



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:24 PM UTC

PDB ID : 7F4G / pdb_00007f4g
EMDB ID : EMD-31450
Title : Structure of RPAP2-bound RNA polymerase II
Authors : Chen, X.; Qi, Y.; Wang, X.; Li, J.; Zhao, D.; Xu, Y.
Deposited on : 2021-06-18
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

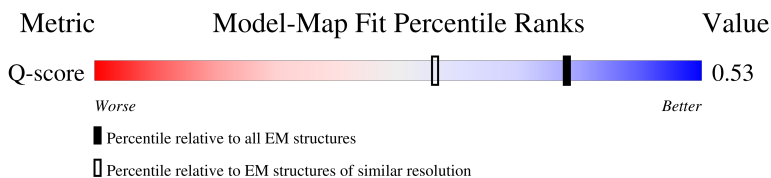
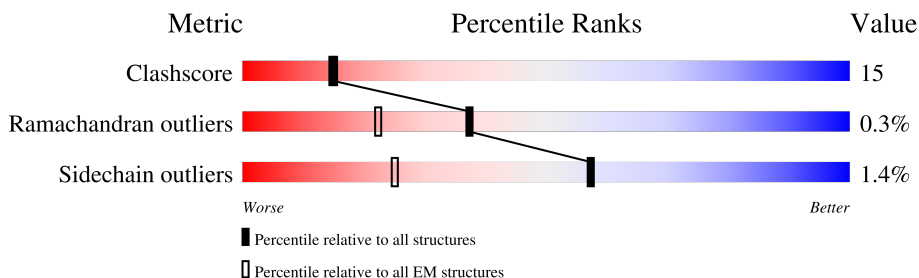
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 Å.

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



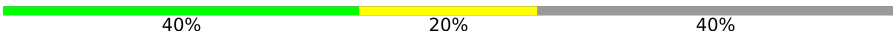
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

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

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	
4	E	210	

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Mol	Chain	Length	Quality of chain
5	F	127	
6	H	150	
7	I	125	
8	J	67	
9	K	117	
10	L	58	
11	R	612	
12	D	142	
13	G	172	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27957 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 RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1026	Total	C	N	O	S	0	0
			8179	5153	1440	1542	44		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	978	Total	C	N	O	S	0	0
			7820	4966	1356	1448	50		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	254	Total	C	N	O	S	0	0
			2038	1282	348	402	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	208	Total	C	N	O	S	0	0
			1703	1080	299	316	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	76	Total	C	N	O	S	0	0
			609	391	103	110	5		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 8 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 9 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 10 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 11 is a protein called RPAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	163	Total	C	N	O	S	0	0
			1335	848	227	253	7		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

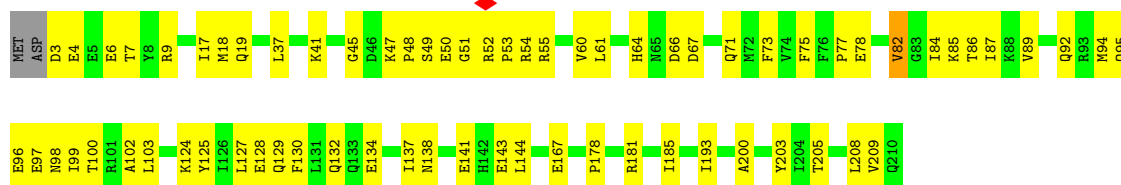
Mol	Chain	Residues	Atoms		AltConf
14	I	2	Total 2	Zn 2	0
14	J	1	Total 1	Zn 1	0
14	L	1	Total 1	Zn 1	0
14	R	1	Total 1	Zn 1	0





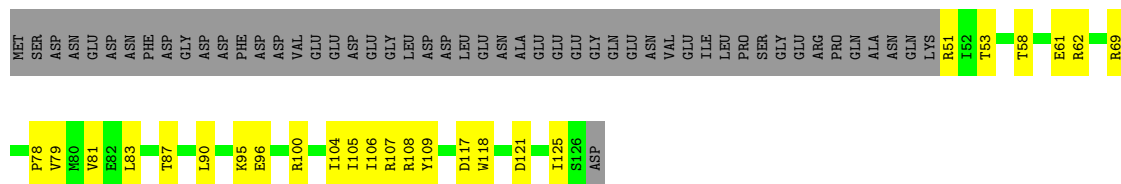
• Molecule 4: DNA-directed RNA polymerase II subunit E

Chain E: 66% 32%



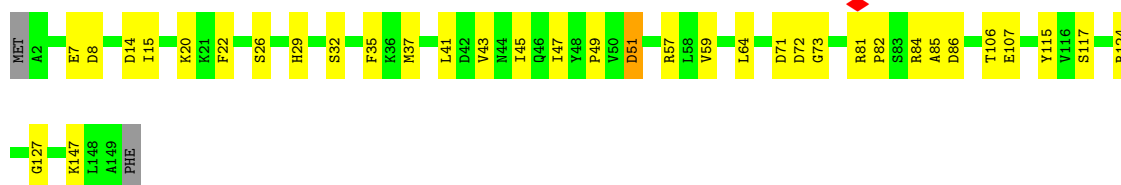
• Molecule 5: DNA-directed RNA polymerase II subunit F

Chain F: 40% 20% 40%



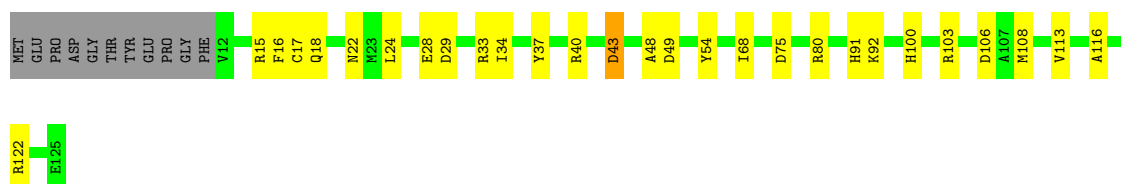
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 75% 23%



• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 69% 22% 9%



• Molecule 8: RPB10

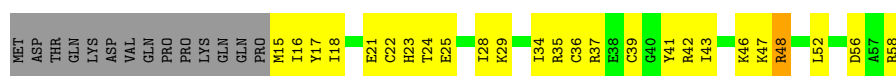
Chain J: 70% 25%



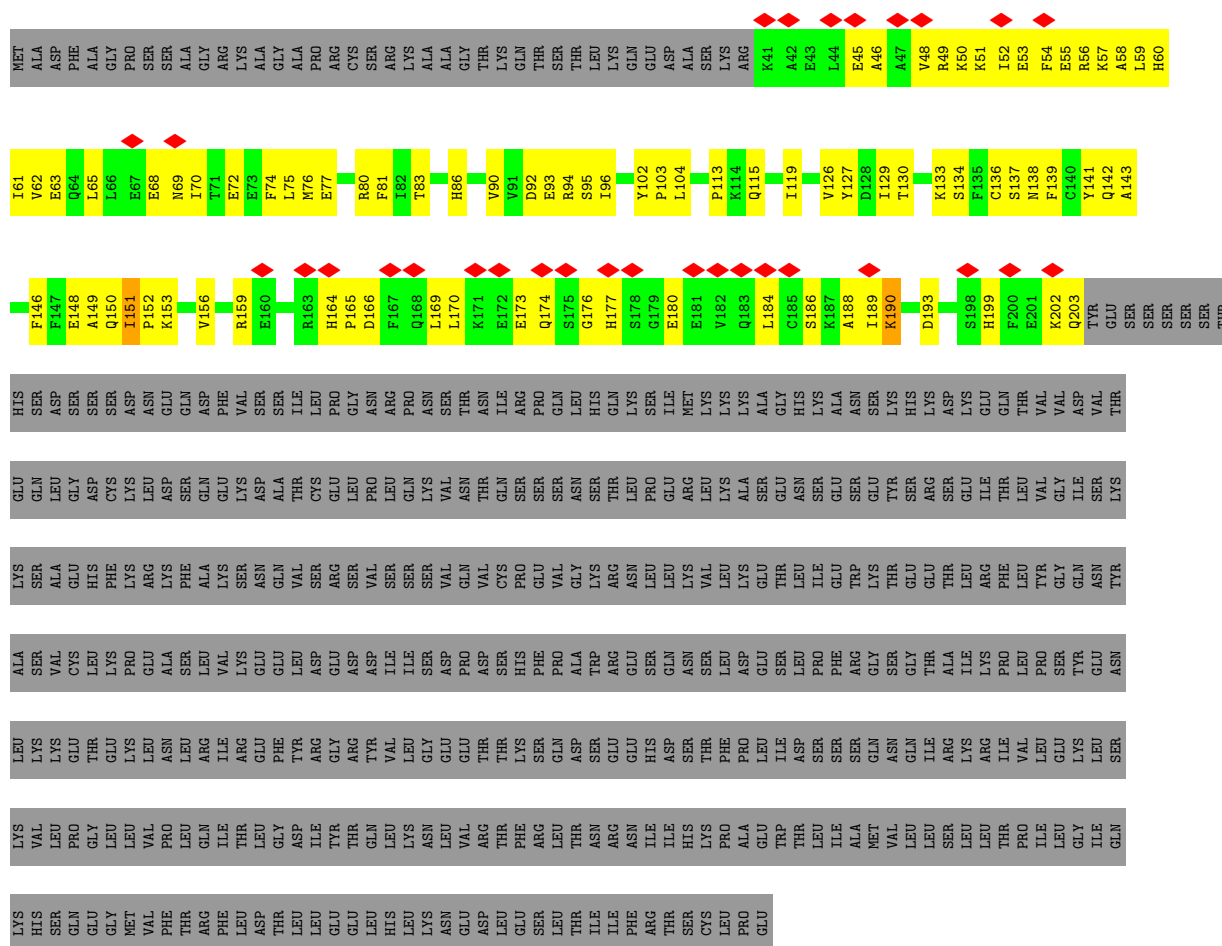
- Molecule 9: RNA_pol_L_2 domain-containing protein



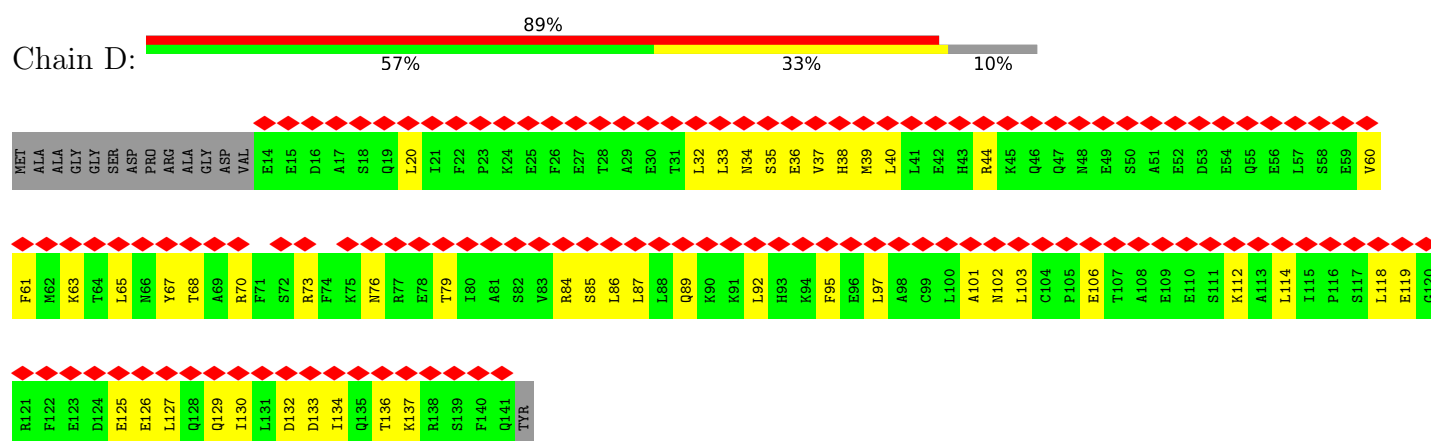
- Molecule 10: RPB12



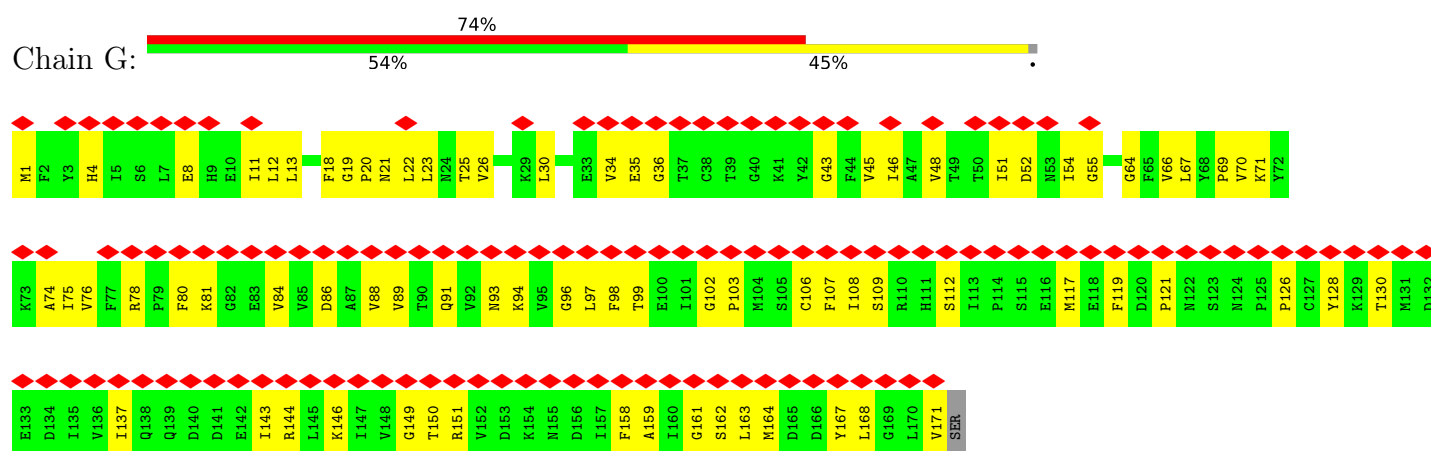
- Molecule 11: RPAP2



- Molecule 12: DNA-directed RNA polymerase II subunit RPB4



• Molecule 13: DNA-directed RNA polymerase II subunit RPB7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	646517	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	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	5.185	Depositor
Minimum map value	-3.433	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.29	Depositor
Map size ($\text{\AA}$)	334.08002, 334.08002, 334.08002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.044, 1.044, 1.044	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/8322	0.64	0/11237
2	B	0.87	1/7978 (0.0%)	0.72	7/10775 (0.1%)
3	C	0.92	0/2081	0.70	2/2828 (0.1%)
4	E	0.55	0/1734	0.62	0/2342
5	F	0.53	0/619	0.66	0/837
6	H	0.73	0/1207	0.59	0/1628
7	I	0.59	0/948	0.54	0/1284
8	J	1.09	1/533 (0.2%)	0.90	2/719 (0.3%)
9	K	0.83	0/939	0.58	0/1271
10	L	0.73	0/377	0.76	0/500
11	R	0.31	0/1362	0.61	1/1829 (0.1%)
12	D	0.17	0/1019	0.51	0/1374
13	G	0.22	0/1365	0.52	0/1853
All	All	0.72	2/28484 (0.0%)	0.66	12/38477 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	24	LEU	C-O	-5.36	1.16	1.24
2	B	304	SER	CA-CB	-5.05	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	556	ILE	CA-C-N	8.63	135.30	121.83
2	B	556	ILE	C-N-CA	8.63	135.30	121.83
2	B	305	LEU	N-CA-C	-7.11	104.49	113.02
2	B	303	PRO	CB-CA-C	-6.55	100.76	111.56
2	B	742	VAL	N-CA-C	-6.42	107.61	113.71
2	B	898	THR	CA-C-O	-6.05	115.25	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	70	LEU	CA-C-N	-5.44	118.67	122.59
3	C	70	LEU	C-N-CA	-5.44	118.67	122.59
11	R	130	THR	N-CA-C	-5.39	107.71	114.56
8	J	24	LEU	N-CA-C	-5.30	106.86	113.38
2	B	163	LEU	CB-CA-C	-5.20	102.76	111.13
8	J	27	ALA	N-CA-C	-5.10	106.81	112.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8179	0	8216	294	0
2	B	7820	0	7823	214	0
3	C	2038	0	1991	52	0
4	E	1703	0	1725	54	0
5	F	609	0	640	23	0
6	H	1186	0	1147	26	0
7	I	927	0	860	24	0
8	J	524	0	540	15	0
9	K	920	0	942	23	0
10	L	372	0	382	23	0
11	R	1335	0	1329	71	0
12	D	1005	0	964	40	0
13	G	1334	0	1333	59	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
14	R	1	0	0	0	0
All	All	27957	0	27892	840	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 15.

