



## Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 03:18 PM JST

PDB ID : 7CUN  
EMDB ID : EMD-30473  
Title : The structure of human Integrator-PP2A complex  
Authors : Zheng, H.; Qi, Y.; Liu, W.; Li, J.; Wang, J.; Xu, Y.  
Deposited on : 2020-08-23  
Resolution : 3.50 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

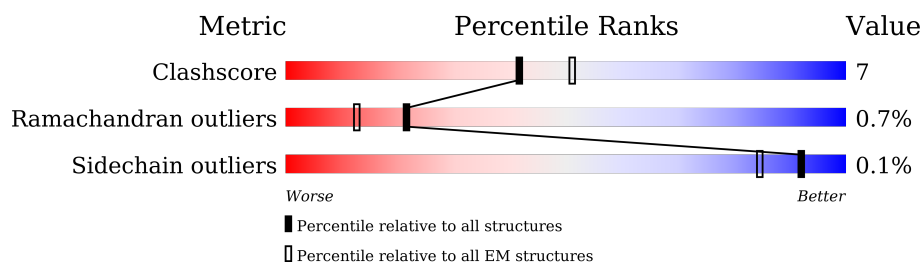
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	2190	
2	B	1204	
3	D	963	
4	E	1019	
5	F	887	
6	G	962	
7	H	995	
8	I	658	

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Mol	Chain	Length	Quality of chain
9	K	600	<div><div></div><div>39%</div><div></div><div>79%</div><div></div><div>18%</div><div></div><div>..</div></div>
10	P	589	<div><div></div><div></div><div></div><div>75%</div><div></div><div>24%</div><div></div><div>.</div></div>
11	Q	309	<div><div></div><div></div><div></div><div>83%</div><div></div><div>12%</div><div></div><div>5%</div></div>
12	U	594	<div><div></div><div>45%</div><div></div><div>51%</div><div></div><div></div><div>49%</div></div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 57642 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 Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	730	Total	C	N	O	S	0	0
			4653	2872	876	880	25		

- Molecule 2 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1058	Total	C	N	O	S	0	0
			7541	4765	1318	1407	51		

- Molecule 3 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	827	Total	C	N	O	S	0	0
			5942	3743	1049	1119	31		

- Molecule 4 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	796	Total	C	N	O	S	0	0
			5288	3321	989	963	15		

- Molecule 5 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	534	Total	C	N	O	S	0	0
			3822	2417	669	715	21		

- Molecule 6 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	895	Total	C	N	O	S	0	0
			6826	4319	1196	1270	41		

- Molecule 7 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	912	Total	C	N	O	S	0	0
			6657	4216	1178	1231	32		

- Molecule 8 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	624	Total	C	N	O	S	0	0
			4701	3004	778	888	31		

- Molecule 9 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	588	Total	C	N	O	S	0	0
			3792	2347	709	721	15		

- Molecule 10 is a protein called PP2A-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	P	582	Total	C	N	O	S	Se	0	0
			4535	2881	764	863	14	13		

- Molecule 11 is a protein called PP2A-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	293	Total	C	N	O	S	0	0
			2366	1497	405	449	15		

- Molecule 12 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	303	Total	C	N	O	0	0
			1515	909	303	303		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	K	2	Total	Zn	0
			2	2	

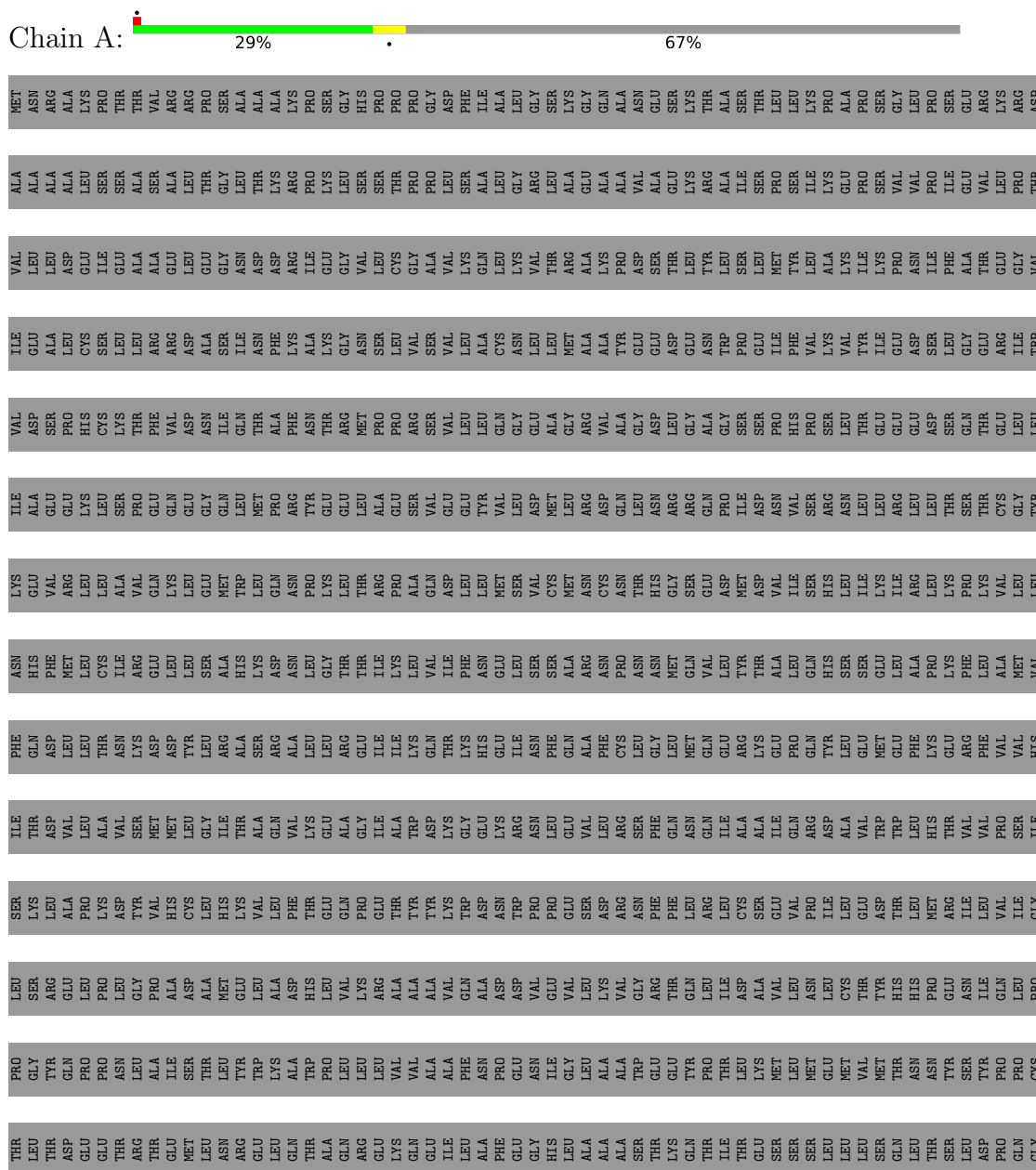
- Molecule 14 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
14	Q	2	Total	Mn	0
			2	2	

### 3 Residue-property plots

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

- Molecule 1: Integrator complex subunit 1





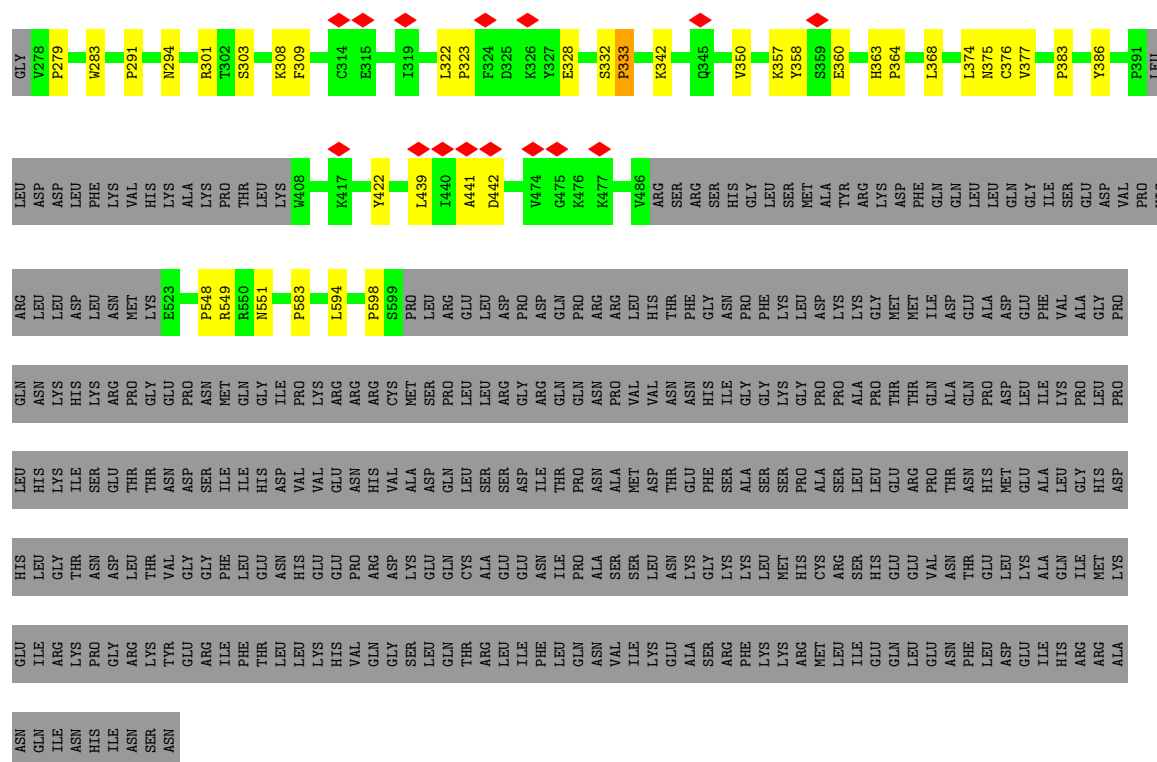
Chain B:  75% 13% 12%





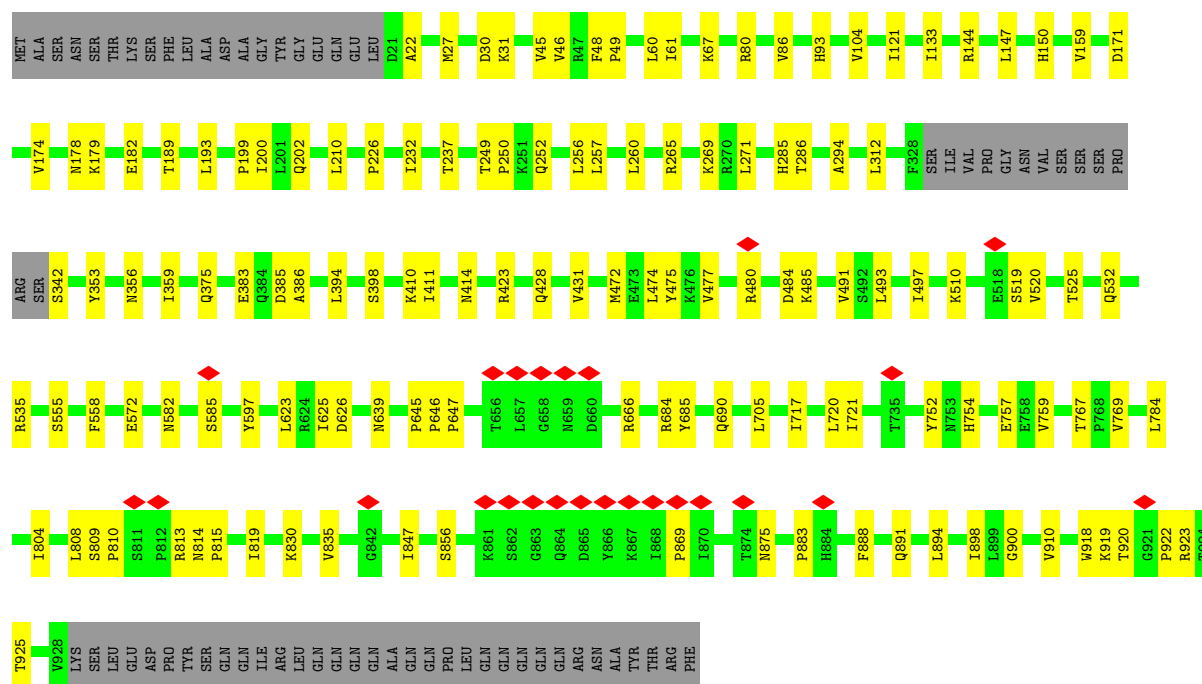






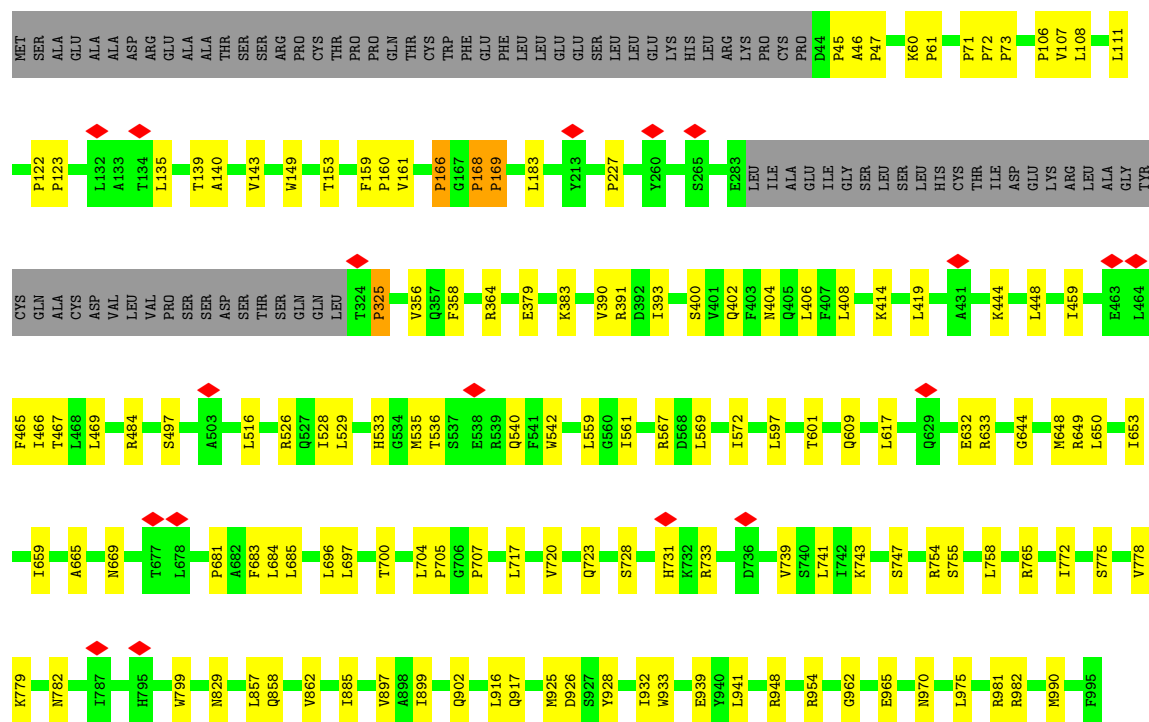
• Molecule 6: Integrator complex subunit 7

