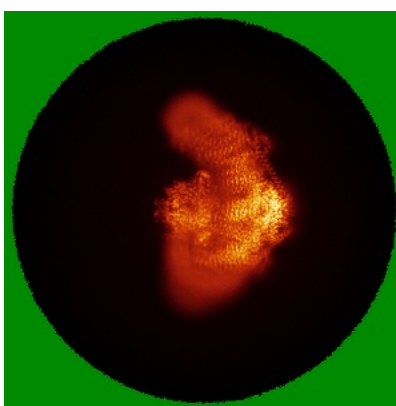
The images above show the largest variance slices of the map in three orthogonal directions.

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

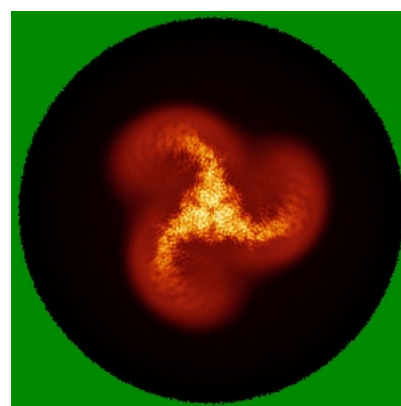
6.4.1 Primary map



X



Y

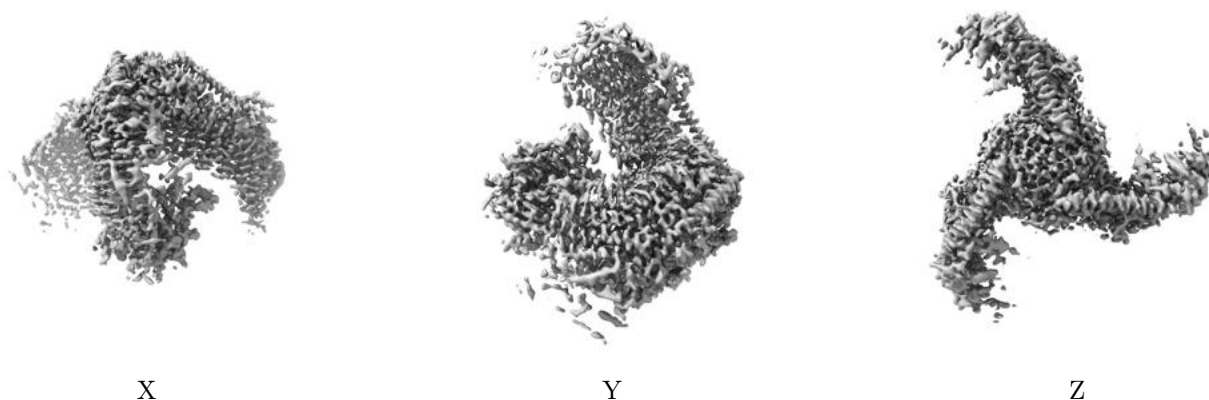


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

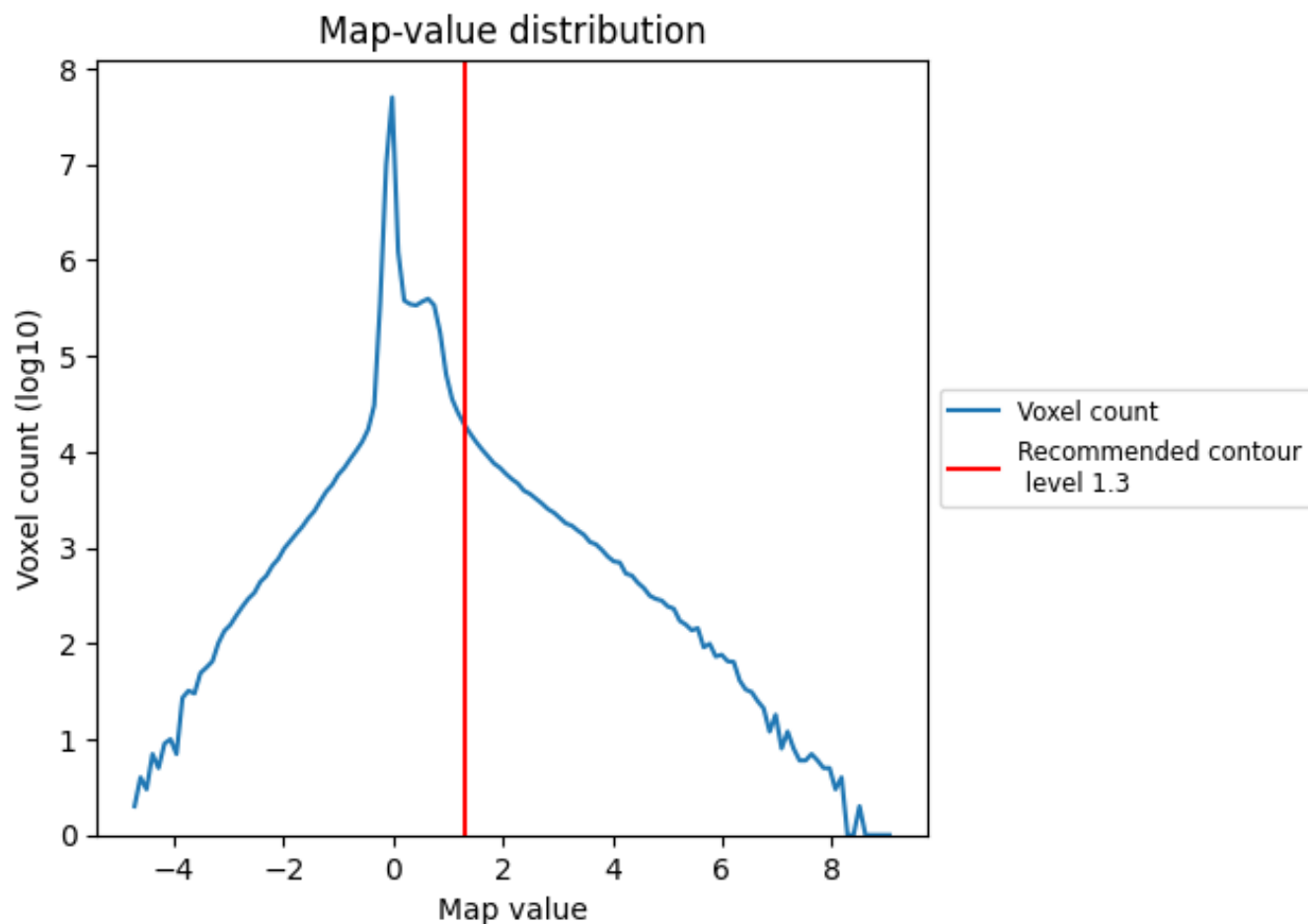
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