All (840) 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)
2:B:721:ARG:HD2	2:B:975:ARG:HB3	1.48	0.94
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.05	0.88
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.07	0.88
1:A:542:LEU:HD21	1:A:642:LYS:HB3	1.56	0.87
11:R:94:ARG:HH12	11:R:103:PRO:HA	1.40	0.85
2:B:984:CYS:SG	2:B:1046:THR:OG1	2.35	0.84
3:C:190:ASN:O	3:C:193:ARG:NH1	2.09	0.84
1:A:388:MET:HE1	1:A:503:LEU:HB3	1.60	0.82
11:R:127:TYR:HB3	11:R:190:LYS:HB2	1.62	0.81
12:D:33:LEU:HD11	12:D:102:ASN:HB3	1.61	0.81
13:G:52:ASP:HB3	13:G:71:LYS:HG3	1.62	0.81
1:A:1248:ASN:HD21	1:A:1255:LEU:HA	1.46	0.81
2:B:984:CYS:HG	2:B:1046:THR:HG1	1.28	0.81
11:R:199:HIS:HB2	11:R:202:LYS:HD3	1.64	0.78
1:A:784:VAL:HG13	2:B:978:ILE:HD11	1.64	0.78
13:G:91:GLN:HB2	13:G:98:PHE:HB2	1.67	0.77
2:B:627:ILE:HD11	2:B:663:GLU:HG3	1.67	0.76
1:A:604:ARG:HH11	1:A:651:SER:H	1.32	0.75
1:A:1005:HIS:HD2	1:A:1006:PRO:HD2	1.51	0.75
2:B:561:ILE:HD11	2:B:573:TRP:HH2	1.50	0.75
1:A:931:ARG:NH1	1:A:936:GLU:OE1	2.20	0.75
1:A:554:PHE:HB3	1:A:585:LEU:HG	1.68	0.75
1:A:904:GLN:NE2	1:A:981:CYS:O	2.20	0.75
12:D:112:LYS:HE3	12:D:127:LEU:HD22	1.69	0.74
3:C:67:ARG:NH1	8:J:3:ILE:O	2.19	0.74
12:D:114:LEU:HB3	13:G:84:VAL:HG11	1.70	0.74
2:B:561:ILE:HD11	2:B:573:TRP:CH2	2.22	0.73
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.69	0.73
1:A:1343:LEU:HD23	1:A:1347:LEU:HD22	1.71	0.73
4:E:95:GLN:NE2	4:E:125:TYR:OH	2.22	0.73
3:C:190:ASN:ND2	3:C:195:THR:O	2.21	0.72
4:E:9:ARG:NH2	4:E:132:GLN:OE1	2.22	0.72
1:A:813:ASP:OD1	7:I:100:HIS:NE2	2.22	0.72
1:A:1054:MET:HE1	1:A:1060:LEU:HD12	1.70	0.72
11:R:68:GLU:HG3	11:R:69:ASN:H	1.52	0.72
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.22	0.72
1:A:481:THR:O	1:A:483:ARG:NH1	2.23	0.71
3:C:13:GLU:HB3	3:C:20:LYS:HB2	1.73	0.71
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.24	0.70
1:A:757:GLN:NE2	1:A:778:LYS:O	2.23	0.70
1:A:1172:ASN:ND2	1:A:1215:GLU:OE2	2.24	0.70
2:B:391:LYS:O	2:B:392:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.23	0.70
7:I:68:ILE:HG13	7:I:122:ARG:HG2	1.73	0.70
1:A:1097:GLU:HG2	1:A:1098:PRO:HD3	1.74	0.70
7:I:29:ASP:O	7:I:33:ARG:HA	1.92	0.70
8:J:7:CYS:HA	8:J:48:MET:HE2	1.74	0.70
2:B:311:ILE:HG23	2:B:316:VAL:HG23	1.74	0.70
1:A:413:TYR:O	1:A:415:GLY:N	2.25	0.70
2:B:352:GLY:O	2:B:361:LYS:NZ	2.25	0.69
8:J:66:GLU:HA	10:L:23:HIS:HB3	1.75	0.69
2:B:296:GLU:OE1	7:I:103:ARG:NH1	2.25	0.69
3:C:99:VAL:HG21	3:C:127:VAL:HG11	1.73	0.69
1:A:522:PRO:O	1:A:662:HIS:NE2	2.26	0.69
1:A:595:ILE:HD11	1:A:675:VAL:HG21	1.73	0.68
2:B:403:LEU:HD21	2:B:447:SER:HB3	1.75	0.68
11:R:174:GLN:HA	11:R:177:HIS:CD2	2.28	0.68
2:B:933:ASP:HA	2:B:1054:MET:HA	1.75	0.68
11:R:149:ALA:O	11:R:153:LYS:NZ	2.27	0.68
4:E:73:PHE:CD2	4:E:99:ILE:HD11	2.29	0.68
1:A:1181:PRO:O	1:A:1184:THR:OG1	2.12	0.68
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.76	0.68
4:E:134:GLU:OE2	4:E:181:ARG:NH1	2.27	0.67
5:F:69:ARG:NH2	5:F:96:GLU:OE2	2.28	0.67
2:B:280:SER:OG	2:B:281:ASP:N	2.26	0.67
1:A:766:PHE:HE1	2:B:973:PRO:HB3	1.59	0.67
4:E:103:LEU:HD12	4:E:128:GLU:HG3	1.77	0.67
11:R:139:PHE:HA	11:R:184:LEU:HD13	1.77	0.67
10:L:18:ILE:HD11	10:L:47:LYS:HD3	1.77	0.66
1:A:418:TYR:OH	1:A:430:ARG:NH2	2.29	0.66
1:A:1365:ILE:HG23	1:A:1369:LEU:HD12	1.77	0.66
2:B:62:ALA:HB1	2:B:412:LEU:HD11	1.76	0.66
9:K:12:LEU:HD11	9:K:18:LYS:HB2	1.77	0.66
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.29	0.66
1:A:593:SER:HB2	1:A:634:GLU:HA	1.77	0.66
6:H:51:ASP:OD1	6:H:51:ASP:N	2.27	0.66
2:B:241:ALA:O	2:B:242:ARG:CB	2.42	0.65
1:A:522:PRO:HG3	1:A:666:ARG:HG3	1.77	0.65
1:A:780:ASN:HA	2:B:976:MET:HE1	1.78	0.65
1:A:1147:SER:OG	1:A:1351:ASP:OD2	2.14	0.65
4:E:138:ASN:HB3	4:E:141:GLU:HG3	1.77	0.65
2:B:90:GLN:HG2	2:B:91:ILE:H	1.60	0.65
1:A:695:ASP:N	1:A:695:ASP:OD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ARG:NH1	2:B:176:GLU:OE2	2.30	0.65
1:A:636:ILE:HG22	1:A:637:MET:HG2	1.79	0.65
1:A:894:ASP:OD1	1:A:1396:ARG:NH2	2.30	0.65
7:I:29:ASP:O	7:I:33:ARG:N	2.30	0.65
1:A:872:MET:HE3	1:A:1084:GLY:HA2	1.78	0.64
13:G:151:ARG:O	13:G:158:PHE:N	2.28	0.64
7:I:29:ASP:O	7:I:33:ARG:CA	2.45	0.64
12:D:44:ARG:NH2	13:G:35:GLU:OE2	2.30	0.64
11:R:174:GLN:HA	11:R:177:HIS:HD2	1.62	0.64
1:A:1377:ALA:O	1:A:1381:GLU:HG2	1.98	0.64
11:R:126:VAL:HG13	11:R:193:ASP:HB3	1.79	0.64
13:G:48:VAL:HG12	13:G:74:ALA:HB2	1.80	0.64
3:C:67:ARG:NH2	3:C:149:LEU:O	2.29	0.63
7:I:113:VAL:HG22	7:I:122:ARG:HG3	1.80	0.63
3:C:77:ASP:OD2	3:C:126:ARG:NH1	2.31	0.63
3:C:158:GLU:OE2	3:C:160:ARG:NH2	2.32	0.63
3:C:56:SER:HB2	3:C:158:GLU:H	1.63	0.63
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.80	0.63
11:R:57:LYS:HE2	11:R:156:VAL:HG21	1.80	0.63
1:A:432:HIS:O	1:A:434:LYS:N	2.32	0.63
1:A:1099:ALA:HA	1:A:1102:MET:HE2	1.80	0.63
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.81	0.63
1:A:936:GLU:HA	1:A:939:VAL:HG12	1.79	0.62
2:B:834:ARG:HH12	2:B:841:ARG:HG3	1.65	0.62
3:C:9:VAL:HG11	9:K:105:PHE:HD1	1.61	0.62
11:R:164:HIS:HB3	11:R:165:PRO:HD3	1.81	0.62
2:B:845:TYR:HA	2:B:865:VAL:HG11	1.81	0.62
3:C:7:PRO:O	9:K:104:ARG:NH1	2.32	0.62
1:A:777:SER:H	1:A:780:ASN:ND2	1.97	0.62
6:H:84:ARG:NH2	6:H:86:ASP:HA	2.13	0.62
1:A:1184:THR:HG23	1:A:1258:ARG:HH12	1.64	0.62
4:E:185:ILE:CG2	4:E:209:VAL:HG21	2.30	0.62
1:A:631:GLU:HB3	1:A:636:ILE:HD12	1.82	0.61
2:B:631:GLN:HG3	2:B:683:GLN:HB3	1.83	0.61
3:C:212:ASP:OD1	3:C:212:ASP:N	2.32	0.61
4:E:55:ARG:HB2	4:E:78:GLU:HG2	1.81	0.61
5:F:62:ARG:HE	5:F:125:ILE:HD11	1.66	0.61
1:A:1027:ASP:HB3	1:A:1030:SER:HB3	1.83	0.60
3:C:10:ARG:NH1	3:C:24:GLU:OE2	2.34	0.60
1:A:732:THR:OG1	1:A:735:GLN:NE2	2.34	0.60
1:A:930:LEU:HB3	1:A:939:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:57:LYS:O	11:R:61:ILE:HG12	2.01	0.60
6:H:49:PRO:O	6:H:147:LYS:NZ	2.19	0.60
13:G:163:LEU:HA	13:G:168:LEU:HD23	1.83	0.60
1:A:417:LYS:HE2	1:A:430:ARG:HH21	1.67	0.60
1:A:1011:GLU:O	1:A:1015:GLU:HG2	2.02	0.60
2:B:548:TRP:HE1	2:B:582:GLN:HE22	1.48	0.60
3:C:72:PRO:HG3	8:J:13:ILE:HD11	1.83	0.60
11:R:45:GLU:HA	11:R:48:VAL:HG22	1.84	0.60
1:A:651:SER:O	1:A:654:HIS:N	2.31	0.60
2:B:180:ASP:OD2	2:B:184:TYR:OH	2.19	0.60
13:G:93:ASN:HB3	13:G:96:GLY:H	1.66	0.60
6:H:37:MET:HE2	6:H:127:GLY:HA3	1.84	0.59
2:B:388:TYR:OH	2:B:524:LYS:HE3	2.02	0.59
9:K:63:VAL:HG22	9:K:71:ILE:HG22	1.82	0.59
2:B:223:SER:HG	2:B:350:HIS:CE1	2.19	0.59
11:R:65:LEU:HD21	11:R:93:GLU:HB3	1.83	0.59
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.84	0.59
13:G:54:ILE:HG22	13:G:70:VAL:HG22	1.84	0.59
1:A:1410:HIS:CD2	1:A:1412:MET:HE3	2.38	0.59
12:D:126:GLU:O	12:D:129:GLN:HG3	2.02	0.59
1:A:391:ALA:HA	1:A:447:GLU:HA	1.84	0.59
1:A:734:ARG:HE	7:I:108:MET:HG2	1.68	0.59
1:A:875:TYR:OH	5:F:61:GLU:OE2	2.13	0.59
6:H:7:GLU:OE1	6:H:57:ARG:NH2	2.36	0.59
6:H:7:GLU:HB2	6:H:59:VAL:HG22	1.83	0.59
2:B:227:ASN:O	2:B:229:SER:N	2.35	0.59
4:E:185:ILE:HG21	4:E:209:VAL:HG21	1.83	0.59
9:K:7:PHE:HA	9:K:10:PHE:CE1	2.38	0.58
5:F:107:ARG:NE	5:F:117:ASP:OD1	2.37	0.58
4:E:6:GLU:HB3	4:E:48:PRO:HG3	1.86	0.58
4:E:37:LEU:HG	4:E:41:LYS:HE2	1.84	0.58
9:K:65:HIS:HE1	9:K:67:LEU:HD12	1.68	0.58
12:D:73:ARG:NH2	13:G:86:ASP:OD2	2.23	0.58
13:G:34:VAL:HG21	13:G:48:VAL:HG11	1.85	0.58
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.85	0.58
3:C:44:ILE:HD12	3:C:178:PRO:HB3	1.86	0.58
1:A:923:ASP:OD1	1:A:924:TYR:N	2.36	0.58
13:G:21:ASN:O	13:G:25:THR:OG1	2.20	0.58
2:B:955:PRO:HB2	2:B:1028:LEU:HD23	1.86	0.57
1:A:1375:ARG:NH1	1:A:1379:GLU:OE1	2.37	0.57
11:R:142:GLN:HE21	11:R:189:ILE:HA	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLN:HA	1:A:406:VAL:HG22	1.85	0.57
13:G:12:LEU:HD21	13:G:67:LEU:HD12	1.85	0.57
1:A:1279:MET:HE3	1:A:1283:VAL:HG12	1.86	0.57
5:F:83:LEU:HA	5:F:95:LYS:HZ2	1.69	0.57
1:A:852:VAL:O	1:A:856:GLU:HG3	2.05	0.57
11:R:46:ALA:O	11:R:49:ARG:HG2	2.04	0.57
3:C:123:ASN:OD1	3:C:124:SER:N	2.37	0.57
1:A:479:TRP:HB2	1:A:483:ARG:HH21	1.70	0.57
2:B:331:THR:HG22	2:B:333:GLU:H	1.69	0.57
2:B:35:ASP:OD2	2:B:646:ARG:NH2	2.36	0.57
2:B:89:GLU:HB3	2:B:127:ASP:HB2	1.86	0.57
2:B:506:TRP:CZ2	2:B:677:MET:HE1	2.40	0.57
2:B:917:LYS:HE3	10:L:34:ILE:HD11	1.85	0.57
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.38	0.57
13:G:30:LEU:O	13:G:34:VAL:HG22	2.04	0.57
2:B:771:GLU:O	8:J:55:LEU:HD21	2.05	0.57
11:R:56:ARG:HA	11:R:59:LEU:HD23	1.87	0.57
12:D:63:LYS:HE2	13:G:103:PRO:HA	1.86	0.57
1:A:646:GLY:O	1:A:651:SER:OG	2.23	0.56
1:A:1102:MET:HE1	1:A:1124:LEU:HD22	1.87	0.56
1:A:1124:LEU:O	1:A:1128:ILE:HG12	2.05	0.56
11:R:46:ALA:HA	11:R:49:ARG:NE	2.19	0.56
10:L:17:TYR:HD2	10:L:28:ILE:HB	1.70	0.56
1:A:762:GLU:OE1	1:A:767:LYS:NZ	2.39	0.56
1:A:766:PHE:CE1	2:B:973:PRO:HB3	2.39	0.56
1:A:1191:GLU:HG2	1:A:1192:TRP:N	2.20	0.56
2:B:1040:GLN:HG2	3:C:203:TRP:CH2	2.40	0.56
6:H:117:SER:OG	6:H:117:SER:O	2.22	0.56
1:A:797:ARG:NH2	1:A:815:TYR:O	2.33	0.56
2:B:752:TYR:HE1	2:B:809:VAL:HG22	1.71	0.56
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.88	0.56
4:E:19:GLN:NE2	4:E:138:ASN:HD22	2.03	0.56
13:G:89:VAL:HA	13:G:99:THR:HA	1.86	0.56
1:A:850:THR:O	1:A:854:THR:HG23	2.05	0.56
4:E:52:ARG:O	4:E:54:ARG:N	2.38	0.56
1:A:383:SER:HB2	9:K:2:ASN:HD21	1.71	0.55
2:B:422:PHE:HB3	2:B:428:ASP:O	2.06	0.55
2:B:941:GLN:HG2	2:B:975:ARG:HE	1.71	0.55
12:D:34:ASN:O	12:D:68:THR:OG1	2.24	0.55
1:A:370:ASP:HB2	1:A:483:ARG:HB3	1.87	0.55
1:A:863:ARG:HH21	1:A:1414:ILE:C	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:PRO:HB3	2:B:87:LYS:HB3	1.88	0.55
2:B:89:GLU:N	2:B:127:ASP:O	2.35	0.55
3:C:77:ASP:OD1	3:C:77:ASP:N	2.38	0.55
3:C:78:ILE:HD11	3:C:126:ARG:HD2	1.89	0.55
13:G:144:ARG:HE	13:G:171:VAL:HG22	1.70	0.55
4:E:45:GLY:HA3	4:E:53:PRO:HD3	1.89	0.55
13:G:23:LEU:HA	13:G:26:VAL:HG12	1.86	0.55
1:A:767:LYS:O	1:A:771:VAL:HG22	2.07	0.55
11:R:77:GLU:O	11:R:80:ARG:HB3	2.07	0.55
1:A:604:ARG:HD3	1:A:651:SER:H	1.72	0.55
1:A:863:ARG:NH1	1:A:1129:ASN:OD1	2.35	0.55
1:A:889:LEU:O	1:A:890:ARG:NH1	2.36	0.55
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.72	0.55
2:B:656:LEU:O	2:B:661:VAL:HG12	2.06	0.55
8:J:24:LEU:O	8:J:29:TYR:HB2	2.06	0.55
7:I:49:ASP:OD1	7:I:49:ASP:N	2.38	0.55
2:B:339:ALA:HA	2:B:342:VAL:HG12	1.88	0.55
1:A:1304:ILE:HG23	1:A:1338:THR:HB	1.88	0.55
2:B:506:TRP:CH2	2:B:677:MET:HE1	2.41	0.55
2:B:817:GLN:OE1	2:B:912:ASN:ND2	2.39	0.55
3:C:9:VAL:HG11	9:K:105:PHE:CD1	2.41	0.55
3:C:72:PRO:HG3	8:J:13:ILE:CD1	2.37	0.55
11:R:146:PHE:O	11:R:150:GLN:HG2	2.06	0.55
12:D:114:LEU:HD11	13:G:167:TYR:HB2	1.89	0.55
1:A:513:ALA:HB2	5:F:90:LEU:HD21	1.89	0.55
2:B:64:PRO:O	2:B:416:ARG:NH2	2.33	0.55
11:R:113:PRO:O	11:R:133:LYS:NZ	2.26	0.55
2:B:694:THR:O	2:B:695:HIS:ND1	2.40	0.54
7:I:43:ASP:OD1	7:I:43:ASP:N	2.33	0.54
12:D:133:ASP:O	12:D:136:THR:OG1	2.19	0.54
4:E:55:ARG:NH2	4:E:132:GLN:HE21	2.06	0.54
10:L:36:CYS:SG	10:L:39:CYS:HB3	2.47	0.54
11:R:51:LYS:HA	11:R:54:PHE:CD2	2.42	0.54
2:B:721:ARG:NE	2:B:940:GLY:O	2.39	0.54
1:A:397:PHE:HB3	5:F:87:THR:HB	1.90	0.54
2:B:344:GLN:HE21	2:B:354:SER:C	2.15	0.54
4:E:55:ARG:HH22	4:E:132:GLN:HE21	1.55	0.54
12:D:70:ARG:HH12	13:G:88:VAL:HG11	1.72	0.54
1:A:1377:ALA:HB2	4:E:144:LEU:HD13	1.88	0.54
2:B:834:ARG:NH1	2:B:841:ARG:HG3	2.22	0.54
1:A:757:GLN:NE2	1:A:778:LYS:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:TYR:CZ	1:A:863:ARG:HD2	2.42	0.54
3:C:40:ALA:O	3:C:41:GLU:HG3	2.08	0.54
11:R:136:CYS:SG	11:R:137:SER:N	2.80	0.54
1:A:962:ASP:HB3	1:A:1043:ILE:HG12	1.90	0.54
2:B:319:ASN:ND2	11:R:203:GLN:OE1	2.41	0.53
12:D:34:ASN:HA	12:D:37:VAL:HG22	1.90	0.53
13:G:18:PHE:HA	13:G:22:LEU:HD13	1.90	0.53
3:C:250:SER:OG	9:K:102:GLU:OE1	2.22	0.53
4:E:94:MET:SD	4:E:102:ALA:HB2	2.49	0.53
13:G:43:GLY:N	13:G:78:ARG:HD2	2.23	0.53
2:B:995:GLU:HG2	2:B:996:ILE:H	1.73	0.53
1:A:947:HIS:NE2	1:A:951:GLU:OE1	2.41	0.53
1:A:582:PRO:HD2	6:H:47:ILE:HD12	1.91	0.53
1:A:752:THR:HB	1:A:786:ALA:HB1	1.91	0.53
1:A:1044:HIS:O	1:A:1048:THR:HG22	2.09	0.53
1:A:896:LEU:HD13	1:A:980:PRO:HB3	1.90	0.53
6:H:14:ASP:HB3	6:H:29:HIS:HB2	1.89	0.53
12:D:20:LEU:HD21	12:D:95:PHE:HD2	1.72	0.53
11:R:58:ALA:O	11:R:62:VAL:HG23	2.08	0.53
1:A:687:ILE:HG22	2:B:782:ILE:HG21	1.91	0.53
1:A:845:GLU:OE1	2:B:500:GLN:NE2	2.42	0.53
1:A:1194:ASN:O	1:A:1198:GLU:N	2.42	0.53
2:B:236:TRP:HB2	2:B:259:THR:HB	1.90	0.53
1:A:732:THR:HG22	1:A:733:LEU:H	1.74	0.53
2:B:624:PRO:HA	2:B:663:GLU:O	2.09	0.53
6:H:64:LEU:HD13	6:H:84:ARG:HD2	1.91	0.53
12:D:20:LEU:HD21	12:D:95:PHE:CD2	2.44	0.53
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.91	0.53
4:E:86:THR:HA	4:E:89:VAL:HG12	1.90	0.53
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.34	0.52
1:A:727:PRO:HD3	1:A:733:LEU:HD12	1.90	0.52
1:A:376:ASP:OD1	1:A:473:ARG:NH2	2.43	0.52
1:A:578:ALA:N	1:A:590:GLN:HE22	2.07	0.52
1:A:1218:ARG:NH2	1:A:1250:ASP:O	2.37	0.52
2:B:393:LEU:HD22	2:B:485:LEU:HD22	1.91	0.52
7:I:91:HIS:CG	7:I:116:ALA:HB2	2.44	0.52
13:G:96:GLY:HA3	13:G:109:SER:HA	1.89	0.52
1:A:549:THR:O	1:A:589:LYS:HE3	2.10	0.52
1:A:1211:LEU:HD12	1:A:1260:ARG:NE	2.25	0.52
1:A:546:ARG:HD3	1:A:772:SER:HB3	1.90	0.52
1:A:1022:ILE:H	1:A:1034:GLN:HE22	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:22:CYS:SG	10:L:24:THR:HG22	2.50	0.52
11:R:53:GLU:HA	11:R:56:ARG:HG2	1.91	0.52
12:D:86:LEU:HA	12:D:89:GLN:HE21	1.74	0.52
4:E:7:THR:HG23	4:E:48:PRO:HD3	1.91	0.52
11:R:166:ASP:O	11:R:170:LEU:HG	2.10	0.52
1:A:472:HIS:CE1	1:A:521:VAL:HG11	2.45	0.52
1:A:788:VAL:HG23	1:A:825:ASN:O	2.10	0.52
8:J:46:ARG:O	8:J:50:LEU:HB2	2.10	0.51
11:R:57:LYS:NZ	11:R:81:PHE:HB3	2.26	0.51
1:A:1136:THR:O	1:A:1136:THR:OG1	2.24	0.51
3:C:115:VAL:HB	3:C:151:VAL:HG12	1.92	0.51
1:A:1192:TRP:O	1:A:1195:VAL:HB	2.09	0.51
4:E:67:ASP:OD1	4:E:67:ASP:N	2.41	0.51
7:I:29:ASP:HB2	7:I:34:ILE:O	2.10	0.51
1:A:1191:GLU:HG2	1:A:1192:TRP:H	1.76	0.51
12:D:85:SER:O	12:D:89:GLN:NE2	2.43	0.51
1:A:691:ASP:CG	1:A:765:ASN:HD22	2.16	0.51
1:A:892:GLY:O	1:A:893:GLU:HG2	2.10	0.51
2:B:718:GLN:HG2	2:B:975:ARG:O	2.09	0.51
2:B:837:CYS:HB2	2:B:889:LYS:HE2	1.93	0.51
1:A:706:ILE:HD11	1:A:787:VAL:HG21	1.90	0.51
1:A:1474:LEU:HD22	5:F:107:ARG:HD3	1.93	0.51
5:F:79:VAL:HG11	5:F:83:LEU:HD23	1.92	0.51
10:L:17:TYR:CD2	10:L:28:ILE:HB	2.46	0.51
10:L:56:ASP:O	10:L:58:ARG:N	2.40	0.51
1:A:419:ILE:HD13	1:A:440:LEU:HD21	1.92	0.51
2:B:110:PRO:HB3	2:B:156:LEU:HD11	1.92	0.51
2:B:699:HIS:HD2	2:B:701:SER:OG	1.94	0.51
4:E:103:LEU:HD11	4:E:130:PHE:HE2	1.76	0.51
13:G:94:LYS:HG2	13:G:119:PHE:CE2	2.45	0.51
1:A:983:LEU:HD12	1:A:1048:THR:HG21	1.93	0.51
11:R:102:TYR:CE2	11:R:104:LEU:HB2	2.46	0.51
13:G:121:PRO:HA	13:G:126:PRO:HA	1.92	0.51
1:A:479:TRP:HB2	1:A:483:ARG:NH2	2.26	0.51
2:B:309:PHE:O	2:B:312:GLN:NE2	2.32	0.51
1:A:962:ASP:OD2	1:A:1046:ARG:NH2	2.28	0.51
1:A:1347:LEU:HG	4:E:137:ILE:HD13	1.93	0.51
1:A:775:LYS:HE3	2:B:974:SER:HB3	1.93	0.50
1:A:926:ASN:C	1:A:928:ARG:H	2.19	0.50
1:A:1486:ILE:HG22	5:F:78:PRO:HA	1.93	0.50
2:B:787:GLY:O	2:B:790:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:56:ARG:HA	11:R:59:LEU:CD2	2.42	0.50
1:A:1218:ARG:O	1:A:1222:THR:HG23	2.10	0.50
7:I:15:ARG:HB3	7:I:24:LEU:HD12	1.93	0.50
11:R:76:MET:SD	11:R:174:GLN:HB2	2.51	0.50
1:A:1315:ASP:HA	1:A:1318:LYS:HG3	1.92	0.50
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.92	0.50
4:E:64:HIS:CD2	4:E:66:ASP:H	2.30	0.50
2:B:542:LEU:O	2:B:546:GLU:HG2	2.12	0.50
9:K:112:LYS:C	9:K:114:GLU:H	2.19	0.50
13:G:86:ASP:HA	13:G:143:ILE:O	2.11	0.50
1:A:1125:LYS:O	1:A:1129:ASN:ND2	2.44	0.50
2:B:910:THR:OG1	2:B:911:LEU:N	2.43	0.50
10:L:16:ILE:HG23	10:L:25:GLU:HB2	1.93	0.50
5:F:100:ARG:NH2	5:F:121:ASP:O	2.45	0.50
1:A:651:SER:O	1:A:653:VAL:N	2.45	0.50
1:A:1262:MET:HE2	1:A:1262:MET:HA	1.93	0.50
1:A:894:ASP:HB3	4:E:200:ALA:HB2	1.93	0.49
2:B:567:ILE:HD11	2:B:577:HIS:HB2	1.93	0.49
2:B:711:ILE:HG12	2:B:725:GLN:HG2	1.94	0.49
13:G:146:LYS:NZ	13:G:164:MET:HB2	2.27	0.49
1:A:1301:ILE:O	1:A:1303:GLN:N	2.45	0.49
1:A:1472:ASP:HB2	5:F:109:TYR:CE2	2.47	0.49
1:A:1286:ARG:HD3	7:I:54:TYR:CE2	2.47	0.49
4:E:96:GLU:C	4:E:98:ASN:H	2.20	0.49
1:A:393:ILE:HG12	1:A:445:LYS:HG2	1.95	0.49
1:A:950:ASN:O	1:A:954:ARG:HG2	2.13	0.49
2:B:285:LEU:HD21	2:B:305:LEU:HD21	1.95	0.49
2:B:325:GLY:HA3	2:B:338:TYR:HE2	1.77	0.49
2:B:629:GLU:HB2	2:B:634:LEU:HD21	1.94	0.49
13:G:43:GLY:HA3	13:G:78:ARG:HB3	1.94	0.49
1:A:757:GLN:HA	1:A:760:LEU:HG	1.94	0.49
2:B:363:TYR:OH	2:B:558:PRO:HG3	2.11	0.49
5:F:51:ARG:HD3	5:F:118:TRP:CZ2	2.48	0.49
5:F:51:ARG:NH2	5:F:117:ASP:O	2.46	0.49
6:H:84:ARG:NH1	6:H:85:ALA:O	2.46	0.49
1:A:757:GLN:HE22	1:A:778:LYS:HB2	1.78	0.49
2:B:129:THR:O	2:B:130:LYS:HE2	2.13	0.49
2:B:721:ARG:NH2	2:B:940:GLY:O	2.45	0.49
9:K:77:THR:OG1	9:K:81:TYR:O	2.28	0.49
1:A:392:GLU:OE2	1:A:402:LEU:HD21	2.12	0.49
9:K:81:TYR:OH	9:K:89:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:25:GLU:OE1	10:L:47:LYS:NZ	2.45	0.49
11:R:150:GLN:CD	11:R:173:GLU:HA	2.38	0.49
4:E:100:THR:OG1	4:E:124:LYS:O	2.29	0.49
9:K:80:ASP:OD1	9:K:80:ASP:N	2.33	0.49
11:R:184:LEU:HD21	11:R:189:ILE:HD11	1.93	0.49
12:D:32:LEU:HD21	12:D:36:GLU:HB3	1.95	0.49
1:A:432:HIS:O	1:A:434:LYS:HG2	2.12	0.49
1:A:775:LYS:HE3	2:B:974:SER:CB	2.42	0.49
2:B:42:GLN:HG2	2:B:43:GLN:N	2.26	0.49
2:B:384:ASP:HB3	2:B:387:HIS:HB2	1.95	0.49
8:J:47:ARG:NH1	8:J:48:MET:SD	2.86	0.49
11:R:95:SER:OG	11:R:134:SER:OG	2.09	0.49
11:R:138:ASN:HB3	11:R:189:ILE:HG13	1.94	0.48
13:G:151:ARG:N	13:G:158:PHE:O	2.38	0.48
1:A:604:ARG:HH11	1:A:651:SER:N	2.07	0.48
2:B:90:GLN:HG2	2:B:91:ILE:N	2.25	0.48
2:B:796:MET:HB2	2:B:948:GLN:HG2	1.94	0.48
1:A:413:TYR:OH	1:A:450:MET:O	2.24	0.48
1:A:865:ILE:O	1:A:869:GLU:HB3	2.13	0.48
1:A:1282:ASP:OD1	1:A:1283:VAL:N	2.46	0.48
3:C:16:ASP:OD1	3:C:240:ARG:NH2	2.47	0.48
3:C:60:HIS:HD2	3:C:62:GLU:OE1	1.96	0.48
11:R:152:PRO:HD3	11:R:169:LEU:HD22	1.95	0.48
11:R:176:GLY:O	11:R:180:GLU:HG2	2.13	0.48
1:A:1194:ASN:HA	1:A:1197:TYR:HB2	1.96	0.48
11:R:60:HIS:HA	11:R:63:GLU:OE1	2.14	0.48
12:D:102:ASN:OD1	12:D:103:LEU:N	2.45	0.48
12:D:133:ASP:O	12:D:137:LYS:HG2	2.12	0.48
13:G:108:ILE:HG12	13:G:161:GLY:H	1.79	0.48
2:B:281:ASP:HB2	7:I:22:ASN:HA	1.95	0.48
8:J:5:VAL:HG12	8:J:6:ARG:HG2	1.96	0.48
1:A:1372:GLU:HG3	4:E:193:ILE:HG12	1.96	0.48
2:B:853:LEU:HD23	2:B:867:ILE:HG23	1.95	0.48
13:G:150:THR:HA	13:G:159:ALA:HA	1.96	0.48
2:B:124:LEU:HD22	2:B:152:ILE:HD11	1.95	0.48
3:C:260:GLN:HE22	9:K:88:THR:HG23	1.77	0.48
1:A:1468:THR:HA	1:A:1471:PHE:HE1	1.78	0.48
2:B:563:ASP:OD1	2:B:563:ASP:N	2.39	0.48
4:E:89:VAL:HA	4:E:92:GLN:HG2	1.96	0.48
1:A:382:ARG:HH12	1:A:478:PRO:HB3	1.79	0.48
1:A:1262:MET:O	1:A:1263:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:ILE:C	1:A:1303:GLN:H	2.22	0.48
2:B:257:VAL:HB	2:B:266:GLU:HB3	1.96	0.48
3:C:72:PRO:O	3:C:130:VAL:HG23	2.13	0.48
1:A:653:VAL:HG11	1:A:669:TYR:CZ	2.49	0.48
3:C:92:GLU:HG3	3:C:93:PHE:CD2	2.49	0.48
1:A:1115:LYS:HE2	1:A:1138:SER:HB2	1.95	0.47
1:A:1355:VAL:O	4:E:143:GLU:HB2	2.13	0.47
5:F:53:THR:HG21	5:F:108:ARG:HD3	1.96	0.47
6:H:20:LYS:NZ	6:H:45:ILE:HD11	2.29	0.47
6:H:26:SER:HB3	6:H:45:ILE:HD13	1.96	0.47
11:R:102:TYR:OH	11:R:177:HIS:HB2	2.13	0.47
13:G:11:ILE:HG21	13:G:26:VAL:HG23	1.95	0.47
13:G:54:ILE:HG13	13:G:54:ILE:O	2.14	0.47
2:B:677:MET:H	2:B:682:LEU:HG	1.78	0.47
3:C:75:SER:HB2	3:C:79:VAL:HG13	1.96	0.47
13:G:162:SER:OG	13:G:164:MET:HG2	2.14	0.47
