



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:33 AM UTC

PDB ID : 9KOX / pdb_00009kox
EMDB ID : EMD-62482
Title : human Hsp90-FKBP51-PINK1 complex
Authors : Tian, X.Y.; Su, J.Y.
Deposited on : 2024-11-21
Resolution : 4.43 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

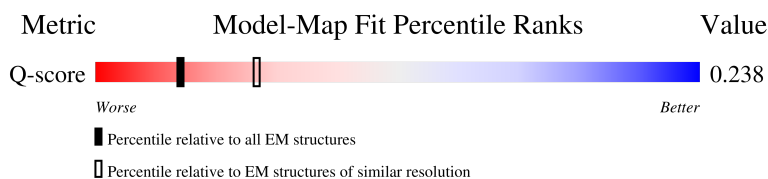
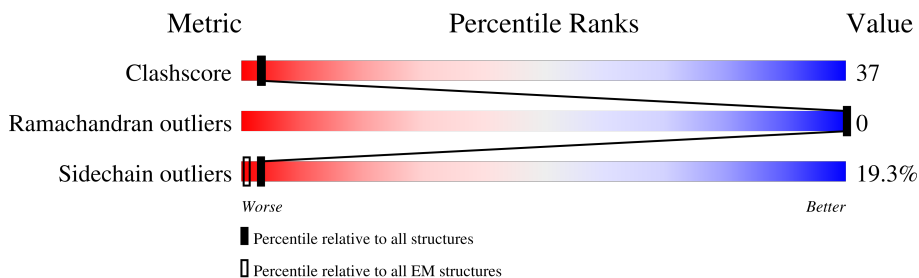
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.43 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	3083 (3.93 - 4.93)

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	D	457	
2	A	732	
2	B	732	
3	C	494	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16257 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 Peptidyl-prolyl cis-trans isomerase FKBP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	409	Total	C	N	O	S	0	0
			3229	2043	550	616	20		

- Molecule 2 is a protein called Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	635	Total	C	N	O	S	0	0
			5168	3278	870	997	23		
2	A	635	Total	C	N	O	S	0	0
			5168	3278	870	997	23		

- Molecule 3 is a protein called Serine/threonine-protein kinase PINK1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	343	Total	C	N	O	S	0	0
			2638	1688	461	470	19		

There are 22 discrepancies between the modelled and reference sequences:

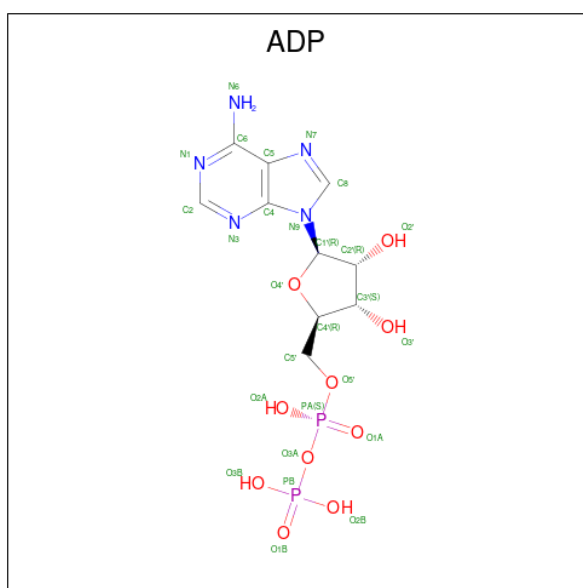
Chain	Residue	Modelled	Actual	Comment	Reference
C	582	ASP	-	expression tag	UNP Q9BXM7
C	583	TYR	-	expression tag	UNP Q9BXM7
C	584	LYS	-	expression tag	UNP Q9BXM7
C	585	ASP	-	expression tag	UNP Q9BXM7
C	586	HIS	-	expression tag	UNP Q9BXM7
C	587	ASP	-	expression tag	UNP Q9BXM7
C	588	GLY	-	expression tag	UNP Q9BXM7
C	589	GLY	-	expression tag	UNP Q9BXM7
C	590	TYR	-	expression tag	UNP Q9BXM7
C	591	LYS	-	expression tag	UNP Q9BXM7
C	592	ASP	-	expression tag	UNP Q9BXM7
C	593	HIS	-	expression tag	UNP Q9BXM7
C	594	ASP	-	expression tag	UNP Q9BXM7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	595	ILE	-	expression tag	UNP Q9BXM7
C	596	ASP	-	expression tag	UNP Q9BXM7
C	597	TYR	-	expression tag	UNP Q9BXM7
C	598	LYS	-	expression tag	UNP Q9BXM7
C	599	ASP	-	expression tag	UNP Q9BXM7
C	600	ASP	-	expression tag	UNP Q9BXM7
C	601	ASP	-	expression tag	UNP Q9BXM7
C	602	ASP	-	expression tag	UNP Q9BXM7
C	603	LYS	-	expression tag	UNP Q9BXM7

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

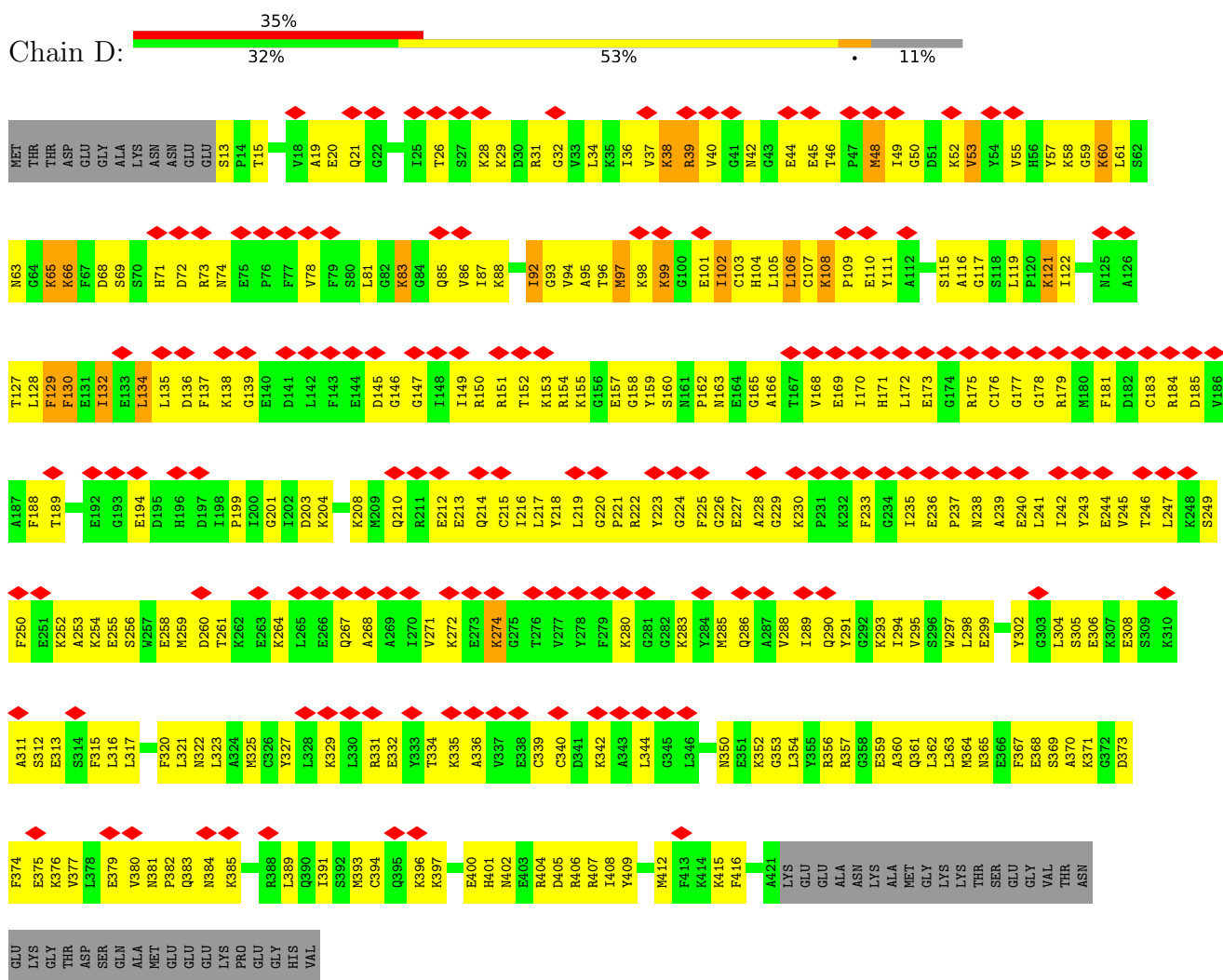


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

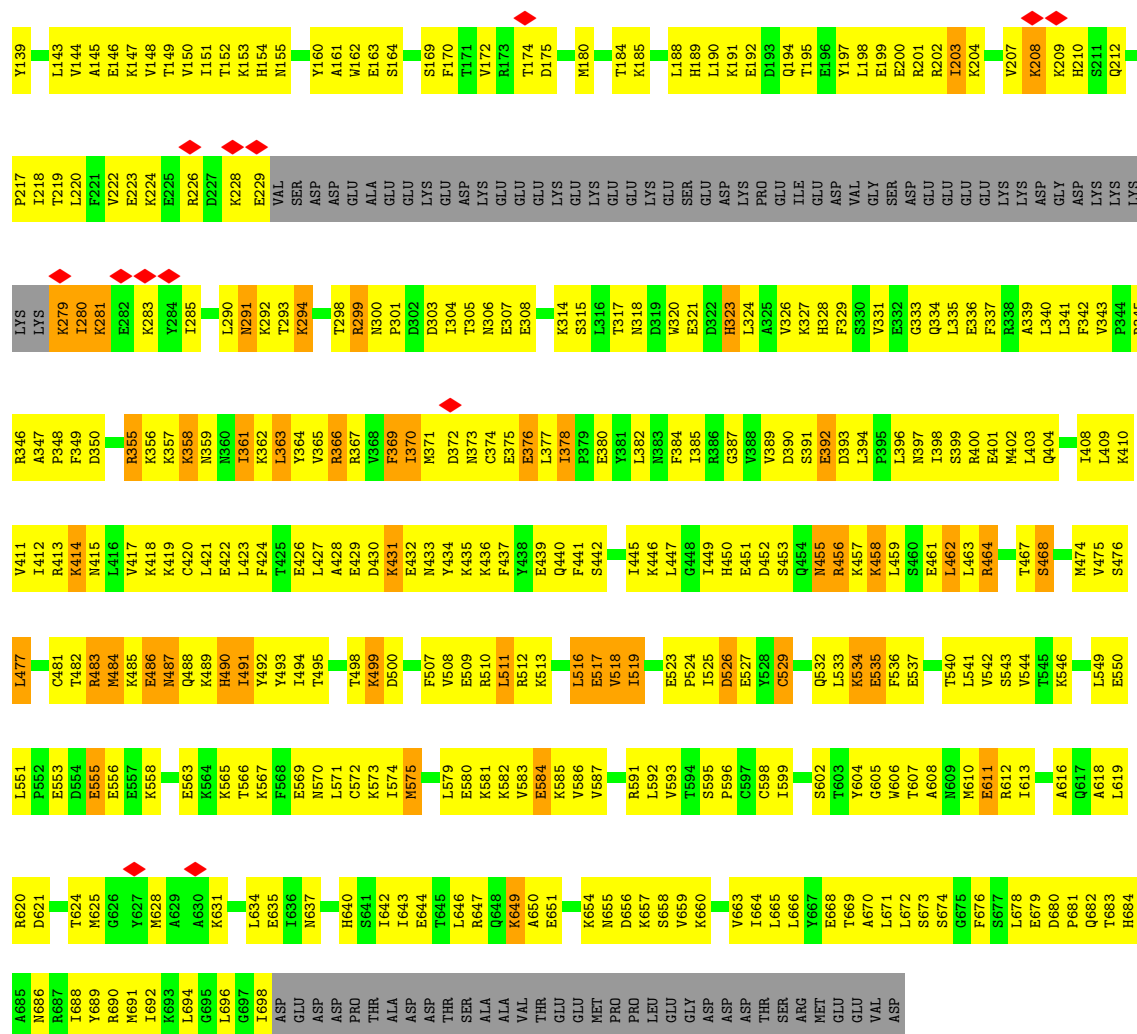
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP5

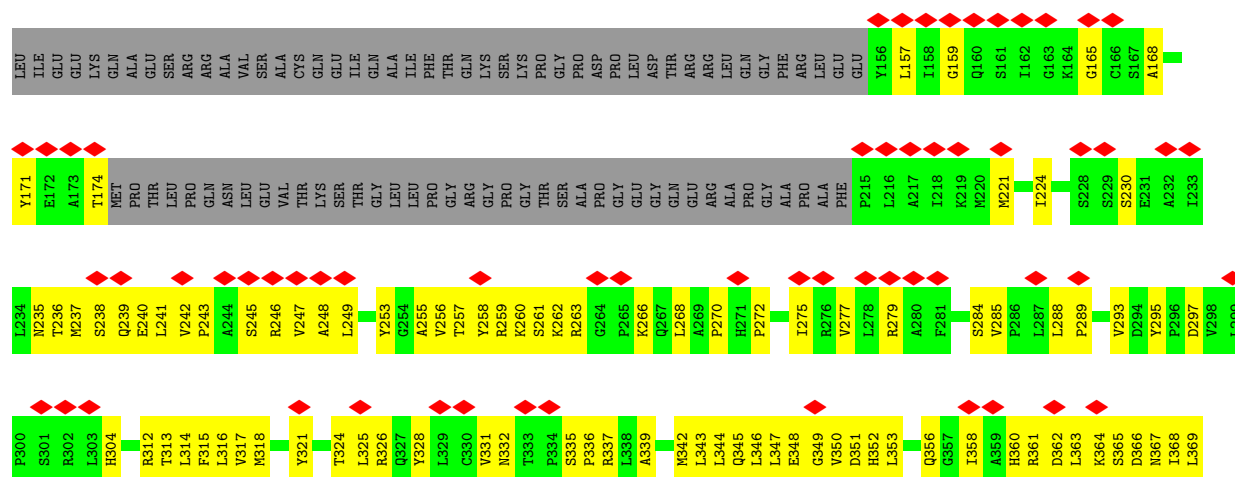


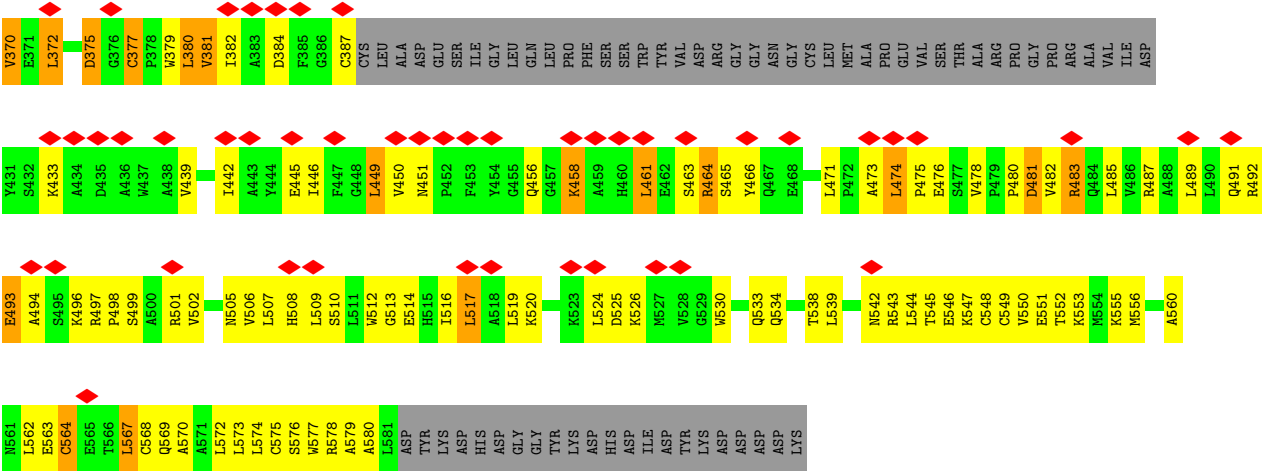
• Molecule 2: Heat shock protein HSP 90-alpha





• Molecule 3: Serine/threonine-protein kinase PINK1, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229994	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.252	Depositor
Minimum map value	-0.731	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.109	Depositor
Map size ($\text{\AA}$)	243.516, 243.516, 243.516	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8697, 0.8697, 0.8697	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: ADP

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	D	0.41	0/3287	0.74	0/4398
2	A	0.60	0/5251	0.85	0/7055
2	B	0.57	0/5251	0.79	0/7055
3	C	0.35	0/2693	0.66	0/3657
All	All	0.52	0/16482	0.78	0/22165

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3229	0	3219	258	0
2	A	5168	0	5221	348	0
2	B	5168	0	5221	454	0
3	C	2638	0	2713	181	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
All	All	16257	0	16398	1199	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 37.