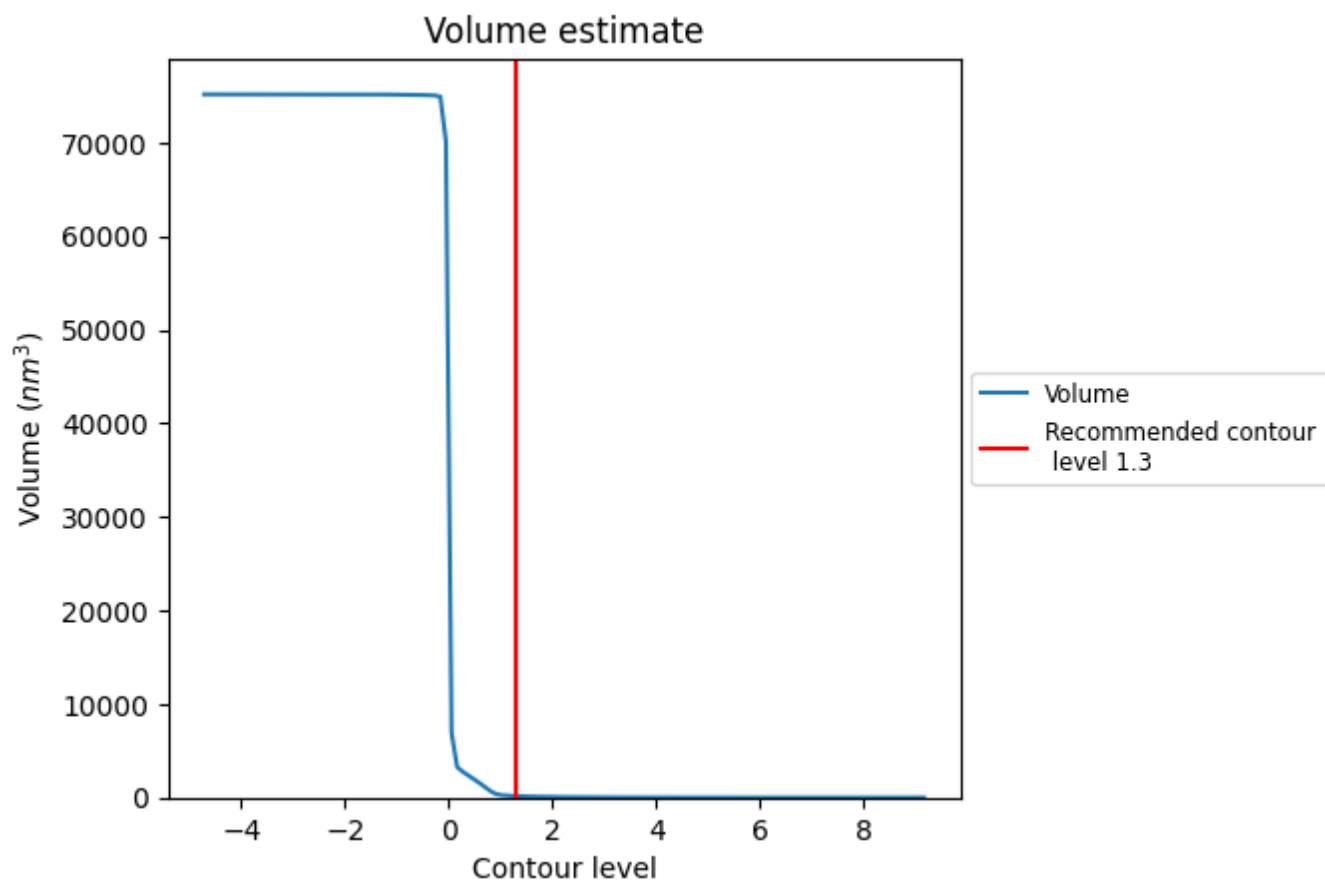
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