1:A:754:SER:O	1:A:758:LYS:HG2	2.14	0.47
11:R:115:GLN:HG3	11:R:129:ILE:HD11	1.96	0.47
1:A:1188:GLU:N	1:A:1188:GLU:OE1	2.47	0.47
2:B:99:TRP:HZ3	2:B:151:LYS:NZ	2.12	0.47
2:B:285:LEU:HD12	7:I:16:PHE:HZ	1.79	0.47
9:K:65:HIS:CE1	9:K:67:LEU:HD12	2.49	0.47
1:A:389:THR:HB	1:A:447:GLU:HG2	1.97	0.47
2:B:430:ASN:O	2:B:433:LEU:HD23	2.14	0.47
2:B:548:TRP:NE1	2:B:582:GLN:HE22	2.11	0.47
10:L:15:MET:N	10:L:29:LYS:HZ3	2.12	0.47
11:R:50:LYS:HG2	11:R:54:PHE:CZ	2.49	0.47
13:G:13:LEU:HB2	13:G:66:VAL:HG12	1.95	0.47
13:G:21:ASN:OD1	13:G:25:THR:OG1	2.32	0.47
1:A:571:ASP:OD1	1:A:571:ASP:N	2.46	0.47
1:A:1139:LEU:HB3	1:A:1338:THR:OG1	2.14	0.47
2:B:666:ASP:OD1	2:B:666:ASP:N	2.46	0.47
2:B:957:THR:HG22	2:B:958:CYS:N	2.30	0.47
3:C:103:LEU:HB3	3:C:161:LEU:HG	1.97	0.47
2:B:21:LEU:HD12	2:B:24:GLU:OE2	2.14	0.47
5:F:62:ARG:NE	5:F:125:ILE:HD11	2.30	0.47
11:R:86:HIS:O	11:R:90:VAL:HG23	2.15	0.47
12:D:106:GLU:N	12:D:106:GLU:OE1	2.48	0.47
1:A:917:GLU:O	1:A:921:ARG:HB2	2.14	0.47
1:A:1163:HIS:CD2	1:A:1297:THR:HG23	2.50	0.47
1:A:1228:MET:HE1	1:A:1248:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:722:ASN:O	2:B:726:SER:OG	2.28	0.47
12:D:61:PHE:O	12:D:65:LEU:HG	2.15	0.47
1:A:790:GLN:NE2	1:A:791:GLN:O	2.44	0.46
1:A:1025:GLY:HA2	1:A:1030:SER:OG	2.15	0.46
1:A:1192:TRP:HZ3	1:A:1246:ILE:HG22	1.80	0.46
1:A:1206:ARG:HG3	1:A:1207:ILE:H	1.80	0.46
1:A:1227:THR:H	1:A:1230:GLN:NE2	2.12	0.46
2:B:169:ARG:O	2:B:173:GLU:HG3	2.15	0.46
2:B:949:TYR:HB3	2:B:953:ASP:HB2	1.96	0.46
3:C:154:ARG:HB2	8:J:60:LEU:HD22	1.97	0.46
2:B:715:ASP:OD1	2:B:715:ASP:N	2.42	0.46
2:B:752:TYR:CE2	2:B:807:ARG:HD2	2.50	0.46
4:E:61:LEU:HD21	4:E:71:GLN:NE2	2.29	0.46
1:A:401:ARG:O	1:A:404:GLU:HG2	2.15	0.46
1:A:617:PRO:HG2	1:A:618:TYR:CD2	2.51	0.46
1:A:732:THR:HG22	1:A:733:LEU:N	2.30	0.46
2:B:782:ILE:HD12	2:B:1042:PHE:CD1	2.51	0.46
11:R:152:PRO:HD3	11:R:169:LEU:CD2	2.45	0.46
1:A:927:GLU:OE2	1:A:931:ARG:NE	2.39	0.46
1:A:988:TRP:HE1	1:A:992:LYS:HE2	1.80	0.46
1:A:1021:VAL:HA	1:A:1034:GLN:HE22	1.81	0.46
1:A:1481:LYS:HD3	13:G:20:PRO:HA	1.98	0.46
2:B:636:LYS:H	2:B:639:HIS:HD2	1.64	0.46
2:B:848:LEU:HD21	2:B:865:VAL:HG13	1.97	0.46
9:K:17:LYS:C	9:K:19:ILE:H	2.23	0.46
1:A:1140:THR:O	1:A:1357:THR:HA	2.16	0.46
1:A:1273:GLU:O	1:A:1276:VAL:HG22	2.15	0.46
10:L:21:GLU:HB2	10:L:41:TYR:CD2	2.51	0.46
12:D:87:LEU:HD13	12:D:97:LEU:HD12	1.97	0.46
13:G:119:PHE:HB2	13:G:128:TYR:HE1	1.80	0.46
1:A:578:ALA:HB2	1:A:590:GLN:HE21	1.80	0.46
1:A:1211:LEU:HD11	1:A:1258:ARG:NE	2.30	0.46
2:B:187:ILE:HD13	2:B:448:LEU:HB3	1.98	0.46
4:E:75:PHE:O	4:E:77:PRO:HD3	2.16	0.46
1:A:1244:ASN:HB2	1:A:1262:MET:HE3	1.97	0.46
2:B:325:GLY:HA3	2:B:338:TYR:CE2	2.50	0.46
9:K:31:CYS:SG	9:K:84:GLN:NE2	2.89	0.46
13:G:55:GLY:HA3	13:G:69:PRO:HG2	1.98	0.46
1:A:376:ASP:HA	1:A:521:VAL:HG23	1.98	0.46
1:A:704:ASN:O	1:A:708:LYS:HG2	2.16	0.46
1:A:1410:HIS:HD2	1:A:1412:MET:HE3	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:VAL:O	2:B:467:SER:HA	2.16	0.46
7:I:17:CYS:SG	7:I:18:GLN:N	2.88	0.46
10:L:46:LYS:O	10:L:46:LYS:HG2	2.16	0.46
11:R:76:MET:SD	11:R:173:GLU:HG3	2.55	0.46
1:A:379:GLY:HA2	1:A:475:ARG:O	2.16	0.46
2:B:1037:ILE:O	3:C:195:THR:HG22	2.16	0.46
3:C:166:LYS:HB2	3:C:166:LYS:HE3	1.60	0.46
4:E:19:GLN:HE21	4:E:138:ASN:HD22	1.62	0.46
11:R:148:GLU:HA	11:R:151:ILE:HG13	1.98	0.46
1:A:775:LYS:HG2	2:B:970:HIS:O	2.16	0.46
1:A:1082:HIS:O	1:A:1085:GLU:HB2	2.16	0.46
3:C:45:ILE:HG22	3:C:73:LEU:HD12	1.97	0.46
12:D:132:ASP:O	12:D:136:THR:HG23	2.16	0.46
1:A:1177:TYR:CE1	7:I:28:GLU:HG3	2.51	0.45
2:B:262:TYR:O	2:B:263:ILE:HG13	2.17	0.45
11:R:159:ARG:HE	11:R:159:ARG:HB2	1.59	0.45
2:B:778:SER:O	2:B:1045:PRO:HA	2.16	0.45
2:B:792:ASP:O	2:B:943:GLY:HA3	2.17	0.45
2:B:856:PRO:HG2	10:L:48:ARG:HA	1.96	0.45
2:B:908:MET:HE2	10:L:43:ILE:HG23	1.98	0.45
13:G:112:SER:HB3	13:G:162:SER:HA	1.99	0.45
1:A:450:MET:SD	1:A:474:VAL:HG21	2.56	0.45
2:B:479:LEU:O	2:B:483:ARG:HG3	2.17	0.45
4:E:103:LEU:HD11	4:E:130:PHE:CE2	2.52	0.45
13:G:97:LEU:O	13:G:107:PHE:HA	2.15	0.45
1:A:592:PHE:O	1:A:595:ILE:N	2.49	0.45
1:A:604:ARG:NH1	1:A:643:LYS:O	2.50	0.45
2:B:262:TYR:CE2	2:B:346:GLU:HG2	2.51	0.45
2:B:851:ASP:N	10:L:15:MET:HE1	2.31	0.45
4:E:47:LYS:O	4:E:51:GLY:HA3	2.16	0.45
4:E:84:ILE:HA	4:E:87:ILE:HG12	1.98	0.45
11:R:83:THR:HG22	11:R:159:ARG:NH2	2.31	0.45
1:A:893:GLU:HB2	4:E:203:TYR:CD1	2.52	0.45
1:A:1242:ASP:HB3	11:R:119:ILE:HG12	1.98	0.45
2:B:274:ARG:NH1	2:B:308:ALA:O	2.50	0.45
2:B:558:PRO:O	2:B:561:ILE:HG22	2.15	0.45
2:B:626:LEU:HB2	2:B:696:CYS:HB3	1.98	0.45
5:F:83:LEU:HA	5:F:95:LYS:NZ	2.31	0.45
5:F:108:ARG:HD2	5:F:118:TRP:CD1	2.52	0.45
13:G:46:ILE:N	13:G:75:ILE:O	2.48	0.45
1:A:365:THR:HG22	1:A:366:VAL:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:PRO:HB2	2:B:675:LEU:HD12	1.99	0.45
1:A:731:ASN:OD1	1:A:731:ASN:N	2.48	0.45
2:B:851:ASP:HB3	10:L:15:MET:SD	2.57	0.45
2:B:907:VAL:HG13	2:B:921:ILE:HG12	1.98	0.45
11:R:102:TYR:HE2	11:R:104:LEU:HB2	1.81	0.45
1:A:361:PHE:HE1	1:A:505:LEU:H	1.64	0.45
1:A:413:TYR:O	1:A:449:HIS:HD2	2.00	0.45
1:A:607:SER:HA	1:A:643:LYS:NZ	2.32	0.45
2:B:860:VAL:O	2:B:901:THR:HA	2.16	0.45
3:C:179:THR:O	3:C:180:ALA:HB3	2.16	0.45
1:A:1139:LEU:HD21	1:A:1346:VAL:HG21	1.98	0.45
1:A:1146:GLN:HA	1:A:1149:ARG:HH11	1.82	0.45
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.52	0.45
11:R:57:LYS:CE	11:R:156:VAL:HG21	2.45	0.45
12:D:76:ASN:HB3	12:D:79:THR:OG1	2.17	0.45
13:G:106:CYS:HA	13:G:159:ALA:O	2.17	0.45
1:A:1123:ARG:NH2	1:A:1360:ASN:O	2.49	0.45
1:A:1230:GLN:O	1:A:1234:LYS:HG2	2.17	0.45
1:A:1244:ASN:OD1	1:A:1245:CYS:N	2.50	0.45
2:B:718:GLN:HB3	2:B:976:MET:HG3	1.99	0.45
2:B:761:THR:H	2:B:764:MET:HE3	1.82	0.45
11:R:92:ASP:O	11:R:96:ILE:HG13	2.17	0.45
11:R:138:ASN:HA	11:R:189:ILE:HG21	1.99	0.45
12:D:130:ILE:O	12:D:134:ILE:HG12	2.17	0.45
1:A:418:TYR:HB2	1:A:447:GLU:HB3	1.99	0.44
1:A:552:ASP:OD1	6:H:22:PHE:HB3	2.17	0.44
2:B:955:PRO:O	2:B:963:PRO:HD2	2.17	0.44
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.53	0.44
1:A:857:THR:HG21	1:A:1100:THR:HG22	1.98	0.44
1:A:1052:ARG:O	1:A:1056:GLU:HG2	2.18	0.44
2:B:386:ASP:OD1	2:B:496:ALA:HB1	2.18	0.44
9:K:23:LYS:HE2	9:K:31:CYS:SG	2.57	0.44
9:K:58:PHE:CE2	9:K:74:ARG:HD3	2.52	0.44
1:A:765:ASN:O	1:A:769:MET:HG2	2.17	0.44
1:A:1177:TYR:HB2	1:A:1210:TRP:CZ3	2.52	0.44
1:A:1235:ILE:HA	1:A:1296:MET:HE2	1.99	0.44
2:B:118:LEU:HD22	2:B:913:GLN:HG3	1.98	0.44
2:B:974:SER:OG	2:B:975:ARG:NH1	2.51	0.44
8:J:53:VAL:HG23	8:J:53:VAL:O	2.18	0.44
11:R:56:ARG:HG3	11:R:60:HIS:CE1	2.52	0.44
2:B:911:LEU:HD12	10:L:42:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:49:SER:C	4:E:50:GLU:HG3	2.42	0.44
13:G:1:MET:HE1	13:G:80:PHE:CD2	2.53	0.44
13:G:128:TYR:O	13:G:137:ILE:HB	2.17	0.44
6:H:14:ASP:OD1	6:H:15:ILE:N	2.51	0.44
1:A:421:ARG:CZ	1:A:427:ILE:HD11	2.48	0.44
6:H:71:ASP:O	6:H:72:ASP:HB3	2.17	0.44
10:L:37:ARG:H	10:L:37:ARG:HD2	1.81	0.44
11:R:142:GLN:NE2	11:R:188:ALA:O	2.50	0.44
1:A:381:PRO:HB3	1:A:479:TRP:O	2.18	0.44
1:A:539:GLN:H	1:A:539:GLN:HG3	1.36	0.44
2:B:425:ARG:HG2	2:B:427:LYS:NZ	2.32	0.44
4:E:3:ASP:OD1	4:E:3:ASP:N	2.49	0.44
4:E:77:PRO:HG2	4:E:82:VAL:HG21	2.00	0.44
1:A:383:SER:CB	9:K:2:ASN:HD21	2.30	0.44
1:A:1121:VAL:N	1:A:1122:PRO:HD2	2.33	0.44
4:E:85:LYS:HE2	4:E:85:LYS:HB2	1.76	0.44
12:D:38:HIS:ND1	12:D:68:THR:HG23	2.32	0.44
1:A:376:ASP:HA	1:A:521:VAL:CG2	2.48	0.44
1:A:1480:CYS:HB3	13:G:19:GLY:HA2	2.00	0.44
2:B:636:LYS:H	2:B:639:HIS:CD2	2.36	0.44
4:E:102:ALA:HB3	4:E:127:LEU:HG	2.00	0.44
11:R:70:ILE:HG23	11:R:74:PHE:HD2	1.83	0.44
11:R:170:LEU:O	11:R:173:GLU:HG2	2.18	0.44
1:A:365:THR:HG22	1:A:366:VAL:N	2.33	0.43
1:A:416:ALA:HA	1:A:448:ARG:HA	1.99	0.43
1:A:1022:ILE:N	1:A:1034:GLN:HE22	2.16	0.43
2:B:978:ILE:O	2:B:982:ILE:HG13	2.18	0.43
6:H:81:ARG:CZ	6:H:82:PRO:HG3	2.47	0.43
11:R:52:ILE:HA	11:R:55:GLU:OE2	2.17	0.43
11:R:141:TYR:CD1	11:R:141:TYR:C	2.96	0.43
12:D:67:TYR:HB2	13:G:102:GLY:HA2	1.99	0.43
12:D:112:LYS:HD2	12:D:119:GLU:HA	1.99	0.43
1:A:506:PRO:HG3	1:A:515:ILE:HD12	1.99	0.43
1:A:731:ASN:O	1:A:732:THR:OG1	2.29	0.43
1:A:1218:ARG:NH1	1:A:1255:LEU:HD23	2.33	0.43
2:B:88:PHE:CD2	2:B:128:ILE:HG12	2.52	0.43
2:B:205:VAL:O	2:B:371:ARG:NH1	2.52	0.43
2:B:255:ARG:HD2	2:B:307:GLU:OE1	2.18	0.43
2:B:831:LYS:HG3	2:B:848:LEU:HB2	2.00	0.43
7:I:29:ASP:CB	7:I:34:ILE:O	2.66	0.43
9:K:82:SER:OG	9:K:85:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:125:GLU:HG2	12:D:126:GLU:N	2.33	0.43
1:A:394:VAL:HG23	1:A:444:TYR:O	2.17	0.43
1:A:784:VAL:HG13	2:B:978:ILE:CD1	2.41	0.43
2:B:490:GLY:O	2:B:494:LYS:HG2	2.19	0.43
2:B:814:TYR:HE2	2:B:897:ARG:HG3	1.82	0.43
2:B:833:THR:HB	2:B:834:ARG:H	1.54	0.43
12:D:38:HIS:HB2	12:D:68:THR:OG1	2.17	0.43
1:A:1211:LEU:HD12	1:A:1260:ARG:HE	1.83	0.43
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.54	0.43
11:R:143:ALA:HA	11:R:180:GLU:HG3	2.00	0.43
12:D:35:SER:O	12:D:38:HIS:HB3	2.19	0.43
1:A:576:GLN:HG3	1:A:577:PRO:HD2	2.00	0.43
2:B:26:CYS:SG	2:B:699:HIS:HB2	2.59	0.43
11:R:52:ILE:HG23	11:R:56:ARG:HH21	1.84	0.43
13:G:45:VAL:HA	13:G:76:VAL:HG12	2.00	0.43
1:A:457:ILE:HD11	1:A:504:HIS:HD2	1.84	0.43
1:A:930:LEU:HB3	1:A:939:VAL:CG2	2.49	0.43
1:A:1189:ASP:OD2	1:A:1258:ARG:HD2	2.19	0.43
2:B:345:LYS:HG2	2:B:353:VAL:HG13	2.00	0.43
6:H:8:ASP:OD2	6:H:35:PHE:HB2	2.19	0.43
7:I:92:LYS:HB3	7:I:92:LYS:HE3	1.69	0.43
11:R:150:GLN:NE2	11:R:173:GLU:HA	2.33	0.43
12:D:60:VAL:HG21	13:G:36:GLY:HA2	2.01	0.43
1:A:580:LEU:HD13	1:A:580:LEU:HA	1.83	0.43
1:A:841:MET:HE2	1:A:841:MET:HB3	1.88	0.43
1:A:872:MET:HA	1:A:1087:VAL:HG22	2.00	0.43
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.15	0.43
2:B:419:ALA:O	2:B:423:ILE:HG12	2.19	0.43
11:R:72:GLU:O	11:R:76:MET:HG2	2.19	0.43
1:A:432:HIS:HD2	1:A:434:LYS:HD3	1.82	0.43
1:A:1017:SER:HB2	1:A:1042:ASN:OD1	2.19	0.43
1:A:1301:ILE:O	1:A:1301:ILE:HG22	2.18	0.43
1:A:1301:ILE:HB	1:A:1304:ILE:HD12	1.99	0.43
2:B:119:THR:HG23	2:B:187:ILE:HA	2.00	0.43
2:B:602:SER:HB3	2:B:615:TYR:HB2	2.00	0.43
11:R:53:GLU:O	11:R:56:ARG:HG2	2.19	0.43
1:A:1244:ASN:CB	1:A:1262:MET:HE3	2.49	0.43
2:B:561:ILE:HD13	2:B:561:ILE:HG21	1.70	0.43
2:B:566:LYS:HB3	2:B:568:PHE:CE1	2.53	0.43
2:B:841:ARG:H	2:B:841:ARG:HG2	1.59	0.43
3:C:47:ILE:HA	3:C:165:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:92:LEU:HD11	12:D:118:LEU:HD21	2.01	0.43
13:G:81:LYS:HD3	13:G:149:GLY:HA2	2.00	0.43
1:A:1207:ILE:HD11	1:A:1260:ARG:HD3	2.01	0.43
8:J:65:LEU:O	10:L:23:HIS:ND1	2.52	0.43
10:L:56:ASP:OD1	10:L:56:ASP:N	2.50	0.43
11:R:129:ILE:CG2	11:R:190:LYS:HG2	2.49	0.43
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.83	0.42
1:A:955:GLU:OE1	1:A:1051:SER:OG	2.24	0.42
1:A:1158:LEU:HD12	1:A:1309:MET:HB3	2.00	0.42
2:B:645:GLU:O	2:B:649:ASN:HB2	2.19	0.42
13:G:51:ILE:HG13	13:G:51:ILE:O	2.19	0.42
1:A:687:ILE:HG21	2:B:972:ILE:HB	2.00	0.42
2:B:834:ARG:HD3	2:B:834:ARG:HA	1.59	0.42
3:C:45:ILE:HB	3:C:75:SER:HB3	2.01	0.42
6:H:106:THR:OG1	6:H:107:GLU:OE1	2.36	0.42
7:I:75:ASP:O	7:I:80:ARG:NH1	2.49	0.42
1:A:401:ARG:O	1:A:405:LEU:HG	2.19	0.42
1:A:922:PHE:CD1	1:A:952:LEU:HD13	2.54	0.42
1:A:1473:LEU:HD22	5:F:104:ILE:HG21	2.01	0.42
2:B:281:ASP:OD1	2:B:305:LEU:HD22	2.20	0.42
2:B:323:SER:HB2	2:B:324:ARG:HH11	1.84	0.42
2:B:448:LEU:O	2:B:467:SER:OG	2.24	0.42
12:D:40:LEU:O	12:D:44:ARG:HG2	2.19	0.42
1:A:1474:LEU:HB2	5:F:105:ILE:HG13	2.02	0.42
3:C:5:ASN:OD1	3:C:5:ASN:N	2.49	0.42
4:E:18:MET:HE3	4:E:60:VAL:HG11	1.99	0.42
9:K:24:ASP:HB3	9:K:30:ALA:HB3	2.01	0.42
13:G:93:ASN:OD1	13:G:94:LYS:N	2.52	0.42
1:A:786:ALA:O	1:A:787:VAL:HG23	2.19	0.42
1:A:1137:PRO:HB2	1:A:1341:VAL:HG13	2.01	0.42
1:A:1271:GLU:HG3	1:A:1272:GLU:H	1.84	0.42
2:B:93:LEU:HD23	2:B:160:TYR:CD2	2.55	0.42
2:B:265:GLN:HB2	2:B:324:ARG:HG2	2.01	0.42
2:B:763:SER:O	2:B:767:LEU:HG	2.20	0.42
2:B:898:THR:O	2:B:1060:HIS:HB3	2.19	0.42
3:C:189:ASP:O	3:C:191:ALA:N	2.52	0.42
13:G:4:HIS:CD2	13:G:75:ILE:HG13	2.54	0.42
1:A:867:SER:HB2	1:A:1414:ILE:HB	2.02	0.42
1:A:950:ASN:OD1	1:A:951:GLU:N	2.53	0.42
1:A:1082:HIS:HB3	5:F:58:THR:HG23	2.00	0.42
2:B:300:MET:HE2	2:B:300:MET:HB3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:818:GLU:HG3	2:B:828:VAL:HA	2.00	0.42
4:E:49:SER:O	4:E:50:GLU:HG3	2.20	0.42
9:K:40:HIS:H	9:K:40:HIS:CD2	2.38	0.42
1:A:434:LYS:O	1:A:438:LEU:HG	2.19	0.42
1:A:537:ILE:HG12	1:A:542:LEU:HD13	2.02	0.42
3:C:52:ILE:HG21	3:C:55:ASN:HB2	2.01	0.42
3:C:154:ARG:HD3	8:J:64:PRO:HD3	2.02	0.42
6:H:64:LEU:HD22	6:H:84:ARG:NH1	2.34	0.42
13:G:8:GLU:HB3	13:G:71:LYS:HB3	2.02	0.42
1:A:421:ARG:HG2	1:A:444:TYR:CE1	2.54	0.42
1:A:1054:MET:HE3	1:A:1054:MET:HB3	1.55	0.42
1:A:1027:ASP:HB3	1:A:1030:SER:CB	2.49	0.42
1:A:1134:PRO:O	1:A:1137:PRO:HD3	2.20	0.42
1:A:1207:ILE:HG13	1:A:1262:MET:CE	2.50	0.42
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.81	0.42
4:E:19:GLN:HE21	4:E:138:ASN:ND2	2.17	0.42
13:G:119:PHE:HB2	13:G:128:TYR:CE1	2.55	0.42
1:A:1008:LYS:HE2	1:A:1008:LYS:HB2	1.86	0.42
1:A:1142:PHE:HD2	1:A:1357:THR:H	1.68	0.42
1:A:1481:LYS:HD3	1:A:1481:LYS:HA	1.86	0.42
2:B:214:LYS:HB2	2:B:214:LYS:HE3	1.76	0.42
2:B:706:VAL:HG22	2:B:767:LEU:HD22	2.02	0.42
2:B:912:ASN:OD1	2:B:912:ASN:N	2.52	0.42
4:E:193:ILE:HB	4:E:205:THR:HG23	2.02	0.42
11:R:49:ARG:O	11:R:52:ILE:HG22	2.20	0.42
1:A:402:LEU:HB3	1:A:446:VAL:HG11	2.02	0.41
1:A:1098:PRO:HG2	1:A:1393:VAL:CG2	2.50	0.41
2:B:268:PRO:HB2	2:B:271:ILE:HG12	2.02	0.41
2:B:592:ARG:NE	2:B:663:GLU:OE2	2.38	0.41
2:B:869:LYS:HE3	2:B:892:CYS:SG	2.59	0.41
3:C:18:ASN:H	3:C:241:PRO:HG3	1.84	0.41
5:F:79:VAL:HG22	5:F:81:VAL:H	1.84	0.41
11:R:184:LEU:HG	11:R:186:SER:H	1.84	0.41
13:G:86:ASP:N	13:G:86:ASP:OD1	2.52	0.41
1:A:477:LEU:HD23	1:A:477:LEU:HA	1.80	0.41
1:A:710:LYS:O	1:A:714:ILE:HG12	2.20	0.41
1:A:1163:HIS:HA	1:A:1300:GLY:HA3	2.02	0.41
2:B:110:PRO:HG2	2:B:163:LEU:HD11	2.02	0.41
2:B:115:LEU:O	2:B:920:LYS:HE3	2.20	0.41
4:E:167:GLU:O	4:E:208:LEU:HD22	2.20	0.41
10:L:16:ILE:CG2	10:L:25:GLU:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:35:ARG:HD3	10:L:42:ARG:CZ	2.50	0.41
1:A:552:ASP:CG	6:H:22:PHE:HB3	2.46	0.41
1:A:578:ALA:HB2	1:A:590:GLN:NE2	2.35	0.41
1:A:598:GLY:HA3	1:A:660:MET:SD	2.61	0.41
1:A:863:ARG:HH12	1:A:1129:ASN:CG	2.25	0.41
1:A:1007:ILE:HD12	1:A:1007:ILE:HA	1.77	0.41
1:A:1272:GLU:HB2	1:A:1275:VAL:HB	2.01	0.41
1:A:1374:VAL:HG21	1:A:1411:LEU:HD11	2.02	0.41
2:B:866:ILE:HD13	2:B:866:ILE:HA	1.80	0.41
2:B:866:ILE:HG12	2:B:896:LEU:HD12	2.02	0.41
11:R:72:GLU:HG3	11:R:104:LEU:HD11	2.03	0.41
1:A:386:ALA:HB2	1:A:413:TYR:HD1	1.85	0.41
1:A:1193:VAL:HG21	1:A:1258:ARG:NH1	2.35	0.41
1:A:521:VAL:H	1:A:521:VAL:HG22	1.61	0.41
2:B:166:LEU:HD23	2:B:166:LEU:HA	1.91	0.41
2:B:177:CYS:HB2	2:B:739:ASN:OD1	2.21	0.41
2:B:337:LYS:HD3	2:B:337:LYS:HA	1.85	0.41
7:I:106:ASP:OD1	7:I:106:ASP:N	2.53	0.41
1:A:651:SER:O	1:A:651:SER:OG	2.35	0.41
1:A:1467:GLY:O	1:A:1468:THR:OG1	2.34	0.41
2:B:40:VAL:HG11	2:B:482:LEU:HD13	2.03	0.41
2:B:653:TRP:CH2	2:B:662:VAL:HG11	2.56	0.41
2:B:941:GLN:HG2	2:B:975:ARG:NE	2.35	0.41
6:H:8:ASP:OD2	6:H:32:SER:HB2	2.20	0.41
1:A:538:VAL:HG13	1:A:540:ASP:H	1.84	0.41
1:A:724:GLU:OE1	1:A:724:GLU:N	2.53	0.41
2:B:206:TYR:HA	2:B:383:ASP:OD2	2.21	0.41
2:B:211:LYS:H	2:B:211:LYS:HG3	1.43	0.41
2:B:529:MET:SD	2:B:702:MET:HG3	2.61	0.41
2:B:972:ILE:N	2:B:973:PRO:HD2	2.36	0.41
4:E:129:GLN:HG2	4:E:130:PHE:N	2.34	0.41
13:G:146:LYS:HZ1	13:G:164:MET:HB2	1.85	0.41
1:A:990:ALA:HB2	1:A:1067:TRP:CZ3	2.56	0.41
11:R:129:ILE:HG22	11:R:190:LYS:HG2	2.03	0.41
11:R:133:LYS:H	11:R:133:LYS:HG3	1.70	0.41
1:A:706:ILE:HD13	1:A:706:ILE:HA	1.91	0.41
1:A:809:HIS:CE1	2:B:677:MET:HE2	2.55	0.41
1:A:903:PHE:HA	1:A:977:VAL:O	2.21	0.41
1:A:1245:CYS:O	1:A:1246:ILE:HD13	2.21	0.41
1:A:1370:GLY:HA2	4:E:178:PRO:HD2	2.03	0.41
2:B:23:GLN:O	2:B:27:TRP:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:PHE:HB2	2:B:397:GLY:HA2	2.03	0.41
2:B:193:VAL:HG13	2:B:482:LEU:HD23	2.03	0.41
2:B:385:ARG:HD3	2:B:492:ASP:OD1	2.21	0.41
2:B:557:SER:O	2:B:559:ALA:N	2.54	0.41
3:C:246:LEU:HD23	3:C:246:LEU:HA	1.80	0.41
6:H:41:LEU:HG	6:H:43:VAL:HG23	2.03	0.41
7:I:37:TYR:CD2	7:I:48:ALA:HB2	2.56	0.41
12:D:36:GLU:O	12:D:39:MET:HB3	2.21	0.41
12:D:61:PHE:CE2	12:D:65:LEU:HD11	2.56	0.41
12:D:127:LEU:HA	12:D:130:ILE:HD12	2.02	0.41
1:A:521:VAL:HG23	1:A:522:PRO:HD3	2.02	0.41
2:B:309:PHE:HE1	7:I:40:ARG:HB2	1.86	0.41
2:B:725:GLN:HE22	2:B:1049:GLN:HE22	1.69	0.41
2:B:1052:LYS:O	2:B:1052:LYS:HG2	2.21	0.41
4:E:17:ILE:HD13	4:E:17:ILE:HA	1.88	0.41
11:R:57:LYS:HZ1	11:R:81:PHE:HB3	1.86	0.41
12:D:84:ARG:HA	12:D:87:LEU:HB2	2.02	0.41
13:G:46:ILE:HB	13:G:75:ILE:HB	2.01	0.41
2:B:331:THR:HG22	2:B:333:GLU:N	2.35	0.40
2:B:388:TYR:HB2	2:B:667:THR:HG21	2.03	0.40
2:B:557:SER:C	2:B:559:ALA:H	2.29	0.40
2:B:835:GLU:HB3	2:B:836:THR:H	1.71	0.40
4:E:185:ILE:HG22	4:E:209:VAL:HG21	2.00	0.40
13:G:117:MET:HA	13:G:130:THR:HA	2.02	0.40
1:A:557:ARG:HH11	1:A:557:ARG:HD3	1.72	0.40
1:A:732:THR:HB	1:A:735:GLN:H	1.85	0.40
1:A:894:ASP:CG	1:A:1396:ARG:NH2	2.79	0.40
1:A:1052:ARG:HE	1:A:1056:GLU:CD	2.29	0.40
2:B:26:CYS:O	2:B:30:ILE:HG13	2.22	0.40
2:B:346:GLU:N	2:B:346:GLU:OE1	2.54	0.40
2:B:647:GLU:O	2:B:648:TYR:CG	2.74	0.40
2:B:838:GLN:H	2:B:838:GLN:HG2	1.54	0.40
6:H:106:THR:OG1	6:H:107:GLU:N	2.54	0.40
11:R:75:LEU:HD13	11:R:103:PRO:HG2	2.04	0.40
12:D:33:LEU:HD22	12:D:101:ALA:HB1	2.03	0.40
1:A:381:PRO:HG2	1:A:384:ILE:HG12	2.03	0.40
1:A:663:ASP:OD1	1:A:666:ARG:NH2	2.51	0.40
1:A:709:ALA:HB2	1:A:748:ALA:HB2	2.03	0.40
1:A:712:ASP:O	1:A:715:GLU:HG2	2.21	0.40
2:B:548:TRP:HE1	2:B:582:GLN:NE2	2.16	0.40
2:B:728:MET:SD	2:B:942:LYS:HB3	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:41:LYS:O	4:E:45:GLY:N	2.52	0.40
4:E:55:ARG:HH11	4:E:55:ARG:HD3	1.75	0.40
8:J:41:LYS:HA	8:J:41:LYS:HD3	1.74	0.40
12:D:36:GLU:O	12:D:40:LEU:HG	2.21	0.40
1:A:402:LEU:HD13	1:A:446:VAL:CG1	2.50	0.40
2:B:550:MET:HG3	2:B:567:ILE:HD12	2.03	0.40
2:B:737:ILE:O	2:B:740:PHE:HD2	2.04	0.40
2:B:982:ILE:HD13	2:B:982:ILE:HG21	1.87	0.40
3:C:43:PRO:HA	3:C:168:GLY:O	2.21	0.40
3:C:44:ILE:HD13	3:C:44:ILE:HG21	1.60	0.40
3:C:63:PHE:O	3:C:67:ARG:HG2	2.21	0.40
6:H:71:ASP:C	6:H:73:GLY:H	2.30	0.40
1:A:542:LEU:HA	1:A:545:VAL:HG12	2.04	0.40
1:A:612:ASP:OD1	1:A:612:ASP:N	2.50	0.40
1:A:962:ASP:CG	1:A:1046:ARG:HH21	2.23	0.40
1:A:1471:PHE:HD2	5:F:106:ILE:HG23	1.86	0.40
2:B:155:MET:HE3	2:B:155:MET:HB2	1.99	0.40
2:B:713:PHE:HB3	2:B:716:HIS:CD2	2.57	0.40
4:E:4:GLU:OE1	4:E:4:GLU:N	2.55	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	1012/1970 (51%)	916 (90%)	92 (9%)	4 (0%)	30 57
2	B	966/1174 (82%)	863 (89%)	98 (10%)	5 (0%)	24 52
3	C	250/275 (91%)	226 (90%)	24 (10%)	0	100 100
4	E	206/210 (98%)	195 (95%)	10 (5%)	1 (0%)	24 52
5	F	74/127 (58%)	70 (95%)	4 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	146/150 (97%)	136 (93%)	10 (7%)	0	100	100
7	I	112/125 (90%)	99 (88%)	13 (12%)	0	100	100
8	J	64/67 (96%)	61 (95%)	3 (5%)	0	100	100
9	K	113/117 (97%)	104 (92%)	9 (8%)	0	100	100
10	L	42/58 (72%)	35 (83%)	6 (14%)	1 (2%)	4	15
11	R	161/612 (26%)	151 (94%)	10 (6%)	0	100	100
12	D	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
13	G	169/172 (98%)	155 (92%)	13 (8%)	1 (1%)	21	47
All	All	3441/5199 (66%)	3130 (91%)	299 (9%)	12 (0%)	37	63

