



# Full wwPDB EM Validation Report ⓘ

Feb 26, 2025 – 02:53 AM JST

PDB ID : 8YJB  
EMDB ID : EMD-39338  
Title : Cryo-EM structure of the human DSS1-INTAC complex  
Authors : Zheng, H.; Xu, Y.; Cheng, J.  
Deposited on : 2024-03-01  
Resolution : 4.10 Å (reported)  
Based on initial model : 7YCX

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

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:

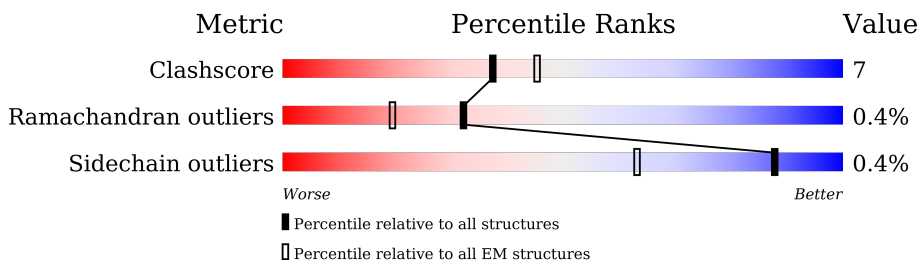
EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

# 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 4.10 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.



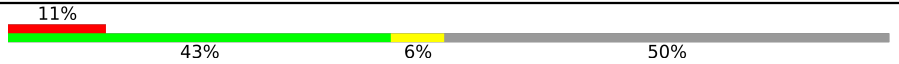



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	70	
2	I	658	
3	K	600	
4	B	1204	
5	D	963	
6	G	962	
7	P	589	
8	Q	309	

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Mol	Chain	Length	Quality of chain
9	A	2190	
10	E	1019	
11	F	887	
12	H	995	

## 2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 62555 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 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	32	275	169	47	58	1	0	0

- Molecule 2 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	633	4985	3210	815	926	34	0	0

- Molecule 3 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	590	4646	2964	806	841	35	0	0

- Molecule 4 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	1061	8328	5322	1412	1530	64	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	817	6108	3872	1065	1140	31	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	901	6873	4348	1202	1282	41	0	0

- Molecule 7 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P	581	4527	2877	763	860	27	0	0

- Molecule 8 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

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

- Molecule 9 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	1091	7530	4708	1373	1410	39	0	0

- Molecule 10 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	E	798	5244	3284	988	958	14	0	0

- Molecule 11 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	F	551	4229	2702	723	782	22	0	0

- Molecule 12 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	937	7440	4761	1274	1361	44	0	0

- 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).

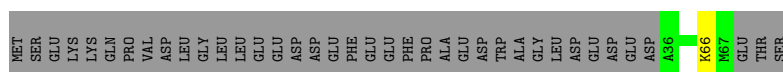
Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
14	Q	2	2	2	0

### 3 Residue-property plots [i](#)


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.

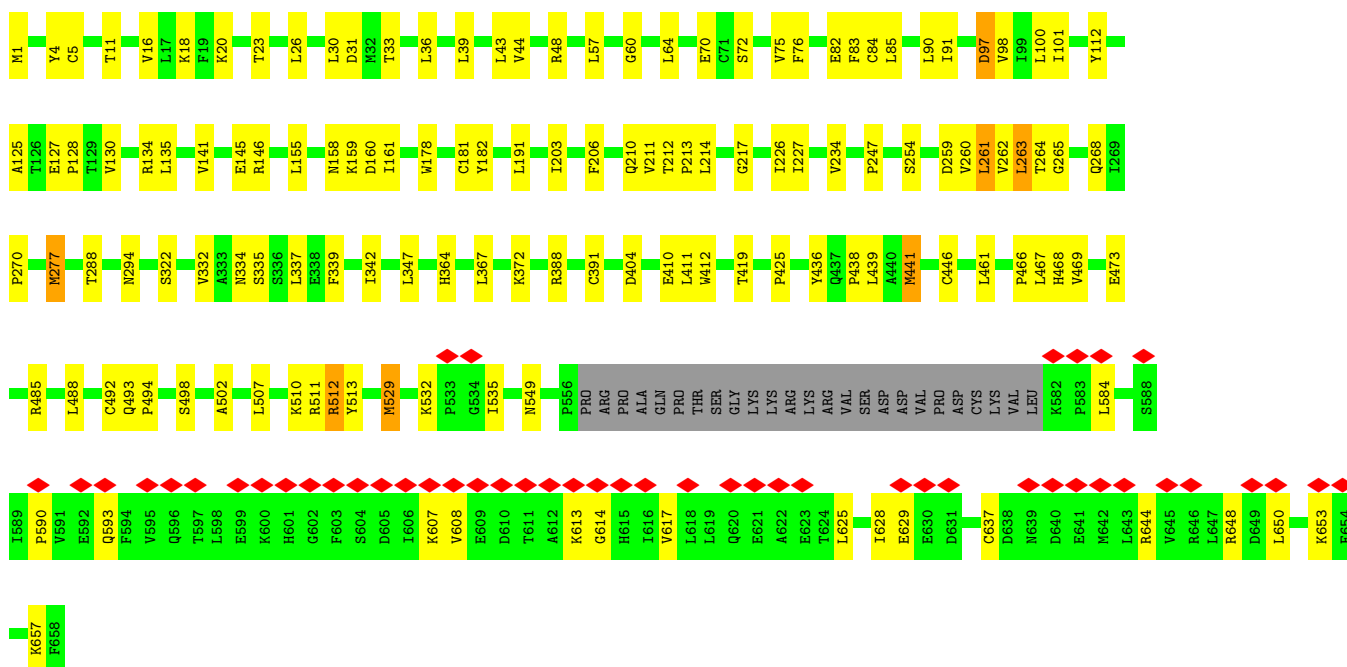
- Molecule 1: 26S proteasome complex subunit DSS1

Chain 0: 




- Molecule 2: Integrator complex subunit 9

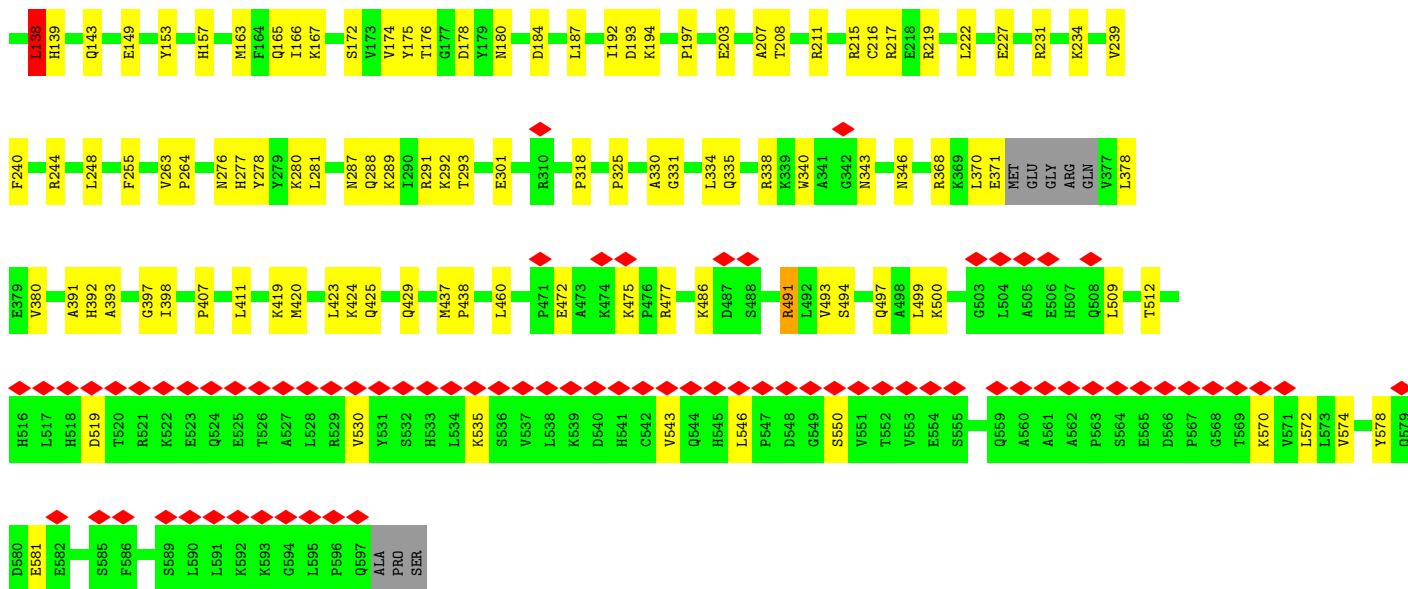
Chain I: 



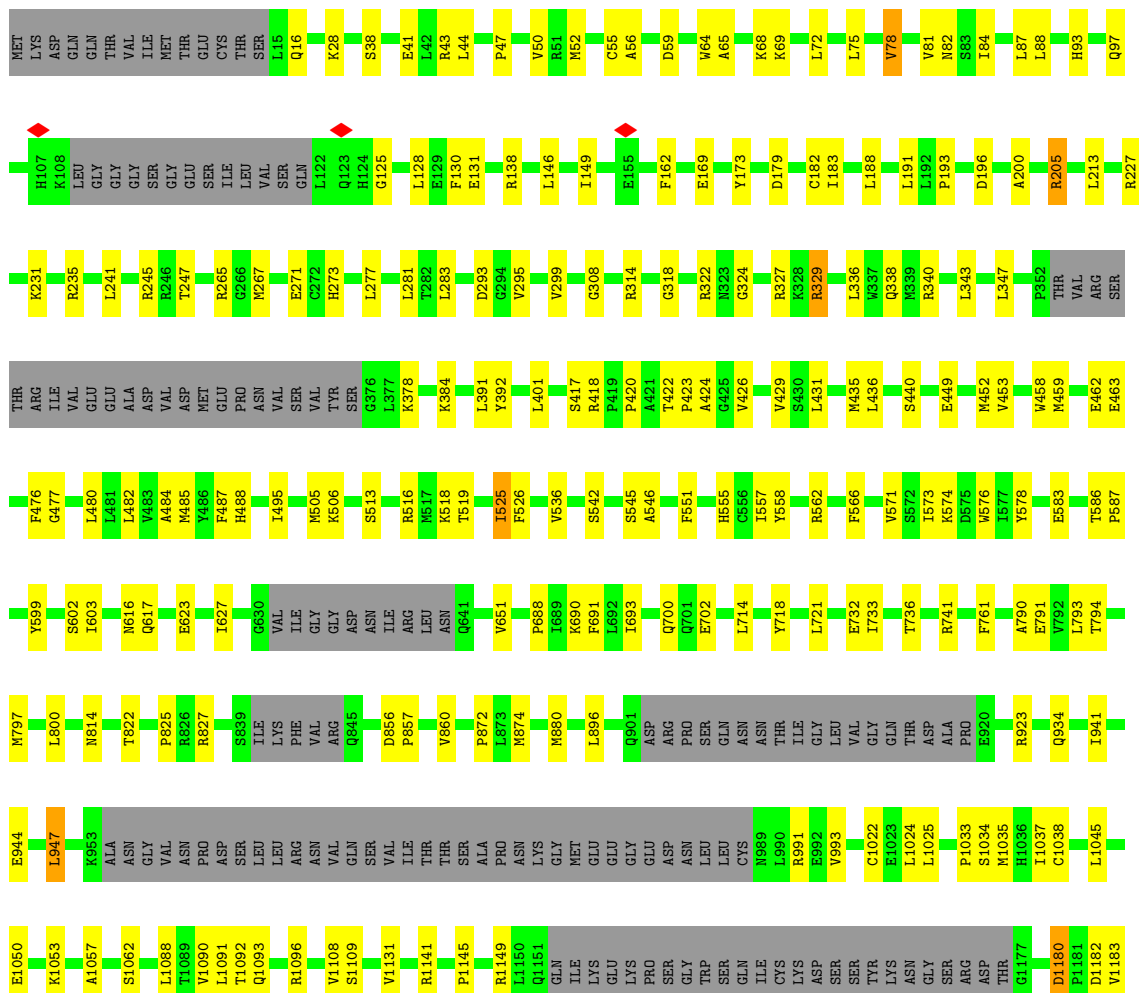
- Molecule 3: Integrator complex subunit 11

Chain K: 





• Molecule 4: Integrator complex subunit 2

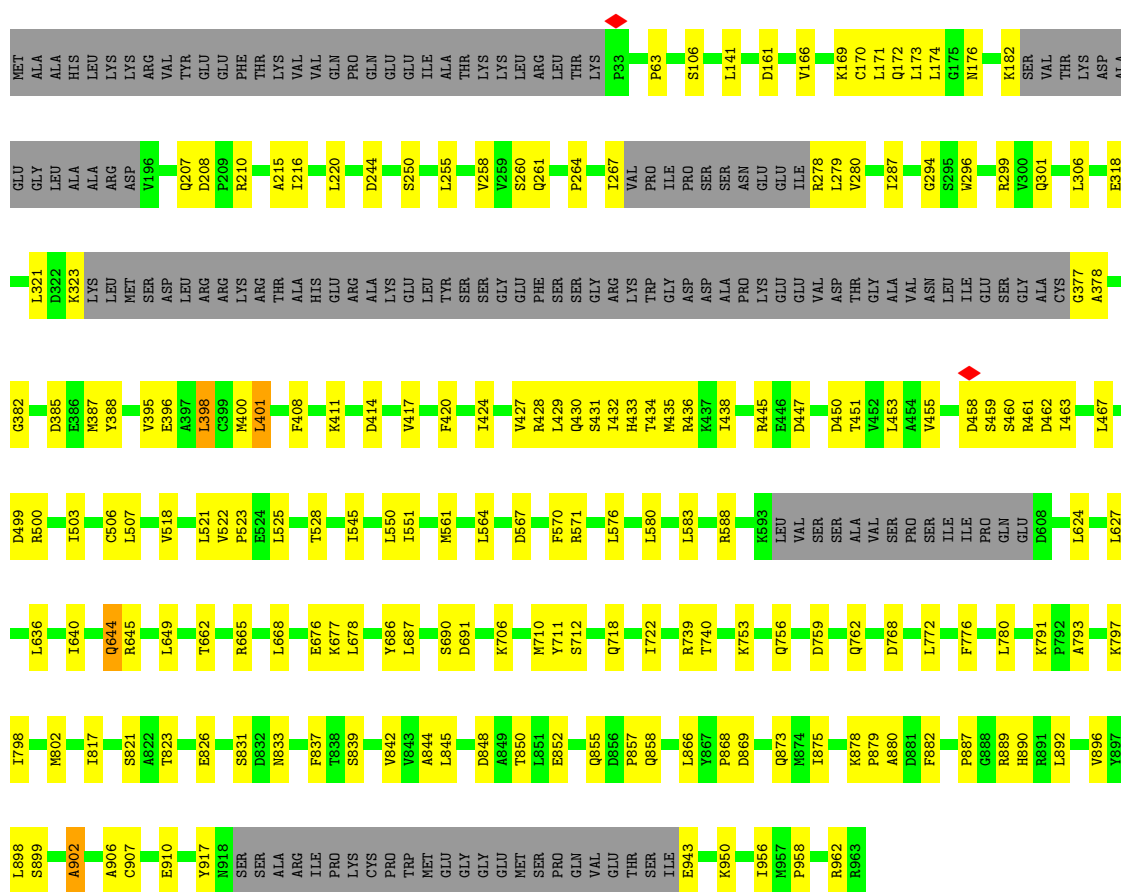






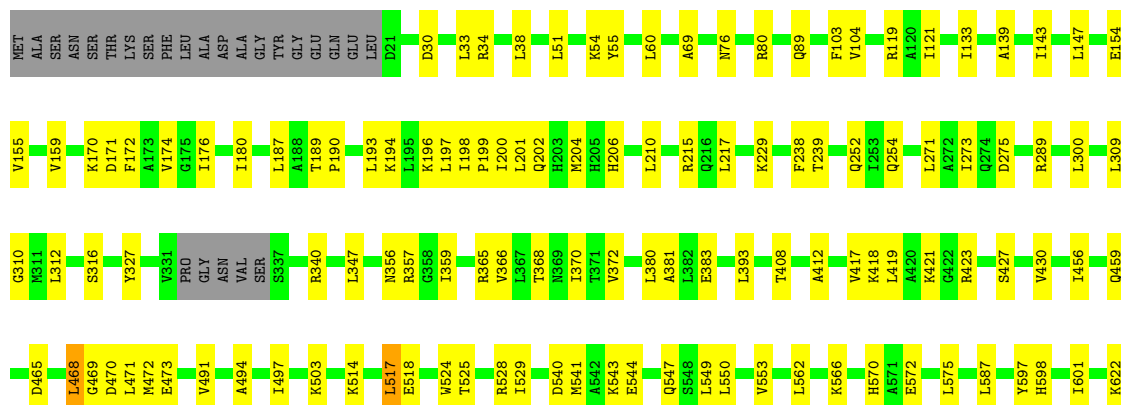
- Molecule 5: Integrator complex subunit 4

Chain D: 66% 19% 15%



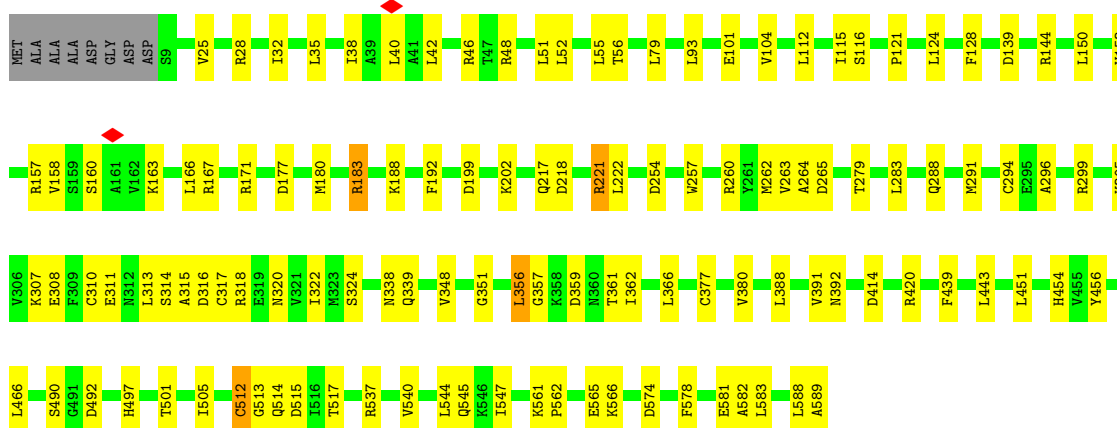
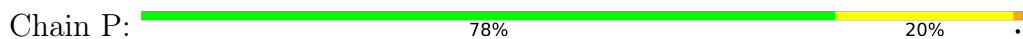
- Molecule 6: Integrator complex subunit 7

Chain G: 76% 17% 6%

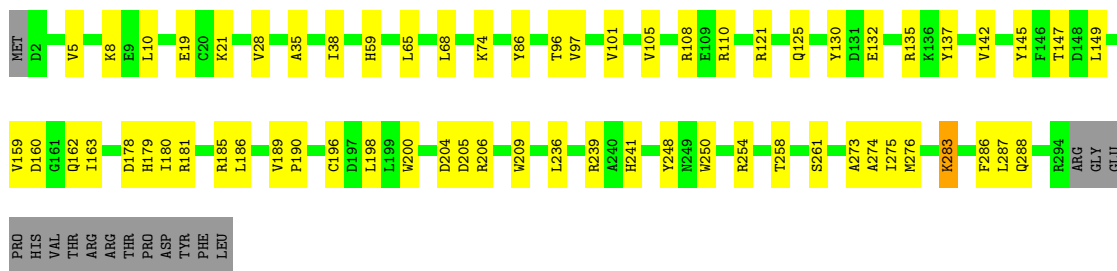




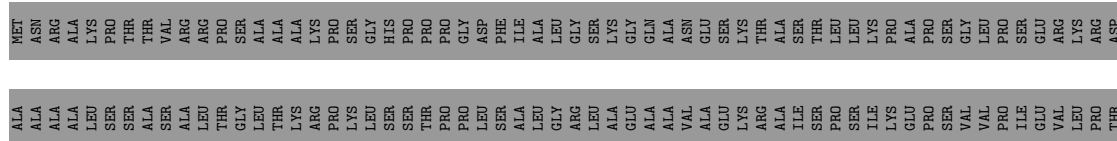
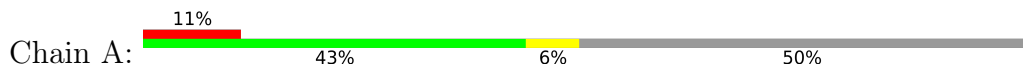
- Molecule 7: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