All (1199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:CYS:SG	1:D:134:LEU:HD11	1.41	1.57
1:D:83:LYS:O	1:D:83:LYS:HD3	1.32	1.30
2:B:180:MET:CE	2:B:185:LYS:HE3	1.74	1.17
1:D:103:CYS:SG	1:D:134:LEU:CD1	2.34	1.16
2:B:151:ILE:HG12	2:B:161:ALA:CB	1.78	1.12
2:A:151:ILE:HG22	2:A:161:ALA:HB2	1.29	1.11
2:B:180:MET:HE1	2:B:185:LYS:CE	1.82	1.07
2:B:151:ILE:HG12	2:B:161:ALA:HB2	1.07	1.07
2:A:84:LYS:HZ3	2:A:224:LYS:HE3	1.17	1.05
1:D:48:MET:CG	1:D:138:LYS:HD3	1.88	1.04
2:A:151:ILE:HG22	2:A:161:ALA:CB	1.89	1.03
1:D:48:MET:HG2	1:D:138:LYS:HD3	1.04	1.02
3:C:516:ILE:HG23	3:C:519:LEU:H	1.22	1.00
1:D:83:LYS:HD3	1:D:83:LYS:C	1.85	0.99
1:D:48:MET:HG2	1:D:138:LYS:CD	1.94	0.96
2:B:337:PHE:HB3	2:B:391:SER:HB2	1.45	0.96
2:B:151:ILE:CG1	2:B:161:ALA:HB2	1.95	0.96
2:A:180:MET:HE1	2:A:185:LYS:HD3	1.45	0.96
2:B:180:MET:HE1	2:B:185:LYS:HE3	0.95	0.95
2:B:160:TYR:HA	2:B:174:THR:HG21	1.48	0.94
2:A:128:ILE:HG22	2:A:130:MET:HG2	1.48	0.94
1:D:103:CYS:HB2	1:D:134:LEU:HD21	1.50	0.94
2:A:329:PHE:HB2	2:A:339:ALA:HB3	1.48	0.93
2:B:329:PHE:HB2	2:B:339:ALA:HB3	1.49	0.92
1:D:97:MET:SD	1:D:134:LEU:HD22	2.08	0.92
1:D:171:HIS:HB2	1:D:246:THR:HB	1.53	0.90
2:B:150:VAL:CG2	2:B:186:VAL:HG22	2.00	0.90
1:D:285:MET:SD	1:D:331:ARG:NH2	2.46	0.89
2:B:491:ILE:HB	2:B:541:LEU:HA	1.52	0.88
1:D:152:THR:HA	1:D:215:CYS:HA	1.53	0.88
2:A:331:VAL:HB	2:A:337:PHE:H	1.39	0.88
2:B:331:VAL:HB	2:B:337:PHE:H	1.39	0.88
2:B:58:LYS:HZ3	2:B:118:PHE:HB3	1.39	0.86
2:A:58:LYS:HZ3	2:A:118:PHE:HB3	1.40	0.85
2:A:128:ILE:CG2	2:A:130:MET:HG2	2.05	0.85
2:B:413:ARG:HA	2:B:416:LEU:HD12	1.57	0.85
2:B:433:ASN:HA	2:B:436:LYS:HE2	1.61	0.83
3:C:550:VAL:HA	3:C:553:LYS:HG2	1.60	0.83
1:D:103:CYS:HG	1:D:134:LEU:HD11	1.38	0.83
2:A:433:ASN:HA	2:A:436:LYS:HE2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLU:HG3	1:D:159:TYR:H	1.44	0.81
2:B:360:ASN:HB3	2:B:386:ARG:HG2	1.63	0.81
1:D:175:ARG:HE	1:D:178:GLY:HA2	1.45	0.80
3:C:353:LEU:HA	3:C:356:GLN:HE21	1.48	0.79
2:A:84:LYS:NZ	2:A:224:LYS:HE3	1.96	0.79
3:C:549:CYS:SG	3:C:553:LYS:NZ	2.55	0.79
3:C:542:ASN:HA	3:C:546:GLU:HG3	1.65	0.78
2:B:87:ARG:HH12	2:B:192:GLU:HG3	1.46	0.78
2:B:308:GLU:N	2:B:308:GLU:OE1	2.17	0.78
2:A:31:SER:HA	2:A:34:ILE:HD12	1.66	0.78
3:C:574:LEU:HG	3:C:577:TRP:CZ2	2.18	0.78
3:C:577:TRP:HB2	3:C:578:ARG:HD3	1.66	0.78
2:B:31:SER:HA	2:B:34:ILE:HD12	1.66	0.78
3:C:562:LEU:HD22	3:C:567:LEU:HD11	1.66	0.78
1:D:219:LEU:HB2	1:D:241:LEU:HB2	1.66	0.78
2:B:689:TYR:HA	2:B:692:ILE:HD12	1.65	0.78
2:B:465:TYR:H	2:B:475:VAL:H	1.32	0.77
2:A:468:SER:HB3	2:A:518:VAL:H	1.50	0.77
2:B:21:ALA:HA	2:A:169:SER:HA	1.66	0.77
2:B:561:GLN:HA	2:B:564:LYS:HD2	1.66	0.77
1:D:28:LYS:HG2	1:D:29:LYS:H	1.48	0.77
2:B:560:LYS:HG3	2:B:564:LYS:HE3	1.67	0.77
2:A:689:TYR:HA	2:A:692:ILE:HD12	1.65	0.76
3:C:165:GLY:HA3	3:C:168:ALA:HB3	1.67	0.75
2:B:208:LYS:HA	2:B:212:GLN:HB3	1.69	0.75
2:B:131:ILE:HA	2:B:366:ARG:HG2	1.69	0.74
3:C:574:LEU:HB3	3:C:578:ARG:HH22	1.49	0.74
2:B:101:ALA:HA	2:B:104:ILE:HD12	1.70	0.74
3:C:325:LEU:HD11	3:C:368:ILE:HB	1.70	0.74
2:A:396:LEU:HB3	2:A:400:ARG:HG3	1.69	0.74
1:D:154:ARG:HB3	1:D:213:GLU:HA	1.70	0.73
2:A:101:ALA:HA	2:A:104:ILE:HD12	1.70	0.73
2:B:512:ARG:NH2	2:B:520:TYR:OH	2.20	0.73
3:C:324:THR:HA	3:C:370:VAL:H	1.54	0.73
1:D:221:PRO:HA	1:D:226:GLY:HA3	1.71	0.73
3:C:241:LEU:HD13	3:C:249:LEU:HD21	1.69	0.73
1:D:83:LYS:O	1:D:83:LYS:CD	2.26	0.72
2:B:511:LEU:HD11	2:B:544:VAL:HG11	1.70	0.72
2:A:76:LEU:O	2:A:217:PRO:HG2	1.89	0.72
2:B:151:ILE:CG1	2:B:161:ALA:CB	2.60	0.72
1:D:97:MET:SD	1:D:134:LEU:CD2	2.77	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LEU:HD13	1:D:320:PHE:HD2	1.55	0.72
3:C:577:TRP:HB2	3:C:578:ARG:HH11	1.55	0.72
3:C:336:PRO:HB2	3:C:337:ARG:HH12	1.54	0.72
3:C:545:THR:HA	3:C:547:LYS:HE2	1.72	0.71
2:B:362:LYS:HB2	2:B:388:VAL:HG22	1.72	0.71
1:D:264:LYS:HZ2	1:D:297:TRP:CG	2.07	0.71
1:D:83:LYS:C	1:D:83:LYS:CD	2.63	0.71
1:D:339:CYS:HA	1:D:342:LYS:HE2	1.71	0.71
2:A:337:PHE:HB3	2:A:391:SER:HB2	1.71	0.71
3:C:501:ARG:HH22	3:C:562:LEU:HD23	1.55	0.71
1:D:48:MET:HE3	1:D:138:LYS:HB2	1.73	0.70
1:D:298:LEU:HD22	1:D:316:LEU:HB2	1.71	0.70
2:B:150:VAL:HG21	2:B:186:VAL:HG22	1.73	0.70
2:A:98:MET:HG3	2:A:103:LEU:HA	1.73	0.70
2:B:663:VAL:HA	2:B:666:LEU:HD12	1.72	0.70
2:A:397:ASN:H	2:A:400:ARG:HA	1.56	0.70
3:C:242:VAL:HA	3:C:266:LYS:HB3	1.73	0.70
3:C:253:TYR:CG	3:C:258:TYR:HA	2.26	0.70
1:D:255:GLU:H	1:D:258:GLU:HB2	1.55	0.70
2:B:348:PRO:HD3	2:B:441:PHE:CZ	2.27	0.70
2:B:397:ASN:H	2:B:400:ARG:HA	1.57	0.70
2:A:146:GLU:N	2:A:189:HIS:O	2.22	0.70
2:A:92:VAL:HG13	2:A:185:LYS:HB3	1.73	0.70
2:A:329:PHE:N	2:A:339:ALA:O	2.23	0.70
1:D:255:GLU:CD	1:D:256:SER:H	2.00	0.70
3:C:576:SER:HA	3:C:579:ALA:HB3	1.74	0.70
2:B:89:LEU:HD12	2:B:188:LEU:HD22	1.74	0.69
2:B:364:TYR:HB2	2:B:390:ASP:HB2	1.74	0.69
1:D:199:PRO:HA	1:D:225:PHE:H	1.56	0.69
2:B:30:MET:HA	2:B:33:ILE:HD12	1.72	0.69
2:B:690:ARG:HH11	2:B:691:MET:HG3	1.57	0.69
3:C:530:TRP:O	3:C:534:GLN:N	2.21	0.69
2:B:56:LEU:HD13	2:B:59:ILE:HD11	1.74	0.69
2:A:690:ARG:HH11	2:A:691:MET:HG3	1.57	0.69
2:A:30:MET:HA	2:A:33:ILE:HD12	1.72	0.69
3:C:544:LEU:HG	3:C:545:THR:HG23	1.72	0.69
2:B:87:ARG:NH2	2:B:192:GLU:OE2	2.24	0.69
3:C:336:PRO:HB2	3:C:337:ARG:NH1	2.06	0.69
2:B:173:ARG:HB2	2:A:17:VAL:HG12	1.74	0.69
1:D:53:VAL:HG13	1:D:136:ASP:O	1.94	0.69
2:A:535:GLU:HA	2:A:540:THR:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ILE:HA	2:B:161:ALA:HA	1.75	0.68
1:D:166:ALA:HB2	1:D:253:ALA:H	1.58	0.68
2:B:682:GLN:N	2:B:682:GLN:OE1	2.27	0.68
2:A:56:LEU:HD13	2:A:59:ILE:HD11	1.75	0.68
2:A:402:MET:HG3	2:A:403:LEU:N	2.09	0.68
2:A:682:GLN:OE1	2:A:682:GLN:N	2.27	0.68
1:D:154:ARG:HB3	1:D:214:GLN:H	1.57	0.68
1:D:409:TYR:HB3	1:D:412:MET:HE2	1.76	0.68
1:D:146:GLY:HA3	1:D:222:ARG:HH12	1.58	0.68
2:B:226:ARG:HB2	2:B:228:LYS:HG3	1.76	0.68
2:A:226:ARG:HB2	2:A:228:LYS:HG3	1.76	0.68
2:B:148:VAL:N	2:B:164:SER:O	2.24	0.68
1:D:103:CYS:CB	1:D:134:LEU:HD21	2.23	0.68
2:B:146:GLU:N	2:B:189:HIS:O	2.22	0.68
2:B:336:GLU:N	2:B:336:GLU:OE1	2.27	0.68
2:A:151:ILE:HA	2:A:161:ALA:HA	1.76	0.68
1:D:34:LEU:HG	1:D:36:ILE:HG12	1.76	0.67
1:D:199:PRO:HG2	1:D:243:TYR:CE1	2.29	0.67
1:D:405:ASP:HA	1:D:408:ILE:HG12	1.75	0.67
2:B:366:ARG:H	2:B:392:GLU:HA	1.58	0.67
3:C:342:MET:SD	3:C:345:GLN:NE2	2.67	0.67
2:A:596:PRO:HA	2:A:637:ASN:HB3	1.76	0.67
1:D:290:GLN:O	1:D:293:LYS:HG2	1.94	0.67
2:B:445:ILE:O	2:B:449:ILE:HG12	1.93	0.67
2:B:172:VAL:O	2:A:17:VAL:HA	1.94	0.67
2:A:145:ALA:HB2	2:A:188:LEU:HG	1.77	0.67
2:A:445:ILE:O	2:A:449:ILE:HG12	1.93	0.67
2:B:98:MET:HG3	2:B:103:LEU:HA	1.77	0.67
2:A:148:VAL:N	2:A:164:SER:O	2.24	0.67
2:A:602:SER:HB2	2:A:631:LYS:HB3	1.76	0.67
2:A:660:LYS:O	2:A:664:ILE:HG13	1.94	0.67
3:C:516:ILE:CG2	3:C:519:LEU:H	2.04	0.67
1:D:108:LYS:H	1:D:127:THR:HG22	1.60	0.67
2:B:145:ALA:HB2	2:B:188:LEU:HG	1.77	0.67
2:A:336:GLU:N	2:A:336:GLU:OE1	2.27	0.67
1:D:268:ALA:HA	1:D:297:TRP:HZ3	1.61	0.66
2:B:402:MET:HG3	2:B:403:LEU:N	2.10	0.66
2:B:450:HIS:NE2	2:B:451:GLU:OE2	2.28	0.66
2:A:450:HIS:NE2	2:A:451:GLU:OE2	2.28	0.66
2:A:596:PRO:O	2:A:637:ASN:N	2.28	0.66
1:D:170:ILE:HA	1:D:247:LEU:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:512:TRP:HB3	3:C:538:THR:HG22	1.77	0.66
3:C:259:ARG:HA	3:C:262:LYS:HB3	1.77	0.66
2:B:169:SER:HA	2:A:21:ALA:HA	1.77	0.66
2:A:103:LEU:HA	2:A:106:ASN:HD21	1.61	0.66
1:D:101:GLU:HB3	1:D:134:LEU:HD12	1.77	0.66
2:B:396:LEU:HB3	2:B:400:ARG:HG3	1.78	0.66
1:D:368:GLU:N	1:D:368:GLU:OE1	2.28	0.66
3:C:505:ASN:O	3:C:509:LEU:HG	1.94	0.66
2:B:547:GLU:HG2	2:B:633:HIS:NE2	2.11	0.65
2:B:449:ILE:HG23	2:B:459:LEU:HB3	1.79	0.65
2:B:391:SER:HB3	2:B:394:LEU:HD21	1.78	0.65
2:B:396:LEU:O	2:B:404:GLN:NE2	2.29	0.65
2:A:574:ILE:HG21	2:A:650:ALA:HB1	1.78	0.65
2:B:171:THR:OG1	2:B:172:VAL:N	2.29	0.65
2:B:396:LEU:N	2:B:404:GLN:HE22	1.93	0.65
2:A:328:HIS:CG	2:A:340:LEU:HD13	2.32	0.65
3:C:530:TRP:HB3	3:C:534:GLN:HE21	1.61	0.65
2:B:329:PHE:N	2:B:339:ALA:O	2.23	0.64
2:B:493:TYR:HB3	2:B:519:ILE:HG23	1.79	0.64
2:B:525:ILE:HG23	2:A:618:ALA:HB1	1.79	0.64
2:B:596:PRO:HA	2:B:637:ASN:HB3	1.78	0.64
2:B:598:CYS:SG	2:B:599:ILE:N	2.70	0.64
2:A:363:LEU:HD23	2:A:389:VAL:HG13	1.79	0.64
2:B:534:LYS:HA	2:B:541:LEU:HD22	1.78	0.64
1:D:150:ARG:NH2	1:D:213:GLU:OE2	2.31	0.64
3:C:268:LEU:HD11	3:C:304:HIS:HE1	1.61	0.64
2:B:304:ILE:HB	2:B:308:GLU:HG2	1.78	0.64
2:B:314:LYS:NZ	2:B:320:TRP:O	2.31	0.64
2:B:440:GLN:HG3	2:B:441:PHE:HD1	1.63	0.64
2:B:328:HIS:CG	2:B:340:LEU:HD13	2.32	0.64
2:B:449:ILE:HD12	2:B:459:LEU:HB3	1.79	0.64
2:A:440:GLN:HG3	2:A:441:PHE:HD1	1.63	0.64
2:A:450:HIS:CE1	2:A:451:GLU:HG2	2.33	0.64
2:A:598:CYS:SG	2:A:599:ILE:N	2.70	0.64
1:D:36:ILE:HD11	1:D:106:LEU:HB2	1.80	0.63
3:C:343:LEU:HD12	3:C:346:LEU:HD12	1.81	0.63
1:D:177:GLY:O	1:D:179:ARG:NH1	2.32	0.63
2:B:450:HIS:CE1	2:B:451:GLU:HG2	2.33	0.63
2:B:571:LEU:HD13	2:B:647:ARG:HA	1.78	0.63
2:A:491:ILE:HG23	2:A:541:LEU:HA	1.80	0.63
3:C:574:LEU:O	3:C:578:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:VAL:HG13	2:B:185:LYS:HB3	1.79	0.63
2:B:364:TYR:CE1	2:B:369:PHE:HA	2.33	0.63
2:B:450:HIS:HB2	2:B:532:GLN:HG3	1.80	0.63
3:C:239:GLN:HA	3:C:242:VAL:HG23	1.79	0.63
2:B:696:LEU:HD11	2:A:642:ILE:HG12	1.80	0.63
1:D:360:ALA:O	1:D:364:MET:N	2.25	0.63
1:D:255:GLU:N	1:D:258:GLU:HB2	2.14	0.63
2:B:508:VAL:HA	2:B:511:LEU:HD12	1.81	0.63
2:B:116:LYS:HG3	2:B:133:GLN:HB2	1.81	0.62
3:C:347:LEU:O	3:C:351:ASP:N	2.23	0.62
1:D:373:ASP:HA	1:D:376:LYS:HE3	1.80	0.62
2:A:418:LYS:HE3	2:A:419:LYS:NZ	2.14	0.62
2:A:346:ARG:NH2	2:A:347:ALA:O	2.33	0.62
2:A:359:ASN:HA	2:A:373:ASN:HB3	1.81	0.62
1:D:97:MET:HG3	1:D:134:LEU:HD13	1.81	0.62
3:C:514:GLU:O	3:C:519:LEU:CD2	2.47	0.62
2:B:583:VAL:HG23	2:B:633:HIS:HA	1.82	0.62
2:A:430:ASP:OD2	2:A:433:ASN:N	2.33	0.62
2:A:447:LEU:O	2:A:450:HIS:ND1	2.33	0.62
1:D:101:GLU:HG2	1:D:102:ILE:H	1.64	0.62
1:D:171:HIS:N	1:D:246:THR:O	2.22	0.62
2:B:397:ASN:HB2	2:B:400:ARG:H	1.65	0.62
2:B:447:LEU:O	2:B:450:HIS:ND1	2.33	0.62
2:B:363:LEU:H	2:B:372:ASP:CG	2.07	0.62
2:B:665:LEU:HD21	2:B:687:ARG:HG2	1.82	0.61
2:B:430:ASP:OD2	2:B:433:ASN:N	2.33	0.61
2:A:204:LYS:HG3	2:A:290:LEU:HD21	1.82	0.61
1:D:304:LEU:HG	1:D:305:SER:N	2.16	0.61
2:B:418:LYS:HE3	2:B:419:LYS:NZ	2.14	0.61
2:A:150:VAL:HG23	2:A:185:LYS:O	2.01	0.61
2:A:291:ASN:C	2:A:293:THR:H	2.07	0.61
2:A:396:LEU:N	2:A:404:GLN:HE22	1.97	0.61
3:C:516:ILE:HG23	3:C:519:LEU:N	2.05	0.61
2:B:346:ARG:NH2	2:B:347:ALA:O	2.33	0.61
3:C:268:LEU:HG	3:C:270:PRO:HD3	1.82	0.61
3:C:498:PRO:HB2	3:C:502:VAL:HB	1.81	0.61
2:B:432:GLU:O	2:B:435:LYS:HG2	2.00	0.61
2:A:402:MET:HG3	2:A:403:LEU:H	1.65	0.61
1:D:99:LYS:HB2	1:D:136:ASP:HA	1.83	0.61
2:A:432:GLU:O	2:A:435:LYS:HG2	2.00	0.61
1:D:291:TYR:HA	1:D:294:ILE:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:291:ASN:HD22	2:A:291:ASN:H	1.49	0.61
3:C:312:ARG:HH22	3:C:314:LEU:HD12	1.65	0.61
2:B:367:ARG:N	2:B:392:GLU:OE2	2.34	0.60
2:B:467:THR:OG1	2:B:470:SER:N	2.26	0.60
3:C:508:HIS:HA	3:C:512:TRP:HE3	1.66	0.60
1:D:57:TYR:HB2	1:D:130:PHE:HB2	1.82	0.60
2:A:34:ILE:HG23	2:A:143:LEU:HD12	1.81	0.60
2:A:397:ASN:HB2	2:A:400:ARG:H	1.65	0.60
2:A:571:LEU:HA	2:A:574:ILE:HD12	1.83	0.60
3:C:347:LEU:HA	3:C:350:VAL:HB	1.83	0.60
1:D:194:GLU:OE2	1:D:286:GLN:N	2.35	0.60
2:B:150:VAL:HG13	2:B:162:TRP:HB3	1.82	0.60
2:B:341:LEU:HD23	2:B:387:GLY:HA3	1.83	0.60
3:C:253:TYR:OH	3:C:261:SER:HB2	2.02	0.60
2:B:297:TRP:CZ2	2:B:364:TYR:HD2	2.19	0.60
3:C:449:LEU:HG	3:C:473:ALA:HA	1.83	0.60
1:D:294:ILE:HA	1:D:297:TRP:CD2	2.37	0.60
1:D:370:ALA:O	1:D:374:PHE:HB2	2.00	0.60
3:C:344:LEU:HD12	3:C:347:LEU:HD11	1.82	0.60
3:C:353:LEU:HB2	3:C:358:ILE:HD11	1.84	0.60
1:D:151:ARG:O	1:D:216:ILE:N	2.35	0.60
2:B:467:THR:O	2:B:471:GLY:N	2.28	0.60
2:A:83:ASN:ND2	2:A:88:THR:OG1	2.29	0.60
1:D:226:GLY:O	1:D:238:ASN:ND2	2.35	0.60
1:D:327:TYR:HD1	1:D:331:ARG:HG3	1.65	0.60
1:D:361:GLN:HA	1:D:364:MET:HE3	1.82	0.60
2:B:210:HIS:HB3	2:B:369:PHE:CD2	2.36	0.60
2:A:640:HIS:HB3	2:A:643:ILE:HG12	1.84	0.60
3:C:256:VAL:HG13	3:C:260:LYS:HD2	1.84	0.60
2:B:365:VAL:O	2:B:368:VAL:HG12	2.02	0.59
3:C:534:GLN:O	3:C:538:THR:HG23	2.02	0.59
2:B:656:ASP:HB3	2:B:659:VAL:HG22	1.84	0.59
2:A:450:HIS:HB2	2:A:532:GLN:HG3	1.84	0.59
3:C:243:PRO:HB2	3:C:277:VAL:O	2.02	0.59
2:B:402:MET:HG3	2:B:403:LEU:H	1.66	0.59
2:B:408:ILE:O	2:B:412:ILE:HG23	2.02	0.59
1:D:225:PHE:HD1	1:D:228:ALA:HB3	1.67	0.59
3:C:325:LEU:HD23	3:C:370:VAL:HG23	1.83	0.59
1:D:28:LYS:HG2	1:D:29:LYS:N	2.16	0.59
2:B:465:TYR:N	2:B:475:VAL:H	1.98	0.59
2:A:150:VAL:HG13	2:A:162:TRP:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:HIS:HB3	2:B:643:ILE:HG12	1.84	0.59
2:A:341:LEU:HD23	2:A:387:GLY:HA3	1.84	0.59
2:A:361:ILE:HD13	2:A:378:ILE:HG13	1.85	0.59
1:D:258:GLU:N	1:D:258:GLU:OE1	2.36	0.59
1:D:393:MET:HA	1:D:396:LYS:HG2	1.85	0.59
2:A:204:LYS:HE3	2:A:290:LEU:HD11	1.85	0.59
3:C:530:TRP:HA	3:C:533:GLN:HB3	1.84	0.59
3:C:312:ARG:NH2	3:C:314:LEU:HA	2.17	0.59
1:D:154:ARG:HB3	1:D:214:GLN:N	2.17	0.59
1:D:352:LYS:O	1:D:356:ARG:HG2	2.03	0.59
2:B:475:VAL:HG22	2:B:479:ASP:OD2	2.03	0.59
2:B:566:THR:C	2:B:567:LYS:HD2	2.28	0.59
2:B:222:VAL:HG11	2:B:224:LYS:HD2	1.85	0.58
2:B:449:ILE:HA	2:B:459:LEU:HD13	1.84	0.58
3:C:348:GLU:O	3:C:352:HIS:N	2.30	0.58
2:B:442:SER:HA	2:B:445:ILE:HD12	1.85	0.58
2:A:222:VAL:HG11	2:A:224:LYS:HD2	1.85	0.58
2:B:25:GLU:OE1	2:B:27:ALA:N	2.36	0.58
2:B:535:GLU:HA	2:B:540:THR:HA	1.83	0.58
2:A:569:GLU:OE1	2:A:569:GLU:N	2.36	0.58
2:B:178:GLU:HG2	2:B:180:MET:HG2	1.83	0.58
2:B:569:GLU:N	2:B:569:GLU:OE1	2.36	0.58
1:D:171:HIS:O	1:D:246:THR:N	2.24	0.58
2:B:126:ALA:O	2:B:127:ASP:OD1	2.21	0.58
2:A:25:GLU:OE1	2:A:27:ALA:N	2.35	0.58
2:B:452:ASP:HB3	2:B:459:LEU:HD11	1.85	0.58
3:C:506:VAL:HA	3:C:574:LEU:HD11	1.84	0.58
1:D:367:PHE:HE2	1:D:401:HIS:HD2	1.52	0.58
1:D:382:PRO:HD2	1:D:383:GLN:HE21	1.68	0.58
2:A:18:GLU:HB3	2:A:20:PHE:CZ	2.39	0.58
2:A:442:SER:HA	2:A:445:ILE:HD12	1.84	0.58
2:B:33:ILE:HA	2:B:37:PHE:CD1	2.39	0.58
2:A:398:ILE:HD12	2:A:398:ILE:H	1.68	0.58
3:C:578:ARG:HD3	3:C:578:ARG:N	2.19	0.58
1:D:371:LYS:HA	1:D:391:ILE:HD11	1.86	0.58
1:D:415:LYS:HG3	2:B:694:LEU:HD11	1.86	0.58
2:A:228:LYS:H	2:A:281:LYS:HD3	1.69	0.58
2:A:524:PRO:C	2:A:526:ASP:H	2.12	0.58
2:B:313:TYR:HB2	2:B:342:PHE:CE2	2.39	0.58
2:B:449:ILE:HD13	2:B:459:LEU:HD22	1.85	0.57
2:B:490:HIS:HB2	2:B:492:TYR:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:331:VAL:C	2:A:336:GLU:HB2	2.29	0.57
3:C:247:VAL:O	3:C:279:ARG:NH1	2.37	0.57
2:B:18:GLU:HB3	2:B:20:PHE:CZ	2.39	0.57
2:B:62:GLU:HB2	2:B:69:LYS:NZ	2.19	0.57
2:B:360:ASN:CB	2:B:386:ARG:HG2	2.34	0.57
1:D:145:ASP:O	1:D:222:ARG:NH2	2.37	0.57
1:D:226:GLY:O	1:D:230:LYS:NZ	2.37	0.57
2:B:470:SER:OG	2:B:471:GLY:N	2.36	0.57
2:A:571:LEU:HD12	2:A:574:ILE:HB	1.87	0.57
3:C:499:SER:OG	3:C:502:VAL:HG23	2.04	0.57
2:B:357:LYS:HA	2:B:373:ASN:HD21	1.69	0.57
2:A:399:SER:HB3	2:A:401:GLU:OE1	2.04	0.57
2:B:580:GLU:O	2:B:581:LYS:HG2	2.05	0.57
2:B:399:SER:HB3	2:B:401:GLU:OE1	2.04	0.57
2:A:115:THR:HB	2:A:130:MET:CE	2.34	0.57
2:A:200:GLU:O	2:A:203:ILE:N	2.38	0.57
2:B:331:VAL:C	2:B:336:GLU:HB2	2.30	0.57
3:C:364:LYS:H	3:C:367:ASN:HD22	1.52	0.57
2:B:501:GLN:HE21	2:A:679:GLU:C	2.13	0.57
3:C:224:ILE:O	3:C:230:SER:OG	2.23	0.57
1:D:31:ARG:HH22	1:D:109:PRO:HB2	1.69	0.56
2:B:314:LYS:HE2	2:B:322:ASP:HA	1.87	0.56
2:B:336:GLU:O	2:B:391:SER:OG	2.21	0.56
2:B:398:ILE:H	2:B:398:ILE:HD12	1.68	0.56
1:D:117:GLY:HA2	3:C:259:ARG:HH22	1.70	0.56
1:D:199:PRO:HG2	1:D:243:TYR:HE1	1.70	0.56
2:B:200:GLU:O	2:B:203:ILE:N	2.38	0.56
2:B:661:ASP:OD1	2:B:662:LEU:N	2.38	0.56
2:A:580:GLU:O	2:A:581:LYS:HG2	2.05	0.56
1:D:99:LYS:HD2	1:D:136:ASP:HA	1.87	0.56
1:D:389:LEU:O	1:D:393:MET:HG2	2.05	0.56
2:B:324:LEU:HB2	2:B:345:ARG:HA	1.87	0.56
2:B:519:ILE:HG12	2:B:520:TYR:N	2.19	0.56
2:A:324:LEU:HB3	2:A:343:VAL:HG13	1.87	0.56
3:C:284:SER:OG	3:C:285:VAL:N	2.38	0.56
3:C:324:THR:HA	3:C:370:VAL:N	2.21	0.56
1:D:36:ILE:O	1:D:104:HIS:HB2	2.05	0.56
2:B:143:LEU:O	2:B:191:LYS:NZ	2.38	0.56
2:B:440:GLN:HG3	2:B:441:PHE:CD1	2.40	0.56
2:B:493:TYR:CZ	2:B:543:SER:HB2	2.40	0.56
3:C:268:LEU:HD11	3:C:304:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:493:GLU:HG3	3:C:496:LYS:HD3	1.87	0.56
1:D:219:LEU:N	1:D:241:LEU:O	2.34	0.56
1:D:294:ILE:O	1:D:297:TRP:HB2	2.05	0.56
2:B:565:LYS:HG2	2:B:588:VAL:HB	1.86	0.56
2:A:190:LEU:HD12	2:A:191:LYS:H	1.71	0.56
2:B:496:GLY:HA3	2:B:502:VAL:HG12	1.87	0.56
3:C:324:THR:OG1	3:C:368:ILE:O	2.24	0.56
1:D:229:GLY:C	1:D:230:LYS:HD3	2.31	0.56
1:D:323:LEU:HG	1:D:327:TYR:CE2	2.41	0.56
2:B:152:THR:HG23	2:B:184:THR:HA	1.88	0.56
2:B:492:TYR:HA	2:B:542:VAL:O	2.05	0.56
2:B:605:GLY:HA3	2:B:631:LYS:HD3	1.88	0.56
3:C:328:TYR:HA	3:C:331:VAL:HB	1.86	0.56
2:B:77:HIS:HA	2:B:217:PRO:HB2	1.86	0.56
2:B:364:TYR:O	2:B:390:ASP:HA	2.06	0.56
3:C:574:LEU:HA	3:C:577:TRP:CE2	2.41	0.56
1:D:218:TYR:HA	1:D:242:ILE:HG22	1.86	0.56
2:B:678:LEU:HD23	2:B:681:PRO:HA	1.88	0.56
2:A:324:LEU:HB2	2:A:345:ARG:HA	1.87	0.56
2:A:671:LEU:HG	2:A:676:PHE:HB2	1.87	0.56
2:B:331:VAL:HG21	2:B:337:PHE:CE2	2.41	0.55
2:B:593:VAL:HG13	2:B:594:THR:HG23	1.88	0.55
2:B:671:LEU:HG	2:B:676:PHE:HB2	1.87	0.55
2:A:543:SER:O	2:A:546:LYS:HD3	2.06	0.55
2:A:440:GLN:HG3	2:A:441:PHE:CD1	2.40	0.55
2:B:47:GLU:CD	2:B:47:GLU:H	2.14	0.55
2:A:47:GLU:H	2:A:47:GLU:CD	2.13	0.55
2:B:69:LYS:HG3	2:B:70:LEU:N	2.21	0.55
2:B:543:SER:O	2:B:546:LYS:HD3	2.06	0.55
2:B:575:MET:O	2:B:579:LEU:HG	2.06	0.55
2:A:89:LEU:HD11	2:A:198:LEU:CD2	2.36	0.55
2:A:688:ILE:HD13	2:A:691:MET:HE2	1.89	0.55
1:D:179:ARG:HH21	1:D:235:ILE:HG23	1.71	0.55
1:D:391:ILE:HA	1:D:394:CYS:SG	2.47	0.55