Chain G: 79% 14% 7%

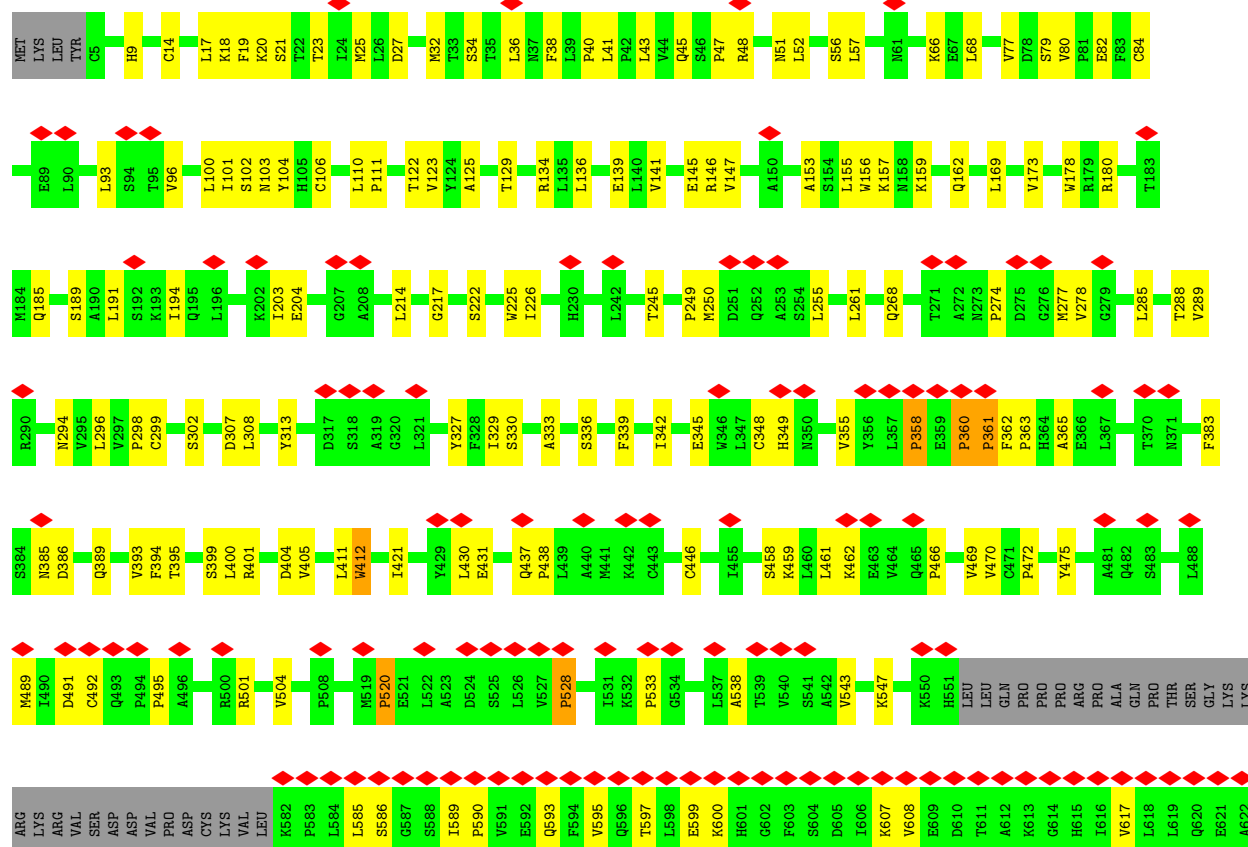


• Molecule 7: Integrator complex subunit 8

Chain H: 78% 13% 8%



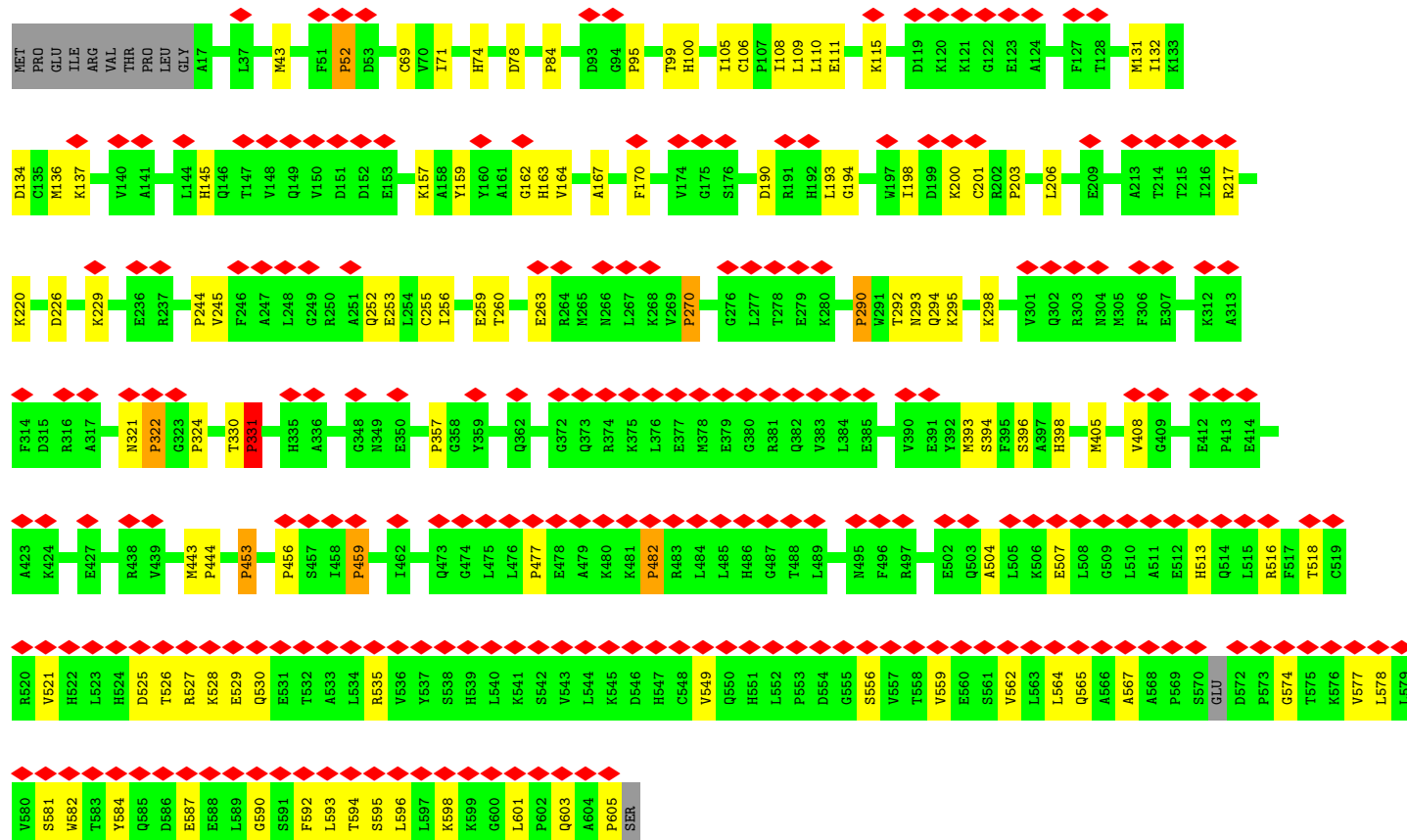
- Molecule 8: Integrator complex subunit 9





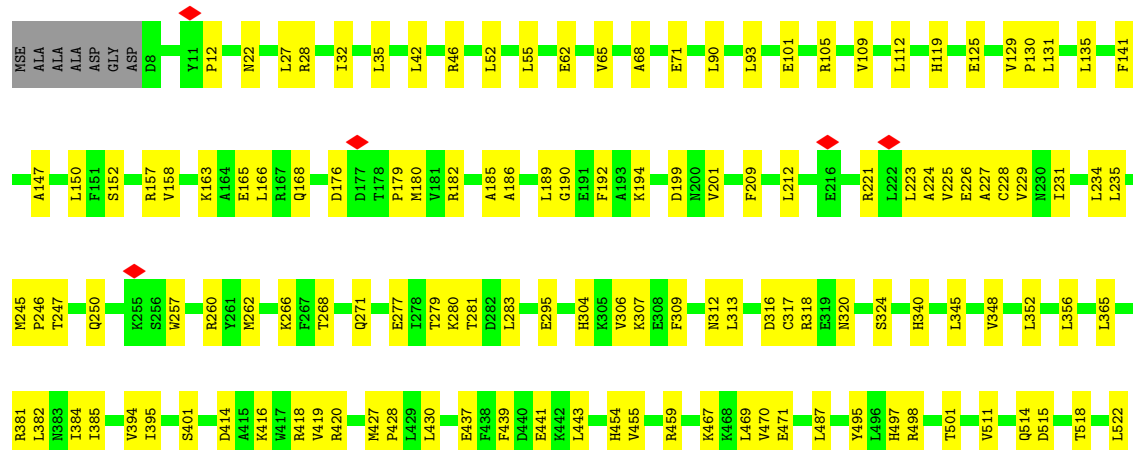
• Molecule 9: Integrator complex subunit 11

Chain K: 39% 79% 18% ..



• Molecule 10: PP2A-A

Chain P: 75% 24% ..





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68378	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 ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size ( $\text{\AA}$ )	506.39996, 506.39996, 506.39996	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.055, 1.055, 1.055	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, ZN

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	0.24	0/4706	0.51	20/6443 (0.3%)
2	B	0.24	0/7651	0.45	9/10439 (0.1%)
3	D	0.24	0/6039	0.47	10/8229 (0.1%)
4	E	0.25	0/5387	0.50	22/7365 (0.3%)
5	F	0.25	0/3903	0.51	9/5328 (0.2%)
6	G	0.23	0/6937	0.40	4/9397 (0.0%)
7	H	0.24	0/6765	0.45	13/9207 (0.1%)
8	I	0.25	0/4807	0.54	7/6562 (0.1%)
9	K	0.25	0/3843	0.59	16/5249 (0.3%)
10	P	0.23	0/4596	0.41	0/6218
11	Q	0.24	0/2423	0.40	0/3285
All	All	0.24	0/57057	0.48	110/77722 (0.1%)

There are no bond length outliers.

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	331	PRO	N-CA-CB	6.96	111.66	103.30
9	K	482	PRO	N-CA-CB	6.92	111.60	103.30
2	B	189	PRO	N-CA-CB	6.89	111.57	103.30
7	H	325	PRO	N-CA-CB	6.88	111.55	103.30
8	I	360	PRO	N-CA-CB	6.87	111.55	103.30
7	H	168	PRO	N-CA-CB	6.81	111.47	103.30
4	E	740	PRO	N-CA-CB	6.80	111.46	103.30
7	H	166	PRO	N-CA-CB	6.78	111.44	103.30
4	E	742	PRO	N-CA-CB	6.73	111.37	103.30
9	K	453	PRO	N-CA-CB	6.72	111.37	103.30
7	H	169	PRO	N-CA-CB	6.69	111.33	103.30
1	A	1816	PRO	N-CA-CB	6.69	111.33	103.30
9	K	52	PRO	N-CA-CB	6.68	111.32	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	827	PRO	N-CA-CB	6.65	111.28	103.30
8	I	520	PRO	N-CA-CB	6.62	111.24	103.30
5	F	333	PRO	N-CA-CB	6.49	111.09	103.30
5	F	242	PRO	N-CA-CB	6.41	110.99	103.30
7	H	122	PRO	N-CA-CB	6.39	110.97	103.30
8	I	358	PRO	N-CA-CB	6.37	110.94	103.30
9	K	244	PRO	N-CA-CB	6.33	110.90	103.30
1	A	1593	PRO	N-CA-CB	6.25	110.79	103.30
9	K	444	PRO	N-CA-CB	6.22	110.77	103.30
1	A	1818	PRO	N-CA-CB	6.22	110.76	103.30
4	E	283	PRO	N-CA-CB	6.21	110.75	103.30
3	D	812	PRO	N-CA-CB	6.19	110.73	103.30
9	K	456	PRO	N-CA-CB	6.19	110.72	103.30
3	D	814	PRO	N-CA-CB	6.18	110.72	103.30
4	E	205	PRO	N-CA-CB	6.15	110.68	103.30
9	K	477	PRO	N-CA-CB	6.15	110.68	103.30
3	D	63	PRO	N-CA-CB	6.07	110.58	103.30
5	F	583	PRO	N-CA-CB	6.06	110.57	103.30
5	F	250	PRO	N-CA-CB	6.04	110.55	103.30
3	D	834	PRO	N-CA-CB	6.02	110.52	103.30
4	E	465	PRO	N-CA-CB	6.01	110.51	103.30
9	K	605	PRO	N-CA-CB	5.99	110.49	103.30
1	A	1579	PRO	N-CA-CB	5.98	110.48	103.30
5	F	240	PRO	N-CA-CB	5.97	110.46	103.30
4	E	349	PRO	N-CA-CB	5.95	110.44	103.30
2	B	258	PRO	N-CA-CB	5.95	110.44	103.30
3	D	49	PRO	N-CA-CB	5.94	110.42	103.30
5	F	279	PRO	N-CA-CB	5.93	110.41	103.30
8	I	533	PRO	N-CA-CB	5.92	110.41	103.30
9	K	290	PRO	N-CA-CB	5.91	110.39	103.30
3	D	33	PRO	N-CA-CB	5.91	110.39	103.30
2	B	193	PRO	N-CA-CB	5.86	110.34	103.30
6	G	645	PRO	N-CA-CB	5.86	110.33	103.30
8	I	528	PRO	N-CA-CB	5.84	110.31	103.30
9	K	357	PRO	N-CA-CB	5.83	110.30	103.30
5	F	244	PRO	N-CA-CB	5.81	110.27	103.30
1	A	1476	PRO	N-CA-CB	5.81	110.27	103.30
2	B	57	PRO	N-CA-CB	5.79	110.25	103.30
9	K	324	PRO	N-CA-CB	5.78	110.24	103.30
4	E	457	PRO	N-CA-CB	5.74	110.19	103.30
1	A	1575	PRO	N-CA-CB	5.74	110.19	103.30
4	E	277	PRO	N-CA-CB	5.74	110.18	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	869	PRO	N-CA-CB	5.73	110.18	103.30
2	B	40	PRO	N-CA-CB	5.72	110.17	103.30
8	I	361	PRO	N-CA-CB	5.71	110.16	103.30
1	A	1811	PRO	N-CA-CB	5.71	110.15	103.30
1	A	1416	PRO	N-CA-CB	5.71	110.15	103.30
4	E	365	PRO	N-CA-CB	5.71	110.15	103.30
4	E	366	PRO	N-CA-CB	5.71	110.15	103.30
4	E	221	PRO	N-CA-CB	5.71	110.15	103.30
2	B	275	PRO	N-CA-CB	5.70	110.14	103.30
4	E	235	PRO	N-CA-CB	5.70	110.14	103.30
4	E	428	PRO	N-CA-CB	5.70	110.14	103.30
2	B	47	PRO	N-CA-CB	5.70	110.14	103.30
7	H	61	PRO	N-CA-CB	5.70	110.14	103.30
7	H	47	PRO	N-CA-CB	5.70	110.13	103.30
7	H	73	PRO	N-CA-CB	5.70	110.14	103.30
7	H	227	PRO	N-CA-CB	5.70	110.14	103.30
2	B	171	PRO	N-CA-CB	5.69	110.13	103.30
3	D	107	PRO	N-CA-CB	5.69	110.13	103.30
1	A	1399	PRO	N-CA-CB	5.69	110.13	103.30
1	A	1554	PRO	N-CA-CB	5.69	110.13	103.30
1	A	1434	PRO	N-CA-CB	5.69	110.13	103.30
4	E	416	PRO	N-CA-CB	5.68	110.12	103.30
1	A	1599	PRO	N-CA-CB	5.68	110.11	103.30
4	E	275	PRO	N-CA-CB	5.68	110.12	103.30
7	H	72	PRO	N-CA-CB	5.67	110.11	103.30
4	E	332	PRO	N-CA-CB	5.67	110.11	103.30
1	A	1470	PRO	N-CA-CB	5.67	110.11	103.30
5	F	598	PRO	N-CA-CB	5.67	110.11	103.30
7	H	45	PRO	N-CA-CB	5.67	110.11	103.30
1	A	1396	PRO	N-CA-CB	5.67	110.10	103.30
1	A	1920	PRO	N-CA-CB	5.67	110.10	103.30
4	E	271	PRO	N-CA-CB	5.67	110.10	103.30
8	I	363	PRO	N-CA-CB	5.67	110.10	103.30
7	H	71	PRO	N-CA-CB	5.67	110.10	103.30
1	A	1573	PRO	N-CA-CB	5.66	110.09	103.30
1	A	1538	PRO	N-CA-CB	5.66	110.09	103.30
2	B	219	PRO	N-CA-CB	5.66	110.09	103.30
4	E	339	PRO	N-CA-CB	5.65	110.08	103.30
4	E	289	PRO	N-CA-CB	5.64	110.07	103.30
6	G	647	PRO	N-CA-CB	5.63	110.06	103.30
1	A	1972	PRO	N-CA-CB	5.63	110.06	103.30
9	K	322	PRO	N-CA-CB	5.63	110.06	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1447	PRO	N-CA-CB	5.63	110.06	103.30
4	E	280	PRO	N-CA-CB	5.62	110.05	103.30
5	F	260	PRO	N-CA-CB	5.62	110.05	103.30
1	A	1984	PRO	N-CA-CB	5.62	110.04	103.30
4	E	380	PRO	N-CA-CB	5.62	110.04	103.30
6	G	646	PRO	N-CA-CB	5.61	110.03	103.30
9	K	84	PRO	N-CA-CB	5.61	110.03	103.30
9	K	459	PRO	N-CA-CB	5.61	110.03	103.30
3	D	86	PRO	N-CA-CB	5.60	110.03	103.30
7	H	123	PRO	N-CA-CB	5.58	109.99	103.30
9	K	270	PRO	N-CA-CB	5.57	109.98	103.30
4	E	464	PRO	N-CA-CB	5.56	109.98	103.30
3	D	142	PRO	N-CA-CB	5.51	109.91	103.30

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	4653	0	3696	41	0
2	B	7541	0	7031	90	0
3	D	5942	0	5402	98	0
4	E	5288	0	4612	51	0
5	F	3822	0	3415	49	0
6	G	6826	0	6830	78	0
7	H	6657	0	6168	80	0
8	I	4701	0	4503	112	0
9	K	3792	0	3006	64	0
10	P	4535	0	4637	87	0
11	Q	2366	0	2269	22	0
12	U	1515	0	322	0	0
13	K	2	0	0	0	0
14	Q	2	0	0	0	0
All	All	57642	0	51891	723	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 7.