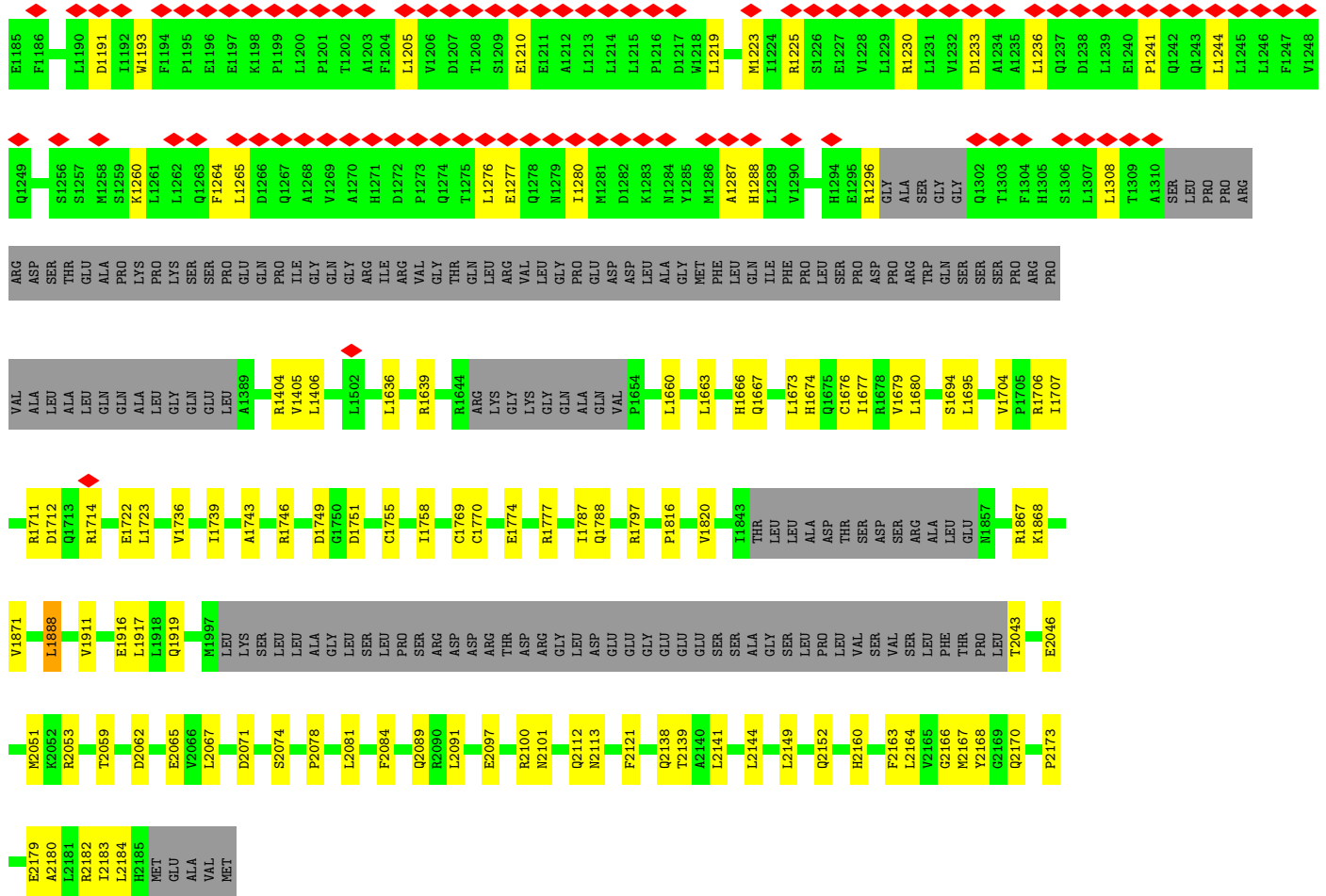
- Molecule 8: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



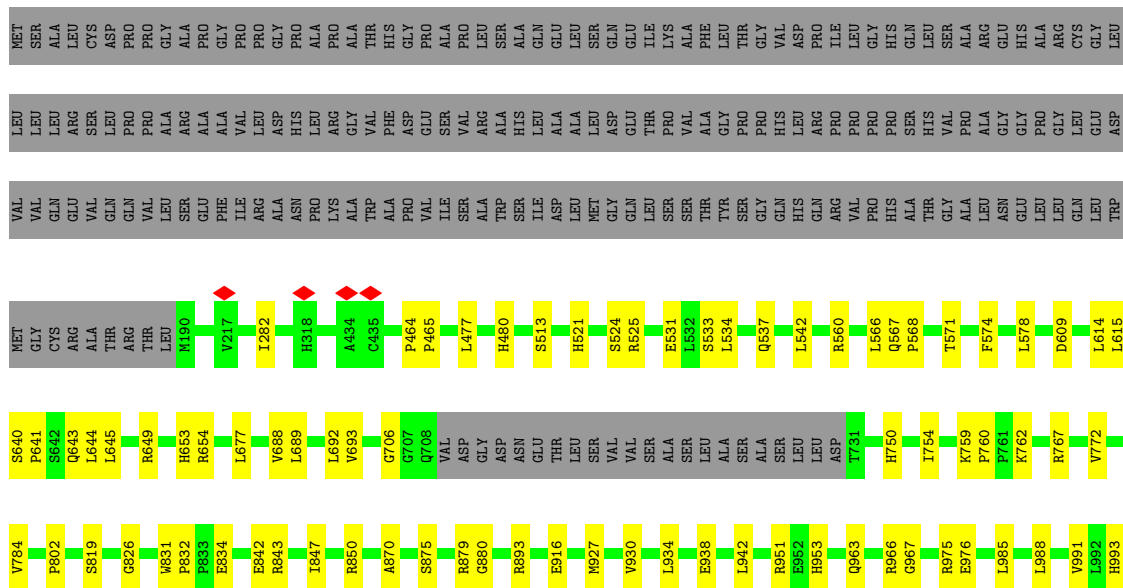
- Molecule 9: Integrator complex subunit 1

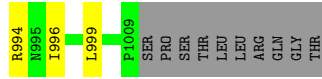






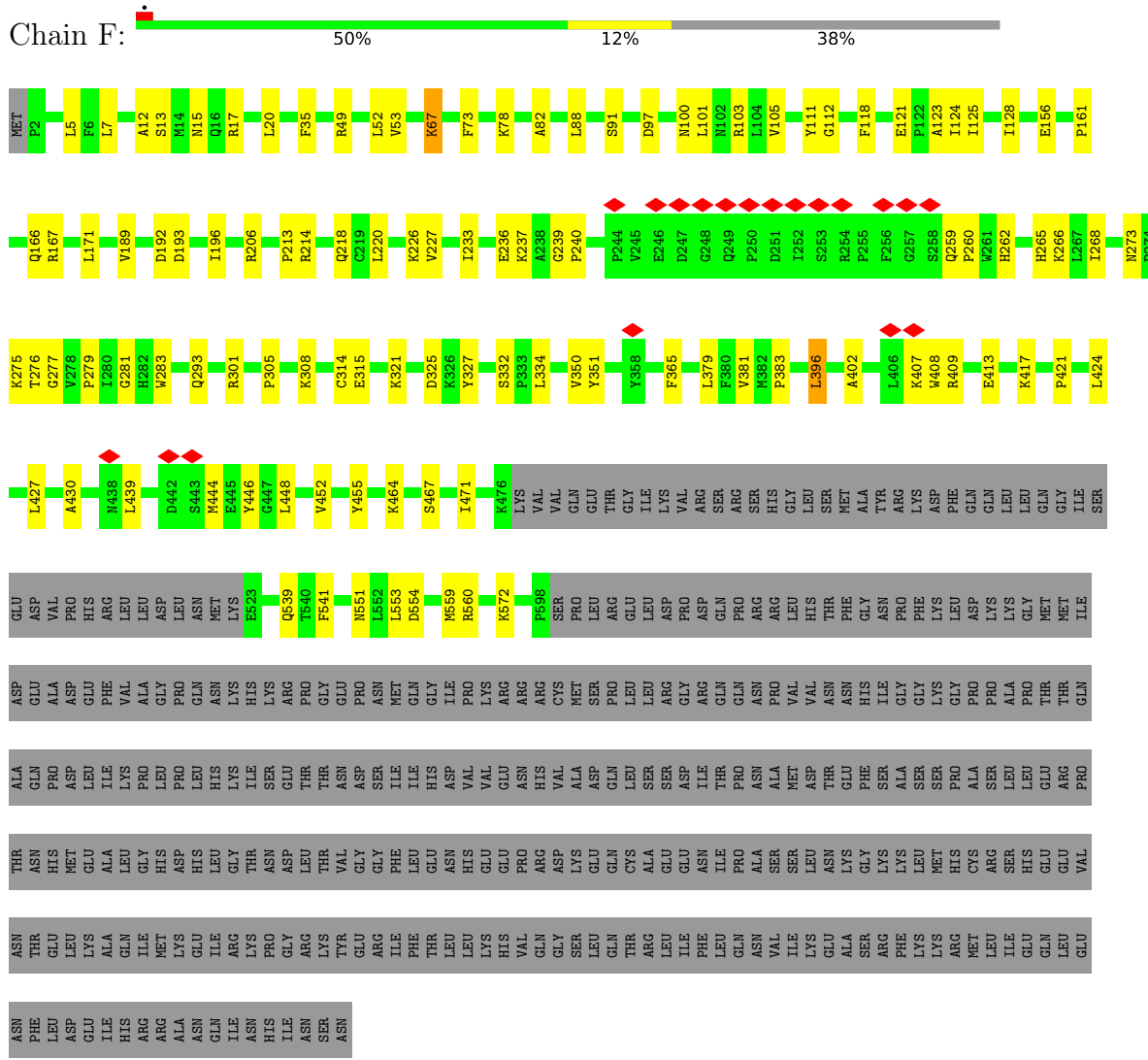
- Molecule 10: Integrator complex subunit 5





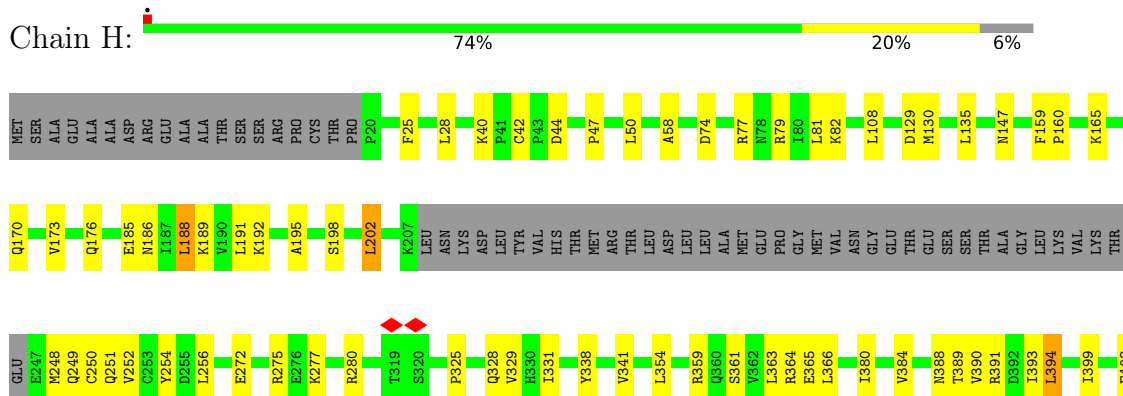
• Molecule 11: Integrator complex subunit 6

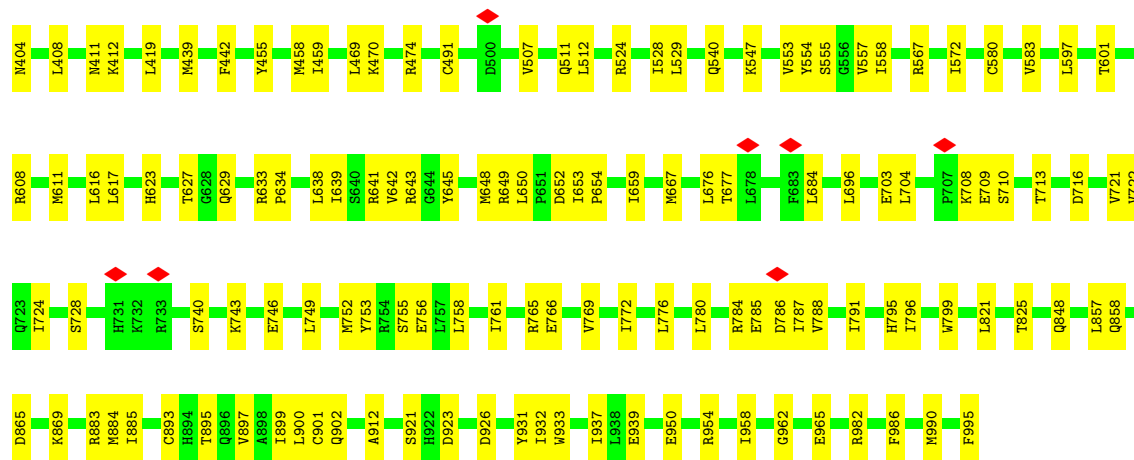
Chain F:



• Molecule 12: Integrator complex subunit 8

Chain H:





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43790	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	443.09998, 443.09998, 443.09998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0	0.27	0/282	0.50	0/381
2	I	0.32	0/5110	0.66	7/6959 (0.1%)
3	K	0.32	0/4747	0.68	2/6412 (0.0%)
4	B	0.31	0/8474	0.64	3/11498 (0.0%)
5	D	0.31	0/6217	0.66	8/8454 (0.1%)
6	G	0.31	0/6981	0.65	5/9452 (0.1%)
7	P	0.30	0/4601	0.68	2/6246 (0.0%)
8	Q	0.32	0/2423	0.68	2/3285 (0.1%)
9	A	0.26	0/7635	0.56	2/10415 (0.0%)
10	E	0.30	0/5344	0.59	2/7312 (0.0%)
11	F	0.30	0/4337	0.65	2/5907 (0.0%)
12	H	0.30	0/7583	0.64	4/10280 (0.0%)
All	All	0.30	0/63734	0.64	39/86601 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1
4	B	0	4
6	G	0	1
8	Q	0	1
10	E	0	1
12	H	0	1
All	All	0	9

There are no bond length outliers.

All (39) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	517	LEU	CA-CB-CG	7.91	133.49	115.30
10	E	609	ASP	CB-CG-OD1	7.25	124.82	118.30
12	H	202	LEU	CA-CB-CG	7.09	131.60	115.30
8	Q	283	LYS	CA-CB-CG	6.64	128.00	113.40
4	B	1180	ASP	CB-CG-OD1	6.44	124.09	118.30
5	D	869	ASP	CB-CG-OD1	6.13	123.82	118.30
6	G	204	MET	CA-CB-CG	6.13	123.72	113.30
9	A	1888	LEU	CA-CB-CG	6.12	129.37	115.30
12	H	394	LEU	CA-CB-CG	6.05	129.22	115.30
9	A	2071	ASP	CB-CG-OD1	6.00	123.70	118.30
7	P	166	LEU	CA-CB-CG	5.98	129.05	115.30
11	F	396	LEU	CA-CB-CG	5.93	128.95	115.30
6	G	772	MET	CG-SD-CE	5.92	109.68	100.20
5	D	564	LEU	CA-CB-CG	5.89	128.86	115.30
7	P	356	LEU	CA-CB-CG	5.81	128.66	115.30
2	I	97	ASP	CB-CG-OD1	5.77	123.49	118.30
2	I	529	MET	CA-CB-CG	5.68	122.95	113.30
2	I	277	MET	CB-CG-SD	-5.46	96.01	112.40
3	K	138	LEU	CA-CB-CG	5.46	127.86	115.30
2	I	441	MET	CA-CB-CG	5.45	122.56	113.30
6	G	187	LEU	CA-CB-CG	5.44	127.81	115.30
2	I	263	LEU	CA-CB-CG	5.43	127.80	115.30
5	D	768	ASP	CB-CG-OD1	5.41	123.17	118.30
12	H	188	LEU	CA-CB-CG	5.34	127.58	115.30
11	F	334	LEU	CA-CB-CG	5.32	127.54	115.30
4	B	88	LEU	CA-CB-CG	5.23	127.33	115.30
5	D	772	LEU	CA-CB-CG	5.19	127.23	115.30
10	E	677	LEU	CA-CB-CG	5.19	127.23	115.30
4	B	947	LEU	CA-CB-CG	5.15	127.14	115.30
6	G	762	LEU	CA-CB-CG	5.14	127.13	115.30
12	H	394	LEU	CB-CG-CD2	5.12	119.70	111.00
5	D	398	LEU	CA-CB-CG	5.11	127.05	115.30
8	Q	160	ASP	CB-CG-OD1	5.09	122.88	118.30
5	D	401	LEU	CA-CB-CG	5.07	126.96	115.30
5	D	220	LEU	CA-CB-CG	5.04	126.90	115.30
3	K	491	ARG	CG-CD-NE	-5.04	101.22	111.80
2	I	261	LEU	CA-CB-CG	5.01	126.83	115.30
2	I	625	LEU	CA-CB-CG	5.01	126.83	115.30
5	D	845	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	169	GLU	Peptide
4	B	205	ARG	Peptide
4	B	573	ILE	Peptide
4	B	586	THR	Peptide
10	E	567	GLN	Peptide
6	G	899	LEU	Peptide
12	H	44	ASP	Peptide
2	I	493	GLN	Peptide
8	Q	283	LYS	Peptide