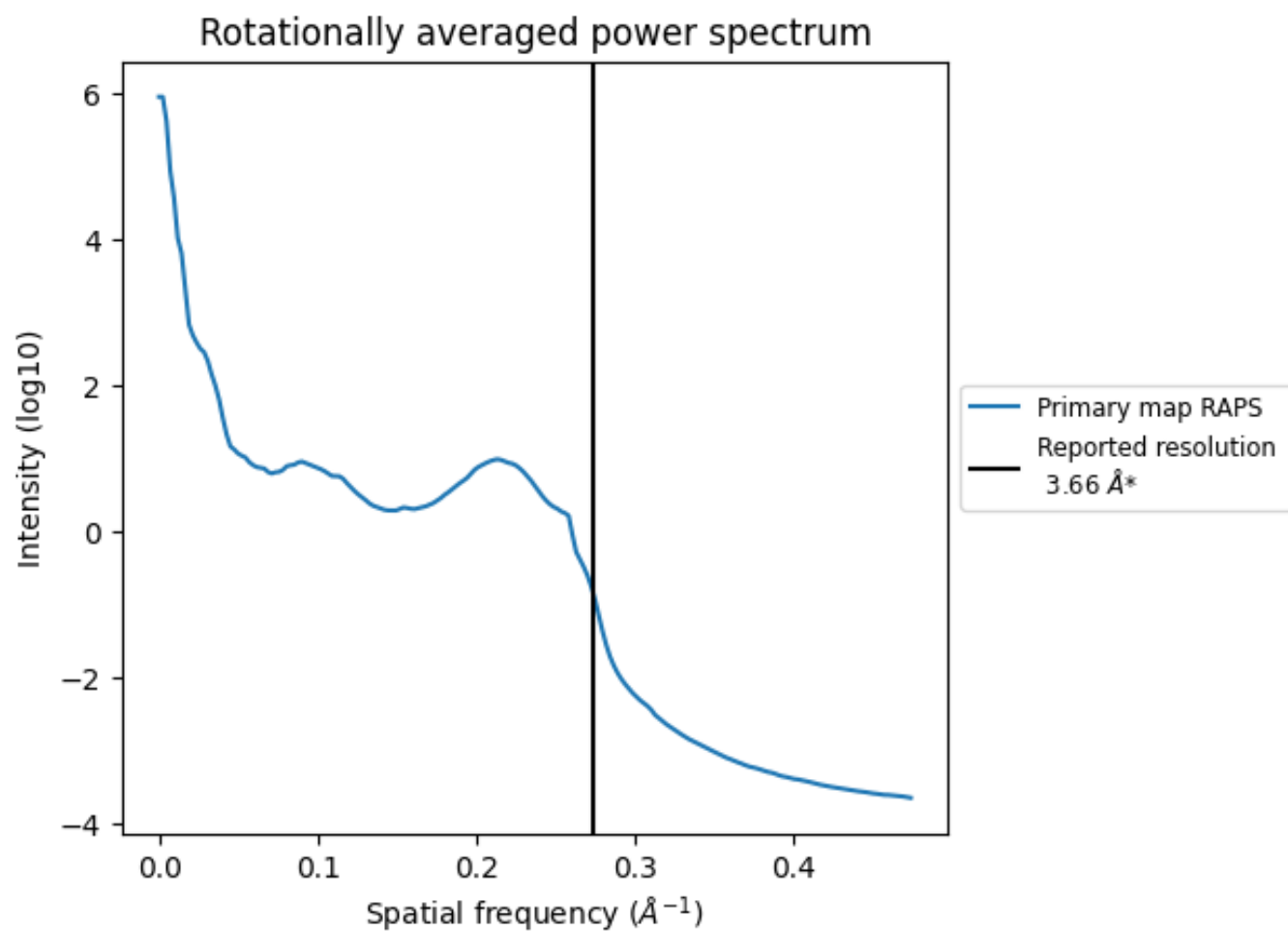
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm^3 ; this corresponds to an approximate mass of 141 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 0.273 Å⁻¹

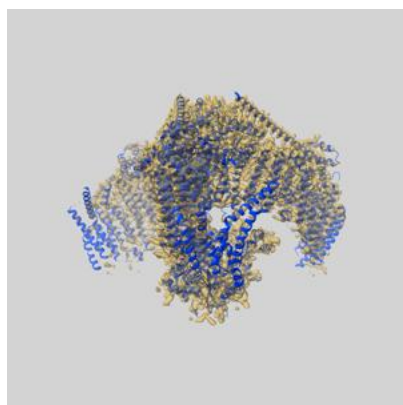
8 Fourier-Shell correlation

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

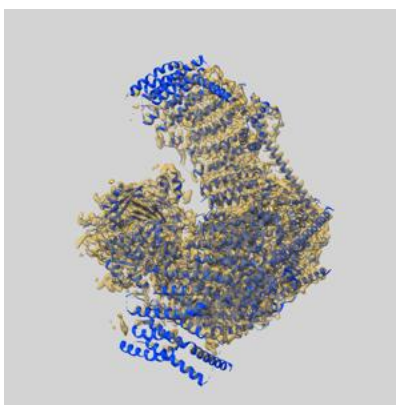
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35577 and PDB model 8IMZ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