All (723) 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)
11:Q:107:TYR:HB3	11:Q:110:ARG:HB2	1.67	0.75
8:I:41:LEU:HD22	8:I:84:CYS:HB2	1.72	0.72
8:I:101:ILE:HD13	8:I:125:ALA:HB2	1.71	0.71
9:K:528:LYS:HD3	9:K:530:GLN:H	1.54	0.71
1:A:2141:LEU:HD11	1:A:2173:PRO:HB3	1.72	0.70
6:G:159:VAL:HG13	6:G:200:ILE:HD11	1.74	0.70
7:H:778:VAL:O	7:H:782:ASN:ND2	2.25	0.69
3:D:172:GLN:O	3:D:176:ASN:ND2	2.25	0.69
6:G:720:LEU:HD22	6:G:759:VAL:HG23	1.73	0.69
2:B:588:LEU:HD22	2:B:703:LEU:HA	1.75	0.68
4:E:777:GLN:HE22	7:H:404:ASN:HD21	1.40	0.67
9:K:162:GLY:HA3	9:K:194:GLY:H	1.59	0.67
10:P:12:PRO:HG2	10:P:42:LEU:HD21	1.74	0.67
9:K:549:VAL:HG22	9:K:559:VAL:HA	1.76	0.67
5:F:357:LYS:HG2	5:F:358:TYR:H	1.60	0.67
9:K:226:ASP:HA	9:K:229:LYS:HG2	1.77	0.67
3:D:669:LEU:HB3	3:D:700:ILE:HD11	1.78	0.66
3:D:538:ASP:HB3	3:D:541:ASP:HB2	1.77	0.65
6:G:375:GLN:HE22	6:G:423:ARG:HH12	1.42	0.65
11:Q:28:VAL:HG11	11:Q:142:VAL:HG13	1.79	0.65
5:F:236:GLU:HB2	5:F:308:LYS:HG2	1.79	0.64
6:G:572:GLU:OE1	6:G:597:TYR:OH	2.12	0.64
8:I:639:ASN:HD21	9:K:521:VAL:HA	1.63	0.64
9:K:74:HIS:NE2	9:K:78:ASP:OD1	2.25	0.64
10:P:135:LEU:HG	10:P:147:ALA:HB2	1.79	0.64
6:G:808:LEU:HG	6:G:810:PRO:HD3	1.79	0.64
4:E:802:PRO:HG2	7:H:408:LEU:HD23	1.79	0.64
9:K:198:ILE:HG23	9:K:200:LYS:H	1.62	0.64
3:D:534:THR:HG22	3:D:535:ALA:H	1.63	0.63
10:P:279:THR:HA	10:P:283:LEU:HB2	1.80	0.63
10:P:90:LEU:HD13	10:P:131:LEU:HD11	1.81	0.63
9:K:203:PRO:HG2	9:K:206:LEU:HD21	1.81	0.63
8:I:82:GLU:HG3	8:I:178:TRP:HE3	1.63	0.63
2:B:1039:LEU:HD23	2:B:1042:ILE:HD12	1.80	0.62
8:I:294:ASN:HB3	8:I:389:GLN:HB3	1.79	0.62
7:H:535:MET:HG3	7:H:536:THR:HG23	1.81	0.62
7:H:741:LEU:HG	7:H:754:ARG:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:330:SER:HB3	8:I:333:ALA:HB2	1.81	0.62
3:D:784:MET:HG3	3:D:785:PRO:HD3	1.80	0.62
5:F:12:ALA:HB3	7:H:939:GLU:HG3	1.81	0.62
2:B:874:MET:HG2	2:B:993:VAL:HG13	1.81	0.62
8:I:626:ILE:HD11	8:I:647:LEU:HD11	1.82	0.62
3:D:424:ILE:HG22	3:D:426:GLU:H	1.65	0.61
8:I:296:LEU:HD23	8:I:298:PRO:HD3	1.83	0.61
10:P:125:GLU:HG2	10:P:158:VAL:HG12	1.83	0.61
2:B:362:GLU:HA	2:B:365:VAL:HG22	1.83	0.61
2:B:1104:LEU:HB3	2:B:1192:THR:HG21	1.83	0.61
5:F:322:LEU:HD12	5:F:323:PRO:HD2	1.83	0.61
8:I:597:THR:HA	8:I:600:LYS:HE2	1.83	0.61
4:E:920:LEU:HD13	4:E:924:LEU:HG	1.82	0.60
3:D:423:GLU:HA	3:D:428:ARG:HH21	1.66	0.60
7:H:516:LEU:HB2	7:H:528:ILE:HG21	1.83	0.60
3:D:208:ASP:HB3	3:D:211:VAL:HG23	1.84	0.59
3:D:417:VAL:HG11	3:D:447:ASP:HB3	1.83	0.59
10:P:176:ASP:O	10:P:182:ARG:NH1	2.35	0.59
6:G:804:ILE:HG12	6:G:835:VAL:HG12	1.85	0.59
7:H:857:LEU:HD11	7:H:990:MET:HG2	1.85	0.59
10:P:572:ASP:HB3	10:P:575:VAL:HG22	1.84	0.59
7:H:448:LEU:O	7:H:484:ARG:NH1	2.36	0.59
3:D:49:PRO:O	8:I:501:ARG:NH2	2.36	0.59
9:K:294:GLN:HG2	9:K:295:LYS:HD3	1.83	0.59
5:F:88:LEU:HD21	5:F:196:ILE:HD13	1.84	0.59
6:G:260:LEU:O	6:G:269:LYS:NZ	2.36	0.59
8:I:302:SER:HB2	8:I:336:SER:HB2	1.84	0.59
3:D:850:THR:OG1	3:D:890:HIS:O	2.21	0.59
2:B:1191:ARG:O	2:B:1195:GLU:HG2	2.02	0.59
3:D:376:CYS:SG	3:D:377:GLY:N	2.76	0.59
3:D:403:GLN:HE21	3:D:437:LYS:HB3	1.67	0.59
3:D:917:TYR:CG	3:D:921:ALA:HB3	2.38	0.59
9:K:134:ASP:HA	9:K:137:LYS:HE2	1.85	0.59
2:B:527:THR:HG22	2:B:528:GLU:H	1.68	0.58
4:E:925:GLY:HA2	4:E:928:HIS:CD2	2.38	0.58
7:H:649:ARG:NH1	7:H:684:LEU:O	2.35	0.58
8:I:595:VAL:O	8:I:599:GLU:HG2	2.02	0.58
4:E:750:HIS:HD2	4:E:752:GLY:H	1.49	0.58
8:I:17:LEU:HD22	8:I:268:GLN:HE21	1.69	0.58
2:B:924:GLU:O	2:B:928:ASN:ND2	2.36	0.58
5:F:99:LEU:HD11	5:F:125:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:994:ARG:HD3	7:H:160:PRO:HD2	1.85	0.58
7:H:419:LEU:HD11	7:H:459:ILE:HA	1.84	0.58
8:I:159:LYS:HG3	8:I:162:GLN:HE21	1.68	0.58
1:A:1864:MET:SD	1:A:2112:GLN:NE2	2.76	0.58
2:B:1040:ASP:OD1	2:B:1072:LYS:NZ	2.37	0.57
3:D:912:ARG:NH2	3:D:926:CYS:O	2.36	0.57
4:E:641:PRO:HD2	7:H:858:GLN:HE21	1.69	0.57
3:D:674:LEU:HD12	3:D:804:ARG:HD2	1.86	0.57
4:E:391:ALA:HB2	4:E:437:ARG:HH12	1.69	0.57
7:H:444:LYS:HG3	7:H:469:LEU:HD11	1.86	0.57
9:K:567:ALA:HB3	9:K:577:VAL:HG13	1.86	0.57
3:D:222:LEU:HD12	3:D:227:LEU:HG	1.86	0.57
11:Q:65:LEU:HD22	11:Q:96:THR:HG23	1.87	0.57
2:B:365:VAL:HG12	2:B:410:GLN:HG2	1.87	0.57
6:G:104:VAL:HG21	6:G:133:ILE:HG21	1.85	0.57
8:I:650:LEU:HA	8:I:653:LYS:HE3	1.87	0.57
10:P:487:LEU:HD22	10:P:524:THR:HG21	1.86	0.57
11:Q:94:VAL:HG23	11:Q:146:PHE:HE2	1.70	0.57
6:G:875:ASN:HD22	6:G:894:LEU:HB2	1.70	0.57
8:I:103:ASN:HB3	8:I:222:SER:HA	1.87	0.57
10:P:260:ARG:NH2	10:P:295:GLU:OE1	2.38	0.56
2:B:344:LEU:HD13	2:B:353:THR:HG21	1.87	0.56
3:D:676:GLU:HG2	3:D:691:ASP:HA	1.87	0.56
10:P:152:SER:HB3	10:P:192:PHE:HA	1.87	0.56
7:H:561:ILE:HB	7:H:567:ARG:HB3	1.87	0.56
3:D:383:LEU:O	3:D:391:ARG:NE	2.38	0.56
6:G:356:ASN:HB3	6:G:359:ILE:HG22	1.88	0.56
7:H:526:ARG:HG3	7:H:569:LEU:HD21	1.86	0.56
9:K:556:SER:OG	9:K:564:LEU:O	2.23	0.56
3:D:851:LEU:HB3	3:D:854:VAL:HG21	1.87	0.56
5:F:291:PRO:HG3	5:F:422:TYR:HE2	1.71	0.56
7:H:700:THR:HG21	7:H:717:LEU:HD22	1.87	0.56
8:I:261:LEU:HD13	8:I:469:VAL:HG12	1.87	0.56
8:I:296:LEU:HD12	8:I:412:TRP:HZ2	1.71	0.56
8:I:45:GLN:HG3	8:I:77:VAL:HB	1.87	0.55
7:H:665:ALA:O	7:H:669:ASN:ND2	2.39	0.55
8:I:23:THR:HG22	8:I:32:MET:HB3	1.89	0.55
8:I:48:ARG:NH2	8:I:147:VAL:O	2.39	0.55
2:B:530:VAL:O	2:B:534:HIS:ND1	2.33	0.55
10:P:28:ARG:O	10:P:32:ILE:HG12	2.06	0.55
9:K:584:TYR:HA	9:K:587:GLU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:271:GLN:HE22	10:P:312:ASN:HB2	1.70	0.55
9:K:259:GLU:O	9:K:263:GLU:HG2	2.06	0.55
3:D:170:CYS:HA	3:D:173:LEU:HB2	1.89	0.55
3:D:172:GLN:HB3	3:D:217:LYS:NZ	2.21	0.55
11:Q:168:GLY:O	11:Q:239:ARG:NH2	2.33	0.55
3:D:724:HIS:HE1	3:D:776:PHE:HB3	1.72	0.55
5:F:57:GLU:O	5:F:61:ALA:N	2.39	0.55
10:P:194:LYS:HD3	10:P:234:LEU:HD11	1.89	0.55
5:F:357:LYS:HB3	5:F:360:GLU:HG2	1.89	0.55
8:I:639:ASN:HD21	9:K:521:VAL:HG12	1.72	0.54
8:I:153:ALA:HB1	8:I:156:TRP:HE1	1.71	0.54
1:A:1704:VAL:HG12	1:A:1706:ARG:H	1.71	0.54
2:B:341:ARG:HH12	2:B:400:GLY:HA2	1.71	0.54
7:H:965:GLU:OE1	7:H:981:ARG:NH1	2.40	0.54
9:K:405:MET:HA	9:K:408:VAL:HG22	1.89	0.54
2:B:586:THR:HB	2:B:587:PRO:HD3	1.90	0.54
3:D:610:SER:OG	3:D:650:GLN:NE2	2.40	0.54
4:E:586:GLN:NE2	4:E:631:ILE:O	2.40	0.54
5:F:103:ARG:NH2	5:F:109:ASP:OD1	2.40	0.54
8:I:437:GLN:HG3	8:I:438:PRO:HD3	1.90	0.54
11:Q:82:PHE:HB2	11:Q:113:ILE:HG22	1.89	0.54
1:A:2089:GLN:HG2	1:A:2124:THR:HG21	1.88	0.54
8:I:100:LEU:HD21	8:I:225:TRP:HB2	1.90	0.54
9:K:105:ILE:HD12	9:K:108:ILE:HD11	1.89	0.54
8:I:217:GLY:HA3	8:I:249:PRO:HA	1.88	0.54
8:I:385:ASN:OD1	8:I:386:ASP:N	2.41	0.54
7:H:681:PRO:HA	7:H:685:LEU:HD13	1.88	0.54
4:E:648:VAL:HG12	4:E:691:LEU:HD12	1.90	0.54
8:I:590:PRO:HG2	8:I:593:GLN:HB3	1.89	0.54
10:P:42:LEU:O	10:P:46:ARG:NE	2.37	0.54
10:P:277:GLU:O	10:P:281:THR:HG23	2.07	0.54
9:K:217:ARG:NH2	9:K:394:SER:OG	2.40	0.54
10:P:101:GLU:O	10:P:105:ARG:NH2	2.41	0.54
2:B:660:GLU:HG2	2:B:717:ASN:HD21	1.71	0.54
4:E:916:GLU:HB3	7:H:364:ARG:HD2	1.91	0.54
2:B:858:LEU:HD13	2:B:861:LEU:HD12	1.91	0.53
5:F:283:TRP:HE1	5:F:323:PRO:HG2	1.72	0.53
3:D:687:LEU:HG	3:D:688:LYS:H	1.73	0.53
6:G:174:VAL:HG12	6:G:210:LEU:HD21	1.90	0.53
6:G:813:ARG:HB2	6:G:819:ILE:HD11	1.90	0.53
10:P:385:ILE:HG21	10:P:419:VAL:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:153:ALA:O	8:I:157:LYS:NZ	2.40	0.53
5:F:267:LEU:N	5:F:328:GLU:O	2.41	0.53
7:H:139:THR:O	7:H:143:VAL:HG23	2.09	0.53
8:I:214:LEU:HD21	8:I:250:MET:HG2	1.90	0.53
4:E:501:GLN:NE2	7:H:497:SER:OG	2.42	0.53
5:F:25:LEU:HD22	5:F:82:ALA:HB2	1.89	0.53
6:G:883:PRO:HB3	6:G:888:PHE:HB3	1.89	0.53
8:I:585:LEU:HG	9:K:513:HIS:HB3	1.90	0.53
10:P:538:PHE:HB3	10:P:575:VAL:HG12	1.90	0.53
8:I:421:ILE:HD11	8:I:446:CYS:HB3	1.90	0.53
10:P:320:ASN:O	10:P:324:SER:OG	2.25	0.53
1:A:2097:GLU:OE1	1:A:2100:ARG:NH1	2.42	0.53
2:B:422:THR:HG22	2:B:424:ALA:H	1.72	0.53
3:D:624:LEU:HD22	3:D:635:LEU:HD22	1.91	0.53
5:F:34:THR:HA	5:F:37:LYS:HG2	1.90	0.53
9:K:256:ILE:O	9:K:260:THR:HG23	2.08	0.53
11:Q:159:VAL:HB	11:Q:163:ILE:HB	1.90	0.53
3:D:644:GLN:OE1	3:D:665:ARG:NH2	2.40	0.53
6:G:510:LYS:H	6:G:510:LYS:HD2	1.74	0.53
8:I:245:THR:HA	8:I:249:PRO:HB3	1.91	0.53
1:A:2171:MET:HG3	1:A:2173:PRO:HD3	1.91	0.53
1:A:1716:PRO:HD2	1:A:1718:LYS:HZ2	1.73	0.53
1:A:1718:LYS:NZ	3:D:567:ASP:OD2	2.42	0.53
8:I:146:ARG:NH1	8:I:404:ASP:OD1	2.42	0.53
7:H:597:LEU:O	7:H:601:THR:HG23	2.09	0.52
3:D:620:ARG:NH1	6:G:285:HIS:O	2.42	0.52
5:F:7:LEU:HB3	5:F:127:THR:HA	1.91	0.52
6:G:428:GLN:HA	6:G:431:VAL:HG12	1.91	0.52
2:B:325:GLN:OE1	2:B:325:GLN:N	2.42	0.52
6:G:147:LEU:HD23	6:G:179:LYS:HD3	1.92	0.52
7:H:917:GLN:O	7:H:948:ARG:NH2	2.36	0.52
8:I:66:LYS:HB3	8:I:68:LEU:HD23	1.92	0.52
8:I:627:GLN:HG2	8:I:634:HIS:HB3	1.90	0.52
11:Q:170:LEU:HD23	11:Q:224:ILE:HG22	1.91	0.52
7:H:970:ASN:HB2	7:H:975:LEU:HG	1.92	0.52
5:F:309:PHE:HA	5:F:350:VAL:HA	1.91	0.52
10:P:141:PHE:HB3	10:P:180:MSE:HE3	1.91	0.52
2:B:734:THR:HB	6:G:199:PRO:HB2	1.91	0.52
3:D:460:SER:HB2	3:D:463:ILE:HB	1.92	0.52
9:K:601:LEU:O	9:K:603:GLN:NE2	2.43	0.52
4:E:921:PRO:HD2	4:E:924:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:898:ILE:HG22	6:G:900:GLY:H	1.75	0.51
8:I:329:ILE:HD11	8:I:383:PHE:HZ	1.76	0.51
9:K:559:VAL:N	9:K:562:VAL:O	2.44	0.51
1:A:1656:PHE:HB3	6:G:226:PRO:HG2	1.92	0.51
10:P:572:ASP:OD1	10:P:573:VAL:N	2.43	0.51
8:I:307:ASP:OD2	8:I:308:LEU:N	2.44	0.51
2:B:589:HIS:HB3	2:B:592:LEU:HG	1.92	0.51
3:D:906:ALA:HB1	3:D:933:GLU:HB3	1.92	0.51
5:F:9:ASP:OD1	5:F:10:THR:N	2.44	0.51
6:G:767:THR:HG23	6:G:769:VAL:HG12	1.92	0.51
8:I:9:HIS:HB3	8:I:504:VAL:HG22	1.92	0.51
8:I:134:ARG:HE	8:I:191:LEU:HD13	1.75	0.51
8:I:636:ILE:HG13	9:K:518:THR:HB	1.91	0.51
3:D:578:ASP:HB3	6:G:144:ARG:HH12	1.76	0.51
9:K:111:GLU:O	9:K:115:LYS:HG2	2.11	0.51
2:B:857:PRO:HG2	2:B:885:LEU:HD23	1.93	0.51
8:I:9:HIS:NE2	8:I:25:MET:SD	2.83	0.51
7:H:149:TRP:O	7:H:153:THR:HG23	2.11	0.51
8:I:36:LEU:HD13	8:I:106:CYS:HA	1.93	0.51
4:E:489:LEU:HD22	4:E:531:GLU:HG3	1.93	0.50
6:G:410:LYS:O	6:G:414:ASN:ND2	2.43	0.50
2:B:582:CYS:SG	2:B:583:GLU:N	2.84	0.50
10:P:190:GLY:O	10:P:194:LYS:NZ	2.44	0.50
10:P:313:LEU:O	10:P:318:ARG:NH2	2.36	0.50
3:D:428:ARG:O	3:D:432:ILE:HG12	2.11	0.50
3:D:724:HIS:CE1	3:D:776:PHE:HB3	2.47	0.50
8:I:348:CYS:SG	8:I:349:HIS:N	2.85	0.50
9:K:582:TRP:HE1	9:K:587:GLU:HG2	1.75	0.50
10:P:112:LEU:HB3	10:P:150:LEU:HD11	1.93	0.50
10:P:381:ARG:HA	10:P:384:ILE:HG22	1.93	0.50
3:D:577:ARG:NH2	3:D:584:VAL:O	2.42	0.50
3:D:869:ASP:OD1	3:D:870:GLY:N	2.42	0.50
5:F:439:LEU:HG	5:F:441:ALA:H	1.76	0.50
3:D:806:SER:OG	3:D:807:ALA:N	2.45	0.50
4:E:851:PHE:HA	4:E:857:LEU:HD12	1.94	0.50
9:K:565:GLN:O	9:K:578:LEU:HD12	2.11	0.50
1:A:1708:TRP:HE3	1:A:1711:ARG:HD2	1.77	0.50
2:B:807:ARG:HH12	2:B:871:PRO:HD2	1.76	0.50
2:B:878:LEU:HB3	2:B:1000:LEU:HD22	1.93	0.50
5:F:7:LEU:HD21	5:F:55:PHE:HE1	1.77	0.50
8:I:627:GLN:HB2	8:I:629:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:69:CYS:HA	9:K:95:PRO:HB2	1.94	0.50
1:A:2139:THR:HG22	1:A:2142:ARG:HH21	1.77	0.50