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	LEU
2	B	832	PRO
2	B	900	GLU
1	A	1302	GLU
2	B	19	PRO
4	E	97	GLU
1	A	910	LYS
2	B	843	ALA
10	L	48	ARG
1	A	433	PRO
13	G	64	GLY
2	B	1001	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	910/1748 (52%)	897 (99%)	13 (1%)	59	82
2	B	857/1027 (83%)	836 (98%)	21 (2%)	42	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	231/252 (92%)	228 (99%)	3 (1%)	61	83
4	E	188/192 (98%)	187 (100%)	1 (0%)	81	92
5	F	66/111 (60%)	66 (100%)	0	100	100
6	H	129/131 (98%)	128 (99%)	1 (1%)	73	89
7	I	103/112 (92%)	102 (99%)	1 (1%)	68	86
8	J	55/56 (98%)	54 (98%)	1 (2%)	51	79
9	K	104/106 (98%)	104 (100%)	0	100	100
10	L	41/55 (74%)	40 (98%)	1 (2%)	43	74
11	R	150/561 (27%)	148 (99%)	2 (1%)	61	83
12	D	106/126 (84%)	106 (100%)	0	100	100
13	G	147/153 (96%)	147 (100%)	0	100	100
All	All	3087/4630 (67%)	3043 (99%)	44 (1%)	57	82