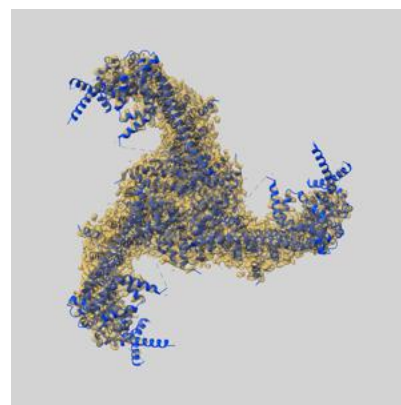
9.1 Map-model overlay [i](#)



X



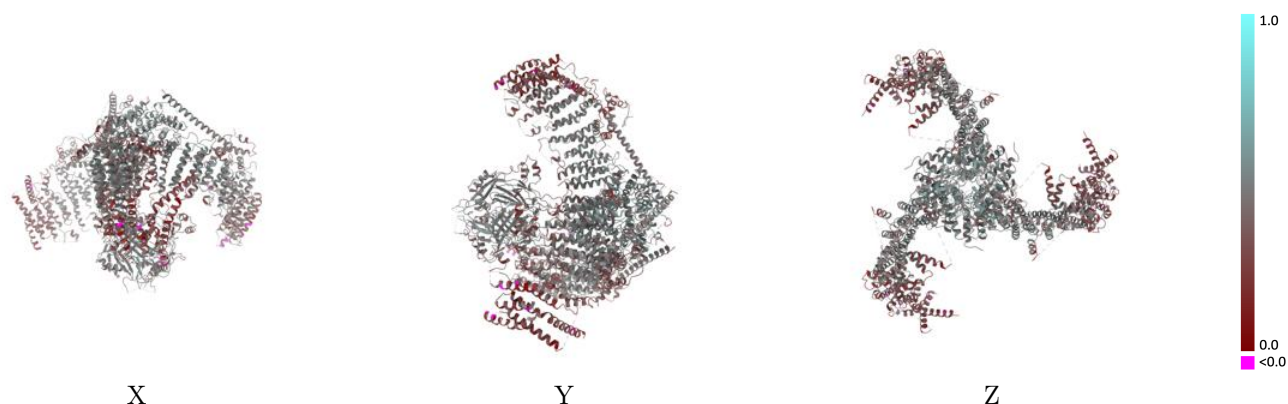
Y



Z

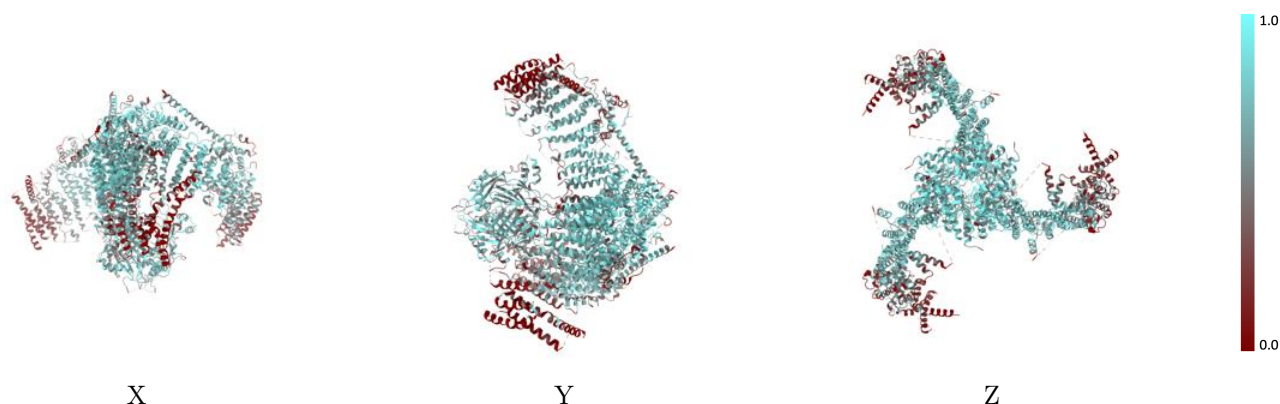
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