8:I:461:LEU:HD22	8:I:466:PRO:HG3	1.92	0.50
10:P:356:LEU:HD12	10:P:365:LEU:HD11	1.93	0.50
1:A:1718:LYS:HD2	1:A:1718:LYS:N	2.27	0.50
9:K:396:SER:HB2	9:K:398:HIS:HD2	1.75	0.50
3:D:902:ALA:HA	3:D:936:PRO:HG2	1.94	0.49
8:I:313:TYR:HE2	8:I:365:ALA:HA	1.77	0.49
8:I:626:ILE:HG12	8:I:635:ILE:HG23	1.93	0.49
10:P:416:LYS:NZ	11:Q:290:ASP:OD2	2.42	0.49
8:I:399:SER:OG	8:I:400:LEU:N	2.44	0.49
1:A:1669:SER:OG	1:A:1671:PRO:HD2	2.12	0.49
2:B:652:LEU:HD22	2:B:692:LEU:HD12	1.94	0.49
5:F:30:GLY:O	5:F:34:THR:HG23	2.11	0.49
4:E:965:GLU:HG2	4:E:966:ARG:HG3	1.94	0.49
7:H:648:MET:HG3	7:H:649:ARG:H	1.78	0.49
10:P:427:MSE:HE2	10:P:469:LEU:HD11	1.93	0.49
11:Q:261:SER:HA	11:Q:273:ALA:HB1	1.95	0.49
8:I:327:TYR:HB2	8:I:393:VAL:HG12	1.94	0.49
8:I:491:ASP:OD1	8:I:492:CYS:N	2.44	0.49
10:P:119:HIS:O	10:P:157:ARG:NH1	2.45	0.49
10:P:280:LYS:NZ	10:P:316:ASP:OD1	2.41	0.49
2:B:781:LEU:HD13	2:B:785:GLU:HB2	1.93	0.49
4:E:817:VAL:HG22	4:E:877:LEU:HD13	1.94	0.49
10:P:257:TRP:HA	10:P:260:ARG:HE	1.77	0.49
4:E:813:ALA:HB1	4:E:874:CYS:HB2	1.94	0.49
6:G:45:VAL:HA	6:G:48:PHE:HD2	1.78	0.49
6:G:519:SER:OG	6:G:520:VAL:N	2.46	0.49
5:F:210:VAL:HG11	5:F:216:LEU:HD12	1.94	0.49
7:H:885:ILE:HG23	7:H:897:VAL:HG13	1.95	0.49
5:F:111:TYR:OH	5:F:163:ARG:NH1	2.46	0.48
6:G:411:ILE:HA	6:G:414:ASN:HD21	1.78	0.48
7:H:108:LEU:HD22	7:H:183:LEU:HA	1.95	0.48
7:H:925:MET:SD	7:H:925:MET:N	2.76	0.48
9:K:159:TYR:OH	9:K:201:CYS:SG	2.67	0.48
10:P:394:VAL:HG23	10:P:395:ILE:HG13	1.95	0.48
2:B:660:GLU:HG3	2:B:713:LEU:HD22	1.96	0.48
8:I:102:SER:OG	8:I:103:ASN:N	2.43	0.48
8:I:411:LEU:HD22	8:I:412:TRP:CE3	2.47	0.48
8:I:470:VAL:HA	8:I:495:PRO:HG2	1.94	0.48
10:P:538:PHE:HZ	11:Q:77:ASP:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:PRO:HG2	2:B:677:LYS:HB2	1.96	0.48
3:D:229:LEU:HD12	3:D:262:LEU:HD11	1.94	0.48
5:F:83:GLU:OE1	7:H:954:ARG:NH2	2.46	0.48
8:I:79:SER:OG	8:I:80:VAL:N	2.46	0.48
1:A:1707:ILE:HG23	2:B:991:ARG:HG2	1.95	0.48
1:A:2171:MET:O	2:B:1130:GLN:NE2	2.46	0.48
4:E:897:THR:OG1	4:E:934:LEU:O	2.31	0.48
9:K:132:ILE:O	9:K:136:MET:HG2	2.13	0.48
9:K:593:LEU:HA	9:K:596:LEU:HD23	1.94	0.48
8:I:339:PHE:HA	8:I:342:ILE:HG22	1.94	0.48
11:Q:129:PHE:HZ	11:Q:146:PHE:HD2	1.60	0.48
11:Q:201:SER:O	11:Q:239:ARG:NH2	2.47	0.48
1:A:2100:ARG:HE	1:A:2139:THR:HG21	1.79	0.48
2:B:449:GLU:O	2:B:452:MET:HG3	2.14	0.48
3:D:693:ALA:HB1	3:D:732:LEU:HD21	1.95	0.48
2:B:369:PRO:O	2:B:373:VAL:HG22	2.14	0.48
3:D:708:GLU:HB2	3:D:722:ILE:HD13	1.95	0.48
7:H:529:LEU:O	7:H:533:HIS:ND1	2.44	0.48
10:P:437:GLU:O	10:P:441:GLU:HB2	2.13	0.48
7:H:617:LEU:HD22	7:H:659:ILE:HG12	1.95	0.48
7:H:696:LEU:HD22	7:H:717:LEU:HD13	1.95	0.48
8:I:274:PRO:O	8:I:278:VAL:HG23	2.14	0.48
8:I:458:SER:O	8:I:462:LYS:HG2	2.14	0.48
2:B:211:LEU:O	6:G:666:ARG:NH1	2.43	0.48
10:P:225:VAL:HG21	10:P:262:MSE:HB3	1.96	0.48
1:A:1785:GLY:O	1:A:1789:GLN:NE2	2.45	0.48
7:H:106:PRO:HB2	7:H:111:LEU:HB2	1.96	0.48
7:H:705:PRO:O	7:H:707:PRO:HD3	2.13	0.48
8:I:298:PRO:HD2	8:I:421:ILE:O	2.14	0.48
5:F:194:SER:OG	5:F:195:ALA:N	2.47	0.47
1:A:1759:GLN:HG3	1:A:1797:ARG:HH12	1.79	0.47
2:B:1042:ILE:HD11	2:B:1064:LEU:HD12	1.97	0.47
2:B:1083:VAL:HA	2:B:1086:THR:HG22	1.96	0.47
4:E:770:GLN:O	4:E:771:GLU:HG2	2.14	0.47
6:G:472:MET:HE2	6:G:497:ILE:HD13	1.95	0.47
6:G:690:GLN:OE1	6:G:919:LYS:NZ	2.41	0.47
10:P:229:VAL:HG11	10:P:266:LYS:HG2	1.96	0.47
3:D:553:ASN:O	3:D:556:LYS:NZ	2.40	0.47
7:H:739:VAL:HB	7:H:743:LYS:HB2	1.95	0.47
5:F:174:ARG:HH12	5:F:192:ASP:HB2	1.79	0.47
3:D:693:ALA:HA	3:D:696:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:852:GLU:HG2	3:D:889:ARG:HG2	1.95	0.47
4:E:489:LEU:HD21	4:E:522:LEU:HD22	1.96	0.47
7:H:406:LEU:O	7:H:414:LYS:NZ	2.47	0.47
3:D:256:ILE:HA	3:D:259:VAL:HG12	1.95	0.47
9:K:526:THR:HG22	9:K:574:GLY:HA2	1.96	0.47
9:K:590:GLY:O	9:K:594:THR:N	2.38	0.47
10:P:495:TYR:HA	10:P:498:ARG:HE	1.80	0.47
2:B:53:ALA:HB1	2:B:56:ALA:HB3	1.97	0.47
2:B:1125:LEU:HD13	2:B:1193:VAL:HG22	1.97	0.47
3:D:865:VAL:HG22	3:D:911:VAL:HG23	1.96	0.47
7:H:135:LEU:HD11	7:H:140:ALA:HB2	1.96	0.47
7:H:159:PHE:HB3	7:H:161:VAL:HG23	1.95	0.47
7:H:390:VAL:HA	7:H:393:ILE:HG22	1.96	0.47
8:I:169:LEU:HD11	8:I:431:GLU:HB2	1.97	0.47
9:K:525:ASP:N	9:K:525:ASP:OD1	2.47	0.47
9:K:592:PHE:O	9:K:595:SER:OG	2.20	0.47
10:P:382:LEU:HD22	10:P:418:ARG:HB2	1.95	0.47
4:E:575:LEU:HD11	4:E:613:LEU:HD13	1.96	0.47
4:E:927:MET:HG3	4:E:942:LEU:HD13	1.97	0.47
5:F:156:GLU:HG2	5:F:157:LEU:HD12	1.96	0.47
9:K:245:VAL:O	9:K:331:PRO:N	2.48	0.47
3:D:464:ARG:O	3:D:468:HIS:ND1	2.48	0.47
3:D:897:TYR:HB3	8:I:51:ASN:HD21	1.80	0.47
3:D:842:VAL:HA	3:D:899:SER:HB3	1.96	0.47
4:E:456:SER:HA	4:E:505:LEU:HD11	1.97	0.47
6:G:27:MET:O	6:G:31:LYS:HG2	2.15	0.47
6:G:178:ASN:O	6:G:182:GLU:HG3	2.14	0.47
10:P:307:LYS:HA	10:P:352:LEU:HD21	1.97	0.47
2:B:724:VAL:HG11	6:G:121:ILE:HD11	1.97	0.46
10:P:32:ILE:HA	10:P:35:LEU:HG	1.97	0.46
1:A:1786:CYS:HA	1:A:1789:GLN:HE21	1.79	0.46
1:A:2072:GLU:OE1	1:A:2075:ARG:NH2	2.49	0.46
2:B:671:ALA:O	2:B:672:MET:HG3	2.15	0.46
3:D:747:LEU:HA	3:D:750:MET:HE3	1.97	0.46
5:F:165:ASP:N	5:F:165:ASP:OD1	2.46	0.46
2:B:692:LEU:HA	2:B:695:GLN:HG2	1.97	0.46
5:F:24:TYR:OH	5:F:175:LEU:O	2.30	0.46
6:G:814:ASN:HB2	6:G:815:PRO:HD3	1.97	0.46
8:I:625:LEU:HG	8:I:636:ILE:HB	1.97	0.46
2:B:602:SER:O	2:B:602:SER:OG	2.33	0.46
7:H:644:GLY:O	7:H:648:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:852:ASP:OD1	2:B:852:ASP:N	2.47	0.46
10:P:165:GLU:O	10:P:168:GLN:HG3	2.16	0.46
10:P:307:LYS:HB2	10:P:348:VAL:HG22	1.97	0.46
11:Q:36:LYS:O	11:Q:40:THR:OG1	2.31	0.46
1:A:1663:LEU:O	1:A:1667:GLN:HB2	2.16	0.46
3:D:715:GLU:O	3:D:719:VAL:HG23	2.15	0.46
7:H:648:MET:HB2	7:H:650:LEU:HG	1.96	0.46
2:B:814:ASN:HB2	2:B:872:PRO:HB3	1.98	0.46
7:H:779:LYS:HG2	7:H:799:TRP:HB2	1.97	0.46
7:H:933:TRP:HB3	7:H:982:ARG:HD2	1.97	0.46
7:H:669:ASN:OD1	7:H:765:ARG:N	2.41	0.46
8:I:14:CYS:SG	8:I:21:SER:OG	2.70	0.46
8:I:80:VAL:HG12	8:I:82:GLU:H	1.80	0.46
11:Q:94:VAL:HG21	11:Q:137:TYR:HE2	1.81	0.46
2:B:868:HIS:O	2:B:993:VAL:HG21	2.15	0.46
3:D:908:GLN:NE2	3:D:930:GLU:OE1	2.48	0.46
6:G:705:LEU:O	6:G:752:TYR:OH	2.33	0.46
6:G:809:SER:OG	6:G:809:SER:O	2.30	0.46
8:I:538:ALA:HA	8:I:547:LYS:HA	1.98	0.46
9:K:131:MET:SD	9:K:132:ILE:HG13	2.56	0.46
9:K:190:ASP:H	9:K:193:LEU:HB2	1.81	0.46
9:K:504:ALA:HA	9:K:507:GLU:HG2	1.98	0.46
2:B:605:THR:HG23	2:B:608:SER:HB3	1.98	0.46
3:D:620:ARG:HH12	6:G:286:THR:HA	1.81	0.46
4:E:868:PRO:HB2	4:E:969:PHE:HB2	1.97	0.46
6:G:626:ASP:OD2	6:G:684:ARG:NH2	2.36	0.46
7:H:916:LEU:HD22	7:H:941:LEU:HD21	1.97	0.46
10:P:514:GLN:O	10:P:518:THR:OG1	2.29	0.46
5:F:238:ALA:HA	5:F:239:GLY:HA2	1.60	0.45
6:G:856:SER:HB3	6:G:875:ASN:HD21	1.81	0.45
7:H:466:ILE:HG22	7:H:467:THR:HG23	1.98	0.45
8:I:617:VAL:HG13	8:I:626:ILE:HB	1.98	0.45
2:B:856:ASP:OD1	2:B:856:ASP:N	2.47	0.45
3:D:566:SER:OG	3:D:569:THR:OG1	2.33	0.45
5:F:229:SER:OG	5:F:268:ILE:N	2.48	0.45
4:E:790:PRO:HA	4:E:791:GLY:HA3	1.47	0.45
8:I:52:LEU:HD12	8:I:57:LEU:HD21	1.98	0.45
3:D:761:PHE:HE2	3:D:777:VAL:HG21	1.81	0.45
6:G:61:ILE:HD13	6:G:93:HIS:HB3	1.97	0.45
10:P:470:VAL:HG13	10:P:511:VAL:HG11	1.98	0.45
2:B:416:THR:HB	2:B:455:TRP:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:19:PHE:CG	8:I:36:LEU:HD23	2.52	0.45
8:I:93:LEU:HD13	8:I:96:VAL:HG21	1.99	0.45
10:P:498:ARG:HB3	10:P:528:MSE:HE1	1.99	0.45
5:F:342:LYS:HB3	5:F:374:LEU:HD22	1.99	0.45
1:A:2122:LEU:HB3	1:A:2123:PRO:HD3	1.99	0.45
3:D:261:GLN:HE21	3:D:324:LYS:HA	1.82	0.45
3:D:431:SER:HA	3:D:434:THR:HG22	1.98	0.45
4:E:753:VAL:HG12	11:Q:283:LYS:HG2	1.98	0.45
8:I:155:LEU:O	8:I:159:LYS:NZ	2.42	0.45
8:I:27:ASP:OD1	8:I:27:ASP:N	2.50	0.45
8:I:122:THR:OG1	8:I:123:VAL:N	2.49	0.45
10:P:382:LEU:HD23	10:P:419:VAL:HG13	1.99	0.45
1:A:2100:ARG:HD3	1:A:2136:VAL:HG12	1.97	0.45
7:H:356:VAL:HG12	7:H:391:ARG:HE	1.81	0.45
1:A:2149:LEU:HD22	1:A:2183:ILE:HG21	1.98	0.45
4:E:524:SER:HA	4:E:574:PHE:HB2	1.99	0.45
10:P:22:ASN:O	10:P:28:ARG:NH2	2.50	0.45
10:P:467:LYS:O	10:P:471:GLU:HG3	2.17	0.45
1:A:1868:LYS:HZ3	1:A:1872:ALA:HB2	1.82	0.44
2:B:1080:ALA:HA	2:B:1083:VAL:HG12	1.99	0.44
3:D:866:LEU:HB3	3:D:910:GLU:HB3	1.98	0.44
4:E:1005:ARG:HE	7:H:358:PHE:HE1	1.65	0.44
1:A:1880:HIS:O	1:A:1883:MET:HG3	2.17	0.44
2:B:817:TRP:HE1	2:B:832:THR:HG21	1.82	0.44
2:B:1046:ILE:HG21	2:B:1083:VAL:HG11	1.98	0.44
3:D:172:GLN:HB3	3:D:217:LYS:HZ1	1.80	0.44
6:G:257:LEU:HD13	6:G:294:ALA:HB3	1.99	0.44
6:G:484:ASP:OD1	6:G:485:LYS:N	2.46	0.44
7:H:107:VAL:HG23	7:H:108:LEU:N	2.33	0.44
8:I:56:SER:O	8:I:56:SER:OG	2.34	0.44
2:B:810:LEU:HB3	2:B:872:PRO:HG2	1.99	0.44
3:D:616:GLN:O	3:D:619:GLU:HG3	2.18	0.44
4:E:511:ARG:HB2	4:E:512:PRO:HD3	2.00	0.44
5:F:594:LEU:H	10:P:340:HIS:CE1	2.36	0.44
8:I:41:LEU:HD11	8:I:173:VAL:HG21	1.98	0.44
9:K:145:HIS:HB3	9:K:157:LYS:HE3	1.99	0.44
2:B:944:GLU:OE2	5:F:549:ARG:NH1	2.50	0.44
2:B:1055:ILE:HD11	2:B:1099:PHE:HA	1.99	0.44
2:B:1093:GLN:N	7:H:926:ASP:OD1	2.50	0.44
3:D:207:GLN:HE21	8:I:543:VAL:H	1.64	0.44
4:E:703:GLU:HA	4:E:707:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:160:GLU:OE1	5:F:303:SER:OG	2.25	0.44
6:G:22:ALA:HB1	6:G:60:LEU:HD22	1.98	0.44
7:H:540:GLN:HB3	7:H:542:TRP:CD1	2.53	0.44
8:I:589:ILE:HD11	8:I:628:ILE:HD12	1.98	0.44
11:Q:263:PRO:HB2	11:Q:291:PRO:HD3	1.98	0.44
2:B:849:THR:OG1	2:B:850:GLN:N	2.50	0.44
2:B:1111:CYS:HB3	2:B:1118:TYR:HE1	1.83	0.44
3:D:216:ILE:O	3:D:219:MET:HG2	2.18	0.44
4:E:685:LEU:HD21	4:E:808:ALA:HB2	1.99	0.44
5:F:442:ASP:OD2	5:F:442:ASP:N	2.45	0.44
8:I:203:ILE:HG13	8:I:204:GLU:N	2.32	0.44
10:P:185:ALA:O	10:P:189:LEU:HG	2.18	0.44
2:B:711:LEU:HD23	6:G:46:VAL:HG11	1.99	0.44
5:F:24:TYR:HE1	5:F:175:LEU:HB2	1.82	0.44
6:G:353:TYR:OH	6:G:385:ASP:OD1	2.22	0.44
6:G:383:GLU:O	6:G:386:ALA:HB3	2.18	0.44
7:H:704:LEU:HB2	7:H:705:PRO:HD3	2.00	0.44
10:P:427:MSE:N	10:P:428:PRO:HD2	2.32	0.44
3:D:915:LEU:HB2	3:D:923:ILE:HB	1.98	0.44
6:G:144:ARG:HE	6:G:179:LYS:HD2	1.83	0.44
8:I:18:LYS:HE2	8:I:268:GLN:OE1	2.18	0.44
8:I:104:TYR:HB3	8:I:129:THR:HA	2.00	0.44
9:K:43:MET:N	9:K:71:ILE:O	2.39	0.44
2:B:331:THR:O	2:B:335:VAL:HG22	2.18	0.44
2:B:341:ARG:HA	2:B:344:LEU:HG	1.99	0.44
2:B:896:LEU:HD13	2:B:927:LYS:HD3	1.99	0.44
3:D:410:GLU:OE2	3:D:411:LYS:NZ	2.41	0.44
6:G:532:GLN:HE22	6:G:535:ARG:HH11	1.64	0.44
6:G:623:LEU:HD23	6:G:685:TYR:CD1	2.52	0.44
8:I:40:PRO:O	8:I:43:LEU:HD22	2.17	0.44
8:I:642:MET:SD	8:I:642:MET:N	2.91	0.44
6:G:171:ASP:OD1	6:G:171:ASP:N	2.51	0.44
8:I:586:SER:HA	9:K:513:HIS:HB2	2.00	0.44
4:E:881:LEU:HD23	4:E:910:LEU:HD13	2.00	0.43
7:H:632:GLU:HG2	7:H:633:ARG:N	2.33	0.43
8:I:285:LEU:HA	8:I:288:THR:HG22	1.99	0.43
9:K:110:LEU:HD13	9:K:132:ILE:HD13	2.00	0.43
9:K:527:ARG:HH22	9:K:535:ARG:HE	1.66	0.43
10:P:186:ALA:HA	10:P:189:LEU:HG	2.00	0.43
1:A:1821:LEU:O	1:A:1879:ARG:NH2	2.39	0.43
1:A:2129:LEU:HA	1:A:2137:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:874:MET:HE2	2:B:945:ILE:HG21	2.00	0.43
3:D:410:GLU:HA	3:D:413:LEU:HD23	2.00	0.43
5:F:375:ASN:OD1	5:F:376:CYS:N	2.47	0.43