2:B:190:LEU:HD12	2:B:191:LYS:H	1.71	0.55
2:B:324:LEU:HB3	2:B:343:VAL:HG13	1.87	0.55
2:B:468:SER:HG	2:B:518:VAL:H	1.52	0.55
1:D:154:ARG:O	1:D:213:GLU:HG3	2.07	0.55
2:A:331:VAL:HG21	2:A:337:PHE:CE2	2.41	0.55
1:D:20:GLU:HG3	1:D:21:GLN:HG2	1.89	0.55
1:D:255:GLU:C	1:D:259:MET:HE2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:HG23	2:B:185:LYS:O	2.06	0.55
2:B:629:ALA:H	3:C:375:ASP:HB3	1.71	0.55
2:A:680:ASP:N	2:A:680:ASP:OD1	2.39	0.55
2:B:688:ILE:HD13	2:B:691:MET:HE2	1.89	0.55
1:D:160:SER:HB2	1:D:250:PHE:CZ	2.41	0.55
1:D:173:GLU:HB2	1:D:244:GLU:HB3	1.88	0.55
1:D:201:GLY:H	1:D:224:GLY:HA2	1.72	0.55
2:B:566:THR:O	2:B:567:LYS:HD2	2.07	0.55
2:A:678:LEU:HD23	2:A:681:PRO:HA	1.88	0.55
1:D:308:GLU:HB3	1:D:311:ALA:HB3	1.89	0.55
2:A:449:ILE:HD13	2:A:459:LEU:HD22	1.87	0.55
1:D:409:TYR:HB2	2:A:694:LEU:HD12	1.88	0.54
2:B:55:ALA:O	2:B:59:ILE:HG23	2.08	0.54
3:C:514:GLU:O	3:C:519:LEU:HD22	2.07	0.54
2:B:341:LEU:HA	2:B:387:GLY:HA3	1.89	0.54
2:A:54:ASP:HB3	2:A:130:MET:CE	2.38	0.54
1:D:50:GLY:HA2	1:D:139:GLY:O	2.08	0.54
1:D:365:ASN:HB2	2:A:657:LYS:HE3	1.89	0.54
2:B:678:LEU:HD12	2:B:679:GLU:H	1.73	0.54
1:D:166:ALA:N	1:D:253:ALA:HB2	2.22	0.54
2:A:102:ASP:HA	2:A:105:ASN:HD22	1.73	0.54
2:B:413:ARG:O	2:B:417:VAL:HG22	2.06	0.54
2:B:501:GLN:NE2	2:A:679:GLU:O	2.37	0.54
2:A:55:ALA:O	2:A:59:ILE:HG23	2.08	0.54
2:B:415:ASN:O	2:B:419:LYS:HG2	2.07	0.54
2:A:449:ILE:HD12	2:A:459:LEU:HB3	1.90	0.54
3:C:353:LEU:O	3:C:358:ILE:HG12	2.08	0.54
3:C:568:CYS:SG	3:C:569:GLN:NE2	2.81	0.54
1:D:375:GLU:O	1:D:379:GLU:HG3	2.08	0.54
2:B:297:TRP:HH2	2:B:364:TYR:HE2	1.56	0.54
2:B:476:SER:N	2:B:479:ASP:OD2	2.40	0.53
2:A:204:LYS:HZ1	2:A:220:LEU:HD13	1.72	0.53
2:A:690:ARG:HH11	2:A:691:MET:CG	2.22	0.53
1:D:376:LYS:HA	1:D:379:GLU:OE2	2.08	0.53
2:A:19:THR:HG23	2:A:19:THR:O	2.08	0.53
2:B:366:ARG:H	2:B:392:GLU:CA	2.21	0.53
2:A:432:GLU:O	2:A:436:LYS:HG3	2.08	0.53
3:C:562:LEU:HD22	3:C:567:LEU:HD21	1.89	0.53
1:D:97:MET:CE	1:D:134:LEU:HD22	2.37	0.53
2:A:678:LEU:HD12	2:A:679:GLU:H	1.73	0.53
3:C:238:SER:O	3:C:242:VAL:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:TYR:CD1	3:C:258:TYR:HA	2.43	0.53
1:D:362:LEU:HD22	1:D:394:CYS:SG	2.49	0.53
2:B:151:ILE:HG12	2:B:161:ALA:CA	2.38	0.53
2:A:89:LEU:HD11	2:A:198:LEU:HD21	1.89	0.53
2:A:452:ASP:HB3	2:A:459:LEU:HD11	1.91	0.53
2:B:33:ILE:HA	2:B:37:PHE:CE1	2.44	0.53
3:C:372:LEU:HA	3:C:377:CYS:O	2.08	0.53
1:D:256:SER:C	1:D:258:GLU:H	2.17	0.53
2:B:297:TRP:CH2	2:B:364:TYR:CE2	2.96	0.53
2:B:28:GLN:NE2	2:A:111:ALA:HB3	2.23	0.53
2:B:102:ASP:HA	2:B:105:ASN:HD22	1.73	0.53
2:B:660:LYS:O	2:B:664:ILE:HG13	2.08	0.53
2:A:33:ILE:HG23	2:A:37:PHE:CD2	2.44	0.53
2:A:149:THR:HG22	2:A:163:GLU:HA	1.91	0.53
2:A:341:LEU:HA	2:A:387:GLY:HA3	1.89	0.53
2:B:37:PHE:O	2:B:399:SER:OG	2.27	0.53
2:B:432:GLU:O	2:B:436:LYS:HG3	2.08	0.53
2:A:96:ILE:O	2:A:154:HIS:HA	2.08	0.53
1:D:154:ARG:CZ	1:D:214:GLN:HE21	2.22	0.53
2:B:327:LYS:HB2	2:B:423:LEU:HD12	1.91	0.53
2:B:643:ILE:HA	2:B:646:LEU:HD12	1.91	0.53
2:A:199:GLU:HG2	2:A:202:ARG:HB3	1.91	0.53
2:A:643:ILE:HA	2:A:646:LEU:HD12	1.91	0.53
2:A:200:GLU:H	2:A:200:GLU:CD	2.15	0.52
3:C:548:CYS:SG	3:C:550:VAL:HG22	2.49	0.52
1:D:225:PHE:CD1	1:D:228:ALA:HB3	2.44	0.52
2:B:149:THR:HG22	2:B:163:GLU:HA	1.91	0.52
2:B:478:LYS:HA	2:B:481:CYS:SG	2.49	0.52
2:B:690:ARG:HH11	2:B:691:MET:CG	2.22	0.52
2:A:152:THR:HG23	2:A:184:THR:HG22	1.92	0.52
3:C:543:ARG:HE	3:C:544:LEU:HB2	1.74	0.52
3:C:360:HIS:NE2	3:C:362:ASP:O	2.43	0.52
2:B:219:THR:OG1	2:B:220:LEU:N	2.43	0.52
2:B:680:ASP:OD1	2:B:680:ASP:N	2.39	0.52
2:A:324:LEU:HD13	2:A:345:ARG:HG3	1.91	0.52
3:C:506:VAL:O	3:C:510:SER:N	2.42	0.52
3:C:574:LEU:HA	3:C:577:TRP:NE1	2.25	0.52
1:D:222:ARG:HA	1:D:227:GLU:CD	2.35	0.52
2:B:297:TRP:CZ2	2:B:364:TYR:CD2	2.97	0.52
2:A:200:GLU:HA	2:A:203:ILE:HG13	1.92	0.52
2:A:334:GLN:H	2:A:334:GLN:CD	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:LEU:HB3	2:B:553:GLU:OE2	2.09	0.52
2:A:348:PRO:HD3	2:A:441:PHE:CZ	2.44	0.52
3:C:505:ASN:ND2	3:C:567:LEU:HA	2.25	0.52
1:D:183:CYS:SG	1:D:184:ARG:N	2.83	0.52
2:B:199:GLU:H	2:B:199:GLU:CD	2.18	0.52
2:B:596:PRO:O	2:B:637:ASN:N	2.43	0.52
2:A:58:LYS:NZ	2:A:118:PHE:HB3	2.18	0.52
2:A:327:LYS:HB2	2:A:423:LEU:HD12	1.91	0.52
2:A:453:SER:HA	2:A:456:ARG:HH21	1.74	0.52
2:A:637:ASN:CG	2:A:640:HIS:HB2	2.35	0.52
2:B:204:LYS:HZ1	2:B:220:LEU:HD13	1.73	0.52
2:B:223:GLU:O	2:B:223:GLU:HG3	2.10	0.52
1:D:416:PHE:HB2	2:B:690:ARG:HD2	1.91	0.52
2:B:199:GLU:HG2	2:B:202:ARG:HB3	1.91	0.52
2:A:219:THR:OG1	2:A:220:LEU:N	2.43	0.52
2:A:223:GLU:O	2:A:223:GLU:HG3	2.10	0.52
2:A:493:TYR:CZ	2:A:543:SER:HB2	2.45	0.52
1:D:34:LEU:O	1:D:36:ILE:HG12	2.10	0.51
2:B:426:GLU:O	2:B:429:GLU:HB3	2.10	0.51
2:A:415:ASN:O	2:A:419:LYS:HG2	2.10	0.51
2:A:318:ASN:HD22	3:C:560:ALA:HA	1.75	0.51
3:C:328:TYR:CZ	3:C:332:ASN:HB2	2.45	0.51
3:C:458:LYS:HE2	3:C:466:TYR:HB3	1.93	0.51
1:D:153:LYS:HG2	1:D:214:GLN:HB2	1.93	0.51
2:B:58:LYS:NZ	2:B:118:PHE:HB3	2.18	0.51
2:B:96:ILE:O	2:B:154:HIS:HA	2.09	0.51
2:B:376:GLU:HB3	2:B:409:LEU:HD13	1.91	0.51
2:A:370:ILE:HG22	2:A:371:MET:H	1.75	0.51
1:D:99:LYS:HB2	1:D:137:PHE:H	1.76	0.51
2:B:324:LEU:HD13	2:B:345:ARG:HG3	1.91	0.51
3:C:575:CYS:O	3:C:578:ARG:N	2.38	0.51
1:D:151:ARG:HB2	1:D:216:ILE:O	2.10	0.51
2:B:313:TYR:HE2	2:B:319:ASP:HB3	1.76	0.51
2:B:347:ALA:HA	2:B:441:PHE:CZ	2.46	0.51
1:D:59:GLY:O	1:D:71:HIS:HB3	2.10	0.51
1:D:340:CYS:HB3	1:D:357:ARG:HG3	1.93	0.51
2:B:200:GLU:H	2:B:200:GLU:CD	2.15	0.51
2:B:334:GLN:H	2:B:334:GLN:CD	2.18	0.51
2:B:456:ARG:HA	2:B:459:LEU:HD12	1.92	0.51
2:A:153:LYS:HG2	2:A:154:HIS:H	1.75	0.51
3:C:513:GLY:H	3:C:538:THR:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:THR:HB	1:D:304:LEU:HD22	1.93	0.51
2:B:200:GLU:HA	2:B:203:ILE:HG13	1.92	0.51
2:B:637:ASN:CG	2:B:640:HIS:HB2	2.35	0.51
3:C:347:LEU:HD21	3:C:507:LEU:HD22	1.93	0.51
2:B:20:PHE:O	2:A:169:SER:OG	2.28	0.51
2:A:426:GLU:O	2:A:429:GLU:HB3	2.11	0.51
2:B:47:GLU:HA	2:B:50:SER:OG	2.11	0.51
2:B:60:ARG:O	2:B:64:LEU:HG	2.11	0.51
2:A:347:ALA:HA	2:A:441:PHE:CZ	2.46	0.51
3:C:525:ASP:OD1	3:C:526:LYS:N	2.39	0.51
1:D:344:LEU:HD21	1:D:354:LEU:HD13	1.93	0.50
2:B:464:ARG:HA	2:B:475:VAL:O	2.10	0.50
2:A:118:PHE:O	2:A:122:LEU:HG	2.11	0.50
2:A:119:MET:HG3	2:A:130:MET:HG3	1.92	0.50
2:A:294:LYS:NZ	2:A:299:ARG:HD3	2.26	0.50
2:A:331:VAL:HG11	2:A:337:PHE:CE1	2.46	0.50
3:C:461:LEU:HB3	3:C:464:ARG:HB2	1.93	0.50
2:A:144:VAL:O	2:A:190:LEU:HA	2.11	0.50
1:D:15:THR:HG21	1:D:129:PHE:CE1	2.47	0.50
1:D:121:LYS:HB2	3:C:297:ASP:HB3	1.92	0.50
1:D:344:LEU:HD11	1:D:354:LEU:HD13	1.94	0.50
2:B:150:VAL:CB	2:B:186:VAL:HG22	2.42	0.50
2:B:180:MET:HE1	2:B:185:LYS:CD	2.40	0.50
2:B:321:GLU:OE2	2:B:345:ARG:HD2	2.12	0.50
2:A:436:LYS:O	2:A:439:GLU:HB2	2.11	0.50
3:C:257:THR:OG1	3:C:260:LYS:HE3	2.11	0.50
2:B:331:VAL:HG11	2:B:337:PHE:CE1	2.46	0.50
2:B:602:SER:HB2	2:B:631:LYS:HB3	1.93	0.50
2:A:155:ASN:N	2:A:155:ASN:OD1	2.44	0.50
2:A:570:ASN:O	2:A:573:LYS:HB3	2.12	0.50
2:B:493:TYR:CE2	2:B:543:SER:HB2	2.46	0.50
2:A:199:GLU:H	2:A:199:GLU:CD	2.18	0.50
1:D:267:GLN:HG3	1:D:297:TRP:CH2	2.47	0.50
1:D:312:SER:HA	1:D:315:PHE:CD2	2.46	0.50
2:B:436:LYS:O	2:B:439:GLU:HB2	2.11	0.50
2:B:150:VAL:HG23	2:B:186:VAL:HG22	1.86	0.50
2:B:173:ARG:HB2	2:A:17:VAL:CG1	2.41	0.50
2:B:200:GLU:OE1	2:B:200:GLU:N	2.26	0.50
2:B:467:THR:N	2:B:470:SER:OG	2.31	0.50
2:B:147:LYS:HG3	2:B:189:HIS:CD2	2.47	0.50
2:B:153:LYS:HG2	2:B:154:HIS:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ARG:HE	1:D:152:THR:HB	1.76	0.50
1:D:158:GLY:H	1:D:210:GLN:HE22	1.58	0.50
1:D:194:GLU:CD	1:D:283:LYS:HD2	2.37	0.50
1:D:317:LEU:HD13	1:D:320:PHE:CD2	2.41	0.50
1:D:391:ILE:HD12	1:D:394:CYS:SG	2.52	0.50
2:B:33:ILE:HG23	2:B:37:PHE:CD2	2.47	0.50
2:B:313:TYR:CE2	2:B:319:ASP:HB3	2.47	0.50
2:B:449:ILE:CD1	2:B:459:LEU:HB3	2.41	0.50
2:A:510:ARG:HG2	2:A:591:ARG:HA	1.94	0.50
3:C:293:VAL:HG22	3:C:295:TYR:H	1.76	0.50
1:D:216:ILE:HA	1:D:244:GLU:HA	1.94	0.49
2:B:329:PHE:CE2	2:B:419:LYS:HB3	2.47	0.49
2:A:321:GLU:OE2	2:A:345:ARG:HD2	2.12	0.49
3:C:570:ALA:O	3:C:574:LEU:N	2.29	0.49
3:C:574:LEU:HG	3:C:577:TRP:CH2	2.46	0.49
1:D:356:ARG:HH22	1:D:359:GLU:HG3	1.77	0.49
2:B:144:VAL:O	2:B:190:LEU:HA	2.11	0.49
2:B:464:ARG:O	2:B:474:MET:HE3	2.12	0.49
2:B:465:TYR:C	2:B:474:MET:HA	2.37	0.49
2:A:45:LEU:HG	2:A:45:LEU:O	2.11	0.49
2:B:62:GLU:HB2	2:B:69:LYS:HZ2	1.75	0.49
2:A:462:LEU:HA	2:A:464:ARG:HH21	1.77	0.49
2:A:492:TYR:HD2	2:A:544:VAL:HG12	1.77	0.49
2:A:508:VAL:HG13	2:A:518:VAL:HG11	1.94	0.49
1:D:179:ARG:NH2	1:D:235:ILE:HG23	2.28	0.49
2:B:118:PHE:O	2:B:122:LEU:HG	2.12	0.49
2:B:366:ARG:N	2:B:392:GLU:HA	2.27	0.49
2:B:500:ASP:O	2:B:503:ALA:N	2.43	0.49
2:A:47:GLU:CD	2:A:47:GLU:N	2.71	0.49
2:A:329:PHE:CE2	2:A:419:LYS:HB3	2.47	0.49
2:A:467:THR:HG22	2:A:519:ILE:HB	1.94	0.49
2:A:692:ILE:O	2:A:696:LEU:HG	2.12	0.49
2:A:80:LEU:HB3	2:A:220:LEU:HD12	1.94	0.49
1:D:374:PHE:HA	1:D:377:VAL:HG22	1.94	0.49
3:C:449:LEU:HD21	3:C:475:PRO:HD2	1.94	0.49
2:A:523:GLU:O	2:A:526:ASP:HB2	2.13	0.49
2:B:153:LYS:HB3	2:B:182:ARG:HA	1.94	0.49
2:B:692:ILE:O	2:B:696:LEU:HG	2.12	0.49
2:A:153:LYS:HG2	2:A:154:HIS:N	2.28	0.49
3:C:326:ARG:HH11	3:C:365:SER:CB	2.26	0.49
2:A:147:LYS:HG3	2:A:189:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:TRP:HB3	2:B:340:LEU:HD23	1.95	0.48
1:D:158:GLY:H	1:D:210:GLN:NE2	2.11	0.48
2:B:153:LYS:HG2	2:B:154:HIS:N	2.28	0.48
2:B:155:ASN:OD1	2:B:155:ASN:N	2.44	0.48
2:B:213:PHE:HD1	2:B:295:PRO:HG3	1.78	0.48
2:B:599:ILE:HA	2:B:634:LEU:HA	1.95	0.48
1:D:323:LEU:HD23	1:D:339:CYS:HB3	1.94	0.48
2:B:170:PHE:CZ	2:A:20:PHE:HB2	2.48	0.48
2:B:204:LYS:HD2	2:B:204:LYS:N	2.28	0.48
2:B:598:CYS:O	2:B:634:LEU:HB2	2.14	0.48
2:A:59:ILE:HG21	2:A:96:ILE:HB	1.93	0.48
1:D:83:LYS:HE2	1:D:83:LYS:HA	1.94	0.48
2:B:89:LEU:HB2	2:B:188:LEU:HB3	1.94	0.48
2:B:204:LYS:HA	2:B:207:VAL:HG22	1.94	0.48
2:B:215:GLY:H	2:B:367:ARG:CZ	2.26	0.48
2:B:427:LEU:HG	2:B:434:TYR:HB2	1.96	0.48
2:A:402:MET:CG	2:A:403:LEU:N	2.76	0.48
3:C:524:LEU:HD23	3:C:524:LEU:H	1.77	0.48
1:D:255:GLU:HB3	1:D:258:GLU:OE1	2.14	0.48
2:B:642:ILE:HG12	2:A:696:LEU:HD11	1.96	0.48
2:A:663:VAL:HA	2:A:666:LEU:HD12	1.94	0.48
3:C:239:GLN:HB3	3:C:272:PRO:HG2	1.96	0.48
3:C:288:LEU:N	3:C:289:PRO:HD3	2.28	0.48
1:D:340:CYS:O	1:D:344:LEU:HG	2.14	0.48
2:B:47:GLU:CD	2:B:47:GLU:N	2.71	0.48
2:B:595:SER:O	2:B:637:ASN:HB2	2.13	0.48
2:A:200:GLU:OE1	2:A:200:GLU:N	2.26	0.48
2:A:204:LYS:HD2	2:A:204:LYS:N	2.28	0.48
2:A:575:MET:O	2:A:579:LEU:HG	2.13	0.48
2:B:431:LYS:HB3	2:B:431:LYS:HE3	1.60	0.48
2:A:599:ILE:HA	2:A:634:LEU:HA	1.95	0.48
3:C:168:ALA:HB2	3:C:221:MET:SD	2.54	0.48
3:C:235:ASN:O	3:C:238:SER:OG	2.21	0.48
3:C:574:LEU:O	3:C:577:TRP:CG	2.67	0.48
1:D:261:THR:CG2	1:D:304:LEU:HD23	2.43	0.48
2:B:70:LEU:O	2:B:71:ASP:C	2.55	0.48
2:B:297:TRP:HH2	2:B:364:TYR:CE2	2.32	0.48
2:B:391:SER:HB3	2:B:394:LEU:CD2	2.43	0.48
3:C:508:HIS:HA	3:C:512:TRP:CE3	2.46	0.48
1:D:244:GLU:OE2	1:D:245:VAL:N	2.47	0.48
2:B:364:TYR:HA	2:B:370:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:LYS:HD2	2:B:567:LYS:N	2.29	0.48
1:D:48:MET:HE2	1:D:48:MET:HB2	1.70	0.48
1:D:402:ASN:O	1:D:406:ARG:HD2	2.13	0.48
2:B:366:ARG:H	2:B:392:GLU:C	2.22	0.48
3:C:255:ALA:HB1	3:C:295:TYR:OH	2.14	0.48
3:C:349:GLY:O	3:C:353:LEU:N	2.33	0.48
1:D:38:LYS:HD2	1:D:38:LYS:HA	1.41	0.47
1:D:181:PHE:HB2	1:D:233:PHE:CD1	2.49	0.47
2:B:629:ALA:N	3:C:375:ASP:HB3	2.29	0.47
2:A:551:LEU:HD13	2:A:551:LEU:HA	1.69	0.47
3:C:285:VAL:HB	3:C:289:PRO:HB3	1.95	0.47
2:B:304:ILE:HD11	2:B:309:TYR:CZ	2.49	0.47
2:A:607:THR:O	2:A:608:ALA:C	2.57	0.47
2:A:656:ASP:HB3	2:A:659:VAL:HG13	1.96	0.47
3:C:260:LYS:HE3	3:C:260:LYS:HB2	1.59	0.47
2:A:427:LEU:HG	2:A:434:TYR:HB2	1.95	0.47
3:C:245:SER:OG	3:C:246:ARG:N	2.47	0.47
3:C:349:GLY:HA2	3:C:352:HIS:HB3	1.96	0.47
1:D:271:VAL:HG21	1:D:293:LYS:HZ1	1.79	0.47
1:D:367:PHE:O	1:D:371:LYS:HG3	2.14	0.47
2:B:478:LYS:HA	2:B:478:LYS:HD2	1.65	0.47
2:A:104:ILE:O	2:A:107:LEU:N	2.47	0.47
2:A:364:TYR:CD1	2:A:369:PHE:HA	2.48	0.47
3:C:574:LEU:HB3	3:C:578:ARG:NH2	2.25	0.47
1:D:13:SER:HB2	1:D:63:ASN:HA	1.96	0.47
1:D:294:ILE:HG23	1:D:297:TRP:CE3	2.49	0.47
1:D:404:ARG:NH1	2:A:658:SER:H	2.13	0.47
2:B:59:ILE:HG21	2:B:96:ILE:HB	1.96	0.47
2:B:199:GLU:OE1	2:B:199:GLU:N	2.38	0.47
2:B:574:ILE:HG21	2:B:650:ALA:HB1	1.97	0.47
2:A:598:CYS:O	2:A:634:LEU:HB2	2.14	0.47
1:D:255:GLU:O	1:D:259:MET:N	2.38	0.47
2:B:375:GLU:O	2:B:413:ARG:NH2	2.48	0.47
2:A:606:TRP:HE3	2:A:611:GLU:HA	1.79	0.47
1:D:188:PHE:CG	1:D:189:THR:N	2.83	0.47
1:D:236:GLU:HB3	1:D:237:PRO:HD3	1.96	0.47
1:D:325:MET:O	1:D:329:LYS:HG2	2.15	0.47
2:B:634:LEU:HD23	2:B:634:LEU:H	1.79	0.47
2:A:151:ILE:CG2	2:A:161:ALA:HB2	2.21	0.47
2:A:358:LYS:HD2	2:A:358:LYS:HA	1.38	0.47
3:C:449:LEU:HD13	3:C:449:LEU:HA	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:480:PRO:HA	3:C:483:ARG:HE	1.79	0.47
3:C:494:ALA:HA	3:C:497:ARG:HB2	1.97	0.47
3:C:577:TRP:H	3:C:577:TRP:CD1	2.33	0.47
1:D:97:MET:HE3	1:D:134:LEU:HD22	1.96	0.47
2:B:328:HIS:CD2	2:B:340:LEU:HB2	2.50	0.47
2:B:402:MET:CG	2:B:403:LEU:N	2.77	0.47
2:A:63:SER:HB2	2:A:70:LEU:HA	1.96	0.47
2:A:328:HIS:CD2	2:A:340:LEU:HB2	2.50	0.47
2:A:607:THR:HG22	2:A:608:ALA:N	2.30	0.47
1:D:157:GLU:OE2	1:D:159:TYR:HB2	2.14	0.47
2:B:87:ARG:NH1	2:B:192:GLU:HG3	2.23	0.47
2:A:229:GLU:HB2	2:A:281:LYS:HZ1	1.80	0.47
2:A:492:TYR:HA	2:A:542:VAL:O	2.14	0.47
3:C:542:ASN:OD1	3:C:555:LYS:NZ	2.42	0.47
1:D:93:GLY:C	1:D:95:ALA:N	2.70	0.47
2:B:96:ILE:HD11	2:B:155:ASN:HB3	1.97	0.47
3:C:326:ARG:HH11	3:C:365:SER:HB2	1.80	0.47
2:B:492:TYR:HA	2:B:542:VAL:HG23	1.98	0.46
2:B:684:HIS:O	2:B:688:ILE:HG12	2.15	0.46
1:D:295:VAL:HG12	1:D:299:GLU:OE2	2.15	0.46
2:B:561:GLN:HB2	2:B:590:ASN:HD21	1.80	0.46
2:B:575:MET:C	2:B:579:LEU:HG	2.39	0.46
2:A:218:ILE:HD11	2:A:291:ASN:HB3	1.98	0.46
2:A:279:LYS:HB3	2:A:280:ILE:H	1.59	0.46
2:B:437:PHE:CE1	2:B:441:PHE:CG	3.03	0.46
2:B:461:GLU:H	2:B:461:GLU:HG2	1.44	0.46
2:A:32:LEU:O	2:A:36:THR:OG1	2.23	0.46
2:A:684:HIS:O	2:A:688:ILE:HG12	2.15	0.46
2:B:39:SER:HB2	2:A:404:GLN:HA	1.96	0.46
2:B:323:HIS:C	2:B:345:ARG:HB2	2.40	0.46
2:B:402:MET:CG	2:B:403:LEU:H	2.29	0.46
2:B:658:SER:O	2:B:662:LEU:HD23	2.16	0.46
2:A:411:VAL:HA	2:A:414:LYS:HE2	1.96	0.46
3:C:257:THR:OG1	3:C:260:LYS:HB2	2.15	0.46
1:D:160:SER:HB2	1:D:250:PHE:HZ	1.79	0.46
2:B:487:ASN:O	2:B:488:GLN:C	2.59	0.46
2:B:493:TYR:O	2:B:543:SER:HA	2.16	0.46
2:B:568:PHE:HB2	2:B:588:VAL:HG21	1.98	0.46
2:B:661:ASP:HA	2:B:664:ILE:HD12	1.97	0.46
2:A:361:ILE:HA	2:A:387:GLY:O	2.16	0.46
3:C:474:LEU:H	3:C:474:LEU:HG	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:THR:HA	1:D:32:GLY:HA3	1.97	0.46
1:D:340:CYS:SG	1:D:357:ARG:HB2	2.56	0.46
2:B:362:LYS:O	2:B:389:VAL:HG12	2.16	0.46
2:B:606:TRP:HD1	2:B:610:MET:HE2	1.81	0.46
2:B:635:GLU:OE1	2:B:635:GLU:N	2.49	0.46
2:A:162:TRP:NE1	2:A:164:SER:OG	2.49	0.46
2:A:327:LYS:HB3	2:A:329:PHE:CZ	2.51	0.46
2:A:534:LYS:HA	2:A:541:LEU:HD22	1.98	0.46
2:A:682:GLN:HG2	2:A:683:THR:N	2.31	0.46
2:B:89:LEU:HD21	2:B:198:LEU:HD22	1.97	0.46
2:B:214:ILE:HA	2:B:367:ARG:CZ	2.46	0.46
2:B:393:ASP:C	2:B:394:LEU:HD22	2.40	0.46
2:B:624:THR:O	2:B:625:MET:C	2.57	0.46
2:A:363:LEU:HD22	2:A:365:VAL:HG23	1.98	0.46
3:C:564:CYS:HA	3:C:567:LEU:HB2	1.96	0.46
1:D:37:VAL:HG23	1:D:103:CYS:HA	1.97	0.46
1:D:154:ARG:NH1	1:D:212:GLU:OE2	2.49	0.46
2:A:323:HIS:C	2:A:345:ARG:HB2	2.40	0.46
2:A:437:PHE:CE1	2:A:441:PHE:CG	3.03	0.46
3:C:577:TRP:CD2	3:C:578:ARG:NH1	2.84	0.46
2:B:637:ASN:HB3	2:B:640:HIS:HB2	1.98	0.46
2:A:524:PRO:C	2:A:526:ASP:N	2.67	0.46
2:A:635:GLU:N	2:A:635:GLU:OE1	2.49	0.46
3:C:505:ASN:HD21	3:C:567:LEU:C	2.23	0.46
1:D:154:ARG:NH1	1:D:214:GLN:HE21	2.14	0.45
1:D:221:PRO:HD3	1:D:239:ALA:HA	1.97	0.45
2:A:571:LEU:HD11	2:A:575:MET:HE3	1.99	0.45
1:D:171:HIS:HA	1:D:185:ASP:HB3	1.99	0.45
1:D:176:CYS:HA	1:D:243:TYR:HB3	1.96	0.45
2:B:152:THR:HG23	2:B:184:THR:HG22	1.98	0.45
2:B:162:TRP:NE1	2:B:164:SER:OG	2.49	0.45
2:B:163:GLU:OE1	2:B:172:VAL:HA	2.16	0.45
2:A:82:PRO:HB2	2:A:198:LEU:HD13	1.98	0.45
3:C:546:GLU:HA	3:C:551:GLU:CD	2.41	0.45
1:D:271:VAL:HG11	1:D:294:ILE:HD11	1.98	0.45
1:D:412:MET:HG3	2:B:690:ARG:HH12	1.82	0.45
2:B:108:GLY:O	2:B:110:ILE:HD12	2.16	0.45
2:B:682:GLN:HG2	2:B:683:THR:N	2.31	0.45
1:D:149:ILE:O	1:D:151:ARG:HG2	2.16	0.45
2:B:421:LEU:HA	2:B:424:PHE:HD2	1.82	0.45
2:B:531:GLN:HE21	3:C:321:TYR:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:30:MET:O	2:A:34:ILE:HG13	2.17	0.45
2:A:366:ARG:H	2:A:392:GLU:HA	1.81	0.45
2:A:402:MET:CG	2:A:403:LEU:H	2.27	0.45
2:A:637:ASN:ND2	2:A:640:HIS:HB2	2.32	0.45
1:D:261:THR:HB	1:D:304:LEU:CD2	2.46	0.45
1:D:268:ALA:HA	1:D:297:TRP:CZ3	2.46	0.45
2:B:19:THR:HA	2:A:170:PHE:O	2.16	0.45
2:B:22:PHE:HB2	2:A:26:ILE:HG21	1.98	0.45
2:B:331:VAL:HB	2:B:337:PHE:N	2.20	0.45
2:B:333:GLY:N	2:B:336:GLU:HB3	2.32	0.45
2:B:596:PRO:HD2	2:A:689:TYR:CE2	2.51	0.45
2:A:690:ARG:NE	2:A:691:MET:SD	2.85	0.45
1:D:39:ARG:HE	1:D:39:ARG:HB3	1.55	0.45
1:D:130:PHE:HD1	1:D:132:ILE:HG12	1.82	0.45
2:B:690:ARG:NE	2:B:691:MET:SD	2.85	0.45
2:A:108:GLY:O	2:A:110:ILE:HD12	2.16	0.45
2:A:376:GLU:H	2:A:376:GLU:HG3	1.39	0.45
2:A:596:PRO:HB3	2:A:640:HIS:CG	2.52	0.45
1:D:147:GLY:O	1:D:220:GLY:N	2.49	0.45
1:D:332:GLU:HG2	1:D:334:THR:HG22	1.98	0.45
2:B:35:ASN:OD1	2:B:36:THR:HG23	2.17	0.45
2:B:472:ASP:OD1	2:B:472:ASP:N	2.50	0.45
2:B:645:THR:HG21	2:A:696:LEU:HD13	1.98	0.45
2:A:359:ASN:HA	2:A:373:ASN:CB	2.46	0.45
2:A:672:LEU:HD13	2:A:672:LEU:HA	1.68	0.45
3:C:363:LEU:HA	3:C:367:ASN:HD22	1.82	0.45
1:D:92:ILE:HA	1:D:92:ILE:HD12	1.64	0.45
1:D:313:GLU:O	1:D:317:LEU:HD23	2.17	0.45