## 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	0	275	0	231	1	0
2	I	4985	0	5012	86	0
3	K	4646	0	4662	90	0
4	B	8328	0	8566	125	0
5	D	6108	0	5810	117	0
6	G	6873	0	6877	96	0
7	P	4527	0	4633	80	0
8	Q	2366	0	2269	41	0
9	A	7530	0	6625	91	0
10	E	5244	0	4501	46	0
11	F	4229	0	4121	61	0
12	H	7440	0	7530	119	0
13	K	2	0	0	0	0
14	Q	2	0	0	0	0
All	All	62555	0	60837	897	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 (897) 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)
7:P:188:LYS:O	7:P:192:PHE:HB2	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:82:GLU:HG2	3:K:125:MET:HB2	1.71	0.72
3:K:108:ARG:HH22	3:K:123:SER:HB3	1.53	0.72
8:Q:196:CYS:O	8:Q:200:TRP:HB2	1.90	0.72
12:H:249:GLN:O	12:H:252:VAL:HB	1.90	0.71
2:I:48:ARG:HH12	2:I:436:TYR:HA	1.56	0.71
4:B:440:SER:HB2	4:B:513:SER:HB2	1.73	0.71
12:H:902:GLN:HE22	12:H:933:TRP:H	1.37	0.70
7:P:362:ILE:HA	7:P:366:LEU:HD23	1.73	0.70
12:H:761:ILE:HD12	12:H:821:LEU:HD13	1.74	0.70
5:D:878:LYS:HG3	5:D:880:ALA:H	1.57	0.69
11:F:97:ASP:O	11:F:101:LEU:HB2	1.92	0.69
3:K:107:TYR:HA	3:K:110:ILE:HD12	1.75	0.68
5:D:866:LEU:HB3	5:D:910:GLU:HB3	1.76	0.68
3:K:40:ASN:HA	3:K:44:ARG:HH21	1.59	0.68
5:D:711:TYR:HB3	5:D:817:ILE:HD11	1.75	0.68
4:B:1090:VAL:HG13	12:H:950:GLU:HG3	1.76	0.68
12:H:191:LEU:O	12:H:195:ALA:HB2	1.95	0.67
5:D:907:CYS:SG	6:G:891:GLN:NE2	2.67	0.67
6:G:514:LYS:NZ	6:G:544:GLU:OE1	2.28	0.67
9:A:1680:LEU:HD21	9:A:1694:SER:HB2	1.75	0.67
3:K:216:CYS:HA	3:K:219:ARG:HE	1.57	0.66
2:I:134:ARG:HE	2:I:191:LEU:HG	1.60	0.66
5:D:169:LYS:HA	5:D:172:GLN:HG3	1.78	0.66
2:I:388:ARG:HH12	5:D:962:ARG:HB2	1.60	0.66
9:A:2051:MET:HB2	9:A:2084:PHE:HE1	1.60	0.66
11:F:124:ILE:HD13	11:F:227:VAL:HG23	1.79	0.65
7:P:492:ASP:OD2	7:P:497:HIS:ND1	2.30	0.65
2:I:5:CYS:O	2:I:502:ALA:HA	1.96	0.65
2:I:650:LEU:HA	2:I:653:LYS:HE3	1.77	0.65
9:A:2170:GLN:NE2	12:H:893:CYS:SG	2.69	0.65
4:B:72:LEU:HD23	9:A:1288:HIS:HE1	1.62	0.65
9:A:2097:GLU:OE2	9:A:2101:ASN:ND2	2.30	0.65
3:K:215:ARG:NH1	5:D:414:ASP:O	2.30	0.65
4:B:944:GLU:HA	4:B:947:LEU:HD23	1.79	0.65
4:B:1035:MET:O	4:B:1038:CYS:HB3	1.97	0.65
7:P:308:GLU:HA	7:P:311:GLU:HG2	1.79	0.65
2:I:64:LEU:HB3	2:I:155:LEU:HD11	1.80	0.64
12:H:704:LEU:HD11	12:H:772:ILE:HD11	1.78	0.64
6:G:383:GLU:OE2	6:G:423:ARG:NH1	2.31	0.64
3:K:216:CYS:SG	3:K:219:ARG:NH2	2.71	0.64
6:G:427:SER:O	6:G:430:VAL:HB	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:324:GLY:HA3	4:B:336:LEU:HD13	1.80	0.63
10:E:934:LEU:HD13	10:E:938:GLU:HG2	1.81	0.63
10:E:537:GLN:NE2	12:H:491:CYS:SG	2.71	0.63
4:B:1091:LEU:HD13	4:B:1096:ARG:HA	1.80	0.63
9:A:1054:ILE:HG22	9:A:1091:ARG:HH22	1.63	0.63
3:K:239:VAL:HG11	3:K:248:LEU:HD21	1.81	0.63
7:P:315:ALA:HA	7:P:318:ARG:HG2	1.81	0.63
9:A:2078:PRO:HB2	9:A:2113:ASN:HD21	1.64	0.63
4:B:896:LEU:HD11	4:B:923:ARG:HB3	1.81	0.63
7:P:314:SER:OG	7:P:317:CYS:SG	2.55	0.63
12:H:650:LEU:HD23	12:H:652:ASP:H	1.63	0.63
11:F:5:LEU:HB3	11:F:125:ILE:HG22	1.81	0.62
4:B:484:ALA:HB2	4:B:526:PHE:HD2	1.65	0.62
6:G:180:ILE:HG13	6:G:200:ILE:HG21	1.81	0.62
12:H:740:SER:HA	12:H:743:LYS:HB2	1.82	0.62
2:I:648:ARG:NH1	3:K:581:GLU:OE2	2.33	0.62
9:A:1023:LEU:HD22	9:A:1061:GLN:HE21	1.63	0.62
9:A:1758:ILE:HG23	9:A:1797:ARG:HH12	1.64	0.62
6:G:851:CYS:HB3	6:G:909:SER:HB2	1.81	0.62
7:P:40:LEU:HB3	7:P:79:LEU:HD21	1.80	0.62
7:P:512:CYS:SG	7:P:513:GLY:N	2.72	0.62
2:I:270:PRO:HB2	2:I:488:LEU:HD13	1.81	0.62
8:Q:19:GLU:HG3	8:Q:21:LYS:HD3	1.81	0.62
2:I:31:ASP:HB3	2:I:84:CYS:HB3	1.81	0.61
2:I:210:GLN:HE22	2:I:212:THR:HB	1.64	0.61
2:I:485:ARG:HH12	2:I:488:LEU:HD12	1.66	0.61
9:A:1769:CYS:SG	9:A:1770:CYS:N	2.73	0.61
12:H:601:THR:HG22	12:H:608:ARG:HH12	1.66	0.61
3:K:207:ALA:HB3	3:K:419:LYS:HB2	1.83	0.61
3:K:289:LYS:HA	3:K:292:LYS:HE3	1.83	0.61
9:A:1277:GLU:HA	9:A:1280:ILE:HD12	1.81	0.61
5:D:525:LEU:HD11	5:D:551:ILE:HD11	1.82	0.61
6:G:469:GLY:O	6:G:472:MET:HB2	2.00	0.61
8:Q:59:HIS:H	8:Q:86:TYR:HA	1.66	0.60
4:B:44:LEU:HD11	4:B:213:LEU:HD21	1.82	0.60
2:I:135:LEU:HD12	2:I:332:VAL:HB	1.83	0.60
3:K:165:GLN:HG3	3:K:174:VAL:HG22	1.83	0.60
4:B:1033:PRO:HG3	9:A:1712:ASP:HB2	1.82	0.60
11:F:35:PHE:HB2	11:F:220:LEU:HD11	1.82	0.60
12:H:469:LEU:O	12:H:474:ARG:NH1	2.33	0.60
4:B:52:MET:O	4:B:68:LYS:NZ	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:409:ARG:HH22	11:F:439:LEU:HD21	1.67	0.60
8:Q:239:ARG:HH21	8:Q:241:HIS:HB3	1.65	0.60
5:D:868:PRO:HB2	6:G:893:LEU:HD23	1.83	0.59
7:P:296:ALA:HA	7:P:299:ARG:HE	1.67	0.59
9:A:1774:GLU:HA	9:A:1777:ARG:HG2	1.84	0.59
12:H:129:ASP:OD1	12:H:130:MET:N	2.32	0.59
6:G:417:VAL:HA	6:G:456:ILE:HD11	1.84	0.59
3:K:70:HIS:CE1	3:K:157:HIS:NE2	2.71	0.59
12:H:251:GLN:O	12:H:254:TYR:HB3	2.01	0.59
2:I:97:ASP:OD1	2:I:98:VAL:N	2.35	0.59
12:H:650:LEU:HD22	12:H:653:ILE:HG23	1.83	0.59
4:B:125:GLY:H	4:B:128:LEU:HD12	1.68	0.59
6:G:201:LEU:HD11	6:G:217:LEU:HD23	1.83	0.59
4:B:16:GLN:NE2	4:B:41:GLU:OE2	2.35	0.58
8:Q:142:VAL:HA	8:Q:145:TYR:HD1	1.68	0.58
2:I:90:LEU:HD23	2:I:91:ILE:HG23	1.85	0.58
7:P:180:MET:HA	7:P:183:ARG:HE	1.68	0.58
9:A:1755:CYS:SG	9:A:1797:ARG:NH2	2.76	0.58
11:F:17:ARG:NH1	12:H:962:GLY:O	2.37	0.58
6:G:189:THR:HB	6:G:193:LEU:HD23	1.86	0.58
8:Q:239:ARG:NH1	8:Q:258:THR:OG1	2.36	0.58
5:D:917:TYR:O	5:D:943:GLU:N	2.37	0.58
12:H:791:ILE:O	12:H:883:ARG:NH2	2.36	0.58
3:K:31:LEU:HD13	3:K:175:TYR:HB2	1.85	0.58
6:G:494:ALA:HB3	6:G:529:ILE:HD12	1.86	0.58
9:A:2078:PRO:O	9:A:2113:ASN:ND2	2.37	0.58
12:H:758:LEU:HD13	12:H:761:ILE:HD11	1.85	0.58
1:O:66:LYS:NZ	6:G:518:GLU:OE2	2.36	0.58
2:I:211:VAL:HG12	2:I:227:ILE:HG13	1.86	0.58
4:B:55:CYS:SG	4:B:56:ALA:N	2.77	0.58
12:H:512:LEU:HD12	12:H:528:ILE:HG23	1.85	0.58
3:K:276:ASN:ND2	3:K:301:GLU:OE1	2.37	0.57
4:B:295:VAL:HG12	4:B:384:LYS:HG3	1.85	0.57
6:G:491:VAL:HA	6:G:529:ILE:HD11	1.84	0.57
3:K:227:GLU:HB3	3:K:231:ARG:HH12	1.69	0.57
7:P:260:ARG:HA	7:P:263:VAL:HG22	1.86	0.57
5:D:172:GLN:O	5:D:176:ASN:ND2	2.38	0.57
6:G:828:ALA:HB1	6:G:891:GLN:HE22	1.68	0.57
12:H:645:TYR:HA	12:H:648:MET:HG2	1.85	0.57
5:D:264:PRO:HA	5:D:279:LEU:HD22	1.86	0.57
7:P:439:PHE:HA	7:P:443:LEU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:834:GLU:OE1	10:E:951:ARG:NH1	2.37	0.57
11:F:100:ASN:ND2	11:F:161:PRO:O	2.37	0.57
9:A:1039:PHE:O	9:A:1043:ARG:CB	2.53	0.57
5:D:507:LEU:HD12	5:D:550:LEU:HD12	1.86	0.57
6:G:491:VAL:HG21	6:G:528:ARG:HE	1.70	0.57
3:K:208:THR:HG23	3:K:419:LYS:HB3	1.86	0.57
11:F:275:LYS:HG3	11:F:276:THR:HG23	1.85	0.57
12:H:540:GLN:HG2	12:H:567:ARG:HH22	1.70	0.57
2:I:158:ASN:OD1	2:I:159:LYS:N	2.38	0.57
2:I:473:GLU:HG3	2:I:498:SER:HB3	1.87	0.57
3:K:475:LYS:HB2	3:K:477:ARG:HH12	1.70	0.57
7:P:112:LEU:HB3	7:P:150:LEU:HD21	1.87	0.57
2:I:439:LEU:HG	2:I:441:MET:H	1.70	0.56
9:A:1074:THR:HG21	9:A:1085:LEU:HD22	1.87	0.56
12:H:277:LYS:O	12:H:280:ARG:HB3	2.04	0.56
3:K:178:ASP:HA	3:K:203:GLU:HG2	1.87	0.56
3:K:208:THR:HG23	3:K:419:LYS:HE3	1.86	0.56
3:K:343:ASN:ND2	3:K:346:ASN:OD1	2.37	0.56
7:P:46:ARG:HH12	7:P:51:LEU:HD12	1.70	0.56
2:I:181:CYS:SG	2:I:182:TYR:N	2.79	0.56
6:G:421:LYS:NZ	6:G:459:GLN:OE1	2.38	0.56
7:P:313:LEU:O	7:P:318:ARG:NH2	2.38	0.56
12:H:629:GLN:HB3	12:H:765:ARG:HH22	1.71	0.56
4:B:82:ASN:OD1	9:A:1225:ARG:NH2	2.39	0.56
6:G:907:GLU:OE2	6:G:923:ARG:NH1	2.38	0.56
4:B:627:ILE:HD13	4:B:651:VAL:HG21	1.87	0.56
5:D:571:ARG:HH21	9:A:1714:ARG:HB3	1.70	0.56
5:D:776:PHE:O	5:D:780:LEU:HB2	2.06	0.56
7:P:583:LEU:HD21	7:P:589:ALA:HB3	1.86	0.56
9:A:907:VAL:HA	9:A:910:LEU:HD12	1.87	0.56
4:B:1141:ARG:NH2	4:B:1182:ASP:OD2	2.39	0.56
6:G:598:HIS:HA	6:G:601:ILE:HG22	1.87	0.56
11:F:273:ASN:HB3	11:F:277:GLY:H	1.71	0.56
12:H:40:LYS:NZ	12:H:42:CYS:O	2.32	0.56
3:K:184:ASP:HB3	3:K:187:LEU:HB2	1.87	0.56
8:Q:276:MET:HG3	8:Q:286:PHE:HE1	1.71	0.56
10:E:963:GLN:HE22	10:E:966:ARG:H	1.52	0.56
11:F:189:VAL:O	11:F:206:ARG:NH2	2.31	0.56
2:I:127:GLU:HA	2:I:130:VAL:HG22	1.88	0.55
3:K:472:GLU:O	3:K:477:ARG:NH1	2.39	0.55
6:G:300:LEU:HD22	6:G:347:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:994:ARG:HD2	12:H:160:PRO:HG2	1.89	0.55
6:G:702:ASN:ND2	6:G:790:SER:O	2.40	0.55
12:H:272:GLU:O	12:H:275:ARG:HG2	2.07	0.55
12:H:393:ILE:HD13	12:H:399:ILE:HD11	1.89	0.55
4:B:733:ILE:HG21	6:G:196:LYS:HE3	1.89	0.55
6:G:372:VAL:HG21	6:G:418:LYS:HG2	1.88	0.55
12:H:899:ILE:HD13	12:H:931:TYR:HB2	1.87	0.55
2:I:637:CYS:SG	2:I:644:ARG:NH1	2.80	0.55
5:D:387:MET:HG3	5:D:388:TYR:H	1.72	0.55
10:E:963:GLN:O	10:E:967:GLY:HA2	2.06	0.55
11:F:539:GLN:NE2	11:F:572:LYS:O	2.40	0.55
3:K:288:GLN:HA	3:K:291:ARG:HD3	1.89	0.55
7:P:537:ARG:HA	7:P:540:VAL:HG12	1.88	0.55
7:P:578:PHE:HA	7:P:581:GLU:HG3	1.88	0.55
12:H:529:LEU:HD11	12:H:572:ILE:HD11	1.89	0.55
3:K:157:HIS:O	3:K:244:ARG:NH2	2.40	0.55
4:B:84:ILE:HA	4:B:87:LEU:HD23	1.89	0.55
4:B:422:THR:HG22	4:B:424:ALA:H	1.71	0.55
7:P:25:VAL:HA	7:P:28:ARG:HH21	1.72	0.55
5:D:624:LEU:HG	5:D:627:LEU:HD11	1.89	0.55
5:D:645:ARG:HH22	5:D:649:LEU:HD21	1.71	0.55
2:I:39:LEU:HD22	2:I:76:PHE:HB2	1.89	0.54
4:B:227:ARG:HH11	4:B:267:MET:HG3	1.72	0.54
4:B:700:GLN:OE1	6:G:89:GLN:NE2	2.39	0.54
5:D:518:VAL:HG21	5:D:550:LEU:HD21	1.89	0.54
5:D:902:ALA:HA	5:D:958:PRO:HB2	1.89	0.54
3:K:287:ASN:OD1	3:K:288:GLN:N	2.40	0.54
6:G:143:ILE:O	6:G:147:LEU:HB2	2.07	0.54
4:B:265:ARG:HB2	4:B:281:LEU:HD11	1.89	0.54
5:D:567:ASP:N	5:D:567:ASP:OD1	2.40	0.54
3:K:398:ILE:HG21	3:K:423:LEU:HD11	1.89	0.54
3:K:425:GLN:OE1	3:K:429:GLN:NE2	2.40	0.54
9:A:1868:LYS:HE3	9:A:2152:GLN:HB3	1.90	0.54
2:I:339:PHE:HA	2:I:342:ILE:HG22	1.90	0.54
3:K:143:GLN:NE2	3:K:149:GLU:OE2	2.38	0.54
4:B:856:ASP:OD2	11:F:560:ARG:NH1	2.41	0.54
5:D:433:HIS:HA	5:D:436:ARG:HG2	1.88	0.54
7:P:218:ASP:OD1	7:P:218:ASP:N	2.41	0.54
4:B:574:LYS:NZ	4:B:616:ASN:OD1	2.39	0.54
6:G:147:LEU:HD21	6:G:180:ILE:HD11	1.89	0.54
8:Q:137:TYR:HD2	8:Q:142:VAL:HG11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:703:GLU:OE1	12:H:713:THR:OG1	2.26	0.54
6:G:174:VAL:HG12	6:G:210:LEU:HD13	1.89	0.54
12:H:784:ARG:HH21	12:H:788:VAL:HG13	1.73	0.54
5:D:395:VAL:HA	5:D:398:LEU:HG	1.89	0.54
5:D:462:ASP:OD1	5:D:462:ASP:N	2.41	0.54
12:H:617:LEU:HD13	12:H:659:ILE:HD13	1.89	0.53
2:I:57:LEU:HG	2:I:60:GLY:H	1.74	0.53
5:D:878:LYS:HD2	5:D:879:PRO:HD2	1.89	0.53
8:Q:132:GLU:OE2	8:Q:135:ARG:NH2	2.36	0.53
9:A:1236:LEU:HD11	9:A:1260:LYS:HD3	1.90	0.53
3:K:331:GLY:O	3:K:335:GLN:N	2.41	0.53
4:B:991:ARG:HG2	9:A:1707:ILE:HG23	1.90	0.53
11:F:236:GLU:O	11:F:308:LYS:HA	2.08	0.53
4:B:1149:ARG:HG2	9:A:2168:TYR:HD2	1.71	0.53
8:Q:206:ARG:HG2	11:F:78:LYS:HB2	1.90	0.53
11:F:233:ILE:HG23	11:F:305:PRO:HB2	1.91	0.53
4:B:690:LYS:HB2	4:B:721:LEU:HD13	1.89	0.53
7:P:310:CYS:O	7:P:318:ARG:NH1	2.41	0.53
12:H:865:ASP:OD1	12:H:869:LYS:NZ	2.41	0.53
3:K:128:ASP:O	3:K:132:LYS:NZ	2.42	0.53
4:B:574:LYS:HE2	4:B:617:GLN:HG2	1.91	0.53
10:E:826:GLY:O	10:E:879:ARG:NH2	2.42	0.53
2:I:26:LEU:HD23	2:I:100:LEU:HB2	1.91	0.53
5:D:791:LYS:HD3	5:D:793:ALA:H	1.73	0.53
6:G:575:LEU:HD11	6:G:628:LEU:HD21	1.90	0.53
9:A:1076:VAL:O	9:A:1130:ARG:NH1	2.42	0.53
10:E:784:VAL:HG11	12:H:404:ASN:HB3	1.90	0.53
4:B:941:ILE:HD11	11:F:553:LEU:HD21	1.89	0.53
7:P:217:GLN:O	7:P:221:ARG:NE	2.38	0.53
8:Q:38:ILE:HD11	8:Q:108:ARG:HB3	1.91	0.53
3:K:277:HIS:HA	3:K:280:LYS:HG2	1.91	0.52
3:K:393:ALA:HB1	3:K:397:GLY:HA3	1.90	0.52
4:B:327:ARG:NH1	4:B:329:ARG:O	2.41	0.52
5:D:821:SER:OG	5:D:852:GLU:OE2	2.27	0.52
9:A:1233:ASP:HA	9:A:1236:LEU:HD12	1.91	0.52
11:F:237:LYS:HE2	11:F:262:HIS:HA	1.89	0.52
4:B:65:ALA:O	4:B:69:LYS:HG2	2.10	0.52
4:B:578:TYR:CZ	4:B:623:GLU:HB3	2.44	0.52
9:A:1167:VAL:HA	9:A:1170:MET:HE2	1.90	0.52
10:E:706:GLY:H	10:E:772:VAL:HG13	1.74	0.52
12:H:965:GLU:OE1	12:H:982:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:186:ASN:HD22	12:H:189:LYS:NZ	2.07	0.52
12:H:921:SER:OG	12:H:923:ASP:OD1	2.28	0.52
2:I:613:LYS:HE2	2:I:629:GLU:HG2	1.92	0.52
12:H:328:GLN:HA	12:H:331:ILE:HG12	1.91	0.52
3:K:59:ASP:OD1	3:K:59:ASP:N	2.39	0.52
4:B:130:PHE:O	4:B:138:ARG:NH1	2.43	0.52
5:D:676:GLU:HG3	5:D:678:LEU:H	1.74	0.52
11:F:551:ASN:O	11:F:554:ASP:HB2	2.10	0.52
12:H:393:ILE:HG12	12:H:442:PHE:HB2	1.92	0.52
4:B:423:PRO:HA	4:B:426:VAL:HG12	1.92	0.52
8:Q:28:VAL:HG11	8:Q:142:VAL:HG23	1.92	0.52
8:Q:101:VAL:HG21	8:Q:149:LEU:HD21	1.91	0.52
9:A:2074:SER:HB2	9:A:2081:LEU:HD11	1.91	0.52
4:B:721:LEU:HD22	4:B:825:PRO:HG2	1.92	0.52
5:D:431:SER:HA	5:D:434:THR:HG22	1.92	0.52
7:P:116:SER:O	7:P:157:ARG:NH1	2.43	0.52
11:F:5:LEU:HD11	11:F:53:VAL:HG23	1.92	0.52
8:Q:185:ARG:HH12	10:E:893:ARG:HH22	1.58	0.52
11:F:156:GLU:OE2	11:F:455:TYR:OH	2.28	0.52
3:K:234:LYS:HD2	3:K:340:TRP:HH2	1.76	0.51
12:H:411:ASN:OD1	12:H:412:LYS:N	2.42	0.51
4:B:241:LEU:HB3	4:B:245:ARG:HH22	1.74	0.51
4:B:761:PHE:HE1	4:B:800:LEU:HD21	1.74	0.51
5:D:267:ILE:O	5:D:278:ARG:N	2.44	0.51
12:H:363:LEU:HD22	12:H:388:ASN:HD22	1.75	0.51
5:D:455:VAL:HG22	5:D:467:LEU:HD13	1.92	0.51
4:B:545:SER:OG	4:B:546:ALA:N	2.43	0.51
4:B:732:GLU:OE2	4:B:736:THR:N	2.42	0.51
9:A:2141:LEU:HA	9:A:2144:LEU:HB2	1.92	0.51
11:F:427:LEU:O	11:F:430:ALA:HB3	2.11	0.51
12:H:895:THR:OG1	12:H:923:ASP:OD2	2.28	0.51
3:K:51:ILE:HG13	3:K:52:THR:HG23	1.92	0.51
4:B:426:VAL:HA	4:B:429:VAL:HG12	1.91	0.51
4:B:874:MET:HG2	4:B:993:VAL:HG13	1.93	0.51
5:D:636:LEU:HB3	5:D:668:LEU:HD12	1.93	0.51
6:G:380:LEU:O	6:G:383:GLU:HB2	2.11	0.51
7:P:296:ALA:HB1	7:P:338:ASN:HD22	1.76	0.51
9:A:1077:GLU:O	9:A:1130:ARG:NH2	2.43	0.51
9:A:1663:LEU:O	9:A:1667:GLN:N	2.44	0.51
12:H:858:GLN:HG3	12:H:995:PHE:HE1	1.76	0.51
4:B:72:LEU:O	9:A:1296:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:356:ASN:HB3	6:G:359:ILE:HG22	1.92	0.51
3:K:512:THR:HA	3:K:574:VAL:O	2.11	0.51
4:B:693:ILE:HD13	4:B:714:LEU:HD22	1.92	0.51
5:D:321:LEU:HD11	5:D:408:PHE:HE1	1.75	0.51
5:D:521:LEU:HB3	5:D:525:LEU:HD23	1.93	0.51
5:D:712:SER:HB2	5:D:855:GLN:HE22	1.76	0.51
4:B:459:MET:HG2	4:B:480:LEU:HD11	1.92	0.51
5:D:461:ARG:HH12	5:D:499:ASP:HB3	1.75	0.51