10:P:199:ASP:OD1	10:P:199:ASP:N	2.51	0.43
10:P:227:ALA:O	10:P:231:ILE:HG12	2.17	0.43
11:Q:203:PRO:HD3	11:Q:239:ARG:CZ	2.48	0.43
2:B:433:PHE:HZ	2:B:483:VAL:HG21	1.82	0.43
2:B:1155:GLU:HA	2:B:1156:LYS:HA	1.50	0.43
3:D:391:ARG:O	3:D:395:VAL:HG22	2.17	0.43
4:E:281:ALA:HA	4:E:282:ILE:HA	1.57	0.43
6:G:49:PRO:HG3	6:G:86:VAL:HG13	2.00	0.43
6:G:474:LEU:HA	6:G:477:VAL:HG22	2.00	0.43
7:H:728:SER:H	7:H:747:SER:HB2	1.82	0.43
10:P:68:ALA:O	10:P:71:GLU:HG3	2.18	0.43
10:P:454:HIS:O	10:P:459:ARG:NH1	2.49	0.43
10:P:522:LEU:N	10:P:523:PRO:HD2	2.34	0.43
2:B:520:ILE:HD12	2:B:520:ILE:H	1.84	0.43
3:D:698:LYS:NZ	3:D:733:GLN:OE1	2.50	0.43
6:G:394:LEU:O	6:G:398:SER:OG	2.29	0.43
8:I:47:PRO:HA	8:I:401:ARG:HB3	2.00	0.43
8:I:639:ASN:ND2	9:K:521:VAL:HA	2.30	0.43
2:B:350:ILE:HG13	2:B:352:PRO:HD2	2.01	0.43
6:G:249:THR:OG1	6:G:250:PRO:HD3	2.18	0.43
6:G:477:VAL:O	6:G:480:ARG:NH1	2.52	0.43
1:A:1746:ARG:HD2	1:A:1754:ALA:HB2	2.01	0.43
3:D:448:GLN:O	3:D:452:VAL:HG22	2.19	0.43
3:D:875:ILE:HD13	3:D:896:VAL:HG23	2.00	0.43
4:E:689:LEU:HD13	4:E:812:VAL:HG23	2.01	0.43
5:F:363:HIS:HD2	5:F:364:PRO:HD2	1.83	0.43
9:K:594:THR:O	9:K:598:LYS:HD3	2.18	0.43
4:E:489:LEU:HD12	4:E:525:ARG:HG3	2.00	0.43
4:E:500:HIS:CE1	4:E:538:LEU:HB2	2.53	0.43
4:E:573:ARG:HA	4:E:576:ARG:HG2	2.01	0.43
6:G:232:ILE:HA	6:G:271:LEU:HD22	1.99	0.43
10:P:22:ASN:HD21	10:P:27:LEU:HB2	1.84	0.43
2:B:541:THR:H	2:B:580:GLN:HE22	1.66	0.43
2:B:1002:HIS:HB2	2:B:1032:ILE:HG23	2.00	0.43
3:D:688:LYS:HD2	3:D:688:LYS:HA	1.91	0.43
6:G:252:GLN:HE21	6:G:256:LEU:HD11	1.84	0.43
9:K:528:LYS:HD3	9:K:529:GLU:N	2.33	0.43
10:P:317:CYS:HA	10:P:320:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:381:ARG:HH12	10:P:419:VAL:HG21	1.83	0.43
2:B:786:LEU:HD23	2:B:789:TYR:HD2	1.82	0.43
2:B:1141:ARG:NH2	2:B:1182:ASP:OD2	2.52	0.43
6:G:920:THR:C	6:G:922:PRO:HD3	2.38	0.43
1:A:1713:GLN:HA	6:G:150:HIS:HD2	1.83	0.43
2:B:1038:CYS:HA	2:B:1041:PHE:CE2	2.54	0.43
7:H:609:GLN:HG2	7:H:653:ILE:HG13	2.01	0.43
9:K:131:MET:HA	9:K:134:ASP:OD2	2.19	0.43
3:D:399:CYS:HB3	3:D:434:THR:OG1	2.19	0.42
7:H:829:ASN:OD1	7:H:829:ASN:N	2.52	0.42
8:I:136:LEU:O	8:I:139:GLU:HG3	2.19	0.42
8:I:226:ILE:HG13	8:I:255:LEU:HD21	2.00	0.42
9:K:516:ARG:HE	9:K:581:SER:HB3	1.84	0.42
4:E:565:THR:HG22	4:E:566:LEU:H	1.83	0.42
5:F:16:GLN:HA	7:H:962:GLY:HA2	2.01	0.42
6:G:189:THR:HB	6:G:193:LEU:HD23	2.01	0.42
7:H:379:GLU:HG2	7:H:383:LYS:HE3	2.01	0.42
8:I:38:PHE:HB2	8:I:84:CYS:HB3	2.01	0.42
9:K:292:THR:OG1	9:K:293:ASN:N	2.53	0.42
10:P:62:GLU:HG2	10:P:65:VAL:HG12	2.00	0.42
10:P:401:SER:HB3	10:P:430:LEU:HG	2.01	0.42
1:A:1820:VAL:O	3:D:588:ARG:NH2	2.52	0.42
2:B:481:LEU:HD21	2:B:534:HIS:HB2	2.02	0.42
6:G:312:LEU:HD12	6:G:359:ILE:HG13	2.02	0.42
6:G:555:SER:HB3	6:G:558:PHE:HD2	1.84	0.42
8:I:125:ALA:N	8:I:194:ILE:HD11	2.33	0.42
10:P:209:PHE:CZ	10:P:228:CYS:HB2	2.54	0.42
1:A:1865:ALA:HB2	1:A:2149:LEU:HD11	2.02	0.42
1:A:2061:GLU:OE1	7:H:755:SER:OG	2.28	0.42
4:E:484:LEU:O	4:E:488:THR:HG23	2.20	0.42
4:E:768:ASN:OD1	4:E:769:GLN:N	2.52	0.42
5:F:31:ALA:HB1	5:F:220:LEU:HD11	2.01	0.42
5:F:548:PRO:HG2	5:F:551:ASN:OD1	2.20	0.42
6:G:754:HIS:O	6:G:757:GLU:HG3	2.19	0.42
8:I:100:LEU:HD11	8:I:225:TRP:CG	2.55	0.42
2:B:756:GLN:O	2:B:759:GLU:HG3	2.19	0.42
2:B:1054:GLN:O	2:B:1058:ILE:HG12	2.20	0.42
3:D:409:ALA:HA	3:D:412:CYS:SG	2.60	0.42
5:F:134:LEU:HD23	5:F:134:LEU:H	1.84	0.42
7:H:559:LEU:HD22	7:H:567:ARG:HH11	1.85	0.42
7:H:731:HIS:CE1	7:H:733:ARG:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:247:THR:O	10:P:250:GLN:HG3	2.19	0.42
1:A:2174:SER:O	1:A:2178:SER:OG	2.19	0.42
4:E:760:PRO:HG2	4:E:761:PRO:HD3	2.00	0.42
8:I:185:GLN:O	8:I:189:SER:OG	2.27	0.42
8:I:462:LYS:NZ	8:I:489:MET:SD	2.93	0.42
5:F:115:ARG:HH21	5:F:301:ARG:HD3	1.85	0.42
9:K:163:HIS:CD2	9:K:164:VAL:HG13	2.53	0.42
9:K:564:LEU:HD12	9:K:578:LEU:HD21	2.01	0.42
3:D:384:GLU:HG3	9:K:220:LYS:HD3	2.02	0.42
6:G:202:GLN:HG3	6:G:237:THR:HG23	2.02	0.42
8:I:66:LYS:HE2	8:I:68:LEU:HD21	2.00	0.42
10:P:105:ARG:O	10:P:109:VAL:HG13	2.18	0.42
2:B:1148:THR:HG22	4:E:615:LEU:HD13	2.02	0.42
3:D:253:VAL:HA	3:D:256:ILE:HG12	2.01	0.42
3:D:687:LEU:HG	3:D:688:LYS:N	2.34	0.42
4:E:991:VAL:HG22	7:H:160:PRO:HG3	2.02	0.42
5:F:368:LEU:HD12	5:F:377:VAL:HG11	2.02	0.42
7:H:414:LYS:HE3	7:H:414:LYS:HB2	1.89	0.42
8:I:20:LYS:HD2	8:I:20:LYS:HA	1.92	0.42
8:I:585:LEU:HD22	9:K:584:TYR:CD2	2.55	0.42
1:A:1611:LEU:O	1:A:1615:SER:HB3	2.20	0.42
1:A:2161:ARG:HH12	4:E:562:HIS:HB3	1.85	0.42
4:E:483:GLU:O	4:E:487:GLU:HG2	2.19	0.42
7:H:697:LEU:HA	7:H:700:THR:HG22	2.02	0.42
8:I:141:VAL:O	8:I:145:GLU:HG2	2.20	0.42
8:I:345:GLU:HG3	9:K:100:HIS:CE1	2.55	0.42
3:D:864:GLN:N	3:D:912:ARG:O	2.52	0.41
6:G:923:ARG:NH1	6:G:925:THR:OG1	2.53	0.41
10:P:129:VAL:HB	10:P:130:PRO:HD3	2.01	0.41
10:P:345:LEU:HD23	10:P:345:LEU:HA	1.90	0.41
3:D:234:TYR:O	3:D:237:ALA:HB3	2.20	0.41
8:I:627:GLN:CG	8:I:634:HIS:HB3	2.50	0.41
9:K:253:GLU:HA	9:K:256:ILE:HG22	2.01	0.41
11:Q:73:GLY:O	11:Q:80:TYR:OH	2.28	0.41
3:D:50:ALA:HA	8:I:501:ARG:NH2	2.35	0.41
3:D:422:ASP:O	3:D:423:GLU:HG3	2.19	0.41
3:D:841:LEU:HD23	3:D:841:LEU:H	1.85	0.41
5:F:54:THR:OG1	5:F:63:LYS:NZ	2.53	0.41
6:G:847:ILE:HG12	6:G:910:VAL:HG21	2.02	0.41
8:I:608:VAL:HG22	8:I:617:VAL:HG23	2.03	0.41
10:P:90:LEU:O	10:P:93:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:257:TRP:HB3	10:P:260:ARG:HH21	1.85	0.41
2:B:527:THR:HG22	2:B:528:GLU:N	2.34	0.41
2:B:899:THR:O	2:B:900:GLU:HG3	2.20	0.41
3:D:409:ALA:HA	3:D:412:CYS:HG	1.85	0.41
3:D:673:ALA:HB1	3:D:693:ALA:HB2	2.02	0.41
6:G:30:ASP:HB2	6:G:67:LYS:HZ3	1.84	0.41
8:I:274:PRO:O	8:I:277:MET:HG2	2.21	0.41
8:I:296:LEU:HD12	8:I:412:TRP:CZ2	2.53	0.41
8:I:430:LEU:H	8:I:430:LEU:HD23	1.85	0.41
9:K:145:HIS:CE1	9:K:159:TYR:HA	2.56	0.41
5:F:383:PRO:HG2	5:F:386:TYR:HB3	2.03	0.41
6:G:491:VAL:HG23	6:G:525:THR:HG23	2.01	0.41
6:G:717:ILE:HD12	6:G:721:ILE:HG13	2.02	0.41
8:I:21:SER:HA	8:I:34:SER:O	2.20	0.41
8:I:299:CYS:SG	8:I:394:PHE:HB3	2.59	0.41
9:K:562:VAL:HG22	9:K:582:TRP:HB3	2.02	0.41
10:P:497:HIS:O	10:P:501:THR:HG23	2.21	0.41
10:P:581:GLU:HA	10:P:584:THR:HG22	2.02	0.41
1:A:1617:LEU:HD13	6:G:265:ARG:HG3	2.02	0.41
4:E:914:MET:O	4:E:919:LEU:HB2	2.21	0.41
5:F:231:VAL:O	5:F:266:LYS:N	2.53	0.41
7:H:649:ARG:NH2	7:H:683:PHE:O	2.53	0.41
7:H:858:GLN:O	7:H:862:VAL:HG23	2.20	0.41
10:P:515:ASP:OD1	10:P:515:ASP:N	2.54	0.41
2:B:889:LYS:HG2	2:B:931:LEU:HD22	2.02	0.41
3:D:167:ARG:HA	3:D:170:CYS:SG	2.60	0.41
6:G:80:ARG:HB3	6:G:121:ILE:HG21	2.03	0.41
7:H:542:TRP:HA	7:H:572:ILE:HD11	2.02	0.41
8:I:472:PRO:HG2	8:I:475:TYR:HE1	1.85	0.41
1:A:2074:SER:O	1:A:2074:SER:OG	2.33	0.41
2:B:943:LEU:HB3	2:B:1024:LEU:HD13	2.01	0.41
3:D:901:THR:HG22	3:D:902:ALA:H	1.86	0.41
7:H:772:ILE:HD13	7:H:772:ILE:HA	1.97	0.41
7:H:899:ILE:HD11	7:H:928:TYR:HB3	2.02	0.41
7:H:902:GLN:HE22	7:H:932:ILE:HG23	1.86	0.41
8:I:82:GLU:OE1	8:I:180:ARG:HB3	2.20	0.41
8:I:110:LEU:HB3	8:I:111:PRO:HD3	2.03	0.41
9:K:99:THR:HB	9:K:170:PHE:HZ	1.86	0.41
9:K:106:CYS:HA	9:K:109:LEU:HG	2.02	0.41
9:K:164:VAL:HG22	9:K:167:ALA:HB2	2.03	0.41
9:K:252:GLN:HA	9:K:255:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:182:ARG:HD2	10:P:212:LEU:HD11	2.03	0.41
11:Q:42:GLU:O	11:Q:185:ARG:NH2	2.53	0.41
2:B:1107:LEU:HD22	2:B:1121:ILE:HD12	2.02	0.41
4:E:674:LEU:O	4:E:678:SER:HB3	2.21	0.41
7:H:107:VAL:HG23	7:H:108:LEU:H	1.84	0.41
8:I:101:ILE:HD11	8:I:123:VAL:CG2	2.50	0.41
9:K:294:GLN:O	9:K:298:LYS:HG3	2.21	0.41
10:P:414:ASP:O	10:P:420:ARG:NH1	2.54	0.41
10:P:439:PHE:HA	10:P:443:LEU:HB2	2.02	0.41
10:P:455:VAL:HG12	11:Q:71:ILE:HG23	2.02	0.41
1:A:1691:PRO:HB3	1:A:1738:LEU:HD13	2.03	0.41
1:A:2154:HIS:O	1:A:2158:LEU:HD23	2.21	0.41
2:B:593:LEU:HB2	2:B:594:PRO:HD3	2.03	0.41
2:B:797:MET:HA	2:B:800:LEU:HD12	2.03	0.41
2:B:801:LEU:HD23	2:B:801:LEU:H	1.86	0.41
3:D:759:ASP:O	3:D:762:GLN:HG3	2.21	0.41
3:D:901:THR:HG22	3:D:902:ALA:N	2.36	0.41
6:G:597:TYR:HB3	6:G:625:ILE:HG12	2.03	0.41
7:H:400:SER:OG	7:H:402:GLN:OE1	2.36	0.41
8:I:395:THR:HB	8:I:405:VAL:HG12	2.02	0.41
10:P:201:VAL:HG11	10:P:235:LEU:HD21	2.03	0.41
10:P:221:ARG:HA	10:P:224:ALA:HB3	2.03	0.41
10:P:304:HIS:HA	10:P:348:VAL:HG21	2.03	0.41
10:P:548:GLY:HA2	10:P:556:LEU:HD21	2.03	0.41
2:B:332:SER:OG	2:B:333:SER:N	2.54	0.40
3:D:687:LEU:HD23	3:D:687:LEU:H	1.86	0.40
3:D:792:PRO:HA	3:D:795:VAL:HB	2.03	0.40
3:D:908:GLN:HE21	3:D:930:GLU:HB3	1.86	0.40
4:E:658:SER:OG	4:E:667:VAL:HG12	2.21	0.40
4:E:797:GLU:OE1	4:E:797:GLU:N	2.52	0.40
6:G:342:SER:O	6:G:342:SER:OG	2.34	0.40
6:G:582:ASN:ND2	6:G:585:SER:OG	2.48	0.40
6:G:910:VAL:O	6:G:918:TRP:HB2	2.22	0.40
10:P:179:PRO:HA	10:P:182:ARG:HB2	2.03	0.40
1:A:2047:MET:HG3	1:A:2080:ILE:HD11	2.02	0.40
2:B:361:GLU:O	2:B:365:VAL:HG13	2.21	0.40
3:D:384:GLU:HA	3:D:391:ARG:NH2	2.37	0.40
3:D:438:ILE:HD12	3:D:438:ILE:HA	1.91	0.40
3:D:499:ASP:N	3:D:499:ASP:OD1	2.54	0.40
3:D:529:HIS:HB3	3:D:532:PHE:HB2	2.03	0.40
4:E:477:LEU:HD13	4:E:502:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:294:ASN:HD22	5:F:294:ASN:HA	1.72	0.40
6:G:784:LEU:HD23	6:G:784:LEU:HA	1.93	0.40
7:H:465:PHE:CZ	7:H:469:LEU:HD22	2.55	0.40
7:H:775:SER:HA	7:H:778:VAL:HG12	2.01	0.40
8:I:285:LEU:O	8:I:289:VAL:HG22	2.22	0.40
9:K:393:MET:N	9:K:393:MET:SD	2.94	0.40
10:P:223:LEU:HA	10:P:226:GLU:HG2	2.04	0.40
2:B:44:LEU:O	6:G:639:ASN:ND2	2.54	0.40
2:B:331:THR:HA	2:B:334:SER:HB3	2.02	0.40
2:B:365:VAL:HA	2:B:368:GLU:HG2	2.02	0.40
3:D:236:GLN:O	3:D:239:LYS:HG2	2.22	0.40
3:D:666:CYS:SG	3:D:700:ILE:HG23	2.61	0.40
6:G:475:TYR:HD1	6:G:493:LEU:HB3	1.86	0.40
6:G:830:LYS:HD3	6:G:891:GLN:HE22	1.86	0.40
7:H:632:GLU:HG2	7:H:633:ARG:H	1.86	0.40
7:H:720:VAL:HA	7:H:723:GLN:HG2	2.04	0.40
7:H:755:SER:HA	7:H:758:LEU:HD12	2.03	0.40
2:B:645:ILE:HG23	2:B:695:GLN:NE2	2.36	0.40
3:D:233:ILE:HD12	3:D:233:ILE:H	1.86	0.40
10:P:52:LEU:HD12	10:P:55:LEU:HD21	2.02	0.40
10:P:306:VAL:HA	10:P:309:PHE:HB3	2.04	0.40
2:B:693:ILE:HG13	2:B:714:LEU:HD22	2.03	0.40
2:B:774:ILE:O	2:B:777:HIS:ND1	2.52	0.40
3:D:780:LEU:HD12	3:D:780:LEU:HA	1.95	0.40
5:F:173:LEU:HA	5:F:210:VAL:HB	2.03	0.40
8:I:17:LEU:CD2	8:I:268:GLN:HE21	2.34	0.40
10:P:163:LYS:O	10:P:166:LEU:HG	2.21	0.40
10:P:245:MSE:HB2	10:P:246:PRO:HD3	2.04	0.40
10:P:268:THR:O	10:P:271:GLN:HG3	2.21	0.40
11:Q:209:TRP:CZ3	11:Q:220:PHE:HB3	2.57	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	722/2190 (33%)	678 (94%)	38 (5%)	6 (1%)	16	51
2	B	1046/1204 (87%)	965 (92%)	78 (8%)	3 (0%)	37	68
3	D	817/963 (85%)	752 (92%)	59 (7%)	6 (1%)	19	53
4	E	790/1019 (78%)	742 (94%)	38 (5%)	10 (1%)	10	41
5	F	524/887 (59%)	466 (89%)	50 (10%)	8 (2%)	8	39
6	G	891/962 (93%)	845 (95%)	46 (5%)	0	100	100
7	H	908/995 (91%)	852 (94%)	50 (6%)	6 (1%)	19	53
8	I	620/658 (94%)	527 (85%)	86 (14%)	7 (1%)	12	45
9	K	584/600 (97%)	522 (89%)	51 (9%)	11 (2%)	6	34
10	P	580/589 (98%)	567 (98%)	13 (2%)	0	100	100
11	Q	291/309 (94%)	280 (96%)	11 (4%)	0	100	100
All	All	7773/10376 (75%)	7196 (93%)	520 (7%)	57 (1%)	21	53