1:D:363:LEU:HD23	1:D:363:LEU:HA	1.85	0.45
2:B:75:GLU:HG2	2:B:77:HIS:HE1	1.82	0.45
2:B:327:LYS:HB3	2:B:329:PHE:CZ	2.51	0.45
2:B:501:GLN:NE2	2:A:679:GLU:C	2.75	0.45
2:A:499:LYS:H	2:A:499:LYS:HG3	1.36	0.45
1:D:99:LYS:CB	1:D:137:PHE:H	2.30	0.45
1:D:264:LYS:HB2	1:D:264:LYS:HE2	1.77	0.45
2:B:74:LYS:HA	2:B:74:LYS:HD3	1.70	0.45
2:B:485:LYS:H	2:B:485:LYS:HG3	1.44	0.45
3:C:517:LEU:H	3:C:517:LEU:HG	1.44	0.45
2:B:197:TYR:O	2:B:203:ILE:HD11	2.17	0.45
2:B:222:VAL:CG1	2:B:224:LYS:HD2	2.47	0.45
2:B:465:TYR:HA	2:B:474:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:209:LYS:HD3	2:A:210:HIS:HD2	1.82	0.45
2:A:218:ILE:CD1	2:A:291:ASN:HB3	2.46	0.45
2:A:477:LEU:H	2:A:477:LEU:HG	1.61	0.45
3:C:573:LEU:HD13	3:C:573:LEU:HA	1.79	0.45
3:C:578:ARG:C	3:C:580:ALA:N	2.73	0.45
2:B:141:ALA:O	2:B:145:ALA:N	2.39	0.44
2:B:616:ALA:HB1	2:A:613:ILE:HG12	1.99	0.44
3:C:159:GLY:H	3:C:171:TYR:HD2	1.63	0.44
3:C:370:VAL:HA	3:C:379:TRP:O	2.18	0.44
3:C:512:TRP:HB3	3:C:538:THR:CG2	2.47	0.44
3:C:574:LEU:O	3:C:575:CYS:C	2.60	0.44
2:B:161:ALA:HB3	2:B:174:THR:HB	1.99	0.44
2:B:408:ILE:HG13	2:B:409:LEU:N	2.33	0.44
2:B:672:LEU:HD13	2:B:672:LEU:HA	1.68	0.44
2:A:599:ILE:HG13	2:A:670:ALA:HB1	1.99	0.44
3:C:237:MET:O	3:C:241:LEU:N	2.50	0.44
1:D:404:ARG:HA	1:D:407:ARG:HH21	1.82	0.44
2:B:99:THR:O	2:B:100:LYS:C	2.59	0.44
2:B:305:THR:OG1	2:B:308:GLU:OE1	2.31	0.44
2:A:333:GLY:N	2:A:336:GLU:HB3	2.32	0.44
2:A:408:ILE:HG13	2:A:409:LEU:N	2.33	0.44
2:A:421:LEU:HA	2:A:424:PHE:HD2	1.82	0.44
2:A:678:LEU:HD21	2:A:684:HIS:HB2	1.99	0.44
3:C:325:LEU:HD12	3:C:365:SER:O	2.17	0.44
1:D:216:ILE:HG13	1:D:244:GLU:OE1	2.17	0.44
2:B:32:LEU:HD23	2:B:33:ILE:N	2.33	0.44
2:B:107:LEU:HD12	2:B:107:LEU:HA	1.72	0.44
2:B:350:ASP:OD1	2:B:350:ASP:O	2.34	0.44
2:B:424:PHE:HE1	2:B:437:PHE:HE2	1.66	0.44
2:B:637:ASN:ND2	2:B:640:HIS:HB2	2.32	0.44
2:B:673:SER:OG	2:B:674:SER:N	2.51	0.44
2:A:637:ASN:HB3	2:A:640:HIS:HB2	1.98	0.44
3:C:326:ARG:N	3:C:366:ASP:OD1	2.37	0.44
1:D:225:PHE:CE2	1:D:230:LYS:HG3	2.52	0.44
1:D:350:ASN:HB3	1:D:353:GLY:H	1.82	0.44
2:B:25:GLU:OE1	2:B:26:ILE:N	2.51	0.44
2:B:41:LYS:HE2	2:B:41:LYS:HB3	1.45	0.44
2:B:139:TYR:C	2:B:141:ALA:H	2.25	0.44
2:B:678:LEU:HD21	2:B:684:HIS:HB2	1.99	0.44
3:C:256:VAL:HG13	3:C:260:LYS:HZ2	1.82	0.44
3:C:568:CYS:O	3:C:572:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:576:SER:HA	3:C:579:ALA:CB	2.44	0.44
1:D:373:ASP:O	1:D:377:VAL:HG13	2.18	0.44
2:A:45:LEU:HD21	2:A:203:ILE:HG23	1.98	0.44
2:A:511:LEU:HD13	2:A:516:LEU:HB3	2.00	0.44
2:A:634:LEU:H	2:A:634:LEU:HD23	1.82	0.44
3:C:270:PRO:HG3	3:C:304:HIS:CE1	2.53	0.44
1:D:304:LEU:HG	1:D:305:SER:H	1.80	0.44
1:D:367:PHE:HA	1:D:370:ALA:HB3	2.00	0.44
2:B:20:PHE:HD2	2:A:170:PHE:CE1	2.35	0.44
2:B:298:THR:HA	2:B:338:ARG:CZ	2.48	0.44
2:B:559:LYS:O	2:B:563:GLU:HG3	2.18	0.44
2:A:420:CYS:O	2:A:423:LEU:HB3	2.18	0.44
2:A:569:GLU:HA	2:A:572:CYS:SG	2.57	0.44
3:C:574:LEU:O	3:C:577:TRP:N	2.49	0.44
1:D:165:GLY:C	1:D:253:ALA:HB2	2.43	0.44
1:D:255:GLU:OE1	1:D:256:SER:N	2.51	0.44
2:B:30:MET:O	2:B:34:ILE:HG13	2.17	0.44
2:A:199:GLU:OE1	2:A:199:GLU:N	2.38	0.44
2:A:222:VAL:CG1	2:A:224:LYS:HD2	2.47	0.44
3:C:352:HIS:O	3:C:356:GLN:HG3	2.18	0.44
3:C:516:ILE:HG12	3:C:517:LEU:N	2.33	0.44
1:D:28:LYS:CG	1:D:29:LYS:H	2.26	0.44
1:D:162:PRO:HA	1:D:252:LYS:HZ3	1.82	0.44
1:D:377:VAL:O	1:D:381:ASN:N	2.43	0.44
2:B:599:ILE:HG13	2:B:670:ALA:HB1	1.99	0.44
2:B:657:LYS:O	2:B:658:SER:C	2.60	0.44
1:D:194:GLU:OE1	1:D:283:LYS:HD2	2.18	0.43
2:B:190:LEU:HD21	2:B:194:GLN:O	2.18	0.43
2:A:25:GLU:OE1	2:A:26:ILE:N	2.51	0.43
2:A:35:ASN:OD1	2:A:36:THR:HG23	2.17	0.43
2:A:69:LYS:HE3	2:A:69:LYS:HB2	1.30	0.43
2:A:115:THR:HB	2:A:130:MET:HE2	2.00	0.43
2:A:436:LYS:O	2:A:440:GLN:HG2	2.18	0.43
2:A:446:LYS:HB3	2:A:529:CYS:SG	2.57	0.43
3:C:255:ALA:O	3:C:295:TYR:HE1	2.00	0.43
1:D:166:ALA:HB2	1:D:253:ALA:N	2.29	0.43
1:D:203:ASP:OD1	1:D:204:LYS:N	2.47	0.43
1:D:240:GLU:O	1:D:241:LEU:HD23	2.18	0.43
2:B:139:TYR:C	2:B:141:ALA:N	2.76	0.43
2:B:356:LYS:HE3	2:B:357:LYS:HD3	2.01	0.43
2:B:362:LYS:HA	2:B:372:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:LEU:HA	2:B:421:LEU:HD23	1.87	0.43
2:B:492:TYR:CD1	2:B:492:TYR:N	2.86	0.43
2:B:527:GLU:O	2:B:528:TYR:C	2.60	0.43
2:B:672:LEU:HD21	2:B:678:LEU:HD22	2.00	0.43
2:B:683:THR:HA	2:B:686:ASN:OD1	2.18	0.43
2:A:107:LEU:HD23	2:A:162:TRP:CZ2	2.53	0.43
3:C:577:TRP:CE3	3:C:578:ARG:NH1	2.86	0.43
2:B:151:ILE:HA	2:B:160:TYR:O	2.19	0.43
2:A:688:ILE:HA	2:A:691:MET:HE2	2.00	0.43
3:C:577:TRP:CD1	3:C:577:TRP:N	2.86	0.43
1:D:288:VAL:HG23	1:D:289:ILE:N	2.33	0.43
2:B:499:LYS:H	2:B:499:LYS:HG3	1.43	0.43
2:A:107:LEU:HD12	2:A:107:LEU:HA	1.82	0.43
2:A:280:ILE:H	2:A:280:ILE:HG12	1.42	0.43
2:A:402:MET:O	2:A:403:LEU:HD22	2.18	0.43
2:A:606:TRP:HB3	2:A:610:MET:HG2	2.00	0.43
1:D:94:VAL:HA	1:D:97:MET:CB	2.48	0.43
1:D:217:LEU:O	1:D:242:ILE:HA	2.19	0.43
2:B:33:ILE:HG23	2:B:37:PHE:CE2	2.53	0.43
2:B:116:LYS:O	2:B:119:MET:HE3	2.18	0.43
2:B:420:CYS:O	2:B:423:LEU:HB3	2.18	0.43
2:B:624:THR:HA	2:B:628:MET:CG	2.48	0.43
2:A:33:ILE:HG23	2:A:37:PHE:CE2	2.54	0.43
2:A:190:LEU:HD21	2:A:194:GLN:O	2.18	0.43
2:A:483:ARG:O	2:A:484:MET:C	2.60	0.43
1:D:172:LEU:N	1:D:185:ASP:OD1	2.47	0.43
1:D:254:LYS:HG2	1:D:259:MET:CG	2.48	0.43
1:D:367:PHE:HB2	1:D:394:CYS:HB3	2.01	0.43
2:B:43:ILE:HD12	2:B:43:ILE:HA	1.70	0.43
2:B:334:GLN:HG2	2:B:335:LEU:H	1.84	0.43
2:B:402:MET:O	2:B:403:LEU:HD22	2.19	0.43
2:B:456:ARG:HH12	2:B:532:GLN:HB3	1.83	0.43
2:A:54:ASP:HB3	2:A:130:MET:HE1	2.00	0.43
2:A:326:VAL:HA	2:A:341:LEU:O	2.19	0.43
2:A:555:GLU:H	2:A:555:GLU:HG3	1.46	0.43
3:C:248:ALA:O	3:C:249:LEU:HD22	2.19	0.43
1:D:368:GLU:HA	1:D:371:LYS:HE2	2.00	0.43
2:B:25:GLU:HB3	2:B:28:GLN:OE1	2.19	0.43
2:B:309:TYR:O	2:B:342:PHE:HZ	2.01	0.43
2:B:599:ILE:HD12	2:B:671:LEU:HA	2.01	0.43
2:A:467:THR:HA	2:A:519:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:570:ASN:O	2:A:574:ILE:HG13	2.18	0.43
2:A:605:GLY:C	2:A:606:TRP:HD1	2.26	0.43
2:A:683:THR:HA	2:A:686:ASN:OD1	2.18	0.43
3:C:236:THR:O	3:C:240:GLU:HG2	2.19	0.43
3:C:562:LEU:HB3	3:C:567:LEU:HD21	2.00	0.43
1:D:103:CYS:HB2	1:D:134:LEU:CD2	2.36	0.43
1:D:169:GLU:HB3	1:D:249:SER:H	1.84	0.43
2:B:326:VAL:HA	2:B:341:LEU:O	2.19	0.43
2:B:397:ASN:HD21	2:B:402:MET:C	2.26	0.43
2:A:208:LYS:HA	2:A:208:LYS:HD3	1.46	0.43
2:A:575:MET:C	2:A:579:LEU:HG	2.43	0.43
2:A:673:SER:OG	2:A:674:SER:N	2.51	0.43
1:D:302:TYR:HB2	1:D:306:GLU:OE2	2.19	0.43
2:B:28:GLN:OE1	2:B:29:LEU:N	2.48	0.43
2:A:32:LEU:HD23	2:A:33:ILE:N	2.33	0.43
2:A:75:GLU:H	2:A:75:GLU:HG3	1.48	0.43
2:A:197:TYR:O	2:A:203:ILE:HD11	2.17	0.43
2:A:301:PRO:C	2:A:303:ASP:H	2.27	0.43
2:A:402:MET:C	2:A:403:LEU:HD22	2.44	0.43
2:A:490:HIS:HB2	2:A:542:VAL:HG21	2.00	0.43
2:A:558:LYS:HB3	2:A:558:LYS:HE3	1.83	0.43
3:C:275:ILE:HG22	3:C:275:ILE:O	2.19	0.43
3:C:574:LEU:C	3:C:578:ARG:NH1	2.77	0.43
1:D:60:LYS:HG2	1:D:71:HIS:HB2	2.00	0.43
1:D:94:VAL:HG22	1:D:97:MET:HE2	2.01	0.43
1:D:97:MET:CG	1:D:134:LEU:HD22	2.49	0.43
1:D:155:LYS:O	1:D:213:GLU:HB2	2.19	0.43
1:D:404:ARG:O	1:D:408:ILE:HG23	2.18	0.43
1:D:409:TYR:HB3	1:D:412:MET:CE	2.48	0.43
2:B:159:GLN:NE2	2:B:174:THR:OG1	2.51	0.43
2:B:370:ILE:HG22	2:B:371:MET:H	1.84	0.43
2:B:637:ASN:H	2:B:643:ILE:HG13	1.84	0.43
2:A:56:LEU:HD13	2:A:56:LEU:HA	1.70	0.43
2:A:384:PHE:CE1	2:A:385:ILE:HG12	2.54	0.43
3:C:325:LEU:HG	3:C:368:ILE:O	2.18	0.43
2:B:75:GLU:HG2	2:B:77:HIS:CE1	2.54	0.42
2:B:592:LEU:HD12	2:B:595:SER:HB3	2.01	0.42
2:A:294:LYS:HE3	2:A:294:LYS:HB3	1.46	0.42
2:A:349:PHE:HB3	3:C:556:MET:CE	2.49	0.42
3:C:360:HIS:HD2	3:C:363:LEU:HD23	1.84	0.42
1:D:19:ALA:HA	1:D:36:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:SER:HB3	1:D:116:ALA:H	1.60	0.42
1:D:179:ARG:HE	1:D:235:ILE:HD13	1.84	0.42
1:D:293:LYS:O	1:D:297:TRP:CD1	2.72	0.42
2:B:436:LYS:O	2:B:440:GLN:HG2	2.18	0.42
2:A:25:GLU:HB3	2:A:28:GLN:OE1	2.19	0.42
2:A:192:GLU:O	2:A:195:THR:HB	2.19	0.42
2:A:637:ASN:H	2:A:643:ILE:HG13	1.84	0.42
3:C:312:ARG:HD2	3:C:313:THR:O	2.19	0.42
3:C:380:LEU:HG	3:C:381:VAL:N	2.32	0.42
3:C:550:VAL:CA	3:C:553:LYS:HG2	2.39	0.42
1:D:93:GLY:O	1:D:97:MET:HB2	2.19	0.42
2:B:144:VAL:C	2:B:191:LYS:HZ3	2.26	0.42
2:B:406:SER:O	2:B:410:LYS:HG2	2.20	0.42
2:B:438:TYR:HE2	2:B:463:LEU:HA	1.84	0.42
2:A:397:ASN:HD21	2:A:402:MET:C	2.27	0.42
1:D:201:GLY:O	1:D:223:TYR:OH	2.36	0.42
1:D:208:LYS:HD2	1:D:208:LYS:HA	1.87	0.42
2:B:150:VAL:HB	2:B:186:VAL:HG22	2.01	0.42
2:B:506:ALA:HB1	2:B:592:LEU:HB2	2.02	0.42
2:A:424:PHE:HE1	2:A:437:PHE:HE2	1.66	0.42
2:A:619:LEU:HA	2:A:619:LEU:HD23	1.69	0.42
3:C:326:ARG:HB3	3:C:366:ASP:OD2	2.19	0.42
1:D:256:SER:C	1:D:258:GLU:N	2.77	0.42
1:D:264:LYS:HZ2	1:D:297:TRP:CD1	2.37	0.42
2:B:657:LYS:HA	2:B:660:LYS:HB3	2.00	0.42
2:A:96:ILE:HD11	2:A:155:ASN:HB3	2.02	0.42
2:A:210:HIS:HB3	2:A:369:PHE:CD2	2.54	0.42
2:A:347:ALA:HB2	2:A:440:GLN:HB2	2.02	0.42
2:A:441:PHE:O	2:A:445:ILE:HG13	2.20	0.42
3:C:157:LEU:HB3	3:C:174:THR:HG22	2.00	0.42
1:D:304:LEU:CG	1:D:305:SER:N	2.82	0.42
2:B:496:GLY:HA3	2:B:502:VAL:CG1	2.50	0.42
2:B:696:LEU:HB2	2:B:698:ILE:HG13	2.01	0.42
3:C:324:THR:OG1	3:C:325:LEU:N	2.49	0.42
3:C:361:ARG:HA	3:C:361:ARG:HD3	1.82	0.42
1:D:168:VAL:HG22	1:D:188:PHE:O	2.19	0.42
2:B:441:PHE:O	2:B:445:ILE:HG13	2.20	0.42
2:A:136:VAL:HA	2:A:139:TYR:CD2	2.54	0.42
2:A:681:PRO:O	2:A:682:GLN:C	2.63	0.42
3:C:542:ASN:ND2	3:C:552:THR:OG1	2.52	0.42
1:D:384:ASN:ND2	1:D:385:LYS:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:LYS:CG	2:B:694:LEU:HD11	2.48	0.42
2:B:215:GLY:H	2:B:367:ARG:NH1	2.18	0.42
1:D:31:ARG:HB3	1:D:108:LYS:HE2	2.01	0.42
2:B:190:LEU:HD12	2:B:191:LYS:N	2.34	0.42
2:B:328:HIS:CD2	2:B:340:LEU:HD13	2.55	0.42
2:B:402:MET:C	2:B:403:LEU:HD22	2.45	0.42
2:A:672:LEU:HD21	2:A:678:LEU:HD22	2.00	0.42
3:C:442:ILE:O	3:C:446:ILE:HG13	2.20	0.42
1:D:61:LEU:HD12	1:D:66:LYS:C	2.44	0.42
1:D:65:LYS:HB2	1:D:65:LYS:HE2	1.34	0.42
1:D:405:ASP:OD1	2:A:694:LEU:HD11	2.20	0.42
2:B:50:SER:O	2:B:53:SER:OG	2.29	0.42
2:B:366:ARG:N	2:B:392:GLU:O	2.53	0.42
2:B:498:THR:O	2:B:502:VAL:HG13	2.20	0.42
2:A:396:LEU:O	2:A:404:GLN:NE2	2.53	0.42
2:A:584:GLU:H	2:A:584:GLU:HG3	1.40	0.42
3:C:520:LYS:HB2	3:C:520:LYS:HE2	1.86	0.42
1:D:254:LYS:HG3	1:D:258:GLU:HB3	2.02	0.41
2:B:326:VAL:HB	2:B:342:PHE:CD1	2.55	0.41
2:B:374:CYS:C	2:B:376:GLU:H	2.28	0.41
2:B:377:LEU:H	2:B:377:LEU:HG	1.51	0.41
2:B:399:SER:C	2:B:401:GLU:H	2.27	0.41
2:B:535:GLU:O	2:B:535:GLU:HG3	2.20	0.41
2:B:688:ILE:HA	2:B:691:MET:HE2	2.00	0.41
2:A:25:GLU:HB3	2:A:28:GLN:CD	2.45	0.41
2:A:103:LEU:HA	2:A:106:ASN:ND2	2.30	0.41
2:A:328:HIS:CD2	2:A:340:LEU:HD13	2.55	0.41
2:A:414:LYS:O	2:A:418:LYS:HE2	2.20	0.41
2:A:599:ILE:HD12	2:A:671:LEU:HA	2.01	0.41
1:D:92:ILE:HG12	1:D:111:TYR:CE2	2.55	0.41
1:D:93:GLY:C	1:D:95:ALA:H	2.27	0.41
1:D:377:VAL:HA	1:D:380:VAL:HG22	2.02	0.41
2:B:69:LYS:CG	2:B:70:LEU:N	2.83	0.41
2:B:179:PRO:O	2:B:180:MET:C	2.62	0.41
2:B:279:LYS:HB3	2:B:280:ILE:H	1.57	0.41
2:B:306:ASN:ND2	2:B:323:HIS:HE1	2.18	0.41
2:A:334:GLN:HG2	2:A:335:LEU:H	1.84	0.41
2:A:399:SER:C	2:A:401:GLU:H	2.27	0.41
3:C:514:GLU:O	3:C:519:LEU:HD23	2.19	0.41
1:D:34:LEU:HG	1:D:36:ILE:CG1	2.47	0.41
1:D:320:PHE:CE1	1:D:342:LYS:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:THR:CG2	2:B:184:THR:HG22	2.49	0.41
2:B:200:GLU:HG2	2:B:201:ARG:N	2.35	0.41
2:B:649:LYS:HB2	2:B:649:LYS:HE2	1.54	0.41
2:B:661:ASP:O	2:B:664:ILE:HB	2.20	0.41
2:A:98:MET:HG3	2:A:106:ASN:HD21	1.85	0.41
2:A:116:LYS:O	2:A:119:MET:HE3	2.19	0.41
2:A:591:ARG:HG3	2:A:592:LEU:HD13	2.02	0.41
1:D:404:ARG:HH22	2:A:657:LYS:CB	2.34	0.41
1:D:404:ARG:HH12	2:A:658:SER:H	1.68	0.41
2:B:678:LEU:HD12	2:B:679:GLU:N	2.35	0.41
2:A:28:GLN:OE1	2:A:29:LEU:N	2.48	0.41
2:A:461:GLU:HG3	2:A:536:PHE:HE1	1.86	0.41
3:C:364:LYS:H	3:C:367:ASN:ND2	2.17	0.41
2:B:25:GLU:HB3	2:B:28:GLN:CD	2.45	0.41
2:B:192:GLU:O	2:B:195:THR:HB	2.19	0.41
2:B:414:LYS:HB2	2:B:414:LYS:HE3	1.85	0.41
2:B:588:VAL:HG13	2:B:636:ILE:HD11	2.02	0.41
2:B:615:LYS:HZ3	2:B:615:LYS:HG2	1.74	0.41
2:A:571:LEU:HA	2:A:571:LEU:HD12	1.82	0.41
3:C:563:GLU:O	3:C:567:LEU:HB2	2.20	0.41
2:B:151:ILE:C	2:B:152:THR:HG1	2.28	0.41
2:B:396:LEU:HD22	2:B:400:ARG:HG3	2.02	0.41
2:A:163:GLU:N	2:A:163:GLU:OE1	2.54	0.41
2:A:228:LYS:HB3	2:A:280:ILE:HB	2.02	0.41
2:A:455:ASN:HB2	2:A:458:LYS:HB2	2.02	0.41
2:A:604:TYR:C	2:A:631:LYS:HD2	2.45	0.41
3:C:356:GLN:C	3:C:358:ILE:H	2.29	0.41
1:D:291:TYR:HB2	1:D:323:LEU:HD13	2.03	0.41
2:B:25:GLU:HB3	2:B:28:GLN:NE2	2.36	0.41
2:B:171:THR:OG1	2:A:17:VAL:HB	2.20	0.41
2:B:297:TRP:HA	2:B:328:HIS:CE1	2.55	0.41
2:B:472:ASP:OD1	2:B:473:GLU:N	2.49	0.41
2:A:151:ILE:HA	2:A:160:TYR:O	2.21	0.41
2:A:486:GLU:O	2:A:487:ASN:C	2.64	0.41
3:C:525:ASP:CG	3:C:526:LYS:HZ1	2.29	0.41
3:C:576:SER:C	3:C:578:ARG:N	2.76	0.41
3:C:577:TRP:HB2	3:C:578:ARG:CD	2.44	0.41
1:D:163:ASN:HD22	1:D:252:LYS:HD2	1.86	0.41
1:D:271:VAL:HA	1:D:274:LYS:HB2	2.03	0.41
2:B:163:GLU:OE1	2:B:163:GLU:N	2.54	0.41
2:B:397:ASN:N	2:B:400:ARG:HA	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:THR:HA	2:B:521:MET:O	2.20	0.41
2:A:200:GLU:HG2	2:A:201:ARG:N	2.36	0.41
2:A:431:LYS:HE3	2:A:431:LYS:HB3	1.61	0.41
2:A:517:GLU:H	2:A:517:GLU:HG2	1.68	0.41
2:A:644:GLU:O	2:A:647:ARG:HB3	2.20	0.41
2:A:649:LYS:HE2	2:A:649:LYS:HB2	1.57	0.41
2:A:696:LEU:HB2	2:A:698:ILE:HG13	2.01	0.41
1:D:336:ALA:HA	1:D:339:CYS:SG	2.61	0.41
2:B:56:LEU:HD11	2:B:94:THR:C	2.46	0.41
2:B:325:ALA:H	2:B:343:VAL:HG13	1.86	0.41
2:B:347:ALA:HB2	2:B:440:GLN:HB2	2.02	0.41
2:B:365:VAL:HG22	2:B:370:ILE:CD1	2.51	0.41
2:B:417:VAL:O	2:B:421:LEU:HB2	2.21	0.41
2:B:435:LYS:HG3	2:B:439:GLU:OE2	2.21	0.41
2:B:523:GLU:HB2	2:B:526:ASP:HB2	2.03	0.41
2:B:551:LEU:HA	2:B:552:PRO:HD3	1.95	0.41
2:A:612:ARG:O	2:A:616:ALA:N	2.44	0.41
3:C:569:GLN:NE2	3:C:569:GLN:H	2.19	0.41
1:D:60:LYS:HD2	1:D:60:LYS:HA	1.78	0.41
1:D:255:GLU:CD	1:D:256:SER:N	2.74	0.41
1:D:335:LYS:HE2	1:D:335:LYS:HB2	1.92	0.41
2:B:327:LYS:HA	2:B:327:LYS:HD3	1.68	0.41
2:B:464:ARG:C	2:B:474:MET:HB3	2.46	0.41
2:B:573:LYS:HD2	2:B:573:LYS:HA	1.55	0.41
2:A:207:VAL:O	2:A:212:GLN:HB3	2.21	0.41
2:A:355:ARG:HE	2:A:355:ARG:HB3	1.35	0.41
2:A:665:LEU:O	2:A:669:THR:HG23	2.21	0.41
3:C:546:GLU:HA	3:C:551:GLU:OE1	2.20	0.41
3:C:562:LEU:CD2	3:C:567:LEU:HD11	2.45	0.41
1:D:31:ARG:HH21	1:D:110:GLU:H	1.68	0.40
1:D:154:ARG:CB	1:D:214:GLN:H	2.29	0.40
1:D:291:TYR:HE2	1:D:322:ASN:HB3	1.85	0.40
1:D:321:LEU:O	1:D:325:MET:HG3	2.21	0.40
1:D:339:CYS:HA	1:D:342:LYS:CE	2.47	0.40
2:B:228:LYS:H	2:B:281:LYS:HD3	1.86	0.40
2:B:301:PRO:HB3	2:B:328:HIS:ND1	2.36	0.40
2:B:331:VAL:HG21	2:B:337:PHE:CD2	2.56	0.40
2:B:331:VAL:HG21	2:B:337:PHE:CZ	2.56	0.40
2:B:415:ASN:HA	2:B:418:LYS:CE	2.51	0.40
2:B:533:LEU:HD22	2:B:533:LEU:HA	1.79	0.40
2:B:620:ARG:HA	2:B:620:ARG:HD2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:662:LEU:O	2:B:666:LEU:HG	2.21	0.40
2:B:665:LEU:O	2:B:669:THR:HG23	2.21	0.40
2:B:681:PRO:O	2:B:682:GLN:C	2.63	0.40
2:A:25:GLU:HB3	2:A:28:GLN:NE2	2.36	0.40
2:A:56:LEU:HD11	2:A:94:THR:C	2.46	0.40
2:A:92:VAL:HA	2:A:185:LYS:HB3	2.03	0.40
2:A:110:ILE:HG13	2:A:139:TYR:CZ	2.55	0.40
2:A:419:LYS:HA	2:A:422:GLU:CD	2.45	0.40
3:C:324:THR:HG1	3:C:369:LEU:HA	1.86	0.40
3:C:335:SER:O	3:C:339:ALA:N	2.45	0.40
2:B:403:LEU:HD13	2:B:403:LEU:HA	1.88	0.40
2:B:419:LYS:HA	2:B:422:GLU:CD	2.45	0.40
2:B:419:LYS:HA	2:B:422:GLU:OE1	2.21	0.40
2:B:550:GLU:C	2:B:551:LEU:HD22	2.46	0.40
2:A:199:GLU:O	2:A:202:ARG:HB3	2.21	0.40
2:A:326:VAL:HB	2:A:342:PHE:CD1	2.55	0.40
2:A:544:VAL:HA	2:A:549:LEU:HD13	2.04	0.40
1:D:157:GLU:HG3	1:D:159:TYR:N	2.24	0.40
1:D:158:GLY:HA2	1:D:210:GLN:HE22	1.86	0.40
1:D:260:ASP:O	1:D:264:LYS:N	2.44	0.40
1:D:397:LYS:HA	1:D:400:GLU:OE1	2.21	0.40
2:B:32:LEU:O	2:B:36:THR:OG1	2.23	0.40
2:B:428:ALA:HA	2:B:434:TYR:CG	2.57	0.40
2:B:687:ARG:HE	2:B:687:ARG:HB2	1.63	0.40
2:A:84:LYS:NZ	2:A:224:LYS:HG3	2.36	0.40
2:A:188:LEU:HD23	2:A:189:HIS:N	2.36	0.40
3:C:315:PHE:CG	3:C:316:LEU:N	2.89	0.40
3:C:481:ASP:HB2	3:C:577:TRP:CE3	2.56	0.40
2:B:544:VAL:HA	2:B:549:LEU:HD13	2.04	0.40
2:B:628:MET:HE3	3:C:375:ASP:N	2.37	0.40
2:B:654:LYS:H	2:B:654:LYS:HG3	1.79	0.40
2:A:320:TRP:HD1	3:C:539:LEU:HG	1.86	0.40
2:A:331:VAL:HG21	2:A:337:PHE:CZ	2.56	0.40
2:A:428:ALA:HA	2:A:434:TYR:CG	2.57	0.40
2:A:550:GLU:C	2:A:551:LEU:HD22	2.46	0.40
3:C:263:ARG:HH11	3:C:263:ARG:HA	1.85	0.40
3:C:317:VAL:HG22	3:C:318:MET:H	1.86	0.40
3:C:547:LYS:N	3:C:547:LYS:HD3	2.37	0.40
1:D:171:HIS:O	1:D:172:LEU:HD23	2.22	0.40
1:D:199:PRO:HA	1:D:225:PHE:HB2	2.02	0.40
1:D:361:GLN:OE1	1:D:369:SER:OG	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:MET:HG3	2:B:690:ARG:NH1	2.37	0.40
2:B:150:VAL:HB	2:B:186:VAL:HG13	2.03	0.40
2:B:199:GLU:O	2:B:202:ARG:HB3	2.21	0.40
2:B:321:GLU:CD	2:B:322:ASP:H	2.30	0.40
2:B:457:LYS:HE3	2:B:457:LYS:HB3	1.78	0.40
2:B:571:LEU:HD22	2:B:647:ARG:HB2	2.04	0.40
2:B:673:SER:C	2:B:675:GLY:H	2.29	0.40
2:A:321:GLU:OE1	2:A:345:ARG:HB3	2.21	0.40
2:A:417:VAL:O	2:A:421:LEU:HB2	2.21	0.40
2:A:435:LYS:HG3	2:A:439:GLU:OE2	2.21	0.40
2:A:678:LEU:HD12	2:A:679:GLU:N	2.35	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	D	407/457 (89%)	360 (88%)	47 (12%)	0	100	100
2	A	631/732 (86%)	560 (89%)	71 (11%)	0	100	100
2	B	631/732 (86%)	554 (88%)	77 (12%)	0	100	100
3	C	286/494 (58%)	253 (88%)	33 (12%)	0	100	100
All	All	1955/2415 (81%)	1727 (88%)	228 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	D	339/378 (90%)	289 (85%)	50 (15%)	3	14
2	A	576/666 (86%)	425 (74%)	151 (26%)	0	3
2	B	576/666 (86%)	471 (82%)	105 (18%)	2	10
3	C	283/406 (70%)	246 (87%)	37 (13%)	4	16
All	All	1774/2116 (84%)	1431 (81%)	343 (19%)	3	8