3:K:9:LEU:HD23	3:K:21:LEU:HD23	1.92	0.51
4:B:193:PRO:HG2	4:B:196:ASP:HB2	1.92	0.51
5:D:906:ALA:HA	5:D:956:ILE:O	2.10	0.51
7:P:322:ILE:HD12	7:P:356:LEU:HD12	1.93	0.51
5:D:518:VAL:HA	5:D:521:LEU:HD23	1.92	0.51
3:K:194:LYS:NZ	5:D:244:ASP:OD1	2.42	0.50
3:K:424:LYS:HD2	3:K:437:MET:SD	2.51	0.50
6:G:470:ASP:OD1	6:G:471:LEU:N	2.45	0.50
7:P:188:LYS:O	7:P:192:PHE:CB	2.51	0.50
12:H:755:SER:OG	12:H:756:GLU:OE1	2.28	0.50
6:G:634:LEU:HD21	6:G:717:ILE:HD11	1.92	0.50
2:I:70:GLU:HA	2:I:75:VAL:HA	1.92	0.50
8:Q:125:GLN:HA	8:Q:130:TYR:HB2	1.94	0.50
9:A:1244:LEU:HD22	9:A:1265:LEU:HG	1.93	0.50
4:B:791:GLU:OE2	4:B:827:ARG:NH2	2.40	0.50
9:A:2149:LEU:HD11	9:A:2183:ILE:HD12	1.93	0.50
11:F:314:CYS:SG	11:F:315:GLU:N	2.83	0.50
3:K:280:LYS:HG3	3:K:281:LEU:HD12	1.93	0.50
10:E:640:SER:H	10:E:643:GLN:HE21	1.58	0.50
5:D:296:TRP:HA	5:D:299:ARG:HE	1.77	0.50
3:K:69:PHE:HA	3:K:74:CYS:HB2	1.93	0.50
3:K:497:GLN:HA	3:K:500:LYS:HG2	1.94	0.50
5:D:395:VAL:HG23	5:D:430:GLN:HE22	1.77	0.50
3:K:34:GLY:HA2	3:K:75:GLY:H	1.77	0.50
5:D:759:ASP:HA	5:D:762:GLN:HE21	1.77	0.50
2:I:614:GLY:CA	2:I:628:ILE:O	2.60	0.49
3:K:288:GLN:NE2	5:D:385:ASP:O	2.44	0.49
3:K:292:LYS:HG3	3:K:293:THR:HG23	1.94	0.49
4:B:340:ARG:HD3	4:B:401:LEU:HD21	1.93	0.49
10:E:568:PRO:HA	10:E:571:THR:HG22	1.94	0.49
4:B:463:GLU:HG3	4:B:477:GLY:HA3	1.94	0.49
5:D:640:ILE:O	5:D:644:GLN:HG2	2.11	0.49
6:G:808:LEU:HD11	6:G:906:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:265:ASP:HA	7:P:305:LYS:HE3	1.93	0.49
9:A:1871:VAL:HB	9:A:1917:LEU:HD21	1.94	0.49
2:I:261:LEU:HG	2:I:466:PRO:HB3	1.93	0.49
3:K:138:LEU:HG	3:K:139:HIS:H	1.77	0.49
3:K:411:LEU:HG	3:K:438:PRO:HG3	1.94	0.49
4:B:93:HIS:O	4:B:97:GLN:HG2	2.12	0.49
5:D:823:THR:OG1	5:D:850:THR:OG1	2.30	0.49
9:A:1746:ARG:HE	9:A:1749:ASP:HB2	1.75	0.49
9:A:2089:GLN:HE21	9:A:2121:PHE:HD1	1.60	0.49
11:F:12:ALA:HB3	12:H:939:GLU:HA	1.93	0.49
11:F:100:ASN:HA	11:F:103:ARG:HB2	1.94	0.49
2:I:388:ARG:HH22	5:D:962:ARG:H	1.61	0.49
6:G:819:ILE:HB	6:G:928:VAL:HG12	1.94	0.49
8:Q:248:TYR:HA	8:Q:258:THR:O	2.12	0.49
9:A:1039:PHE:O	9:A:1043:ARG:HB2	2.12	0.49
10:E:533:SER:O	10:E:537:GLN:HG3	2.11	0.49
3:K:66:ILE:HB	3:K:92:MET:HG3	1.93	0.49
8:Q:10:LEU:HD21	8:Q:105:VAL:HG23	1.94	0.49
4:B:28:LYS:HE3	6:G:587:LEU:HB2	1.95	0.49
10:E:934:LEU:HD21	10:E:999:LEU:HD11	1.94	0.49
2:I:214:LEU:HD11	2:I:254:SER:HB2	1.95	0.49
6:G:170:LYS:HD3	6:G:206:HIS:HB3	1.94	0.49
7:P:545:GLN:HG3	7:P:582:ALA:HA	1.93	0.49
4:B:299:VAL:HG13	4:B:391:LEU:HD22	1.95	0.49
4:B:1088:LEU:HD11	4:B:1131:VAL:HG11	1.94	0.49
9:A:2138:GLN:NE2	12:H:848:GLN:OE1	2.40	0.49
12:H:147:ASN:OD1	12:H:198:SER:HB2	2.12	0.49
2:I:11:THR:HG22	2:I:265:GLY:HA2	1.94	0.49
2:I:512:ARG:HG2	2:I:513:TYR:CD1	2.47	0.49
4:B:557:ILE:HG21	4:B:576:TRP:CZ3	2.48	0.49
4:B:1141:ARG:NE	4:B:1180:ASP:OD2	2.45	0.49
11:F:192:ASP:OD1	11:F:193:ASP:N	2.46	0.49
9:A:1098:THR:O	9:A:1102:HIS:ND1	2.40	0.49
12:H:202:LEU:HB3	12:H:256:LEU:HD22	1.95	0.49
9:A:2166:GLY:HA3	9:A:2173:PRO:HG3	1.95	0.48
11:F:118:PHE:HD1	11:F:279:PRO:HB2	1.78	0.48
12:H:633:ARG:HE	12:H:634:PRO:HD2	1.78	0.48
12:H:821:LEU:O	12:H:825:THR:OG1	2.26	0.48
3:K:222:LEU:HD13	3:K:255:PHE:HD2	1.78	0.48
4:B:814:ASN:HB2	4:B:872:PRO:HB3	1.95	0.48
8:Q:178:ASP:OD1	8:Q:181:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:649:ARG:HH21	12:H:684:LEU:HD13	1.78	0.48
2:I:82:GLU:HB3	2:I:178:TRP:HB3	1.94	0.48
2:I:334:ASN:OD1	2:I:335:SER:N	2.46	0.48
5:D:166:VAL:HG22	5:D:170:CYS:HB3	1.95	0.48
5:D:826:GLU:HG3	5:D:848:ASP:HB3	1.93	0.48
11:F:128:ILE:HG12	11:F:171:LEU:HB2	1.96	0.48
3:K:56:ARG:NH1	3:K:85:GLY:O	2.43	0.48
4:B:1145:PRO:HG3	4:B:1183:VAL:HG12	1.96	0.48
8:Q:261:SER:HA	8:Q:273:ALA:HB1	1.95	0.48
11:F:123:ALA:O	11:F:166:GLN:HA	2.12	0.48
12:H:721:VAL:HA	12:H:724:ILE:HG22	1.95	0.48
3:K:211:ARG:HE	3:K:217:ARG:HH21	1.62	0.48
3:K:331:GLY:HA2	3:K:334:LEU:HB2	1.95	0.48
4:B:426:VAL:HG23	4:B:476:PHE:HD1	1.78	0.48
9:A:2180:ALA:O	9:A:2184:LEU:HB2	2.13	0.48
4:B:271:GLU:HB3	4:B:273:HIS:HD2	1.79	0.48
4:B:436:LEU:HD11	4:B:452:MET:HE3	1.96	0.48
8:Q:159:VAL:HB	8:Q:163:ILE:HB	1.95	0.48
12:H:676:LEU:HG	12:H:677:THR:HG23	1.95	0.48
12:H:455:TYR:HA	12:H:458:MET:SD	2.53	0.48
12:H:524:ARG:O	12:H:528:ILE:HG13	2.13	0.48
5:D:431:SER:O	5:D:435:MET:HG2	2.14	0.48
6:G:912:ASP:OD2	6:G:918:TRP:NE1	2.35	0.48
10:E:843:ARG:O	10:E:847:ILE:HG13	2.14	0.48
12:H:390:VAL:HA	12:H:393:ILE:HG22	1.94	0.48
12:H:766:GLU:HB3	12:H:769:VAL:HG22	1.96	0.48
7:P:313:LEU:H	7:P:318:ARG:HH22	1.62	0.48
7:P:388:LEU:HA	7:P:391:VAL:HG12	1.94	0.48
12:H:325:PRO:HB2	12:H:354:LEU:HD11	1.95	0.48
4:B:1092:THR:O	4:B:1096:ARG:N	2.43	0.48
6:G:316:SER:HB2	6:G:365:ARG:HD2	1.94	0.48
7:P:451:LEU:HD11	7:P:466:LEU:HD11	1.96	0.48
12:H:643:ARG:NH1	12:H:667:MET:SD	2.87	0.48
2:I:44:VAL:HG21	5:D:899:SER:HB3	1.95	0.47
3:K:197:PRO:HG2	3:K:407:PRO:HB3	1.96	0.47
6:G:550:LEU:HD22	6:G:566:LYS:HE2	1.96	0.47
9:A:1244:LEU:HD21	9:A:1264:PHE:HD2	1.79	0.47
9:A:1888:LEU:HD22	9:A:1911:VAL:HG21	1.96	0.47
4:B:860:VAL:HG13	4:B:880:MET:HE2	1.95	0.47
6:G:289:ARG:NH1	6:G:327:TYR:O	2.47	0.47
12:H:784:ARG:HA	12:H:788:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:410:GLU:O	2:I:412:TRP:N	2.47	0.47
11:F:259:GLN:H	11:F:262:HIS:CE1	2.31	0.47
7:P:359:ASP:HA	7:P:362:ILE:HD12	1.96	0.47
4:B:551:PHE:O	4:B:555:HIS:ND1	2.40	0.47
4:B:1108:VAL:HG22	4:B:1196:ILE:HG13	1.97	0.47
9:A:1287:ALA:HB2	9:A:1308:LEU:HB3	1.96	0.47
11:F:101:LEU:HD21	11:F:467:SER:HA	1.96	0.47
3:K:234:LYS:H	3:K:346:ASN:HD22	1.61	0.47
3:K:370:LEU:H	3:K:378:LEU:H	1.63	0.47
4:B:690:LYS:NZ	4:B:822:THR:O	2.46	0.47
12:H:359:ARG:HH11	12:H:391:ARG:HH11	1.63	0.47
2:I:16:VAL:HG21	2:I:91:ILE:HD11	1.97	0.47
3:K:519:ASP:O	3:K:570:LYS:NZ	2.45	0.47
4:B:482:LEU:HA	4:B:485:MET:HE2	1.96	0.47
5:D:458:ASP:OD1	5:D:459:SER:N	2.46	0.47
7:P:279:THR:HA	7:P:283:LEU:HB2	1.97	0.47
7:P:414:ASP:O	7:P:420:ARG:NH1	2.48	0.47
9:A:1070:LEU:O	9:A:1074:THR:OG1	2.27	0.47
11:F:49:ARG:NH2	11:F:121:GLU:OE2	2.47	0.47
6:G:190:PRO:HB3	9:A:1666:HIS:CG	2.50	0.47
9:A:2053:ARG:NH2	9:A:2065:GLU:OE1	2.48	0.47
9:A:2160:HIS:CE1	9:A:2164:LEU:HD13	2.50	0.47
4:B:241:LEU:HB3	4:B:245:ARG:NH2	2.29	0.47
4:B:487:PHE:O	4:B:518:LYS:NZ	2.37	0.47
4:B:516:ARG:O	4:B:519:THR:OG1	2.29	0.47
6:G:139:ALA:O	6:G:143:ILE:HG12	2.15	0.47
6:G:194:LYS:O	6:G:198:ILE:HG13	2.15	0.47
6:G:340:ARG:HH22	6:G:381:ALA:H	1.62	0.47
9:A:1205:LEU:N	9:A:1210:GLU:O	2.47	0.47
5:D:255:LEU:HA	5:D:258:VAL:HG12	1.96	0.47
5:D:450:ASP:HA	5:D:453:LEU:HG	1.97	0.47
6:G:180:ILE:HD12	6:G:197:LEU:HD12	1.96	0.47
4:B:688:PRO:HB2	4:B:691:PHE:HB3	1.97	0.46
5:D:294:GLY:O	5:D:299:ARG:NH2	2.47	0.46
5:D:396:GLU:OE2	5:D:430:GLN:NE2	2.44	0.46
6:G:30:ASP:HA	6:G:33:LEU:HB2	1.96	0.46
6:G:543:LYS:HE2	6:G:570:HIS:HA	1.97	0.46
7:P:357:GLY:O	7:P:361:THR:HG23	2.15	0.46
8:Q:179:HIS:ND1	10:E:842:GLU:OE2	2.48	0.46
10:E:942:LEU:HD11	10:E:991:VAL:HG11	1.96	0.46
12:H:884:MET:HB3	12:H:900:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:608:VAL:HG22	2:I:617:VAL:HG23	1.98	0.46
3:K:153:TYR:CE2	3:K:192:ILE:HG13	2.50	0.46
5:D:424:ILE:HG22	5:D:427:VAL:H	1.81	0.46
6:G:705:LEU:O	6:G:752:TYR:OH	2.33	0.46
9:A:904:VAL:HG12	9:A:906:PRO:HD2	1.98	0.46
9:A:2043:THR:N	9:A:2046:GLU:OE2	2.48	0.46
11:F:111:TYR:HA	11:F:301:ARG:HH21	1.81	0.46
2:I:217:GLY:HA2	2:I:247:PRO:HG2	1.98	0.46
3:K:338:ARG:NH2	3:K:371:GLU:O	2.47	0.46
4:B:308:GLY:O	4:B:314:ARG:NH2	2.44	0.46
8:Q:35:ALA:HA	8:Q:38:ILE:HG22	1.97	0.46
12:H:419:LEU:HD11	12:H:459:ILE:HA	1.97	0.46
2:I:203:ILE:HG23	2:I:211:VAL:HG23	1.96	0.46
5:D:580:LEU:HD13	5:D:583:LEU:HD12	1.96	0.46
6:G:80:ARG:HB3	6:G:121:ILE:HG21	1.97	0.46
5:D:166:VAL:O	5:D:170:CYS:N	2.38	0.46
7:P:160:SER:HA	7:P:163:LYS:HE3	1.96	0.46
7:P:313:LEU:H	7:P:318:ARG:NH2	2.14	0.46
9:A:1751:ASP:N	9:A:1751:ASP:OD1	2.48	0.46
12:H:366:LEU:HD12	12:H:384:VAL:HG11	1.97	0.46
2:I:72:SER:HB3	2:I:438:PRO:HD3	1.97	0.46
4:B:318:GLY:O	4:B:322:ARG:HG2	2.16	0.46
4:B:1050:GLU:HB2	4:B:1053:LYS:HD2	1.97	0.46
5:D:400:MET:HG3	5:D:401:LEU:N	2.31	0.46
9:A:1660:LEU:HD23	9:A:1663:LEU:HD12	1.97	0.46
11:F:167:ARG:NH2	11:F:226:LYS:O	2.48	0.46
8:Q:250:TRP:CE3	8:Q:254:ARG:HD3	2.51	0.46
9:A:2067:LEU:HD11	9:A:2091:LEU:HD21	1.98	0.46
12:H:795:HIS:CE1	12:H:796:ILE:HG12	2.50	0.46
4:B:347:LEU:HD21	4:B:392:TYR:HE2	1.81	0.46
5:D:842:VAL:HA	5:D:898:LEU:O	2.16	0.46
12:H:728:SER:HA	12:H:749:LEU:HG	1.98	0.46
5:D:678:LEU:HD21	5:D:739:ARG:HG2	1.97	0.46
6:G:702:ASN:HD22	6:G:792:GLN:HG2	1.80	0.46
8:Q:274:ALA:HB2	8:Q:288:GLN:HG3	1.96	0.46
12:H:28:LEU:HD21	12:H:77:ARG:HG3	1.97	0.46
12:H:79:ARG:HA	12:H:82:LYS:HD2	1.97	0.46
2:I:211:VAL:HA	2:I:226:ILE:O	2.16	0.46
5:D:171:LEU:HD23	5:D:174:LEU:HD21	1.97	0.46
6:G:119:ARG:NE	6:G:154:GLU:OE2	2.43	0.46
6:G:540:ASP:OD1	6:G:541:MET:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1722:GLU:HG2	9:A:1723:LEU:H	1.80	0.46
12:H:394:LEU:HD22	12:H:439:MET:HE1	1.98	0.46
2:I:33:THR:HA	2:I:36:LEU:HD13	1.97	0.45
7:P:221:ARG:NH1	7:P:254:ASP:OD2	2.50	0.45
11:F:421:PRO:O	11:F:424:LEU:CB	2.64	0.45
12:H:361:SER:O	12:H:365:GLU:HG3	2.16	0.45
2:I:43:LEU:HD11	5:D:842:VAL:HG11	1.98	0.45
2:I:277:MET:HE2	2:I:446:CYS:HA	1.98	0.45
4:B:179:ASP:O	4:B:183:ILE:HG12	2.17	0.45
4:B:599:TYR:O	4:B:603:ILE:HG12	2.16	0.45
7:P:320:ASN:O	7:P:324:SER:OG	2.33	0.45
11:F:214:ARG:O	11:F:218:GLN:HG3	2.17	0.45
2:I:30:LEU:HD11	2:I:83:PHE:HB3	1.98	0.45
7:P:316:ASP:OD1	7:P:316:ASP:N	2.49	0.45
12:H:74:ASP:O	12:H:79:ARG:NH1	2.45	0.45
12:H:185:GLU:HA	12:H:188:LEU:HG	1.97	0.45
5:D:260:SER:HA	5:D:279:LEU:HD21	1.99	0.45
12:H:25:PHE:HA	12:H:28:LEU:HB3	1.98	0.45
12:H:931:TYR:HB3	12:H:986:PHE:HB2	1.99	0.45
6:G:393:LEU:HD21	6:G:408:THR:HG22	1.98	0.45
8:Q:186:LEU:HD23	12:H:165:LYS:HE2	1.97	0.45
11:F:118:PHE:CD2	11:F:281:GLY:HA3	2.52	0.45
4:B:431:LEU:O	4:B:435:MET:HB2	2.16	0.45
4:B:458:TRP:CZ2	4:B:462:GLU:HG2	2.52	0.45
5:D:287:ILE:HG21	5:D:306:LEU:HB3	1.99	0.45
6:G:215:ARG:HG3	6:G:238:PHE:HE1	1.82	0.45
9:A:1867:ARG:NH2	9:A:2112:GLN:O	2.49	0.45
5:D:839:SER:HB2	5:D:902:ALA:HB2	1.99	0.45
6:G:51:LEU:HD11	6:G:60:LEU:HD21	1.99	0.45
7:P:257:TRP:HA	7:P:260:ARG:HE	1.82	0.45
7:P:388:LEU:O	7:P:392:ASN:HB2	2.16	0.45
11:F:351:TYR:HA	11:F:365:PHE:HD1	1.82	0.45
12:H:785:GLU:HG2	12:H:786:ASP:H	1.82	0.45
4:B:343:LEU:HD13	4:B:392:TYR:HE1	1.82	0.45
5:D:837:PHE:HE1	5:D:956:ILE:HG23	1.82	0.45
9:A:1674:HIS:HA	9:A:1677:ILE:HG22	1.99	0.45
2:I:18:LYS:HG2	2:I:23:THR:HG22	1.99	0.45
2:I:268:GLN:HG3	2:I:425:PRO:HB2	1.98	0.45
3:K:368:ARG:HA	3:K:380:VAL:HG23	1.99	0.45
5:D:460:SER:HB3	5:D:463:ILE:HB	1.99	0.45
6:G:524:TRP:CD1	6:G:528:ARG:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:101:GLU:HB2	7:P:104:VAL:HG22	1.98	0.45
11:F:67:LYS:HG2	11:F:471:ILE:HG23	1.98	0.45
12:H:634:PRO:HB2	12:H:639:ILE:HD11	1.99	0.45
12:H:885:ILE:HG23	12:H:897:VAL:HG13	1.98	0.45
2:I:288:THR:HG21	2:I:419:THR:HG22	1.98	0.45
3:K:117:GLU:HG2	3:K:119:ASN:H	1.82	0.45
3:K:166:ILE:O	3:K:172:SER:HA	2.17	0.45
4:B:50:VAL:HG12	4:B:75:LEU:HD11	1.98	0.45
5:D:208:ASP:OD2	5:D:210:ARG:NH2	2.50	0.45
5:D:686:TYR:OH	5:D:691:ASP:OD2	2.28	0.45
7:P:307:LYS:HB2	7:P:348:VAL:HB	1.99	0.45
12:H:616:LEU:HD21	12:H:642:VAL:HA	1.98	0.45
12:H:722:VAL:HG12	12:H:780:LEU:HD13	1.97	0.45
4:B:69:LYS:HD3	9:A:1288:HIS:CD2	2.52	0.44
4:B:149:ILE:HG23	4:B:200:ALA:HB1	1.99	0.44
4:B:558:TYR:OH	4:B:562:ARG:NH2	2.45	0.44
5:D:844:ALA:HA	5:D:896:VAL:O	2.17	0.44
7:P:124:LEU:HA	7:P:128:PHE:CD1	2.52	0.44
9:A:1241:PRO:HB3	9:A:1276:LEU:HD13	1.98	0.44
9:A:1676:CYS:HA	9:A:1679:VAL:HG12	1.99	0.44
9:A:2059:THR:HG23	9:A:2062:ASP:H	1.82	0.44
3:K:6:VAL:HG23	3:K:22:VAL:HG12	1.98	0.44
7:P:35:LEU:HA	7:P:38:ILE:HD12	1.98	0.44
12:H:507:VAL:O	12:H:511:GLN:HG2	2.17	0.44
2:I:4:TYR:HB2	2:I:16:VAL:HB	1.98	0.44
2:I:160:ASP:OD1	2:I:161:ILE:HD12	2.17	0.44
7:P:48:ARG:HH21	7:P:52:LEU:HD11	1.83	0.44
12:H:338:TYR:HB3	12:H:380:ILE:HG21	2.00	0.44
4:B:47:PRO:HA	4:B:50:VAL:HG22	1.98	0.44
4:B:1022:CYS:O	4:B:1025:LEU:HB2	2.17	0.44
5:D:662:THR:HG22	5:D:665:ARG:HH12	1.82	0.44
7:P:150:LEU:HA	7:P:153:VAL:HG12	2.00	0.44
8:Q:65:LEU:HD22	8:Q:96:THR:HG23	1.98	0.44
12:H:597:LEU:HA	12:H:611:MET:HE1	1.99	0.44
4:B:59:ASP:HB3	4:B:64:TRP:CD1	2.53	0.44
5:D:798:ILE:O	5:D:802:MET:HB2	2.17	0.44
5:D:848:ASP:HA	5:D:892:LEU:O	2.17	0.44
7:P:139:ASP:O	7:P:144:ARG:NH2	2.50	0.44
7:P:288:GLN:HA	7:P:291:MET:SD	2.57	0.44
9:A:1039:PHE:O	9:A:1043:ARG:HB3	2.17	0.44
11:F:105:VAL:HG21	11:F:467:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:248:MET:SD	12:H:248:MET:N	2.90	0.44
4:B:1062:SER:HB2	4:B:1109:SER:HB2	1.99	0.44
4:B:1190:GLU:O	4:B:1194:ILE:HG12	2.18	0.44
7:P:167:ARG:O	7:P:171:ARG:HG2	2.17	0.44
9:A:1128:VAL:HG21	9:A:1193:TRP:HH2	1.82	0.44
12:H:638:LEU:HA	12:H:641:ARG:HG2	1.98	0.44
12:H:932:ILE:HD11	12:H:937:ILE:HB	1.99	0.44
5:D:318:GLU:HG2	5:D:411:LYS:HE2	2.00	0.44
7:P:456:TYR:HE2	8:Q:74:LYS:HG3	1.81	0.44
7:P:574:ASP:OD2	8:Q:110:ARG:NH1	2.50	0.44
3:K:234:LYS:HE2	3:K:346:ASN:HD21	1.82	0.44
3:K:420:MET:O	3:K:424:LYS:HG3	2.17	0.44
5:D:588:ARG:NH2	9:A:1820:VAL:O	2.51	0.44
6:G:514:LYS:HA	6:G:517:LEU:HD23	1.99	0.44
6:G:717:ILE:HG12	6:G:777:LEU:HD21	1.99	0.44
10:E:985:LEU:HD12	10:E:988:LEU:HD23	2.00	0.44
2:I:26:LEU:HD21	2:I:227:ILE:HD11	2.00	0.44
2:I:492:CYS:HB2	2:I:494:PRO:HD2	1.99	0.44
5:D:950:LYS:HE2	5:D:950:LYS:HB2	1.84	0.44
6:G:54:LYS:HD3	6:G:55:TYR:CE2	2.53	0.44
6:G:171:ASP:OD1	6:G:172:PHE:N	2.51	0.44
11:F:464:LYS:HD2	11:F:464:LYS:HA	1.84	0.44
2:I:1:MET:HG3	2:I:507:LEU:HB2	1.99	0.43
3:K:460:LEU:HD12	3:K:494:SER:HB2	1.99	0.43
3:K:535:LYS:NZ	3:K:543:VAL:O	2.38	0.43
4:B:78:VAL:HG13	4:B:81:VAL:HG23	1.98	0.43
4:B:241:LEU:HD12	4:B:245:ARG:HH12	1.81	0.43
7:P:124:LEU:HA	7:P:128:PHE:HD1	1.83	0.43
7:P:501:THR:O	7:P:505:ILE:HG12	2.18	0.43
8:Q:236:LEU:HD12	8:Q:236:LEU:HA	1.90	0.43
10:E:993:HIS:HA	10:E:996:ILE:HD11	1.99	0.43