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1593	PRO
1	A	1816	PRO
2	B	47	PRO
2	B	189	PRO
3	D	49	PRO
3	D	814	PRO
3	D	827	PRO
4	E	464	PRO
4	E	740	PRO
4	E	742	PRO
5	F	240	PRO
5	F	242	PRO
5	F	243	SER
5	F	259	GLN
5	F	260	PRO
5	F	333	PRO
7	H	166	PRO
7	H	168	PRO
7	H	169	PRO
7	H	325	PRO

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Mol	Chain	Res	Type
8	I	355	VAL
8	I	358	PRO
8	I	360	PRO
8	I	361	PRO
8	I	520	PRO
8	I	528	PRO
9	K	52	PRO
9	K	322	PRO
9	K	331	PRO
9	K	443	MET
9	K	453	PRO
9	K	482	PRO
1	A	1405	VAL
1	A	1447	PRO
4	E	349	PRO
9	K	321	ASN
4	E	279	SER
9	K	290	PRO
9	K	459	PRO
7	H	46	ALA
9	K	330	THR
2	B	193	PRO
3	D	141	LEU
3	D	142	PRO
4	E	282	ILE
4	E	283	PRO
4	E	348	SER
4	E	380	PRO
5	F	332	SER
1	A	1403	VAL
7	H	60	LYS
1	A	1446	VAL
8	I	362	PHE
4	E	465	PRO
5	F	244	PRO
9	K	270	PRO
3	D	147	ILE