All (343) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	38	LYS
1	D	39	ARG
1	D	40	VAL
1	D	42	ASN
1	D	44	GLU
1	D	45	GLU
1	D	46	THR
1	D	48	MET
1	D	49	ILE
1	D	52	LYS
1	D	53	VAL
1	D	55	VAL
1	D	58	LYS
1	D	60	LYS
1	D	65	LYS
1	D	66	LYS
1	D	68	ASP
1	D	69	SER
1	D	72	ASP
1	D	73	ARG
1	D	74	ASN
1	D	78	VAL
1	D	81	LEU
1	D	83	LYS
1	D	85	GLN
1	D	86	VAL
1	D	87	ILE
1	D	88	LYS
1	D	92	ILE
1	D	96	THR

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Mol	Chain	Res	Type
1	D	97	MET
1	D	98	LYS
1	D	99	LYS
1	D	102	ILE
1	D	105	LEU
1	D	106	LEU
1	D	107	CYS
1	D	108	LYS
1	D	119	LEU
1	D	121	LYS
1	D	122	ILE
1	D	128	LEU
1	D	129	PHE
1	D	130	PHE
1	D	132	ILE
1	D	134	LEU
1	D	135	LEU
1	D	272	LYS
1	D	274	LYS
1	D	280	LYS
2	B	16	GLU
2	B	32	LEU
2	B	39	SER
2	B	40	ASN
2	B	41	LYS
2	B	42	GLU
2	B	43	ILE
2	B	45	LEU
2	B	49	ILE
2	B	74	LYS
2	B	75	GLU
2	B	78	ILE
2	B	98	MET
2	B	99	THR
2	B	100	LYS
2	B	107	LEU
2	B	113	SER
2	B	116	LYS
2	B	130	MET
2	B	131	ILE
2	B	133	GLN
2	B	136	VAL