2:I:529:MET:HE3	2:I:657:LYS:HB2	2.00	0.43
4:B:449:GLU:HA	4:B:452:MET:HG2	1.99	0.43
5:D:686:TYR:CE2	5:D:740:THR:HG22	2.53	0.43
5:D:887:PRO:HD2	5:D:889:ARG:HH12	1.83	0.43
8:Q:5:VAL:HA	8:Q:8:LYS:HE3	2.00	0.43
8:Q:163:ILE:HD11	10:E:754:ILE:HG21	2.00	0.43
9:A:1636:LEU:HA	9:A:1639:ARG:HG2	2.00	0.43
10:E:645:LEU:O	10:E:649:ARG:HG2	2.18	0.43
2:I:141:VAL:O	2:I:145:GLU:HB2	2.18	0.43
2:I:584:LEU:HD11	3:K:499:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:790:ALA:O	4:B:794:THR:OG1	2.34	0.43
6:G:549:LEU:HB3	6:G:562:LEU:HD13	1.99	0.43
6:G:572:GLU:OE1	6:G:597:TYR:OH	2.36	0.43
9:A:910:LEU:HD22	9:A:950:LEU:HD13	2.00	0.43
10:E:614:LEU:HD23	10:E:614:LEU:HA	1.85	0.43
11:F:259:GLN:HA	11:F:260:PRO:HD3	1.91	0.43
2:I:535:ILE:HG13	3:K:486:LYS:HZ3	1.84	0.43
5:D:161:ASP:H	5:D:166:VAL:HG12	1.83	0.43
6:G:846:LYS:HE2	6:G:846:LYS:HB2	1.80	0.43
7:P:112:LEU:HD13	7:P:115:ILE:HD12	2.00	0.43
10:E:524:SER:HA	10:E:574:PHE:HB2	2.00	0.43
11:F:52:LEU:HB2	11:F:73:PHE:HE1	1.83	0.43
12:H:553:VAL:HB	12:H:654:PRO:HB3	1.99	0.43
12:H:633:ARG:HD2	12:H:633:ARG:HA	1.86	0.43
5:D:429:LEU:O	5:D:433:HIS:ND1	2.40	0.43
5:D:503:ILE:HA	5:D:506:CYS:SG	2.59	0.43
7:P:307:LYS:HE2	7:P:351:GLY:HA3	2.00	0.43
7:P:338:ASN:OD1	7:P:339:GLN:N	2.50	0.43
9:A:1704:VAL:HG12	9:A:1706:ARG:H	1.82	0.43
12:H:329:VAL:HG23	12:H:341:VAL:HG13	2.01	0.43
12:H:709:GLU:HG2	12:H:710:SER:H	1.82	0.43
2:I:259:ASP:HA	2:I:467:LEU:H	1.82	0.43
3:K:180:ASN:HD22	3:K:391:ALA:HB1	1.83	0.43
4:B:557:ILE:HG13	4:B:566:PHE:HZ	1.83	0.43
5:D:858:GLN:HG3	5:D:882:PHE:HD2	1.83	0.43
9:A:1043:ARG:HD2	9:A:1073:HIS:HB3	2.00	0.43
9:A:2179:GLU:HA	9:A:2182:ARG:HG2	2.01	0.43
11:F:239:GLY:HA3	11:F:240:PRO:HD3	1.89	0.43
12:H:649:ARG:NH2	12:H:684:LEU:HB2	2.33	0.43
12:H:746:GLU:OE1	12:H:753:TYR:OH	2.35	0.43
5:D:166:VAL:HG23	5:D:169:LYS:HZ2	1.83	0.43
6:G:491:VAL:HG23	6:G:525:THR:HG23	2.01	0.43
11:F:7:LEU:HD11	11:F:91:SER:HB2	2.00	0.43
3:K:157:HIS:HE1	3:K:392:HIS:CE1	2.37	0.43
3:K:263:VAL:HA	3:K:264:PRO:HD3	1.91	0.43
5:D:523:PRO:HA	5:D:528:THR:HG21	2.00	0.43
6:G:199:PRO:HA	6:G:202:GLN:HB3	2.01	0.43
9:A:958:LEU:HD22	9:A:968:THR:HG23	1.99	0.43
9:A:1736:VAL:HA	9:A:1739:ILE:HG22	2.00	0.43
12:H:58:ALA:HB2	12:H:81:LEU:HD22	2.01	0.43
2:I:259:ASP:O	2:I:468:HIS:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:614:GLY:HA3	2:I:628:ILE:O	2.19	0.43
3:K:491:ARG:HG2	3:K:493:VAL:HG23	2.00	0.43
3:K:530:VAL:HG21	3:K:572:LEU:HD22	2.00	0.43
4:B:1034:SER:O	4:B:1037:ILE:HG12	2.19	0.43
5:D:161:ASP:HB2	5:D:166:VAL:HG12	2.00	0.43
8:Q:86:TYR:HE1	8:Q:97:VAL:HG23	1.84	0.43
10:E:802:PRO:HG2	12:H:408:LEU:HB2	2.00	0.43
4:B:162:PHE:HD1	4:B:205:ARG:HH12	1.66	0.43
4:B:293:ASP:OD1	4:B:293:ASP:N	2.51	0.43
5:D:171:LEU:HD13	5:D:215:ALA:HB2	2.00	0.43
7:P:566:LYS:HA	7:P:566:LYS:HD2	1.85	0.43
8:Q:162:GLN:HB2	10:E:759:LYS:HE2	2.00	0.43
12:H:47:PRO:HA	12:H:50:LEU:HD12	2.01	0.43
2:I:337:LEU:HD12	2:I:364:HIS:CD2	2.54	0.42
4:B:525:ILE:HG22	4:B:526:PHE:HD1	1.83	0.42
6:G:524:TRP:NE1	6:G:528:ARG:HD2	2.34	0.42
7:P:515:ASP:OD1	7:P:515:ASP:N	2.50	0.42
9:A:974:TYR:HA	9:A:977:ARG:HG2	2.01	0.42
10:E:615:LEU:HD13	10:E:653:HIS:CE1	2.53	0.42
11:F:266:LYS:HD2	11:F:332:SER:HB2	2.01	0.42
2:I:212:THR:HA	2:I:213:PRO:HD3	1.90	0.42
2:I:364:HIS:HA	2:I:367:LEU:HD12	2.01	0.42
2:I:535:ILE:HG13	3:K:486:LYS:NZ	2.34	0.42
5:D:522:VAL:HA	5:D:525:LEU:HG	2.01	0.42
6:G:215:ARG:HG3	6:G:238:PHE:CE1	2.54	0.42
8:Q:180:ILE:HD12	8:Q:198:LEU:HD11	2.00	0.42
10:E:688:VAL:O	10:E:692:LEU:HB2	2.19	0.42
3:K:128:ASP:HA	3:K:131:LYS:NZ	2.34	0.42
4:B:47:PRO:HB2	4:B:182:CYS:SG	2.59	0.42
4:B:131:GLU:HB2	4:B:173:TYR:HE2	1.84	0.42
4:B:793:LEU:O	4:B:797:MET:HG2	2.20	0.42
8:Q:121:ARG:HH11	8:Q:147:THR:HB	1.84	0.42
9:A:2100:ARG:HE	9:A:2139:THR:HG21	1.84	0.42
10:E:521:HIS:CE1	10:E:525:ARG:HH21	2.37	0.42
12:H:554:TYR:HA	12:H:557:VAL:HG12	2.01	0.42
12:H:857:LEU:HD21	12:H:990:MET:HB3	2.01	0.42
4:B:247:THR:HA	4:B:277:LEU:HD12	2.02	0.42
6:G:368:THR:HG23	6:G:419:LEU:HB2	2.01	0.42
7:P:294:CYS:O	7:P:299:ARG:NH2	2.53	0.42
2:I:322:SER:HA	2:I:372:LYS:HE2	2.00	0.42
3:K:163:MET:HB2	3:K:176:THR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1045:LEU:HG	4:B:1057:ALA:HB2	2.02	0.42
5:D:718:GLN:O	5:D:722:ILE:HG12	2.20	0.42
5:D:831:SER:OG	5:D:833:ASN:OD1	2.36	0.42
8:Q:206:ARG:NH1	8:Q:209:TRP:O	2.52	0.42
10:E:654:ARG:HA	10:E:654:ARG:HD2	1.92	0.42
12:H:192:LYS:HB2	12:H:192:LYS:HE2	1.81	0.42
12:H:250:CYS:SG	12:H:251:GLN:N	2.92	0.42
12:H:786:ASP:OD1	12:H:787:ILE:N	2.47	0.42
4:B:1093:GLN:N	12:H:926:ASP:OD2	2.48	0.42
6:G:468:LEU:HB3	6:G:469:GLY:H	1.48	0.42
7:P:562:PRO:HA	7:P:565:GLU:HG2	2.02	0.42
12:H:108:LEU:HD23	12:H:108:LEU:HA	1.72	0.42
3:K:278:TYR:HD1	3:K:278:TYR:HA	1.70	0.42
5:D:250:SER:HB2	5:D:301:GLN:HG3	2.00	0.42
5:D:323:LYS:HZ1	5:D:377:GLY:N	2.18	0.42
5:D:435:MET:HA	5:D:438:ILE:HG12	2.01	0.42
7:P:514:GLN:O	7:P:517:THR:OG1	2.33	0.42
9:A:1663:LEU:O	9:A:1666:HIS:N	2.53	0.42
9:A:1711:ARG:HE	9:A:1711:ARG:HB2	1.73	0.42
10:E:531:GLU:HA	10:E:534:LEU:HG	2.01	0.42
10:E:831:TRP:NE1	10:E:875:SER:OG	2.51	0.42
11:F:325:ASP:OD1	11:F:381:VAL:HB	2.19	0.42
12:H:170:GLN:HB2	12:H:173:VAL:HG12	2.00	0.42
2:I:5:CYS:O	2:I:502:ALA:CA	2.66	0.42
2:I:590:PRO:HG2	2:I:593:GLN:HB3	2.02	0.42
3:K:167:LYS:HE2	3:K:167:LYS:HB2	1.95	0.42
6:G:312:LEU:HD11	6:G:347:LEU:HD11	2.02	0.42
6:G:465:ASP:OD1	6:G:503:LYS:NZ	2.53	0.42
6:G:715:HIS:HA	6:G:718:GLU:HG2	2.02	0.42
6:G:832:GLU:OE1	6:G:887:TYR:OH	2.27	0.42
7:P:93:LEU:HB3	7:P:112:LEU:HD21	2.00	0.42
11:F:112:GLY:HA3	11:F:448:LEU:HD11	2.02	0.42
12:H:752:MET:HE2	12:H:752:MET:HB3	1.91	0.42
4:B:487:PHE:CE1	4:B:495:ILE:HG13	2.54	0.42
4:B:536:VAL:HG21	4:B:571:VAL:HB	2.02	0.42
5:D:873:GLN:HG3	5:D:875:ILE:HG13	2.02	0.42
7:P:544:LEU:HA	7:P:547:ILE:HG22	2.01	0.42
11:F:20:LEU:HD11	11:F:213:PRO:HG3	2.01	0.42
12:H:901:CYS:SG	12:H:912:ALA:HB2	2.60	0.42
4:B:38:SER:OG	4:B:41:GLU:OE1	2.38	0.42
5:D:753:LYS:HA	5:D:756:GLN:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:155:VAL:O	6:G:159:VAL:HG23	2.20	0.42
6:G:622:LYS:HE2	6:G:622:LYS:HB2	1.66	0.42
6:G:769:VAL:HG23	6:G:770:SER:H	1.84	0.42
6:G:896:PHE:CE2	6:G:928:VAL:HG21	2.55	0.42
7:P:490:SER:HA	7:P:501:THR:HG21	2.02	0.42
9:A:1758:ILE:HG23	9:A:1797:ARG:NH1	2.33	0.42
10:E:542:LEU:HD23	10:E:542:LEU:HA	1.87	0.42
12:H:547:LYS:HA	12:H:547:LYS:HD3	1.74	0.42
2:I:127:GLU:HG2	2:I:128:PRO:HD3	2.02	0.41
2:I:261:LEU:O	2:I:263:LEU:HD22	2.20	0.41
2:I:294:ASN:HA	2:I:391:CYS:O	2.20	0.41
3:K:193:ASP:N	3:K:193:ASP:OD1	2.53	0.41
4:B:283:LEU:HD13	4:B:338:GLN:OE1	2.20	0.41
4:B:1025:LEU:HA	4:B:1025:LEU:HD23	1.84	0.41
8:Q:276:MET:HG3	8:Q:286:PHE:CE1	2.52	0.41
2:I:85:LEU:HD21	2:I:112:TYR:CD2	2.54	0.41
2:I:206:PHE:CE2	5:D:210:ARG:HD3	2.56	0.41
2:I:532:LYS:HD2	2:I:535:ILE:HD13	2.02	0.41
3:K:509:LEU:HD23	3:K:578:TYR:HB2	2.02	0.41
5:D:428:ARG:O	5:D:432:ILE:HG12	2.20	0.41
6:G:172:PHE:CZ	6:G:176:ILE:HG13	2.55	0.41
7:P:377:CYS:HB3	7:P:380:VAL:HG12	2.03	0.41
11:F:283:TRP:CE2	11:F:383:PRO:HD3	2.56	0.41
2:I:263:LEU:HD21	2:I:461:LEU:HD21	2.02	0.41
3:K:263:VAL:HG23	3:K:318:PRO:HB2	2.02	0.41
4:B:146:LEU:HA	4:B:149:ILE:HG22	2.01	0.41
4:B:417:SER:OG	4:B:418:ARG:N	2.53	0.41
4:B:602:SER:HB2	4:B:616:ASN:HD22	1.86	0.41
4:B:714:LEU:HD12	4:B:718:TYR:HB2	2.02	0.41
4:B:947:LEU:HD22	4:B:1024:LEU:HD21	2.01	0.41
5:D:710:MET:HB3	5:D:711:TYR:CD1	2.55	0.41
6:G:38:LEU:HD22	6:G:76:ASN:HD21	1.85	0.41
7:P:199:ASP:HA	7:P:202:LYS:HG2	2.02	0.41
9:A:1916:GLU:HA	9:A:1919:GLN:HG2	2.02	0.41
10:E:566:LEU:HA	10:E:566:LEU:HD12	1.82	0.41
10:E:689:LEU:O	10:E:693:VAL:HG22	2.21	0.41
11:F:15:ASN:ND2	11:F:82:ALA:O	2.48	0.41
11:F:448:LEU:HD12	11:F:452:VAL:HG21	2.00	0.41
12:H:389:THR:HG21	12:H:403:PHE:CD1	2.55	0.41
12:H:580:CYS:HA	12:H:583:VAL:HG12	2.03	0.41
4:B:741:ARG:NH1	6:G:229:LYS:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:470:ASP:O	6:G:473:GLU:HG2	2.20	0.41
7:P:121:PRO:HB3	7:P:157:ARG:HB3	2.02	0.41
7:P:222:LEU:HD22	7:P:262:MET:HG3	2.03	0.41
7:P:414:ASP:OD1	7:P:414:ASP:N	2.51	0.41
10:E:560:ARG:HG2	10:E:566:LEU:HB2	2.03	0.41
3:K:153:TYR:HE2	3:K:192:ILE:HG13	1.85	0.41
4:B:227:ARG:HB3	4:B:231:LYS:NZ	2.36	0.41
5:D:216:ILE:HG23	5:D:255:LEU:HD21	2.02	0.41
5:D:264:PRO:HB3	5:D:280:VAL:HG13	2.02	0.41
6:G:525:THR:O	6:G:529:ILE:HG12	2.21	0.41
7:P:158:VAL:HG23	7:P:163:LYS:HG3	2.02	0.41
8:Q:68:LEU:HD11	8:Q:275:ILE:HD13	2.03	0.41
9:A:1695:LEU:HG	9:A:1739:ILE:HD13	2.02	0.41
2:I:101:ILE:HB	2:I:125:ALA:HB2	2.02	0.41
2:I:247:PRO:HA	2:I:347:LEU:HA	2.03	0.41
4:B:378:LYS:HD3	4:B:378:LYS:HA	1.94	0.41
5:D:170:CYS:HA	5:D:173:LEU:HD12	2.02	0.41
5:D:414:ASP:HA	5:D:417:VAL:HG22	2.03	0.41
5:D:420:PHE:HE2	5:D:451:THR:HA	1.85	0.41
6:G:547:GLN:NE2	6:G:566:LYS:HD2	2.35	0.41
9:A:1787:ILE:HG13	9:A:1788:GLN:HG2	2.02	0.41
10:E:831:TRP:HA	10:E:832:PRO:HD3	1.93	0.41
11:F:13:SER:H	12:H:939:GLU:HG3	1.86	0.41
11:F:424:LEU:HD21	11:F:444:MET:HG2	2.03	0.41
2:I:262:VAL:HG12	2:I:264:THR:HG23	2.03	0.41
2:I:510:LYS:HA	2:I:510:LYS:HD2	1.87	0.41
2:I:549:ASN:N	5:D:207:GLN:OE1	2.35	0.41
3:K:424:LYS:HE2	3:K:424:LYS:HB3	1.92	0.41
4:B:188:LEU:HD23	4:B:191:LEU:HB3	2.03	0.41
4:B:506:LYS:HE3	4:B:506:LYS:HB3	1.95	0.41
5:D:567:ASP:HA	5:D:570:PHE:HD2	1.86	0.41
5:D:571:ARG:NH2	9:A:1714:ARG:O	2.54	0.41
6:G:273:ILE:HD13	6:G:310:GLY:HA3	2.02	0.41
6:G:393:LEU:HD22	6:G:412:ALA:HB2	2.02	0.41
6:G:514:LYS:O	6:G:518:GLU:HG2	2.20	0.41
7:P:28:ARG:O	7:P:32:ILE:HG12	2.21	0.41
9:A:1219:LEU:O	9:A:1223:MET:HG2	2.21	0.41
9:A:2163:PHE:O	9:A:2167:MET:HB2	2.20	0.41
10:E:953:HIS:CD2	10:E:976:GLU:HG3	2.55	0.41
12:H:623:HIS:O	12:H:627:THR:OG1	2.35	0.41
2:I:20:LYS:HD3	2:I:511:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:325:PRO:HD3	3:K:330:ALA:HB3	2.02	0.41
5:D:500:ARG:HA	5:D:503:ILE:HG12	2.02	0.41
5:D:545:ILE:HG23	5:D:576:LEU:HD11	2.03	0.41
5:D:687:LEU:HB3	5:D:690:SER:HB3	2.02	0.41
5:D:857:PRO:HG3	5:D:890:HIS:ND1	2.36	0.41
6:G:104:VAL:HG21	6:G:133:ILE:HG21	2.02	0.41
9:A:1064:SER:HB3	9:A:1116:VAL:HG21	2.02	0.41
9:A:1205:LEU:HB3	9:A:1210:GLU:H	1.86	0.41
10:E:847:ILE:HD12	10:E:880:GLY:HA3	2.03	0.41
11:F:413:GLU:O	11:F:417:LYS:HG3	2.21	0.41
12:H:173:VAL:HG23	12:H:176:GLN:HE21	1.86	0.41
12:H:954:ARG:O	12:H:958:ILE:HG12	2.21	0.41
2:I:158:ASN:HB3	2:I:161:ILE:HD13	2.03	0.41
3:K:124:GLN:NE2	3:K:128:ASP:OD2	2.53	0.41
6:G:309:LEU:HA	6:G:359:ILE:HD13	2.02	0.41
6:G:366:VAL:O	6:G:370:ILE:HG12	2.21	0.41
6:G:497:ILE:HD13	6:G:497:ILE:HA	1.88	0.41
6:G:847:ILE:HG12	6:G:910:VAL:HG11	2.02	0.41
7:P:42:LEU:HD23	7:P:42:LEU:HA	1.96	0.41
7:P:52:LEU:O	7:P:56:THR:HG23	2.21	0.41
7:P:177:ASP:OD1	7:P:177:ASP:N	2.49	0.41
8:Q:204:ASP:OD1	8:Q:205:ASP:N	2.53	0.41
10:E:994:ARG:HA	12:H:159:PHE:CE2	2.55	0.41
11:F:541:PHE:HE1	11:F:559:MET:HA	1.86	0.41
12:H:555:SER:HA	12:H:558:ILE:HG22	2.03	0.41
4:B:542:SER:HA	4:B:583:GLU:HB3	2.03	0.41
5:D:417:VAL:HG11	5:D:447:ASP:HB2	2.03	0.41
7:P:454:HIS:HB3	8:Q:287:LEU:HD11	2.03	0.41
9:A:1743:ALA:O	9:A:1746:ARG:NH1	2.53	0.41
10:E:927:MET:O	10:E:930:VAL:HG22	2.20	0.41
12:H:130:MET:HB3	12:H:135:LEU:HD11	2.02	0.41
12:H:617:LEU:HD12	12:H:617:LEU:HA	1.90	0.41
3:K:123:SER:HA	3:K:126:ILE:HG22	2.02	0.40
4:B:453:VAL:HG13	4:B:525:ILE:HD11	2.02	0.40
4:B:857:PRO:HG3	4:B:934:GLN:HE21	1.85	0.40
5:D:166:VAL:HG23	5:D:169:LYS:NZ	2.36	0.40
6:G:790:SER:OG	6:G:792:GLN:OE1	2.35	0.40
7:P:51:LEU:HD23	7:P:55:LEU:HD23	2.03	0.40
10:E:477:LEU:HA	10:E:480:HIS:HB2	2.03	0.40
10:E:819:SER:O	10:E:850:ARG:NH1	2.46	0.40
11:F:268:ILE:HD12	11:F:327:TYR:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:396:LEU:HB3	11:F:408:TRP:CZ2	2.56	0.40
12:H:696:LEU:HD22	12:H:716:ASP:OD1	2.21	0.40
2:I:263:LEU:HD23	2:I:469:VAL:HG13	2.03	0.40
3:K:234:LYS:HD2	3:K:340:TRP:CH2	2.54	0.40
3:K:546:LEU:HB2	3:K:550:SER:HB3	2.03	0.40
6:G:239:THR:HB	6:G:252:GLN:HE21	1.85	0.40
7:P:561:LYS:HD3	7:P:588:LEU:HB3	2.04	0.40
9:A:1160:ALA:HB1	9:A:1162:MET:HG2	2.03	0.40
3:K:240:PHE:HA	3:K:325:PRO:HA	2.03	0.40
7:P:264:ALA:O	7:P:305:LYS:HG3	2.22	0.40
8:Q:189:VAL:HA	8:Q:190:PRO:HD3	1.92	0.40
9:A:1191:ASP:HA	9:A:1230:ARG:HH22	1.85	0.40
9:A:1673:LEU:HD12	9:A:1673:LEU:HA	1.94	0.40
4:B:235:ARG:HA	4:B:273:HIS:HD1	1.86	0.40
5:D:378:ALA:O	5:D:382:GLY:N	2.55	0.40
5:D:677:LYS:HA	5:D:677:LYS:HD2	1.92	0.40
5:D:706:LYS:HB2	5:D:706:LYS:HE3	1.89	0.40
6:G:69:ALA:HB2	6:G:103:PHE:CD1	2.57	0.40
6:G:805:LYS:HD2	6:G:805:LYS:HA	1.85	0.40
9:A:1404:ARG:O	9:A:1406:LEU:N	2.53	0.40
9:A:2179:GLU:O	9:A:2183:ILE:HG12	2.21	0.40
10:E:750:HIS:NE2	11:F:554:ASP:OD2	2.54	0.40
11:F:350:VAL:HG21	11:F:379:LEU:HD11	2.04	0.40
2:I:146:ARG:NH1	2:I:404:ASP:OD1	2.35	0.40
2:I:234:VAL:HG13	2:I:260:VAL:HB	2.03	0.40
4:B:702:GLU:OE1	4:B:702:GLU:N	2.54	0.40
5:D:583:LEU:HD23	5:D:583:LEU:HA	1.96	0.40
5:D:636:LEU:O	5:D:640:ILE:HG12	2.20	0.40
6:G:271:LEU:O	6:G:275:ASP:HB2	2.21	0.40
10:E:578:LEU:HD12	10:E:578:LEU:HA	1.83	0.40
10:E:641:PRO:HA	10:E:644:LEU:HB3	2.04	0.40
10:E:916:GLU:OE2	12:H:364:ARG:HD3	2.21	0.40
11:F:88:LEU:HD21	11:F:196:ILE:HD12	2.03	0.40
11:F:293:GLN:HE22	11:F:446:TYR:HD1	1.70	0.40
12:H:776:LEU:HD13	12:H:799:TRP:CZ3	2.56	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	0	30/70 (43%)	28 (93%)	2 (7%)	0	100	100
2	I	629/658 (96%)	585 (93%)	43 (7%)	1 (0%)	44	77
3	K	586/600 (98%)	528 (90%)	57 (10%)	1 (0%)	44	77
4	B	1045/1204 (87%)	977 (94%)	64 (6%)	4 (0%)	30	67
5	D	805/963 (84%)	749 (93%)	51 (6%)	5 (1%)	22	59
6	G	893/962 (93%)	819 (92%)	65 (7%)	9 (1%)	13	48
7	P	579/589 (98%)	564 (97%)	14 (2%)	1 (0%)	44	77
8	Q	291/309 (94%)	274 (94%)	17 (6%)	0	100	100
9	A	1073/2190 (49%)	1010 (94%)	60 (6%)	3 (0%)	37	71
10	E	794/1019 (78%)	740 (93%)	47 (6%)	7 (1%)	14	50
11	F	547/887 (62%)	523 (96%)	23 (4%)	1 (0%)	44	77
12	H	933/995 (94%)	880 (94%)	53 (6%)	0	100	100
All	All	8205/10446 (78%)	7677 (94%)	496 (6%)	32 (0%)	32	67