### 5.3.2 Protein sidechains [i](#)

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	313/1907 (16%)	313 (100%)	0	100	100
2	B	711/1072 (66%)	711 (100%)	0	100	100
3	D	543/845 (64%)	542 (100%)	1 (0%)	92	97
4	E	410/812 (50%)	410 (100%)	0	100	100
5	F	353/796 (44%)	353 (100%)	0	100	100
6	G	734/840 (87%)	734 (100%)	0	100	100
7	H	624/896 (70%)	624 (100%)	0	100	100
8	I	505/600 (84%)	502 (99%)	3 (1%)	84	91
9	K	258/520 (50%)	258 (100%)	0	100	100
10	P	509/498 (102%)	509 (100%)	0	100	100
11	Q	259/274 (94%)	259 (100%)	0	100	100
All	All	5219/9060 (58%)	5215 (100%)	4 (0%)	92	97

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

Mol	Chain	Res	Type
3	D	182	LYS
8	I	412	TRP
8	I	459	LYS
8	I	607	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1728	GLN
1	A	1919	GLN
1	A	2112	GLN
1	A	2154	HIS
2	B	323	ASN
2	B	338	GLN
2	B	413	GLN
2	B	448	GLN
2	B	580	GLN
2	B	591	GLN

*Continued on next page...*



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Mol	Chain	Res	Type
2	B	648	GLN
2	B	717	ASN
2	B	758	GLN
2	B	770	GLN
2	B	1002	HIS
2	B	1063	HIS
2	B	1067	GLN
2	B	1187	HIS
3	D	176	ASN
3	D	235	ASN
3	D	261	GLN
3	D	403	GLN
3	D	441	ASN
3	D	650	GLN
3	D	667	GLN
3	D	724	HIS
3	D	771	HIS
3	D	873	GLN
3	D	884	ASN
3	D	908	GLN
4	E	501	GLN
4	E	708	GLN
4	E	750	HIS
4	E	926	ASN
4	E	963	GLN
4	E	984	HIS
4	E	989	HIS
5	F	145	HIS
5	F	293	GLN
5	F	294	ASN
6	G	89	GLN
6	G	150	HIS
6	G	252	GLN
6	G	414	ASN
6	G	437	GLN
6	G	451	HIS
6	G	532	GLN
6	G	539	HIS
6	G	557	HIS
6	G	633	GLN
6	G	670	GLN
6	G	673	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
6	G	814	ASN
6	G	823	ASN
6	G	826	GLN
6	G	853	ASN
6	G	891	GLN
7	H	404	ASN
7	H	405	GLN
7	H	609	GLN
7	H	730	GLN
7	H	731	HIS
7	H	782	ASN
7	H	858	GLN
7	H	894	HIS
7	H	902	GLN
7	H	955	GLN
8	I	162	GLN
8	I	246	HIS
8	I	252	GLN
8	I	294	ASN
8	I	468	HIS
8	I	482	GLN
8	I	639	ASN
9	K	171	GLN
9	K	192	HIS
9	K	304	ASN
9	K	398	HIS
9	K	550	GLN
10	P	211	ASN
10	P	230	ASN
10	P	233	GLN
10	P	237	GLN
10	P	271	GLN
10	P	320	ASN
10	P	340	HIS
10	P	392	ASN
10	P	399	GLN
10	P	402	GLN
10	P	557	GLN
11	Q	12	GLN
11	Q	44	ASN
11	Q	59	HIS
11	Q	79	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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-30473. These allow visual inspection of the internal detail of the map and identification of artifacts.

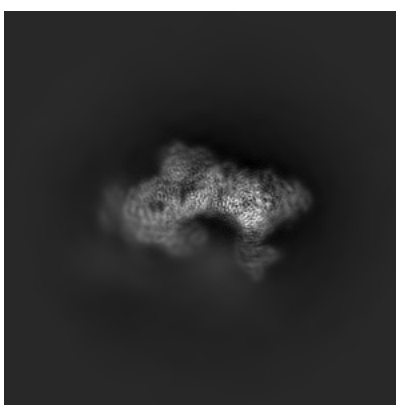
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

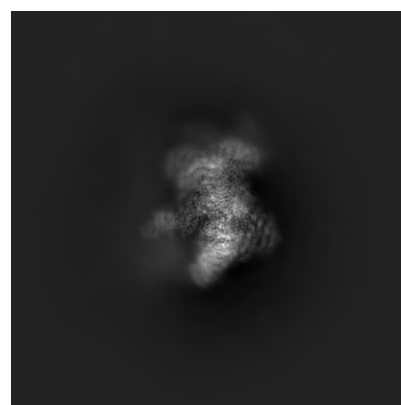
#### 6.1.1 Primary map



X



Y

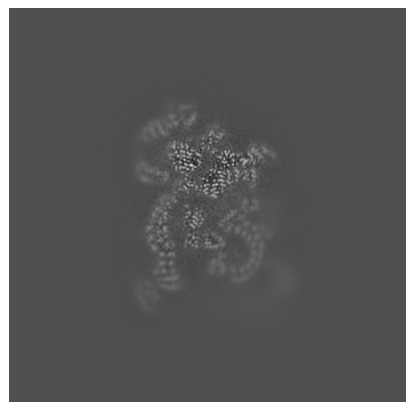


Z

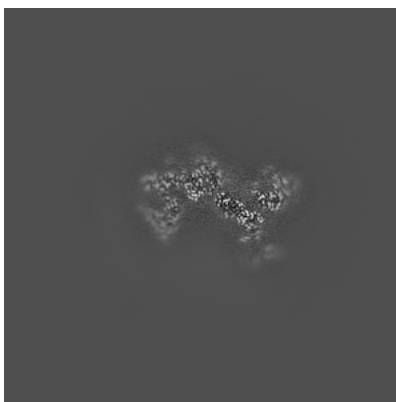
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 240



Y Index: 240

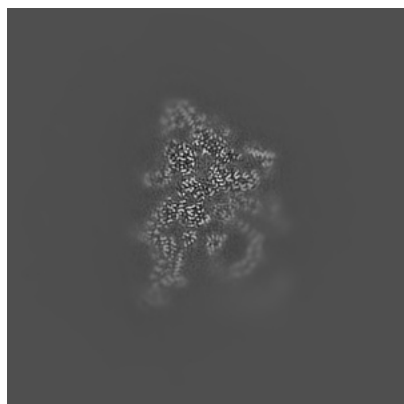


Z Index: 240

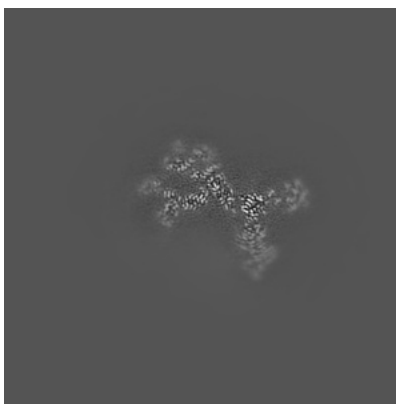
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

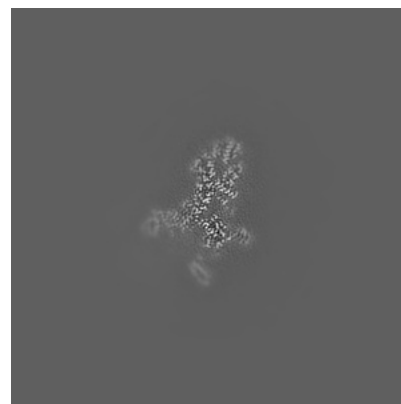
### 6.3.1 Primary map



X Index: 251



Y Index: 220

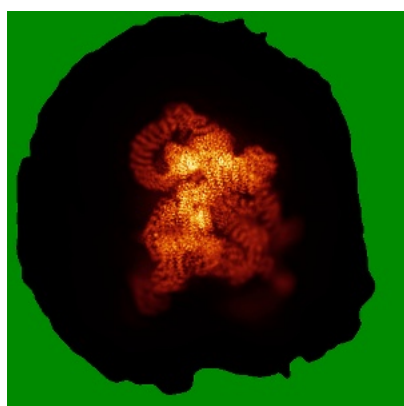


Z Index: 297

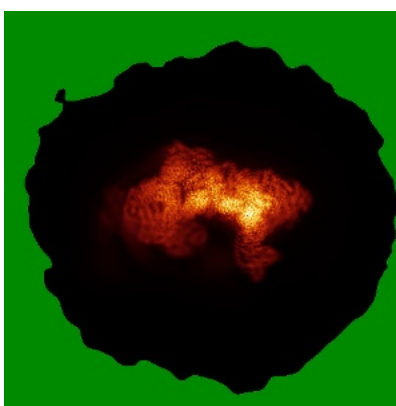
The images above show the largest variance slices of the map in three orthogonal directions.

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

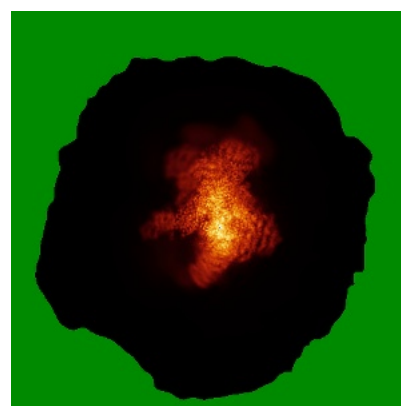
### 6.4.1 Primary map



X



Y

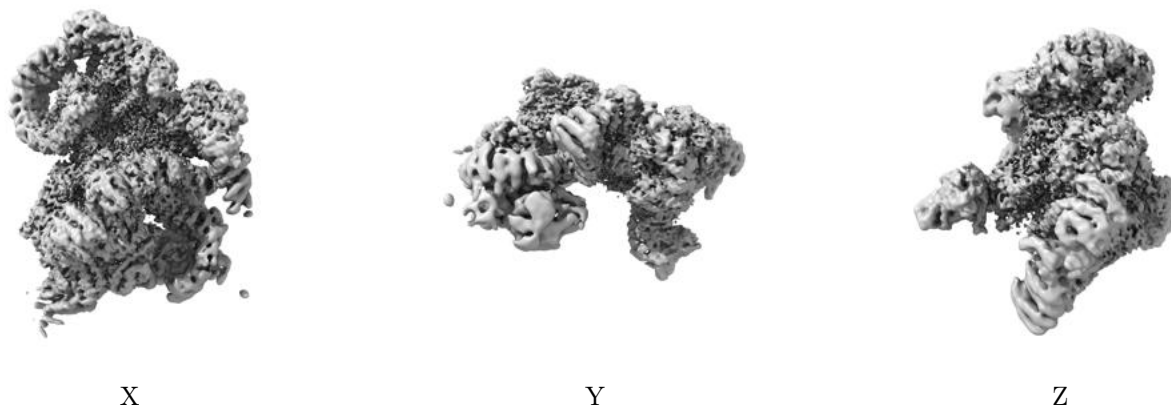


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

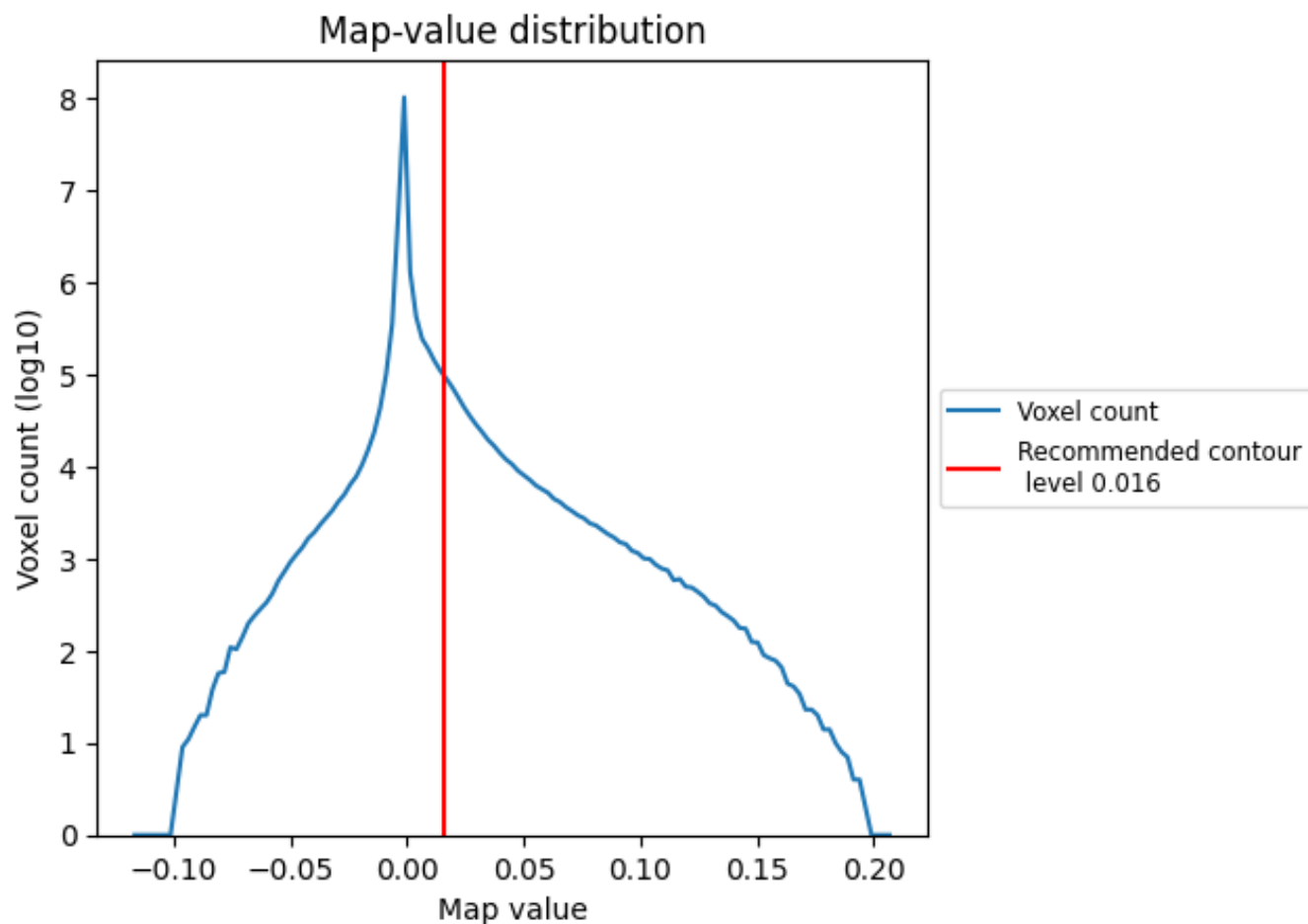
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

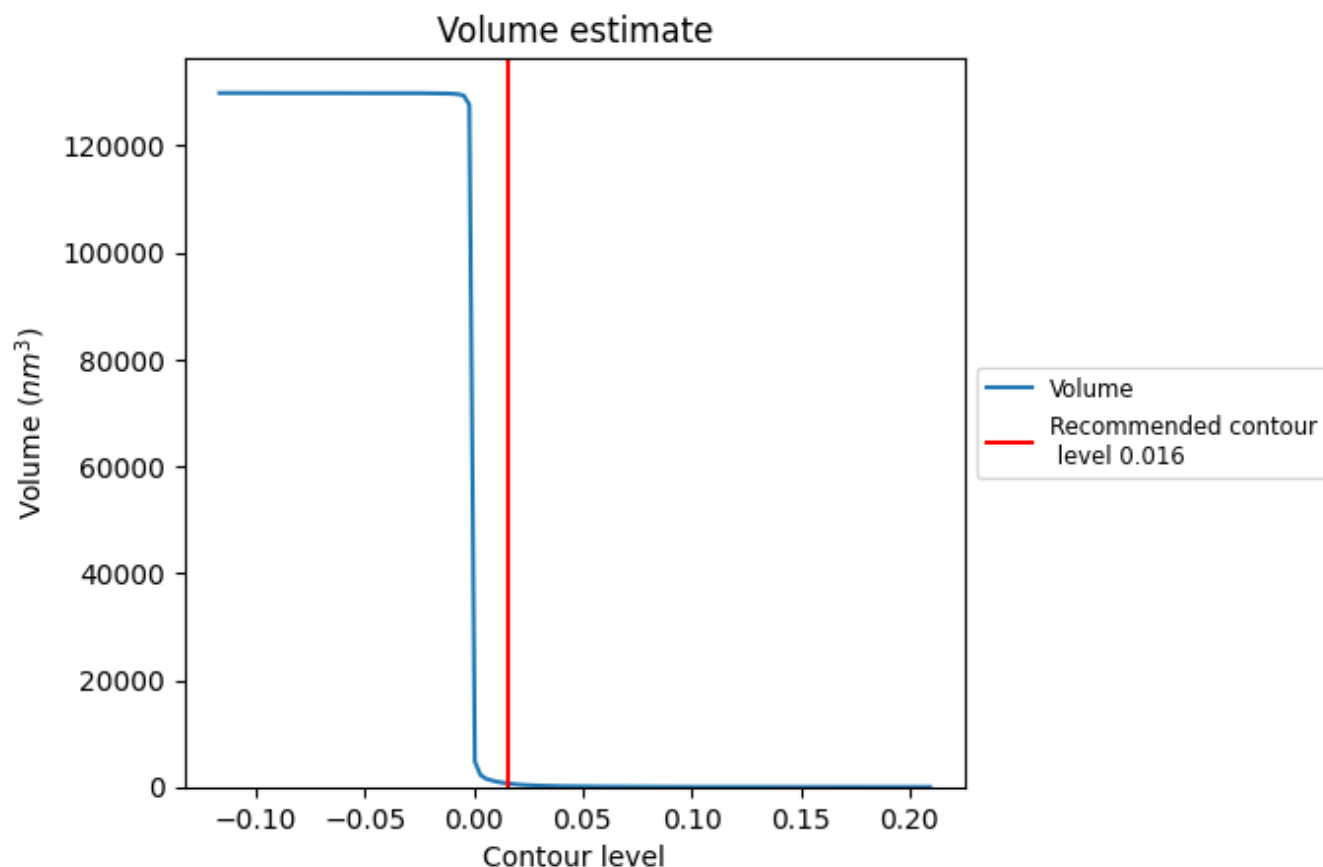
This section contains the results of statistical analysis of the map.