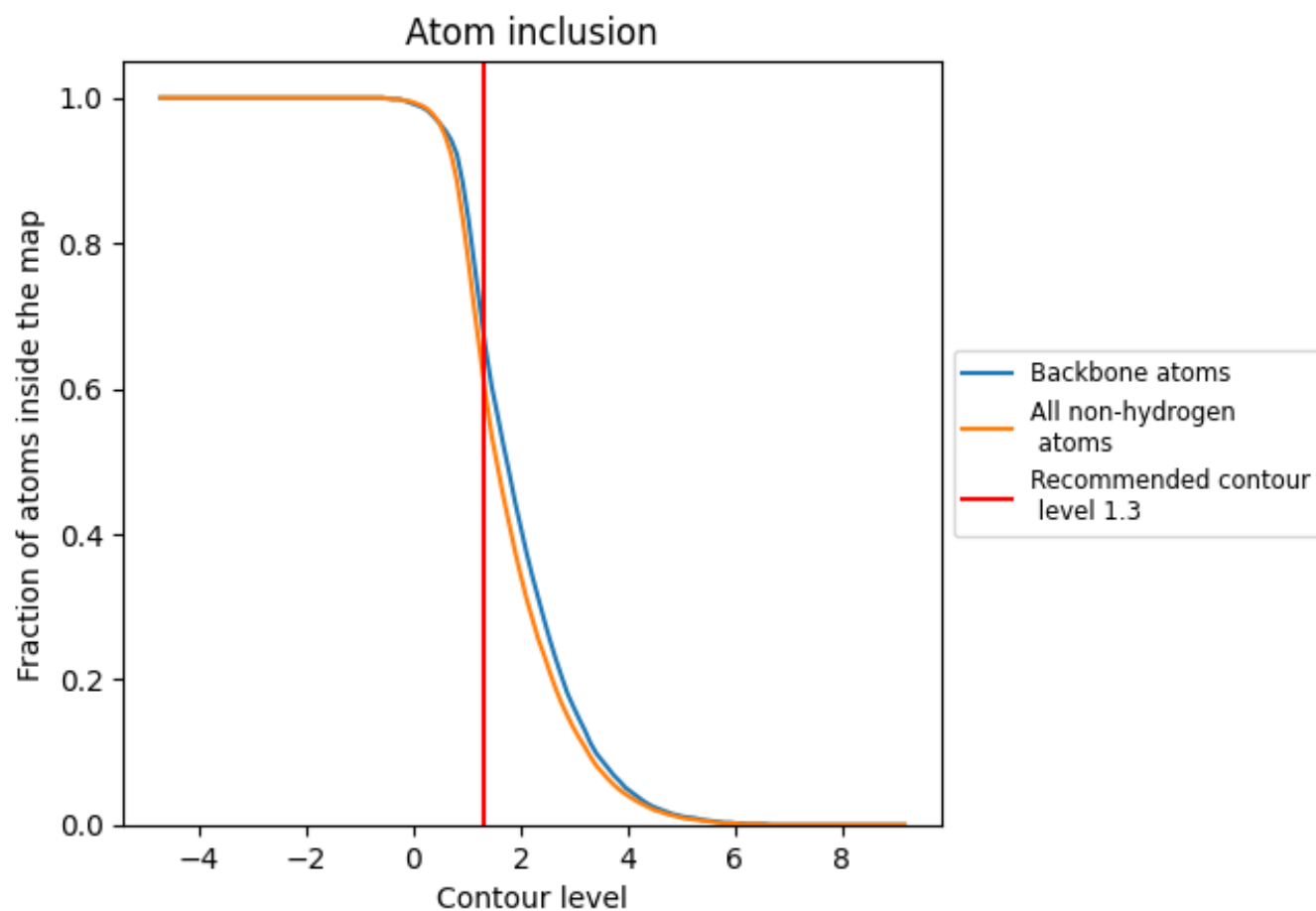
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 62% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6170	0.4240
A	0.6170	0.4220
B	0.6150	0.4240
C	0.6160	0.4240
D	0.6930	0.4750
E	0.7000	0.4780
F	0.6800	0.4710

1.0

0.0

<0.0