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	78	VAL
5	D	63	PRO
5	D	106	SER
5	D	561	MET
6	G	647	PRO
6	G	811	SER
6	G	812	PRO
6	G	815	PRO
6	G	841	PRO
9	A	1816	PRO
10	E	282	ILE
10	E	464	PRO

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Mol	Chain	Res	Type
10	E	760	PRO
4	B	525	ILE
6	G	553	VAL
6	G	788	PRO
9	A	904	VAL
10	E	513	SER
10	E	870	ALA
2	I	411	LEU
3	K	138	LEU
5	D	141	LEU
6	G	814	ASN
7	P	512	CYS
4	B	420	PRO
10	E	465	PRO
10	E	762	LYS
11	F	402	ALA
6	G	468	LEU
5	D	902	ALA
4	B	587	PRO
9	A	1405	VAL

### 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	0	29/63 (46%)	29 (100%)	0	100	100
2	I	575/600 (96%)	573 (100%)	2 (0%)	91	92
3	K	505/520 (97%)	505 (100%)	0	100	100
4	B	946/1072 (88%)	942 (100%)	4 (0%)	89	91
5	D	607/845 (72%)	602 (99%)	5 (1%)	79	84
6	G	742/840 (88%)	737 (99%)	5 (1%)	81	86
7	P	508/512 (99%)	506 (100%)	2 (0%)	89	91
8	Q	259/274 (94%)	259 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	A	636/1907 (33%)	636 (100%)	0	100	100
10	E	395/812 (49%)	393 (100%)	2 (0%)	86	90
11	F	454/796 (57%)	450 (99%)	4 (1%)	75	83
12	H	822/896 (92%)	820 (100%)	2 (0%)	92	94
All	All	6478/9137 (71%)	6452 (100%)	26 (0%)	88	91

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	512	ARG
2	I	607	LYS
4	B	43	ARG
4	B	329	ARG
4	B	488	HIS
4	B	505	MET
5	D	182	LYS
5	D	261	GLN
5	D	445	ARG
5	D	644	GLN
5	D	797	LYS
6	G	34	ARG
6	G	254	GLN
6	G	357	ARG
6	G	845	ARG
6	G	933	ASP
7	P	183	ARG
7	P	221	ARG
10	E	767	ARG
10	E	975	ARG
11	F	67	LYS
11	F	265	HIS
11	F	321	LYS
11	F	407	LYS
12	H	470	LYS
12	H	708	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	210	GLN

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Mol	Chain	Res	Type
3	K	392	HIS
5	D	176	ASN
6	G	670	GLN
6	G	702	ASN
6	G	891	GLN
8	Q	241	HIS
9	A	1288	HIS
9	A	2113	ASN
10	E	537	GLN
12	H	176	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](#)

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

There are no chain breaks in this entry.

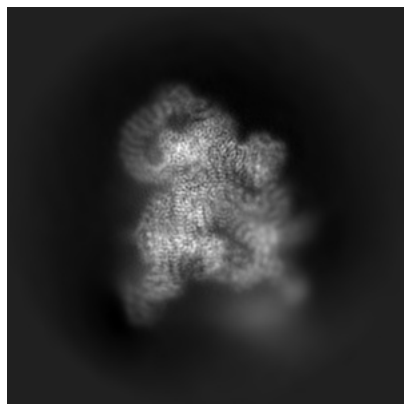
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39338. These allow visual inspection of the internal detail of the map and identification of artifacts.