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	ARG
1	A	539	GLN
1	A	540	ASP
1	A	580	LEU
1	A	581	LYS
1	A	675	VAL
1	A	731	ASN
1	A	811	ILE
1	A	909	LEU
1	A	910	LYS
1	A	912	SER
1	A	1157	ILE
1	A	1293	LEU
2	B	167	THR
2	B	211	LYS
2	B	212	ASP
2	B	213	SER
2	B	214	LYS
2	B	302	LYS
2	B	303	PRO
2	B	433	LEU
2	B	574	VAL

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Mol	Chain	Res	Type
2	B	630	LYS
2	B	809	VAL
2	B	833	THR
2	B	834	ARG
2	B	836	THR
2	B	838	GLN
2	B	840	MET
2	B	841	ARG
2	B	898	THR
2	B	899	SER
2	B	923	VAL
2	B	978	ILE
3	C	79	VAL
3	C	80	ASP
3	C	127	VAL
4	E	82	VAL
6	H	51	ASP
7	I	43	ASP
8	J	5	VAL
10	L	52	LEU
11	R	151	ILE
11	R	190	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	HIS
1	A	504	HIS
1	A	590	GLN
1	A	599	HIS
1	A	632	ASN
1	A	654	HIS
1	A	711	GLN
1	A	721	HIS
1	A	735	GLN
1	A	791	GLN
1	A	839	HIS
1	A	949	GLN
1	A	1005	HIS
1	A	1034	GLN
1	A	1190	GLN
1	A	1230	GLN