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Mol	Chain	Res	Type
2	B	203	ILE
2	B	210	HIS
2	B	279	LYS
2	B	280	ILE
2	B	281	LYS
2	B	282	GLU
2	B	283	LYS
2	B	285	ILE
2	B	323	HIS
2	B	351	LEU
2	B	355	ARG
2	B	356	LYS
2	B	357	LYS
2	B	358	LYS
2	B	361	ILE
2	B	363	LEU
2	B	374	CYS
2	B	376	GLU
2	B	377	LEU
2	B	378	ILE
2	B	382	LEU
2	B	412	ILE
2	B	431	LYS
2	B	455	ASN
2	B	457	LYS
2	B	461	GLU
2	B	462	LEU
2	B	463	LEU
2	B	464	ARG
2	B	483	ARG
2	B	484	MET
2	B	485	LYS
2	B	489	LYS
2	B	494	ILE
2	B	498	THR
2	B	499	LYS
2	B	500	ASP
2	B	502	VAL
2	B	505	SER
2	B	508	VAL
2	B	509	GLU
2	B	510	ARG

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Mol	Chain	Res	Type
2	B	516	LEU
2	B	518	VAL
2	B	519	ILE
2	B	522	ILE
2	B	525	ILE
2	B	527	GLU
2	B	529	CYS
2	B	533	LEU
2	B	534	LYS
2	B	561	GLN
2	B	567	LYS
2	B	570	ASN
2	B	571	LEU
2	B	573	LYS
2	B	584	GLU
2	B	585	LYS
2	B	586	VAL
2	B	587	VAL
2	B	589	SER
2	B	591	ARG
2	B	601	THR
2	B	607	THR
2	B	611	GLU
2	B	612	ARG
2	B	613	ILE
2	B	615	LYS
2	B	617	GLN
2	B	620	ARG
2	B	622	ASN
2	B	623	SER
2	B	624	THR
2	B	625	MET
2	B	631	LYS
2	B	647	ARG
2	B	648	GLN
2	B	649	LYS
2	B	651	GLU
2	B	654	LYS
2	B	657	LYS
2	B	668	GLU
2	B	687	ARG
2	A	32	LEU