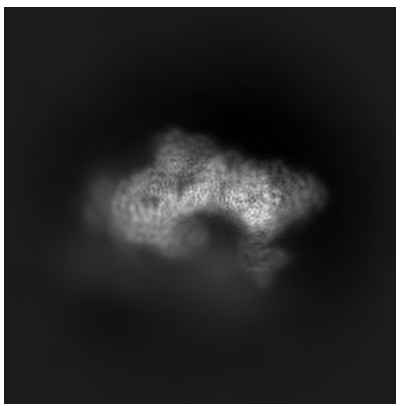
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

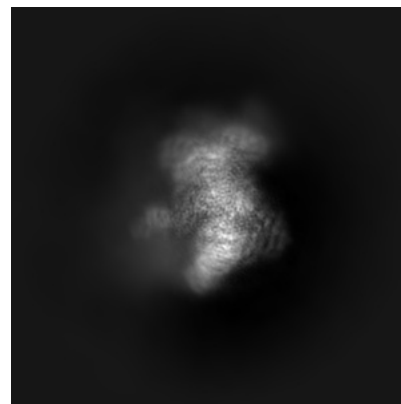
#### 6.1.1 Primary map



X

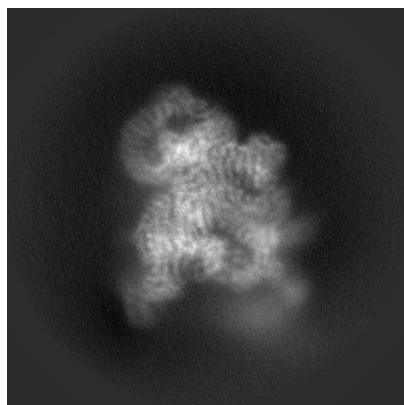


Y

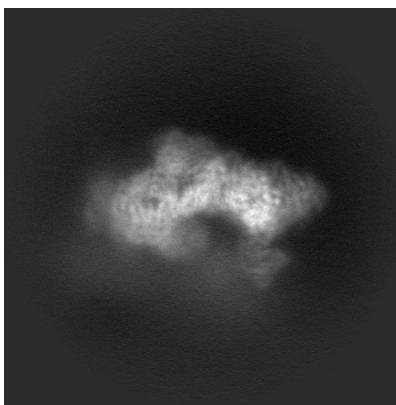


Z

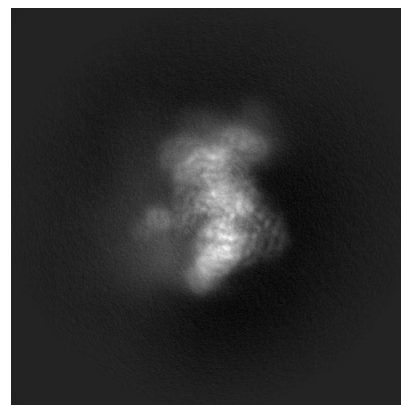
#### 6.1.2 Raw map



X



Y

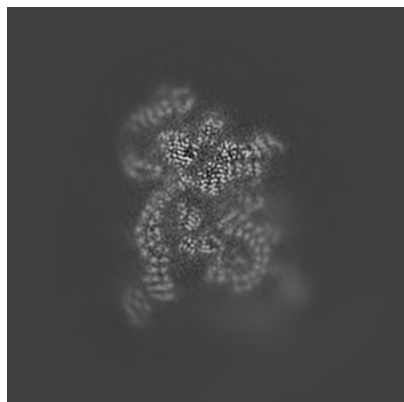


Z

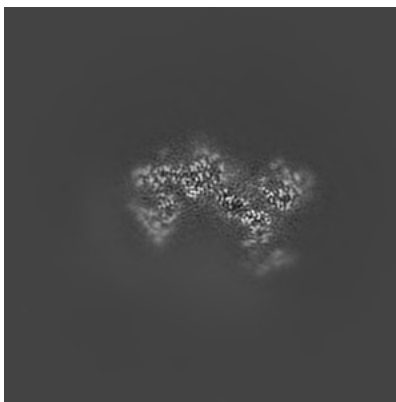
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

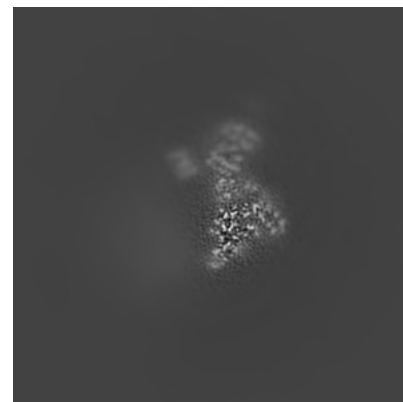
### 6.2.1 Primary map



X Index: 210

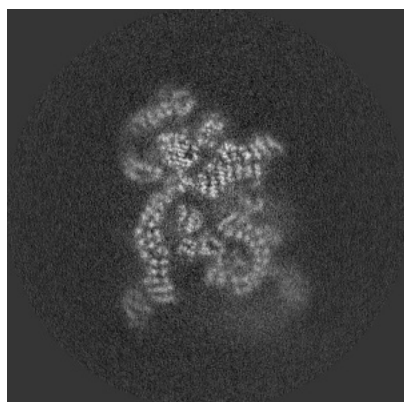


Y Index: 210

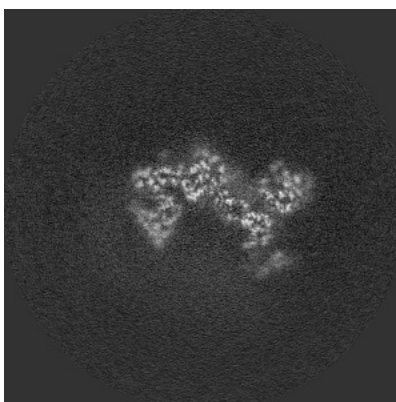


Z Index: 210

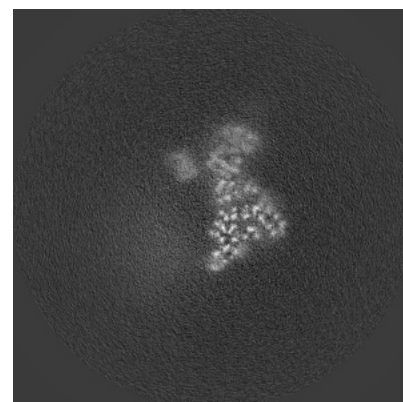
### 6.2.2 Raw map



X Index: 210



Y Index: 210

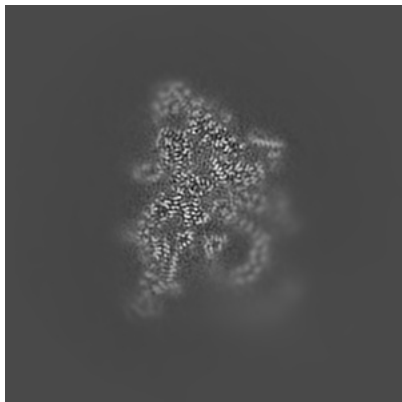


Z Index: 210

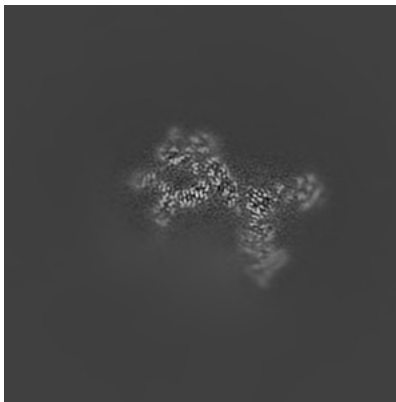
The images above show central slices of the map in three orthogonal directions.

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

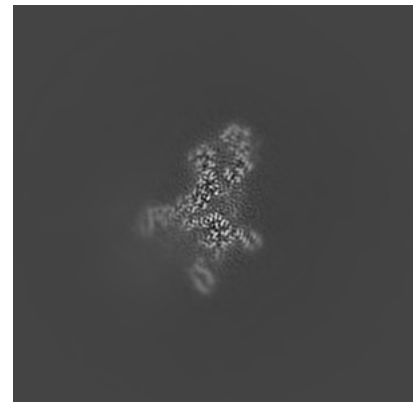
### 6.3.1 Primary map



X Index: 222

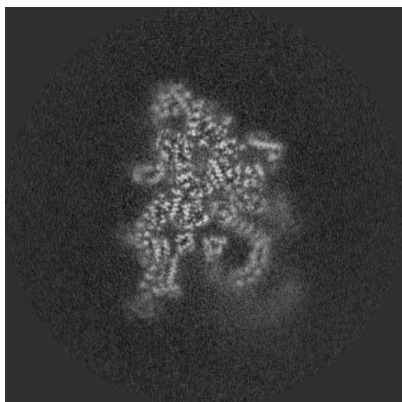


Y Index: 191

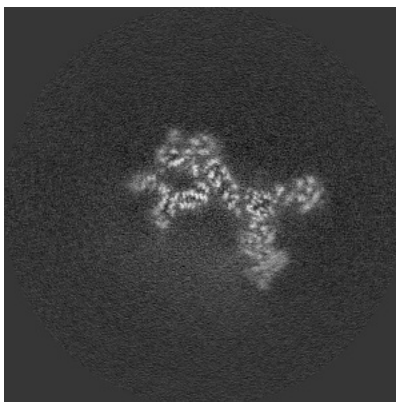


Z Index: 263

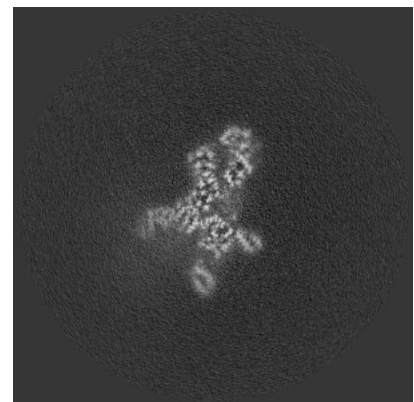
### 6.3.2 Raw map



X Index: 221



Y Index: 191



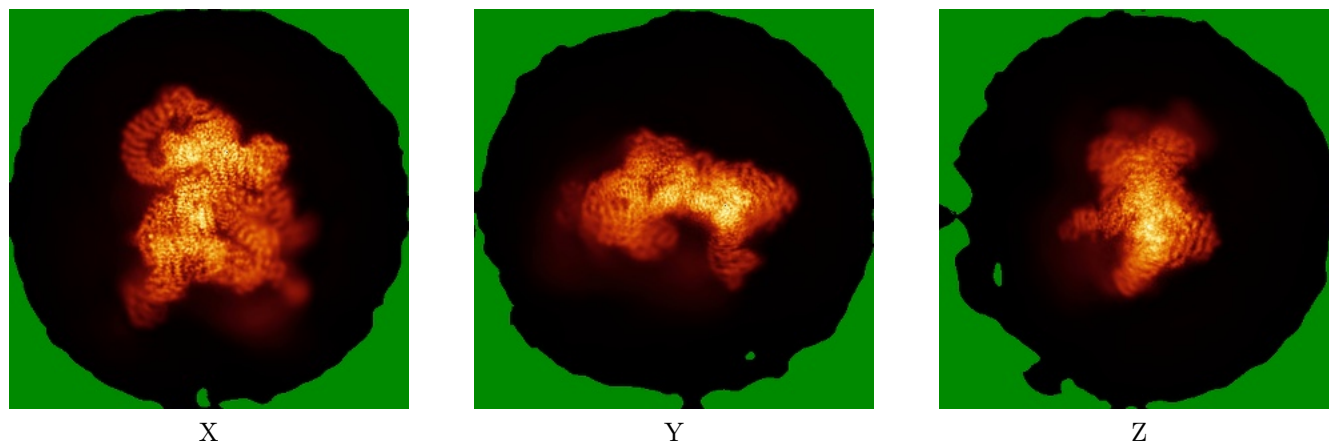
Z Index: 262

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

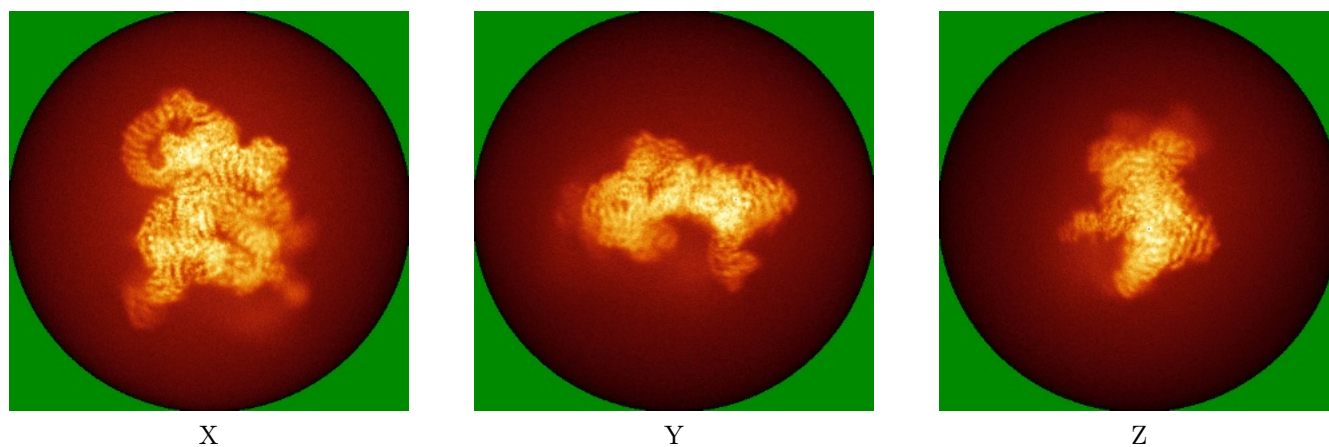


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



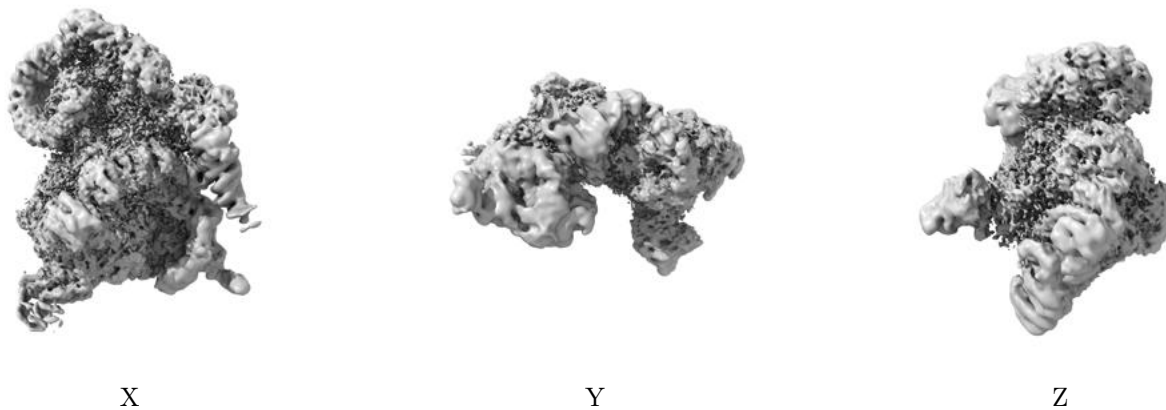
### 6.4.2 Raw map



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.

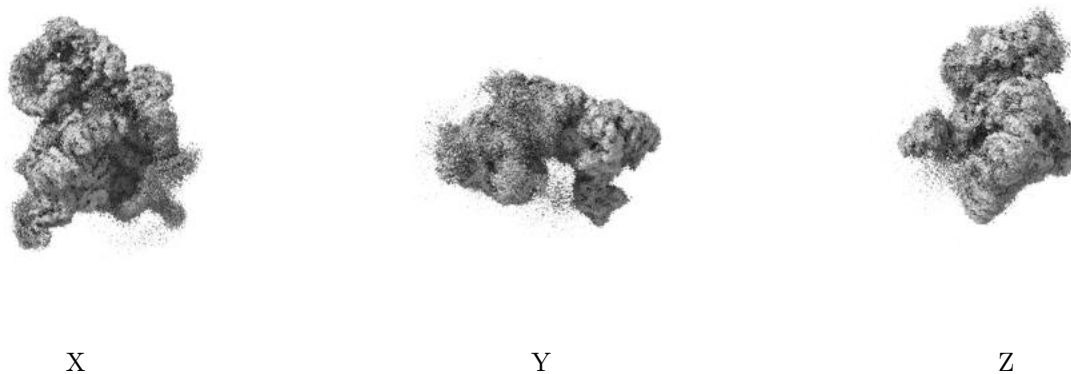
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

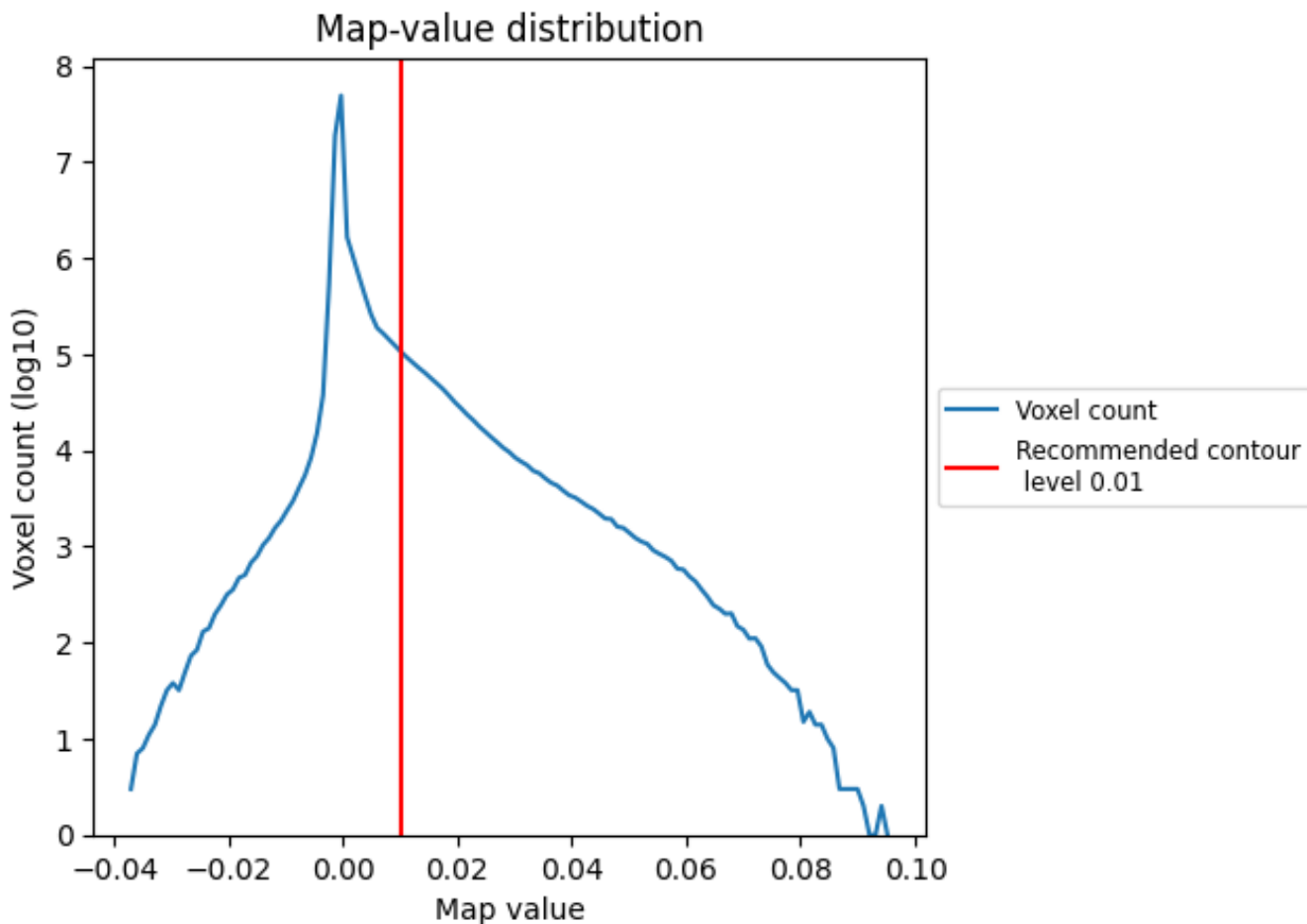
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