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Mol	Chain	Res	Type
1	A	1310	HIS
1	A	1410	HIS
2	B	43	GLN
2	B	319	ASN
2	B	370	HIS
2	B	471	ASN
2	B	500	GLN
2	B	582	GLN
2	B	631	GLN
2	B	639	HIS
2	B	654	GLN
2	B	699	HIS
2	B	725	GLN
2	B	749	HIS
2	B	838	GLN
2	B	986	GLN
2	B	1007	ASN
2	B	1021	HIS
2	B	1030	ASN
2	B	1053	HIS
3	C	60	HIS
3	C	66	HIS
3	C	223	ASN
3	C	260	GLN
4	E	19	GLN
4	E	64	HIS
4	E	95	GLN
4	E	107	GLN
4	E	108	GLN
4	E	116	GLN
4	E	174	GLN
7	I	22	ASN
7	I	41	ASN
7	I	67	GLN
7	I	91	HIS
8	J	52	HIS
9	K	2	ASN
9	K	29	ASN
9	K	69	HIS
9	K	84	GLN
11	R	64	GLN
11	R	86	HIS

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Mol	Chain	Res	Type
11	R	142	GLN
11	R	174	GLN
11	R	177	HIS
11	R	199	HIS
11	R	203	GLN
12	D	34	ASN
12	D	89	GLN
13	G	60	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 5 ligands modelled in this entry, 5 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.