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Mol	Chain	Res	Type
2	A	41	LYS
2	A	42	GLU
2	A	43	ILE
2	A	44	PHE
2	A	49	ILE
2	A	52	SER
2	A	65	THR
2	A	68	SER
2	A	69	LYS
2	A	70	LEU
2	A	74	LYS
2	A	75	GLU
2	A	76	LEU
2	A	77	HIS
2	A	78	ILE
2	A	79	ASN
2	A	80	LEU
2	A	81	ILE
2	A	98	MET
2	A	99	THR
2	A	100	LYS
2	A	113	SER
2	A	116	LYS
2	A	131	ILE
2	A	172	VAL
2	A	174	THR
2	A	175	ASP
2	A	203	ILE
2	A	208	LYS
2	A	279	LYS
2	A	280	ILE
2	A	281	LYS
2	A	283	LYS
2	A	285	ILE
2	A	291	ASN
2	A	292	LYS
2	A	294	LYS
2	A	298	THR
2	A	299	ARG
2	A	300	ASN
2	A	304	ILE
2	A	305	THR

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Mol	Chain	Res	Type
2	A	306	ASN
2	A	307	GLU
2	A	308	GLU
2	A	314	LYS
2	A	315	SER
2	A	317	THR
2	A	323	HIS
2	A	350	ASP
2	A	355	ARG
2	A	356	LYS
2	A	357	LYS
2	A	358	LYS
2	A	361	ILE
2	A	362	LYS
2	A	363	LEU
2	A	366	ARG
2	A	367	ARG
2	A	369	PHE
2	A	370	ILE
2	A	372	ASP
2	A	374	CYS
2	A	375	GLU
2	A	376	GLU
2	A	377	LEU
2	A	378	ILE
2	A	380	GLU
2	A	382	LEU
2	A	390	ASP
2	A	392	GLU
2	A	393	ASP
2	A	394	LEU
2	A	410	LYS
2	A	412	ILE
2	A	413	ARG
2	A	414	LYS
2	A	431	LYS
2	A	455	ASN
2	A	456	ARG
2	A	457	LYS
2	A	458	LYS
2	A	462	LEU
2	A	463	LEU

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Mol	Chain	Res	Type
2	A	464	ARG
2	A	468	SER
2	A	474	MET
2	A	475	VAL
2	A	476	SER
2	A	477	LEU
2	A	481	CYS
2	A	482	THR
2	A	483	ARG
2	A	484	MET
2	A	485	LYS
2	A	486	GLU
2	A	487	ASN
2	A	488	GLN
2	A	489	LYS
2	A	490	HIS
2	A	491	ILE
2	A	494	ILE
2	A	495	THR
2	A	498	THR
2	A	499	LYS
2	A	500	ASP
2	A	507	PHE
2	A	509	GLU
2	A	511	LEU
2	A	512	ARG
2	A	513	LYS
2	A	516	LEU
2	A	517	GLU
2	A	518	VAL
2	A	519	ILE
2	A	525	ILE
2	A	526	ASP
2	A	527	GLU
2	A	529	CYS
2	A	533	LEU
2	A	534	LYS
2	A	535	GLU
2	A	537	GLU
2	A	553	GLU
2	A	555	GLU
2	A	556	GLU

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Mol	Chain	Res	Type
2	A	563	GLU
2	A	565	LYS
2	A	566	THR
2	A	567	LYS
2	A	575	MET
2	A	582	LYS
2	A	583	VAL
2	A	584	GLU
2	A	585	LYS
2	A	586	VAL
2	A	587	VAL
2	A	593	VAL
2	A	595	SER
2	A	611	GLU
2	A	620	ARG
2	A	621	ASP
2	A	624	THR
2	A	625	MET
2	A	628	MET
2	A	649	LYS
2	A	651	GLU
2	A	654	LYS
2	A	655	ASN
2	A	668	GLU
3	C	370	VAL
3	C	372	LEU
3	C	375	ASP
3	C	377	CYS
3	C	380	LEU
3	C	381	VAL
3	C	382	ILE
3	C	384	ASP
3	C	387	CYS
3	C	433	LYS
3	C	439	VAL
3	C	445	GLU
3	C	449	LEU
3	C	450	VAL
3	C	451	ASN
3	C	456	GLN
3	C	458	LYS
3	C	461	LEU

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Mol	Chain	Res	Type
3	C	463	SER
3	C	464	ARG
3	C	465	SER
3	C	471	LEU
3	C	474	LEU
3	C	476	GLU
3	C	478	VAL
3	C	481	ASP
3	C	482	VAL
3	C	483	ARG
3	C	485	LEU
3	C	487	ARG
3	C	489	LEU
3	C	491	GLN
3	C	492	ARG
3	C	493	GLU
3	C	517	LEU
3	C	564	CYS
3	C	567	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	21	GLN
1	D	85	GLN
1	D	163	ASN
1	D	210	GLN
1	D	238	ASN
1	D	350	ASN
1	D	365	ASN
1	D	383	GLN
1	D	384	ASN
1	D	395	GLN
2	B	23	GLN
2	B	77	HIS
2	B	85	GLN
2	B	105	ASN
2	B	300	ASN
2	B	323	HIS
2	B	328	HIS
2	B	487	ASN
2	B	561	GLN