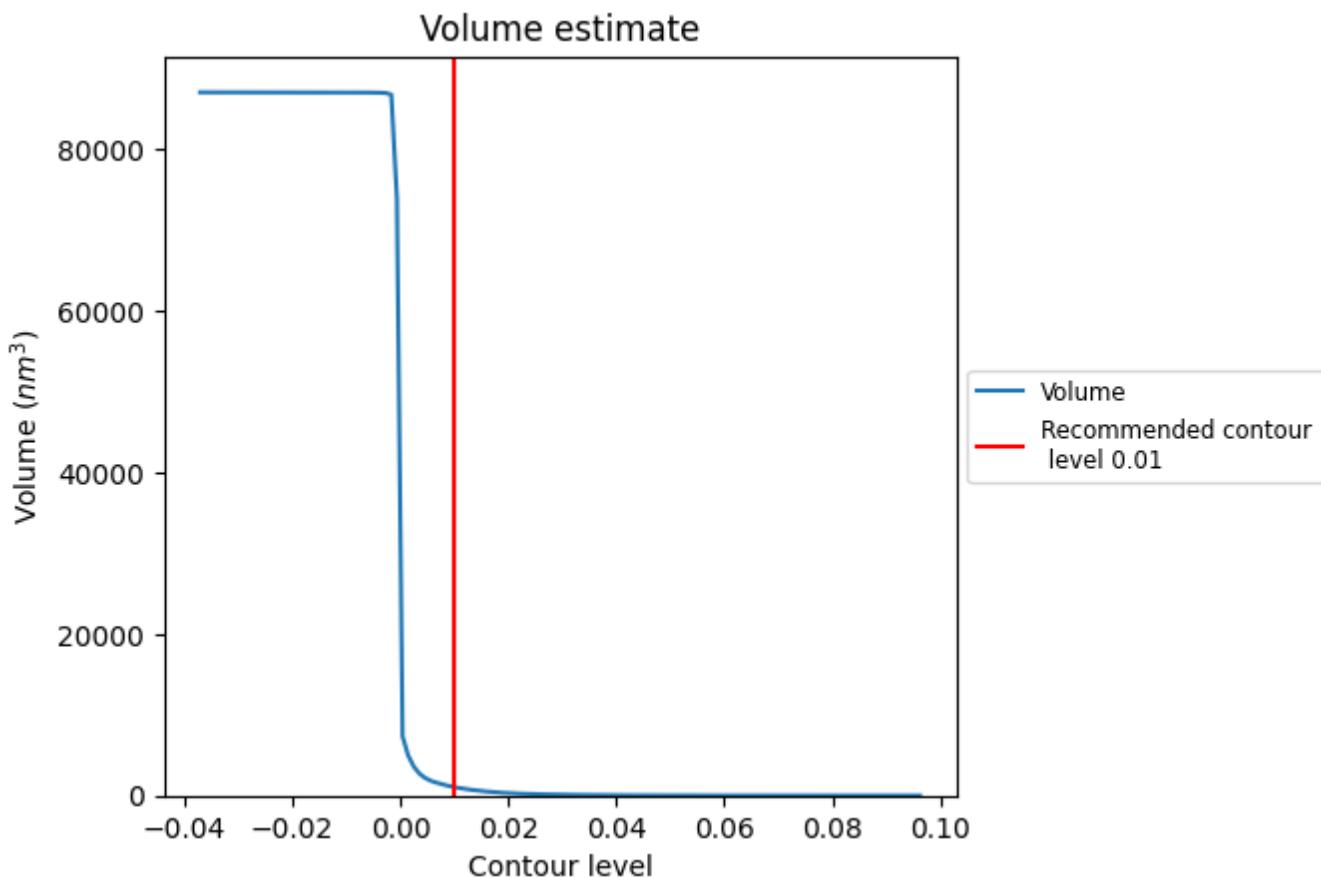
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

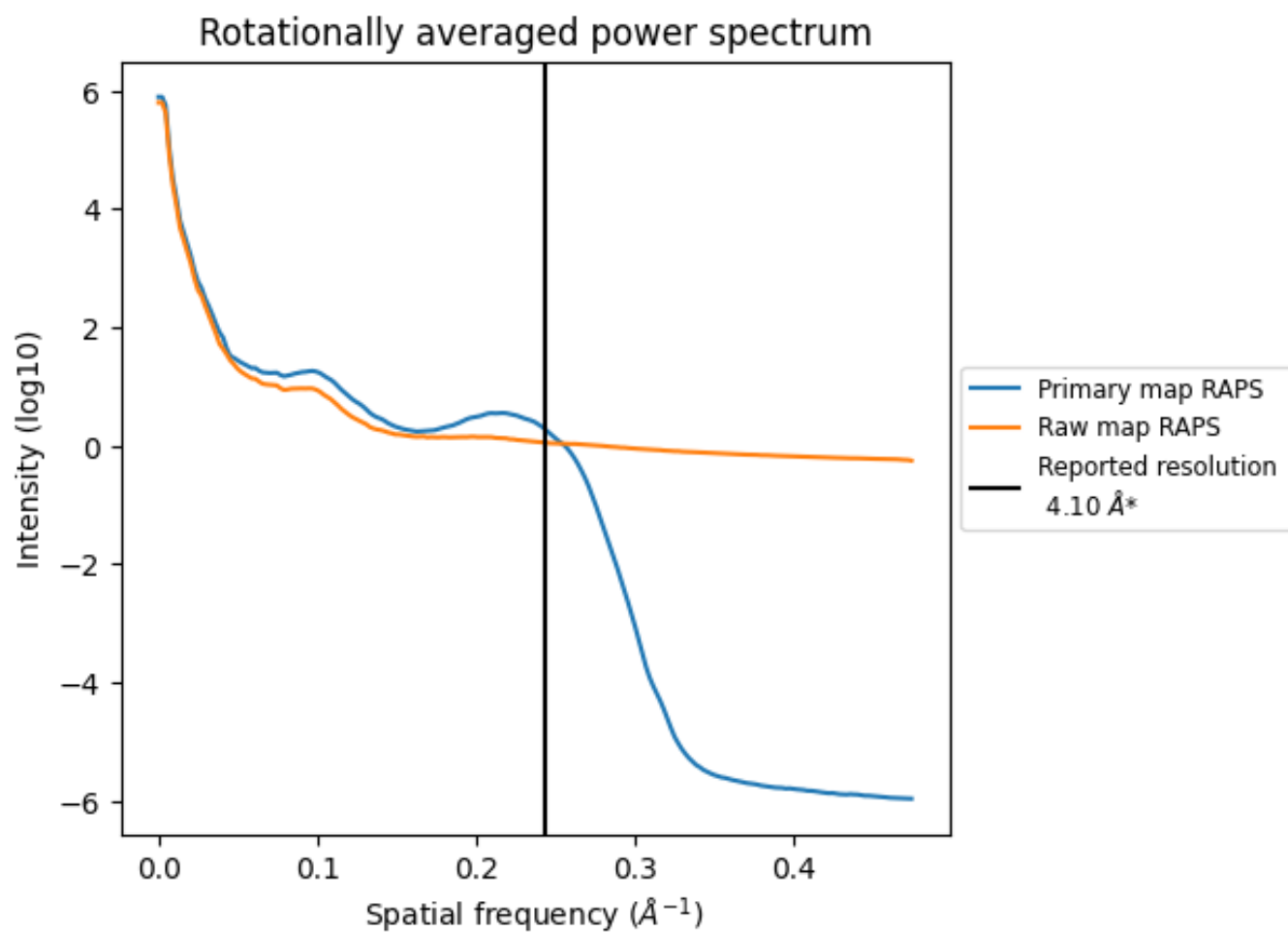
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1048  $\text{nm}^3$ ; this corresponds to an approximate mass of 946 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 i

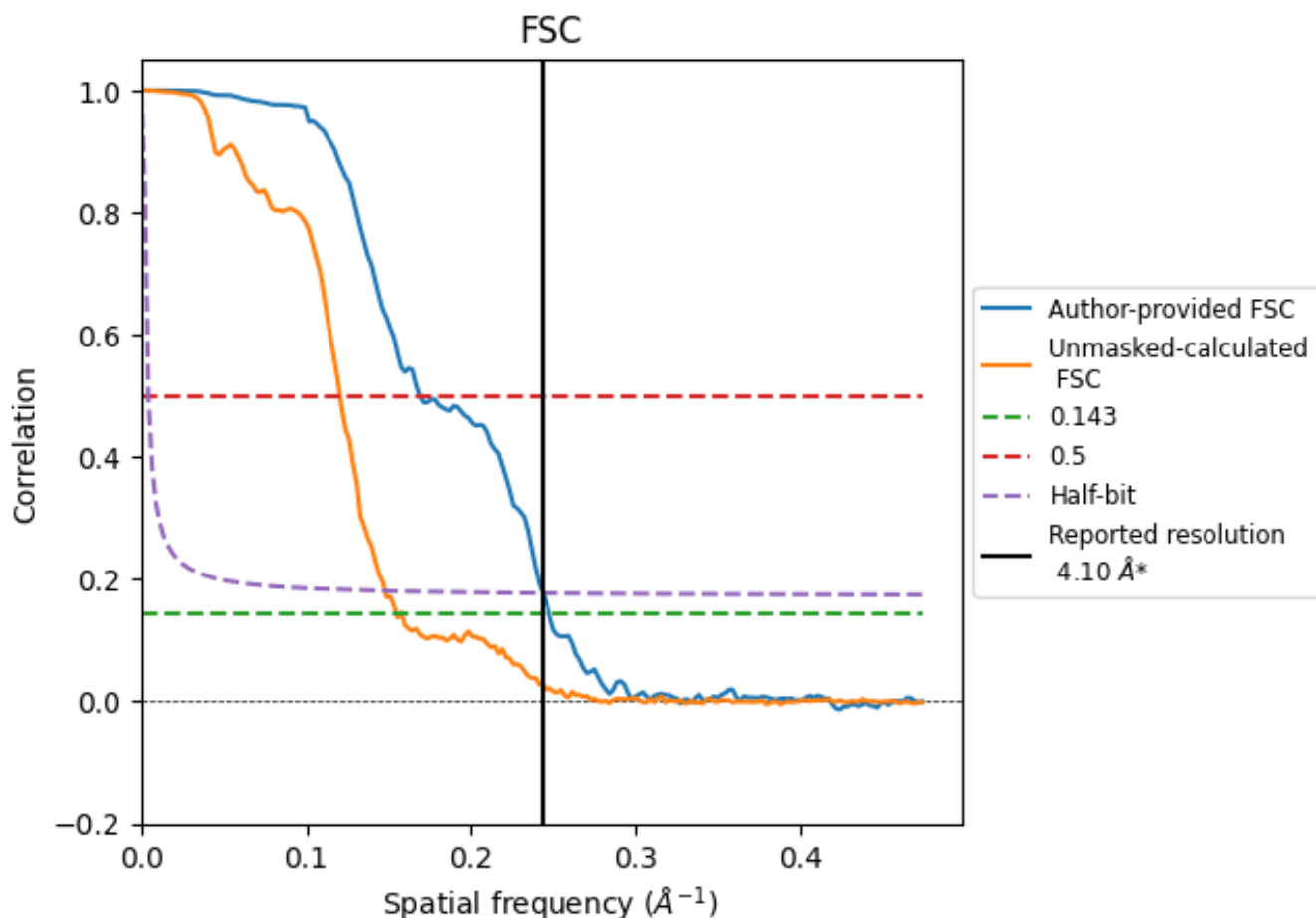


\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

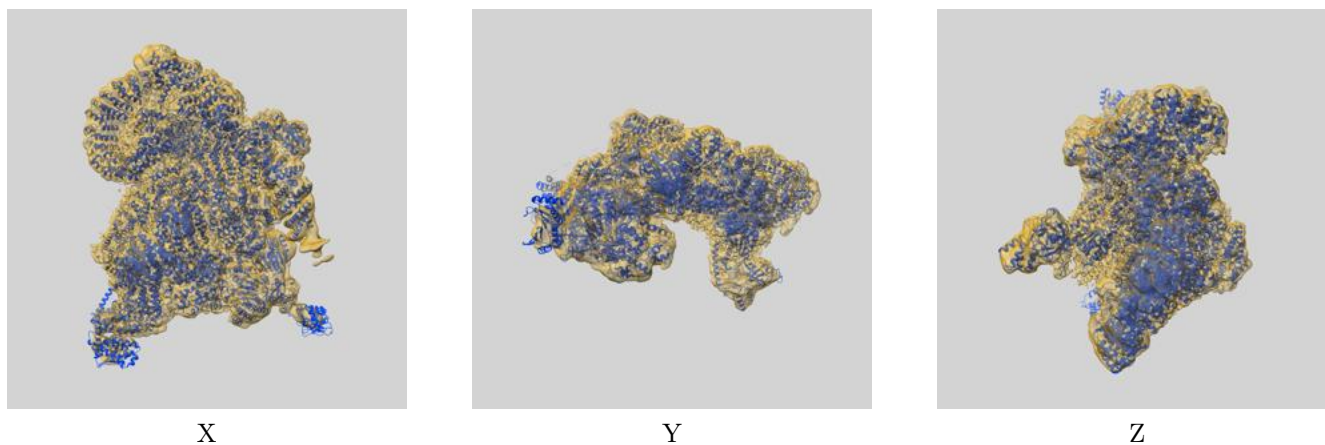
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.04	5.91	4.10
Unmasked-calculated*	6.45	8.29	6.75

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.45 differs from the reported value 4.1 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-39338 and PDB model 8YJB. Per-residue inclusion information can be found in section 3 on page 7.

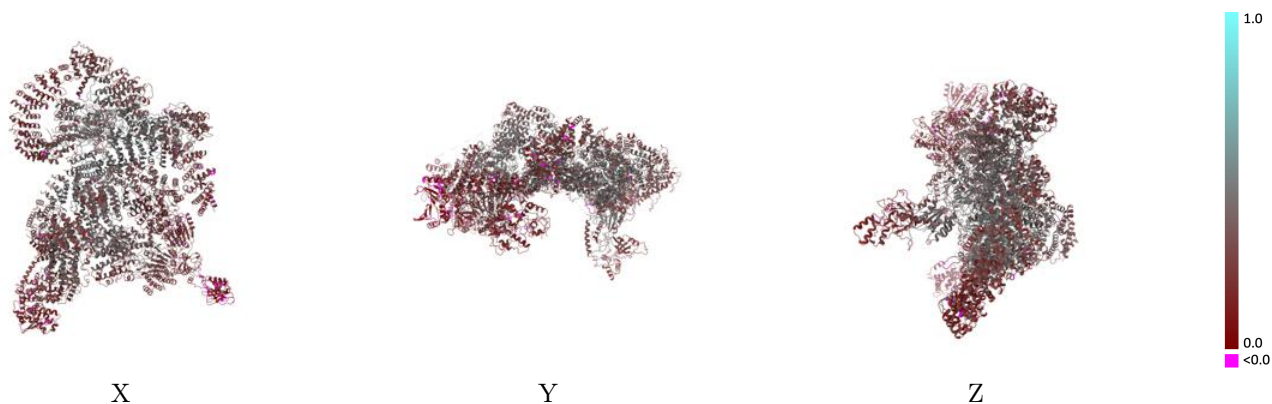
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

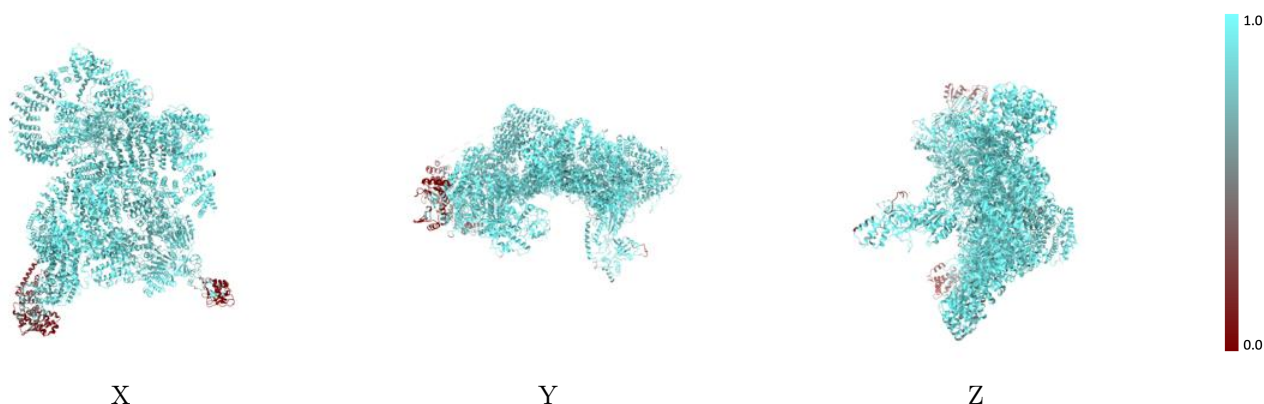


## 9.2 Q-score mapped to coordinate model [i](#)



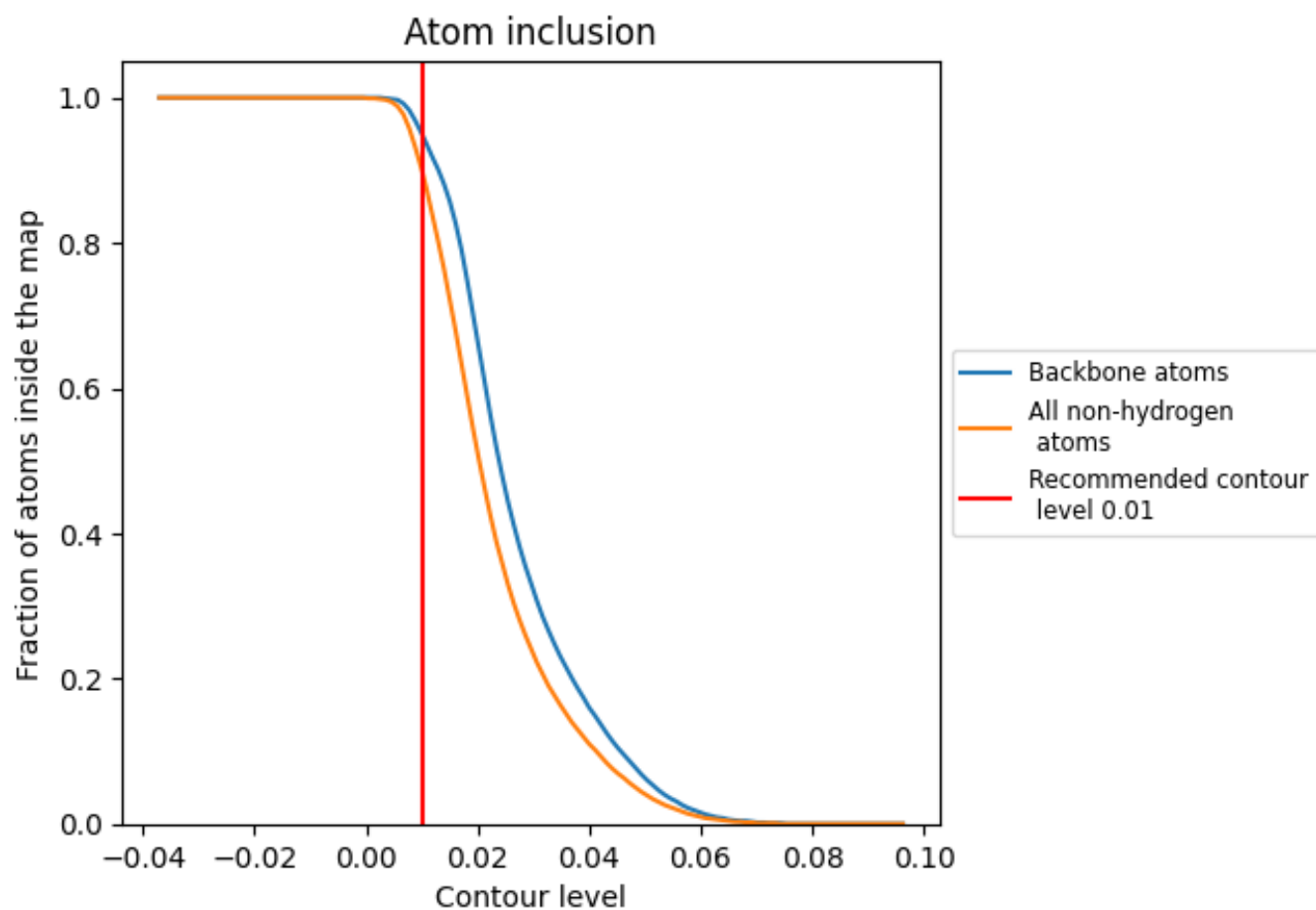
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.3200
O	 0.9040	 0.3850
A	 0.6930	 0.2640
B	 0.9380	 0.3700
D	 0.9560	 0.3080
E	 0.9740	 0.3830
F	 0.9140	 0.3110
G	 0.9580	 0.4090
H	 0.9380	 0.3360
I	 0.8730	 0.2580
K	 0.8290	 0.1690
P	 0.9140	 0.2540
Q	 0.9620	 0.4610