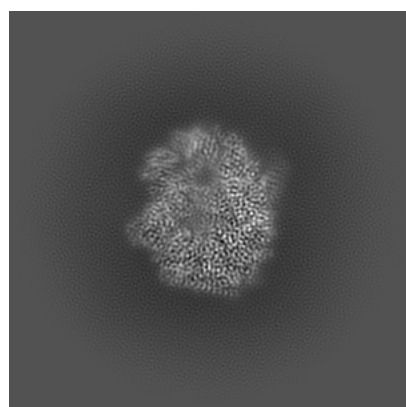
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31450. These allow visual inspection of the internal detail of the map and identification of artifacts.

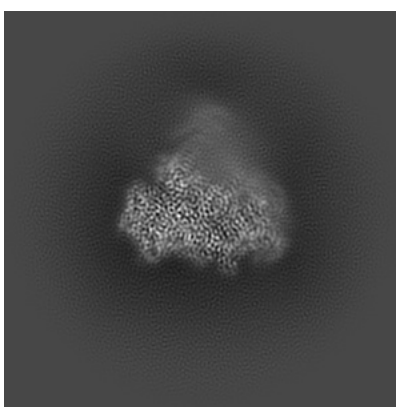
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

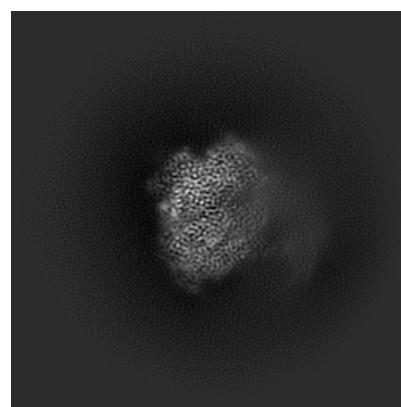
6.1.1 Primary map



X



Y

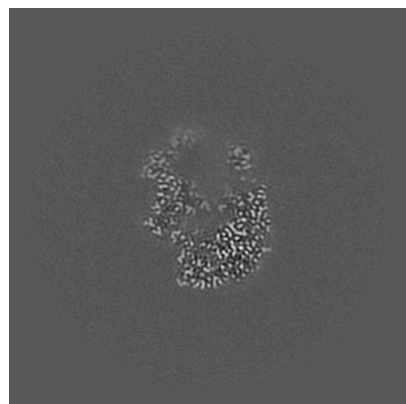


Z

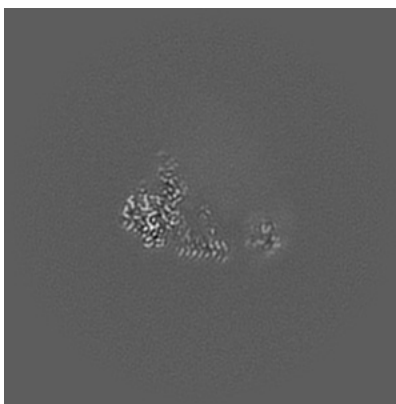
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

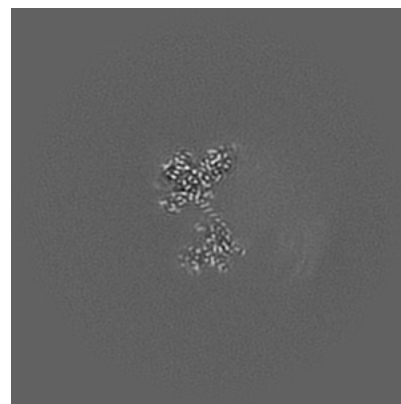
6.2.1 Primary map



X Index: 160



Y Index: 160

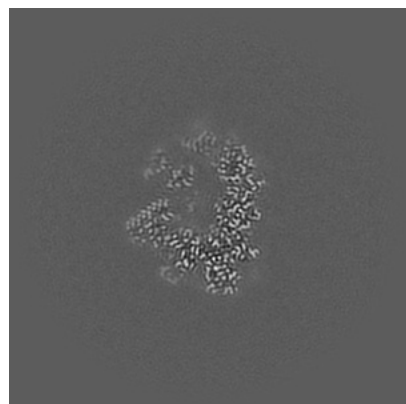


Z Index: 160

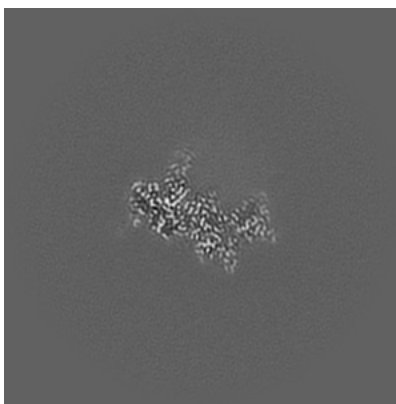
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

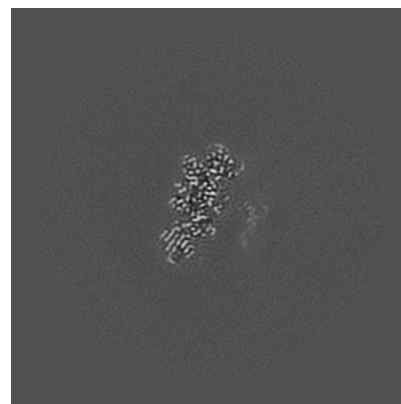
6.3.1 Primary map



X Index: 147



Y Index: 184

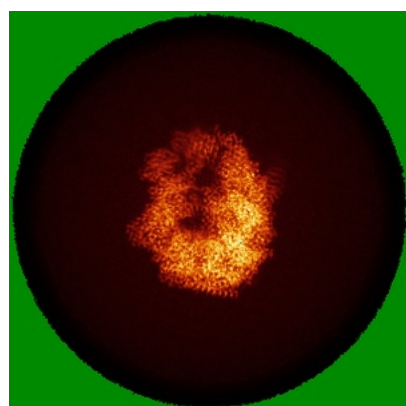


Z Index: 124

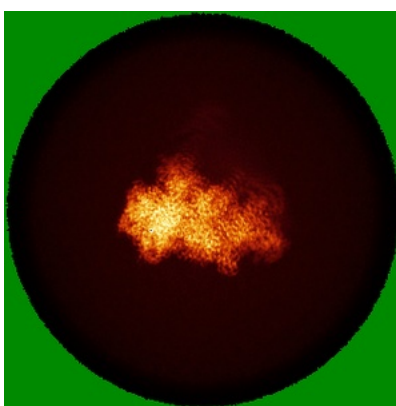
The images above show the largest variance slices of the map in three orthogonal directions.

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

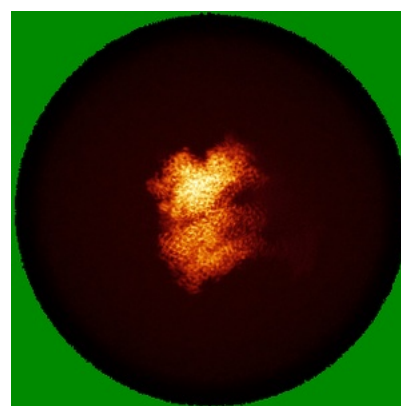
6.4.1 Primary map



X



Y

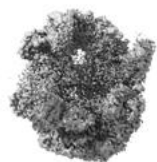


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

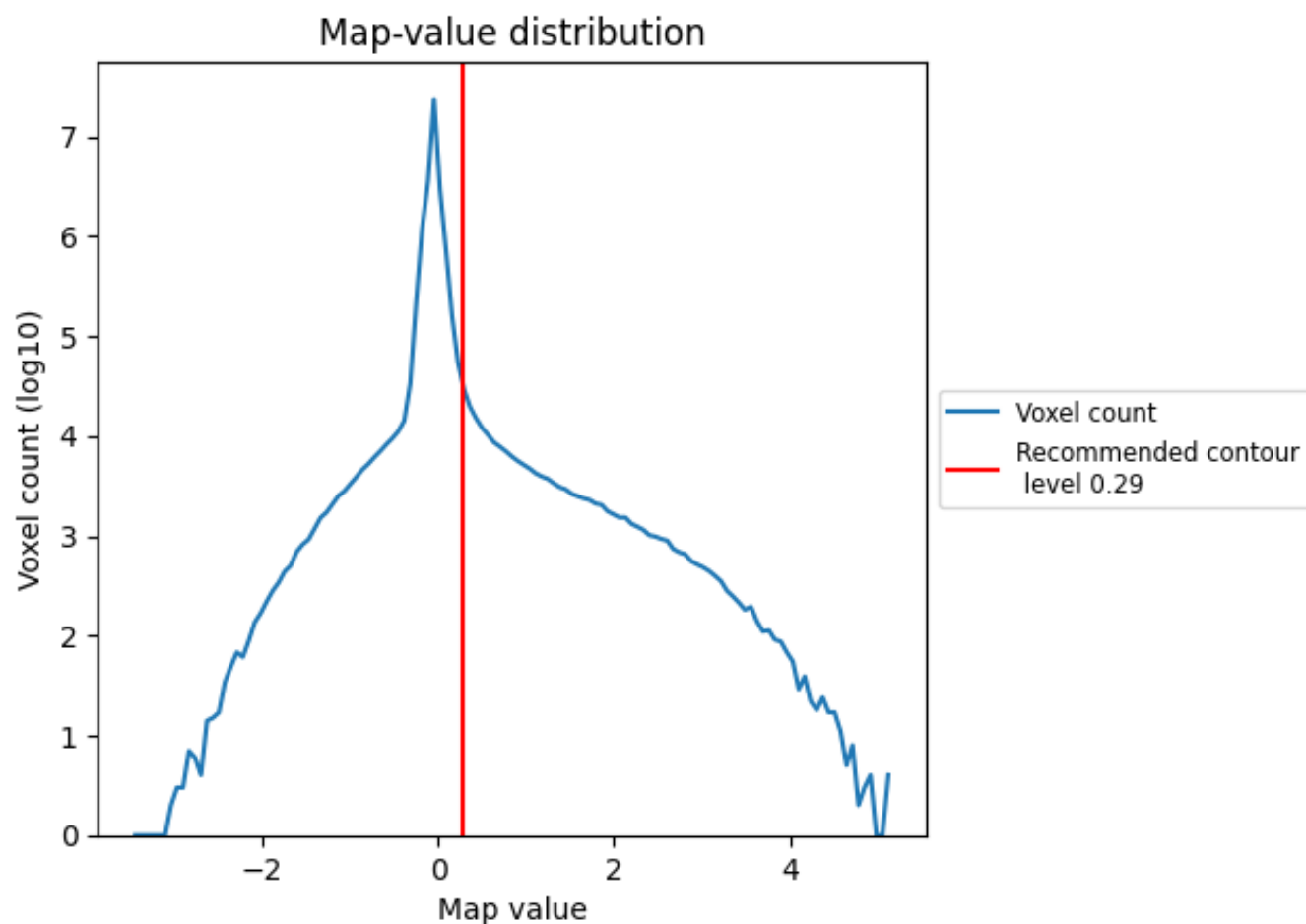
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

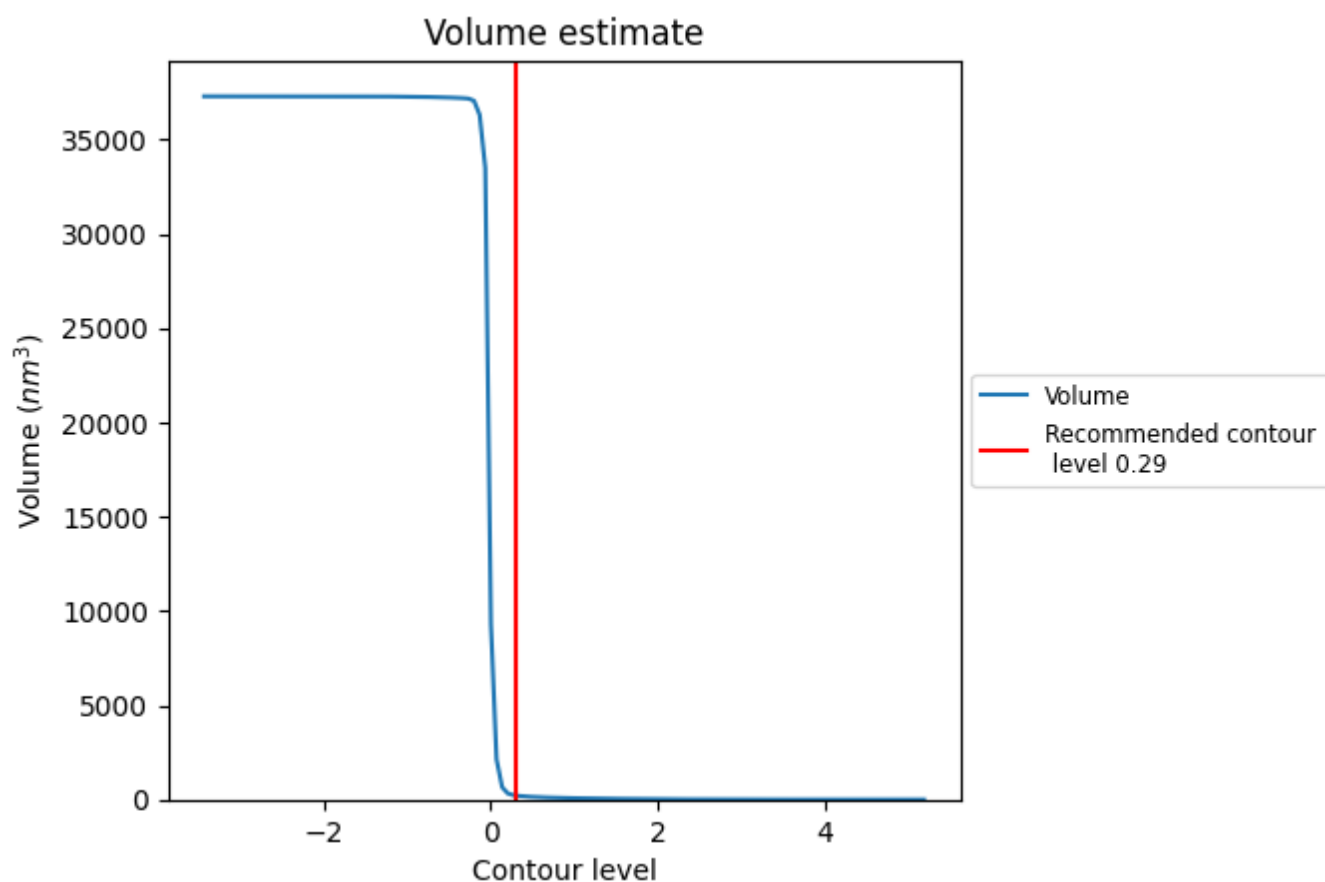
This section contains the results of statistical analysis of the map.