### 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](#)

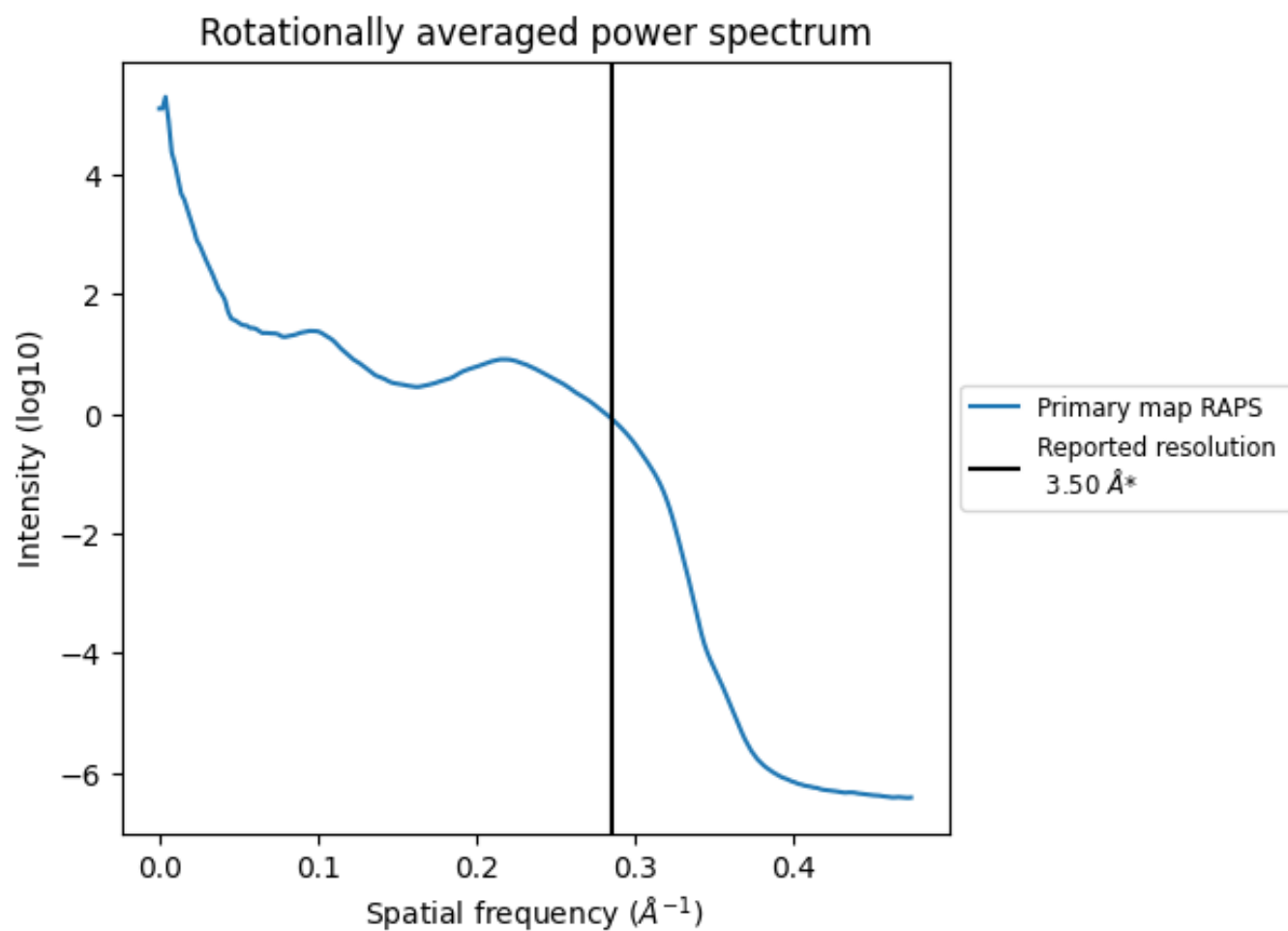


The volume at the recommended contour level is 642  $\text{nm}^3$ ; this corresponds to an approximate mass of 580 kDa.

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 0.286 Å<sup>-1</sup>

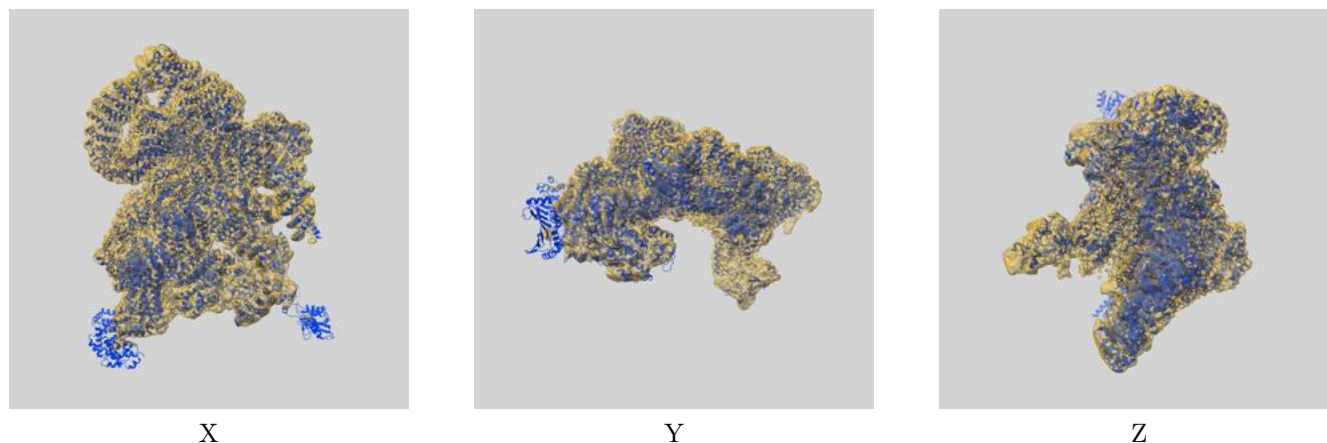
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

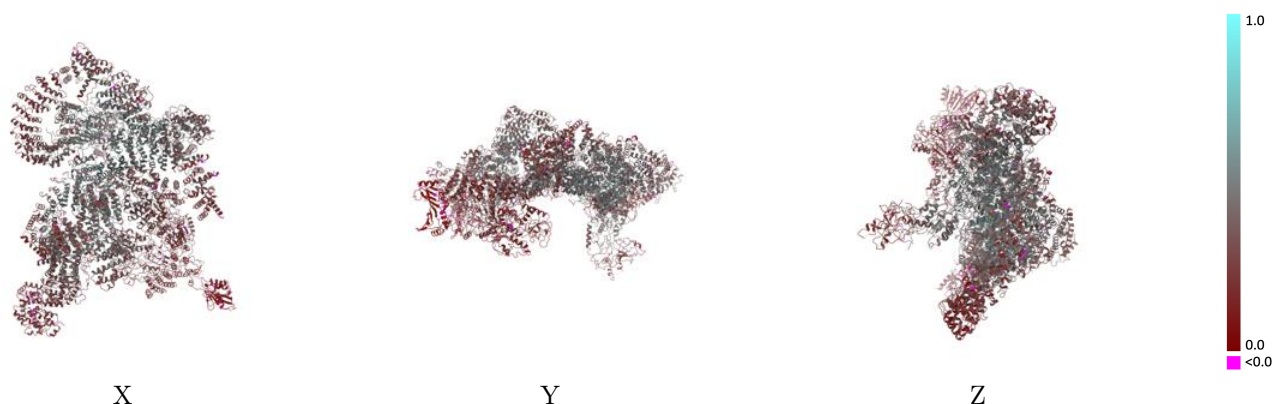
This section contains information regarding the fit between EMDB map EMD-30473 and PDB model 7CUN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



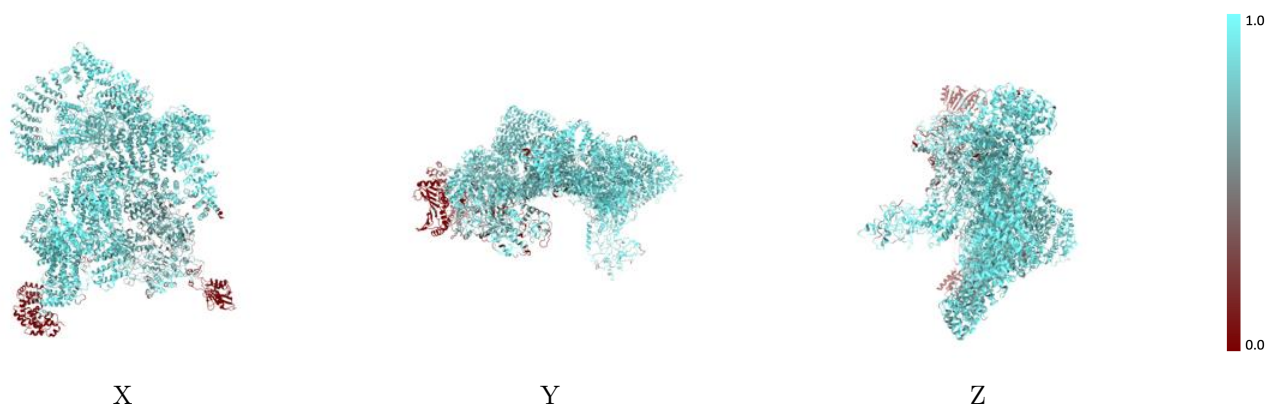
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



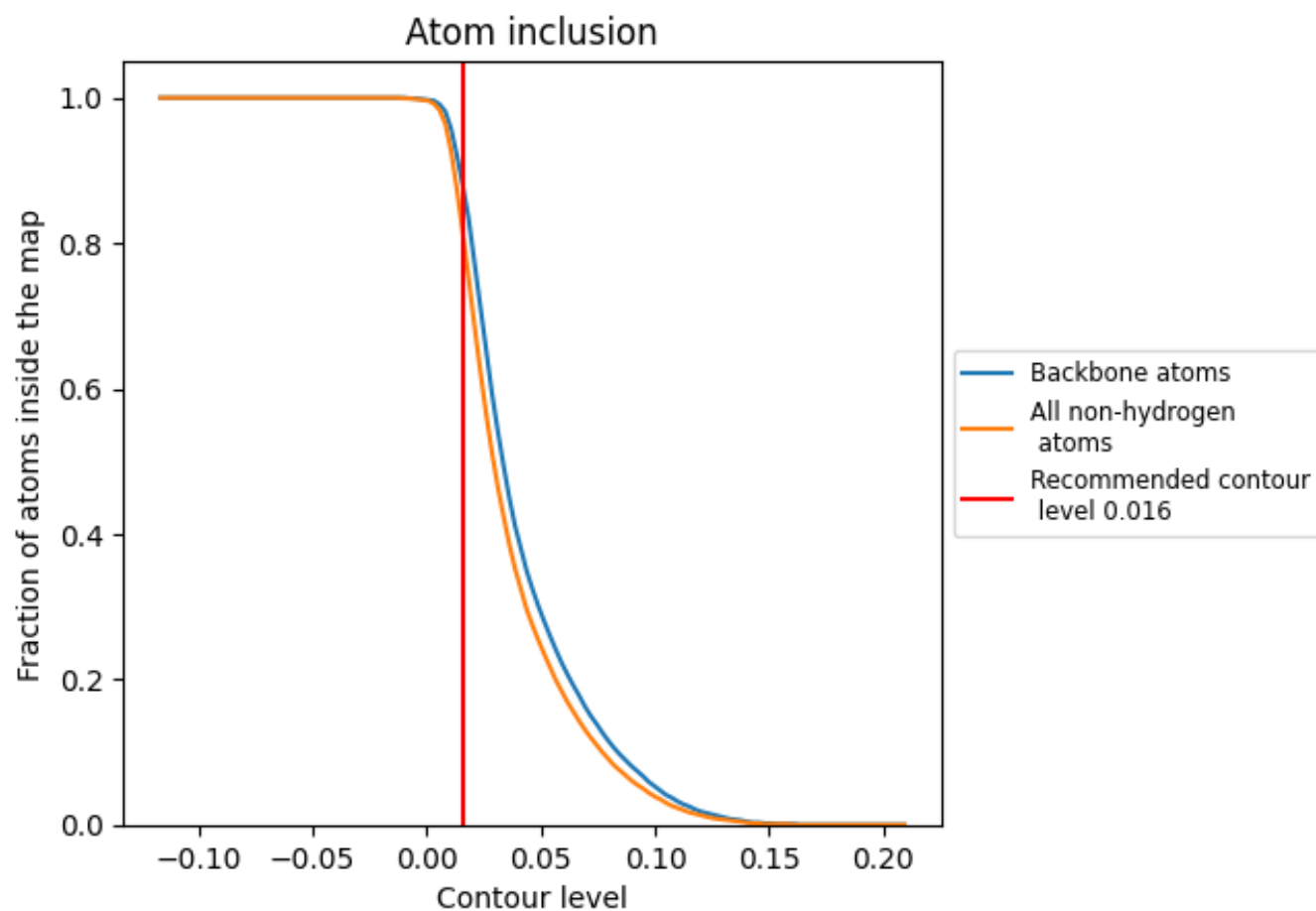
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8090	<div></div> 0.3500
A	<div></div> 0.8810	<div></div> 0.3750
B	<div></div> 0.8790	<div></div> 0.3980
D	<div></div> 0.8020	<div></div> 0.3170
E	<div></div> 0.9000	<div></div> 0.4070
F	<div></div> 0.8630	<div></div> 0.3560
G	<div></div> 0.8850	<div></div> 0.4230
H	<div></div> 0.8990	<div></div> 0.3900
I	<div></div> 0.6190	<div></div> 0.2110
K	<div></div> 0.5140	<div></div> 0.1700
P	<div></div> 0.8400	<div></div> 0.3000
Q	<div></div> 0.9310	<div></div> 0.5100
U	<div></div> 0.1300	<div></div> 0.2180