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.

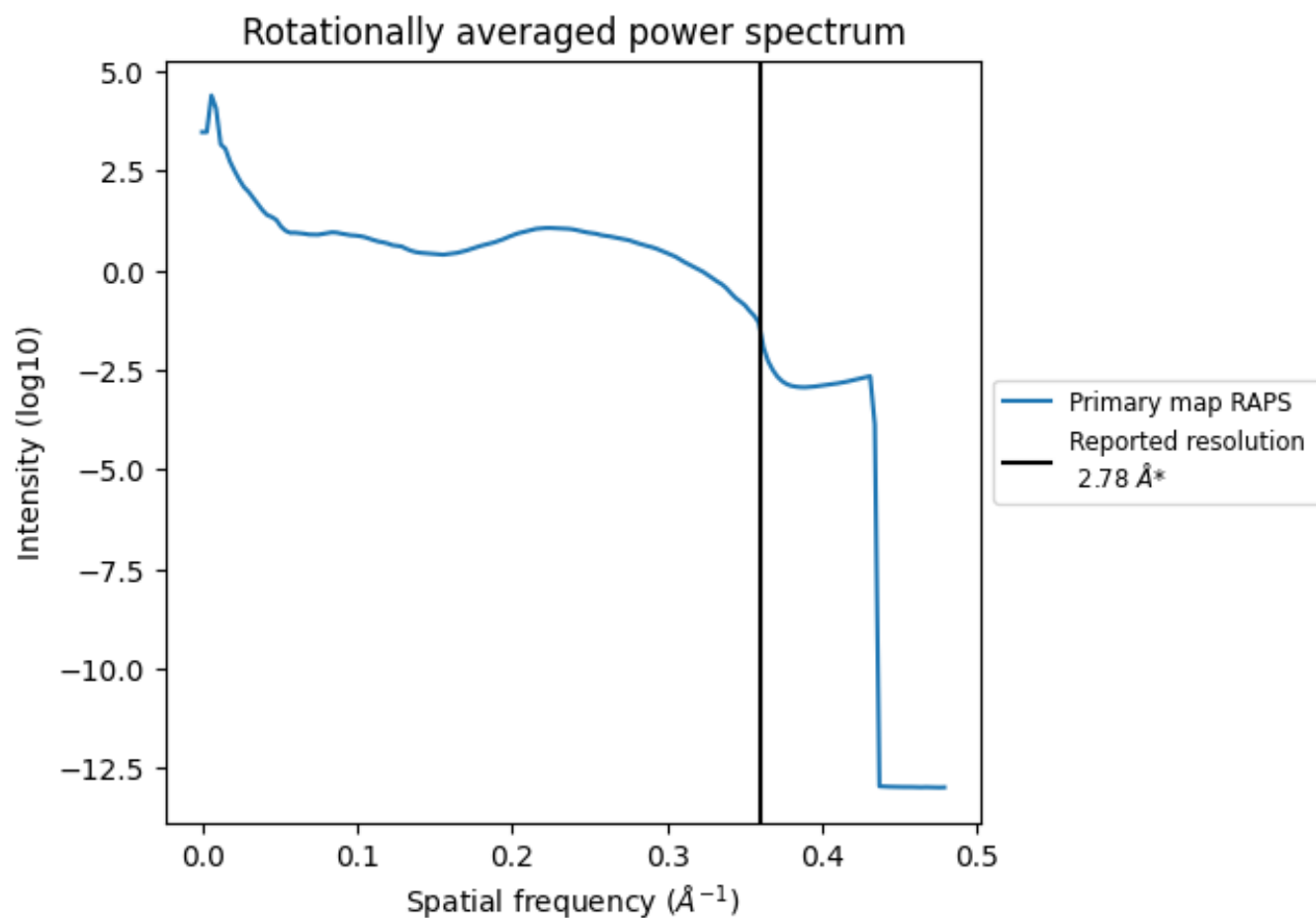
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm³; this corresponds to an approximate mass of 200 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 0.360 Å⁻¹

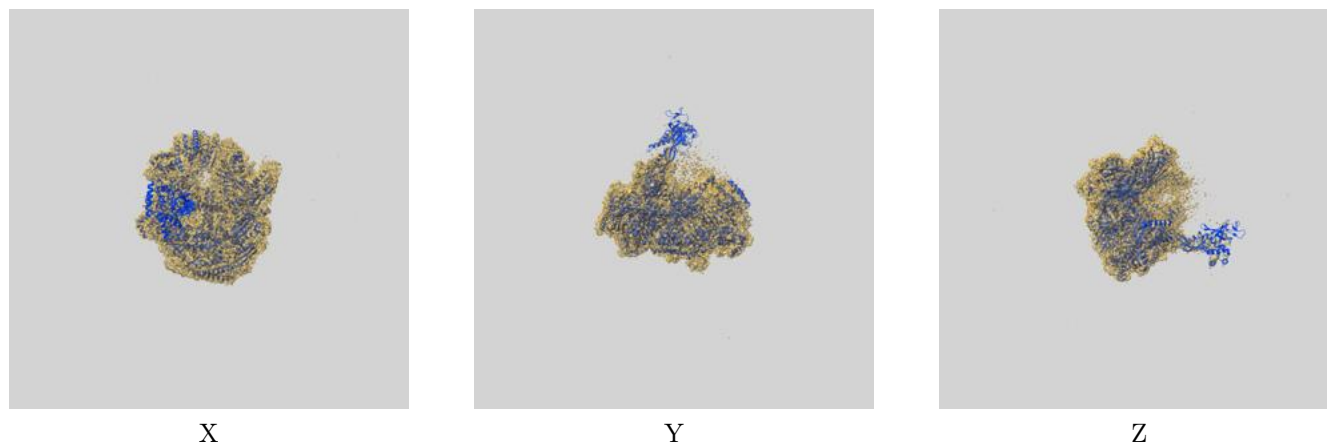
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

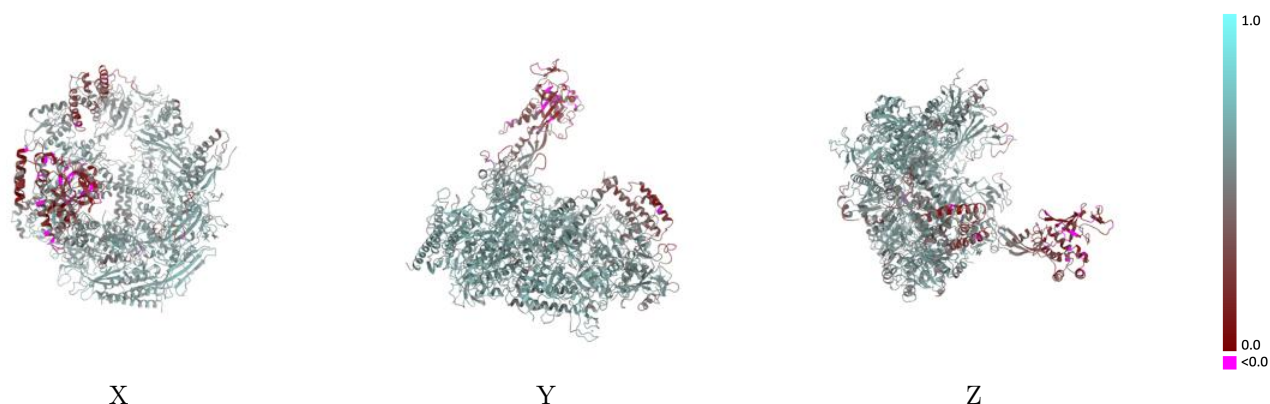
This section contains information regarding the fit between EMDB map EMD-31450 and PDB model 7F4G. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



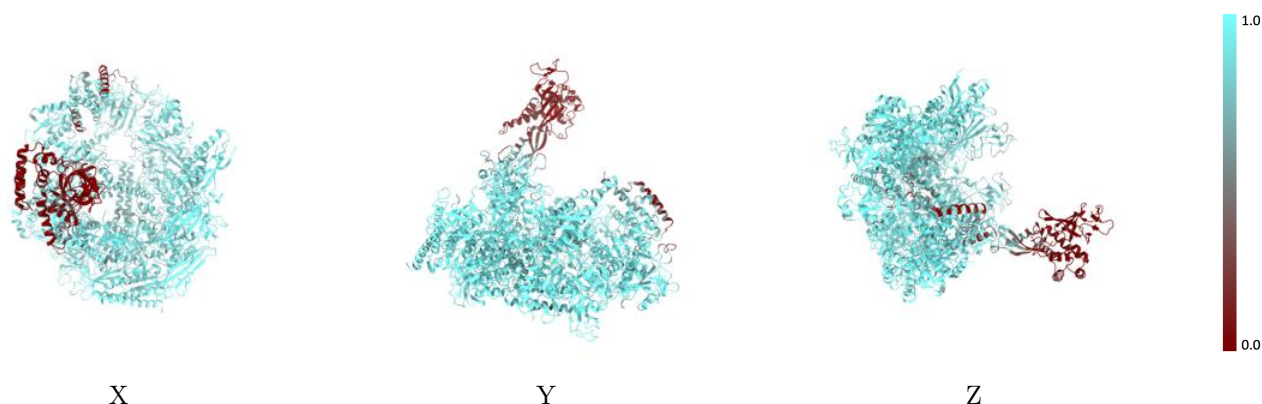
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



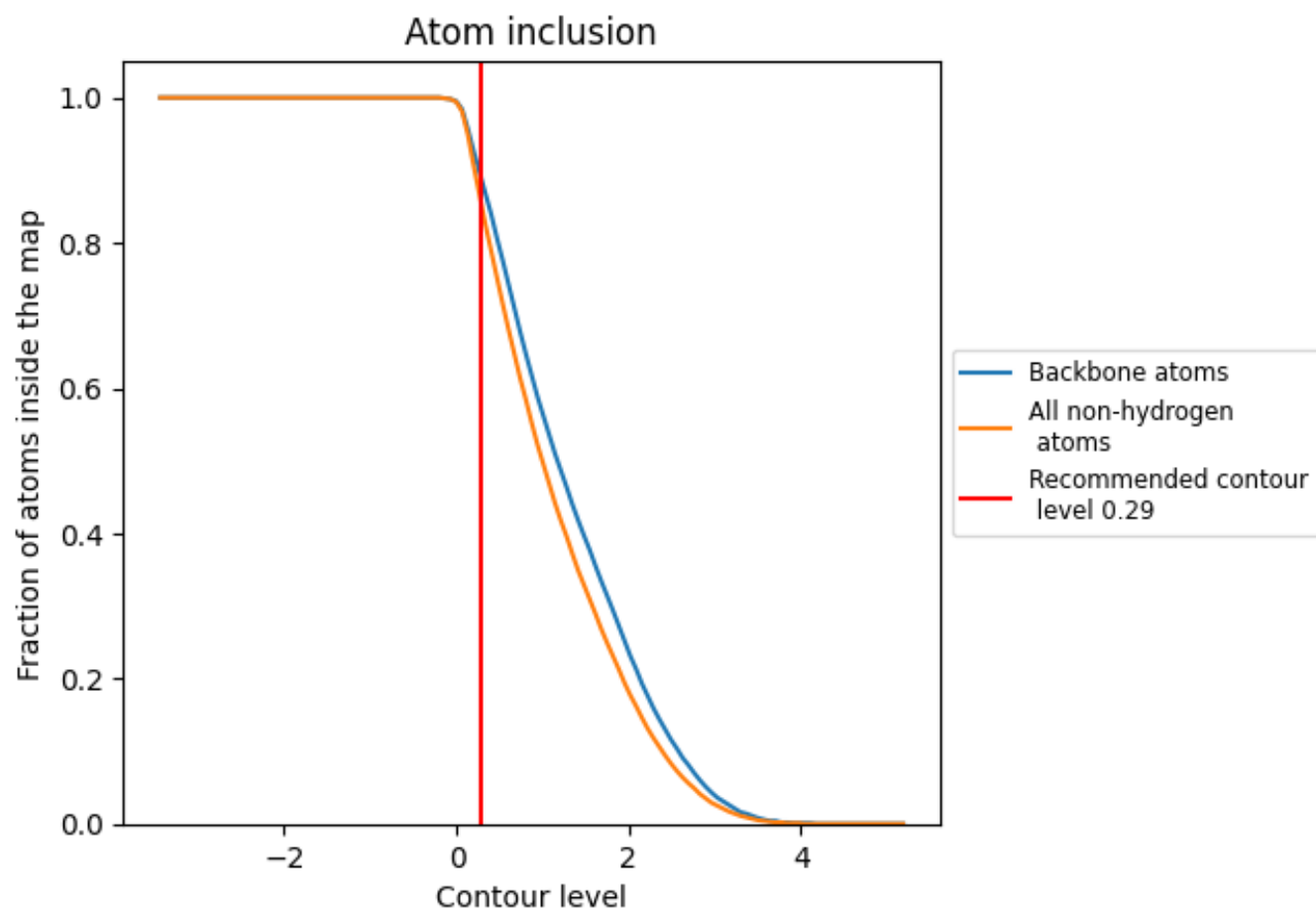
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.29).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8540	0.5300
A	0.9030	0.5520
B	0.9430	0.5780
C	0.9680	0.6000
D	0.0540	0.2140
E	0.9360	0.5480
F	0.8930	0.5370
G	0.2280	0.2600
H	0.9550	0.5770
I	0.9340	0.5550
J	0.9730	0.6190
K	0.9610	0.5930
L	0.9580	0.5510
R	0.6740	0.3370