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Mol	Chain	Res	Type
2	B	570	ASN
2	B	590	ASN
2	B	617	GLN
2	A	23	GLN
2	A	83	ASN
2	A	105	ASN
2	A	106	ASN
2	A	133	GLN
2	A	291	ASN
2	A	318	ASN
2	A	323	HIS
2	A	359	ASN
2	A	514	HIS
2	A	622	ASN
3	C	235	ASN
3	C	304	HIS
3	C	332	ASN
3	C	356	GLN
3	C	367	ASN
3	C	467	GLN
3	C	505	ASN
3	C	534	GLN
3	C	569	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	B	801	-	28,29,29	1.36	5 (17%)	43,45,45	1.90	12 (27%)
4	ADP	A	801	-	28,29,29	1.36	5 (17%)	43,45,45	1.90	12 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	B	801	-	-	1/16/32/32	0/3/3/3
4	ADP	A	801	-	-	1/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	ADP	C5-C4	4.06	1.46	1.39
4	B	801	ADP	C5-C4	4.00	1.46	1.39
4	B	801	ADP	C4-N9	-2.82	1.31	1.37
4	A	801	ADP	C4-N9	-2.82	1.31	1.37
4	B	801	ADP	C5-N7	-2.63	1.34	1.39
4	A	801	ADP	C5-N7	-2.62	1.34	1.39
4	B	801	ADP	C5-C6	2.34	1.47	1.41
4	A	801	ADP	C5-C6	2.32	1.47	1.41
4	A	801	ADP	C8-N9	-2.07	1.34	1.37
4	B	801	ADP	C8-N9	-2.07	1.34	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	ADP	C5-C4-N3	-5.16	119.61	126.72
4	B	801	ADP	C5-C4-N3	-5.16	119.61	126.72
4	B	801	ADP	N3-C4-N9	4.38	134.62	127.17
4	A	801	ADP	N3-C4-N9	4.37	134.60	127.17
4	A	801	ADP	C2'-C1'-N9	-3.90	103.62	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	ADP	C2'-C1'-N9	-3.89	103.64	113.30
4	B	801	ADP	C4-N9-C8	3.66	109.58	105.74
4	A	801	ADP	C4-N9-C8	3.65	109.57	105.74
4	A	801	ADP	C2-N3-C4	3.44	120.23	111.83
4	B	801	ADP	C2-N3-C4	3.43	120.21	111.83
4	A	801	ADP	N3-C2-N1	-3.23	123.69	128.58
4	B	801	ADP	N3-C2-N1	-3.22	123.71	128.58
4	A	801	ADP	C4-C5-N7	-3.18	106.95	110.58
4	B	801	ADP	C4-C5-N7	-3.15	106.98	110.58
4	B	801	ADP	N9-C8-N7	-2.42	110.50	113.94
4	A	801	ADP	N9-C8-N7	-2.40	110.53	113.94
4	A	801	ADP	C5-N7-C8	2.36	107.17	103.45
4	B	801	ADP	C5-N7-C8	2.36	107.16	103.45
4	B	801	ADP	C3'-C2'-C1'	2.15	105.54	101.46
4	A	801	ADP	C3'-C2'-C1'	2.14	105.52	101.46
4	B	801	ADP	O4'-C1'-N9	-2.12	104.02	108.09
4	A	801	ADP	O4'-C1'-N9	-2.11	104.04	108.09
4	A	801	ADP	C6-C5-N7	2.03	136.00	132.09
4	B	801	ADP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

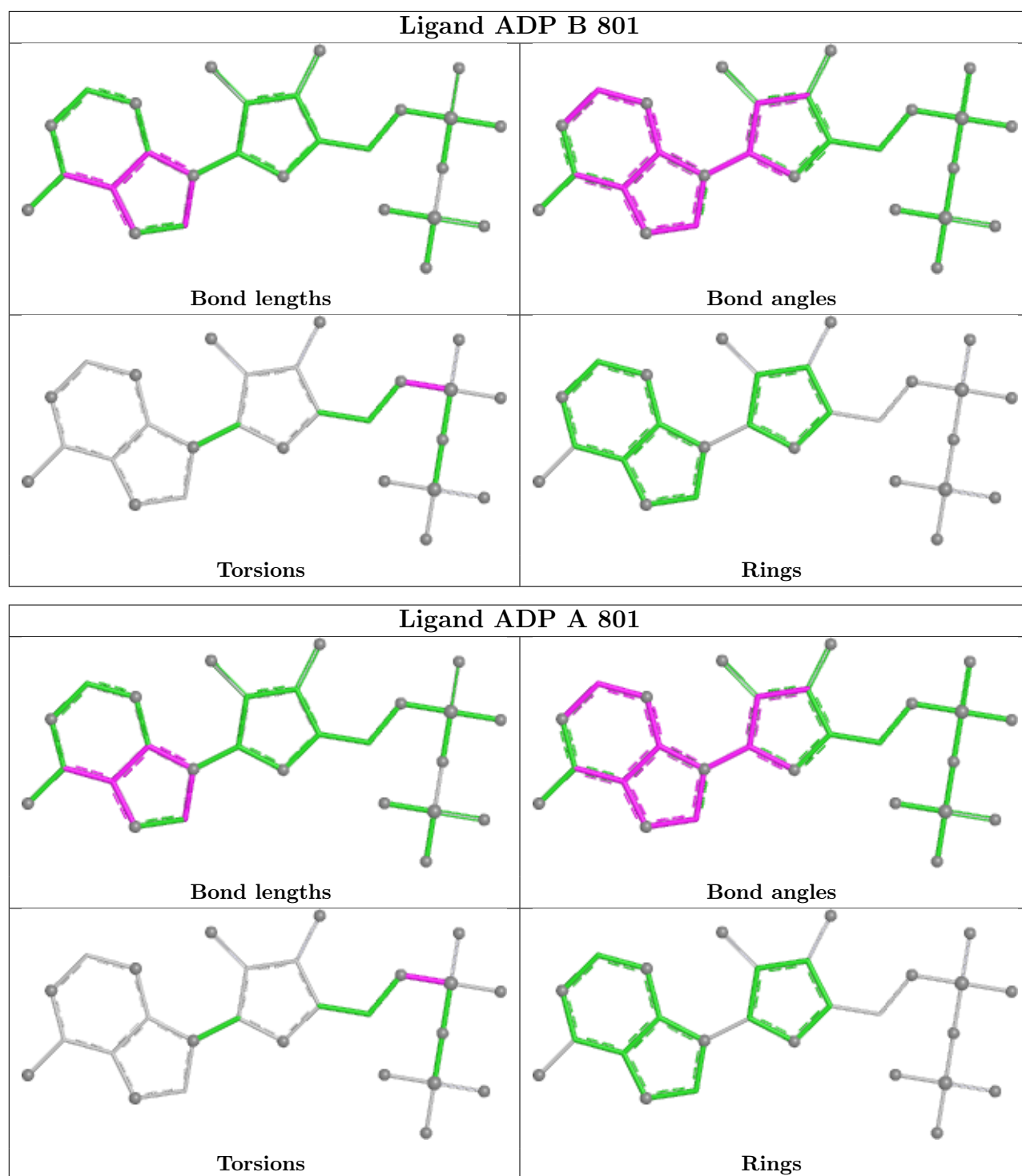
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	ADP	C5'-O5'-PA-O1A
4	A	801	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

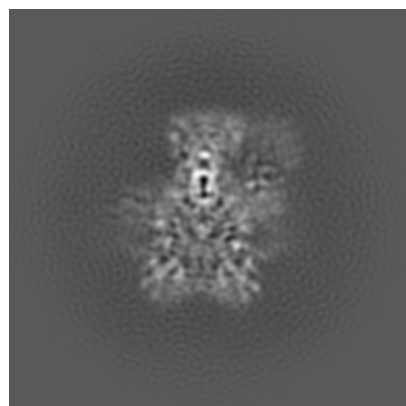
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62482. These allow visual inspection of the internal detail of the map and identification of artifacts.

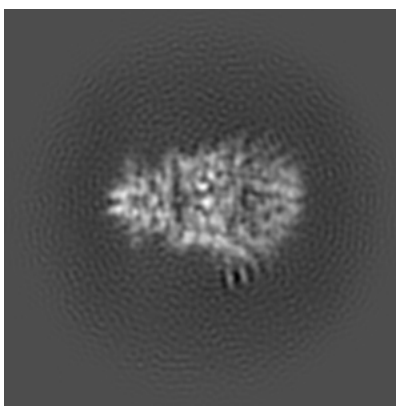
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

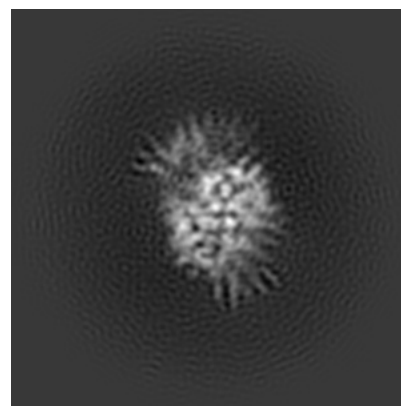
6.1.1 Primary map



X

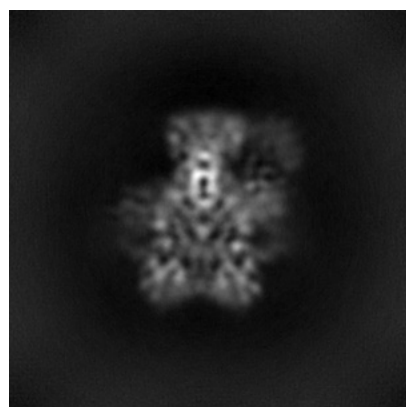


Y

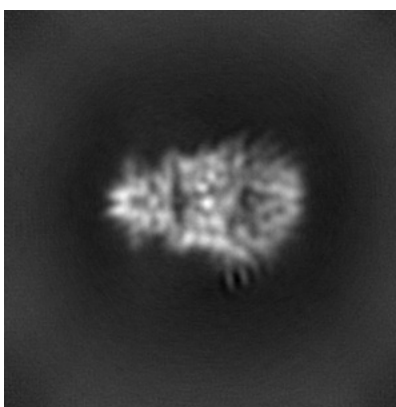


Z

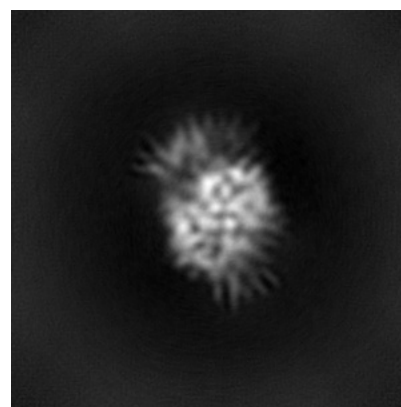
6.1.2 Raw map



X



Y

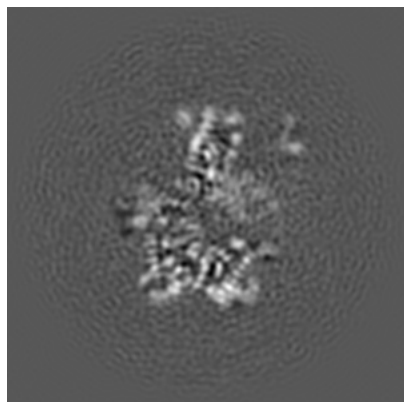


Z

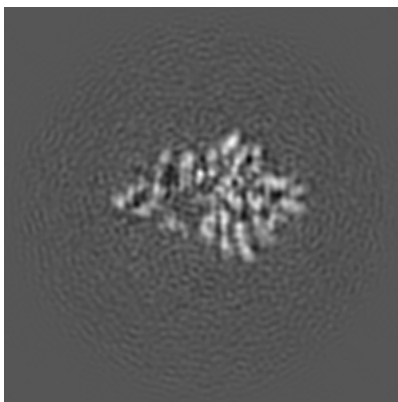
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

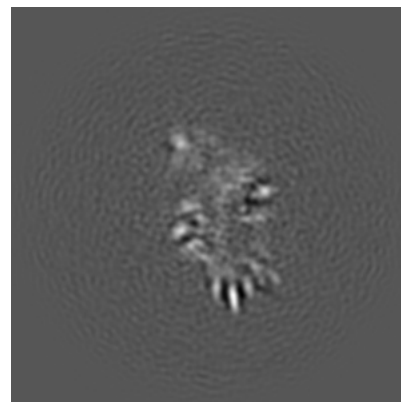
6.2.1 Primary map



X Index: 140

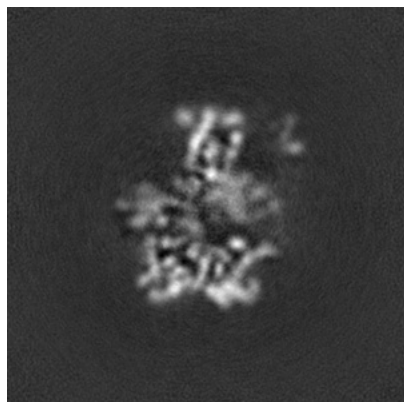


Y Index: 140

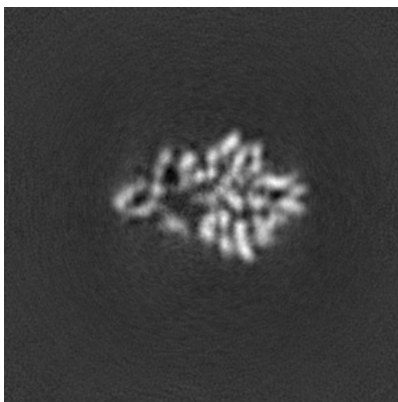


Z Index: 140

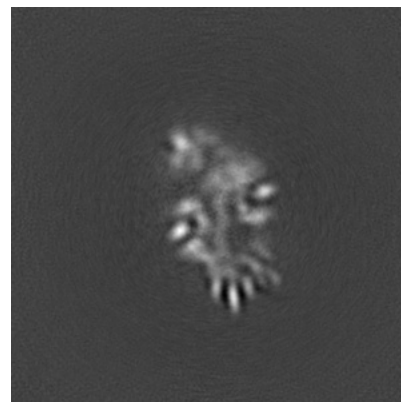
6.2.2 Raw map



X Index: 140



Y Index: 140

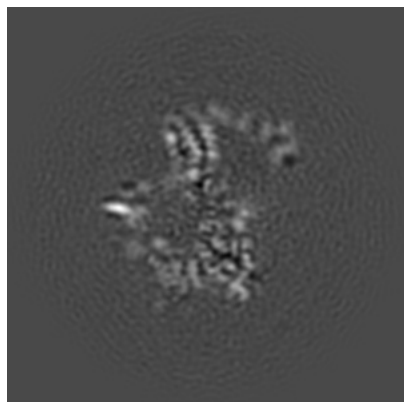


Z Index: 140

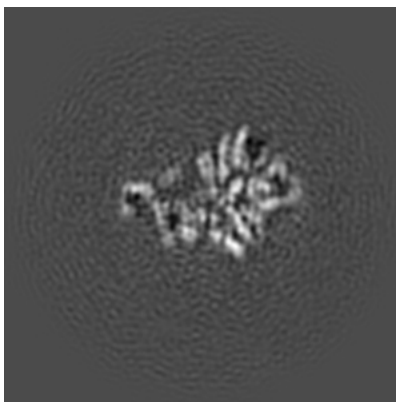
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

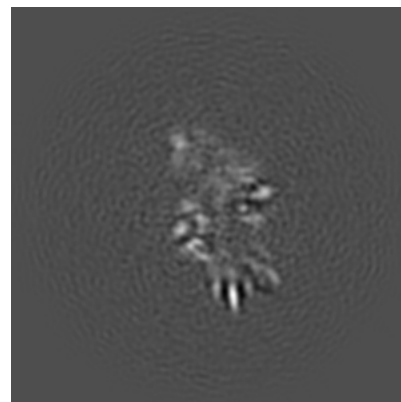
6.3.1 Primary map



X Index: 155

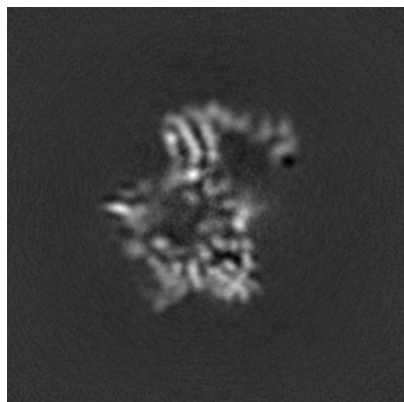


Y Index: 131

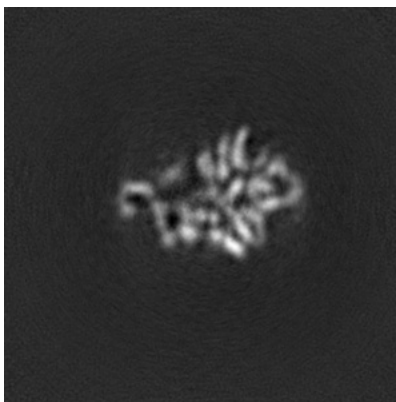


Z Index: 139

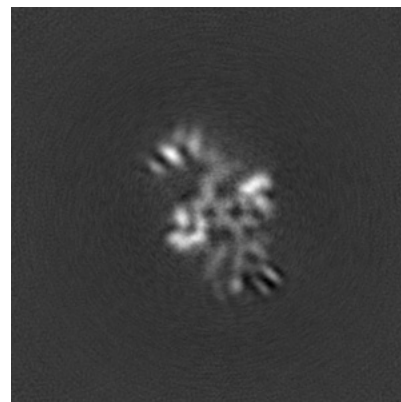
6.3.2 Raw map



X Index: 154



Y Index: 131

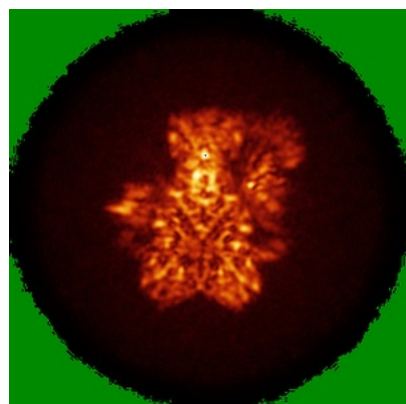


Z Index: 148

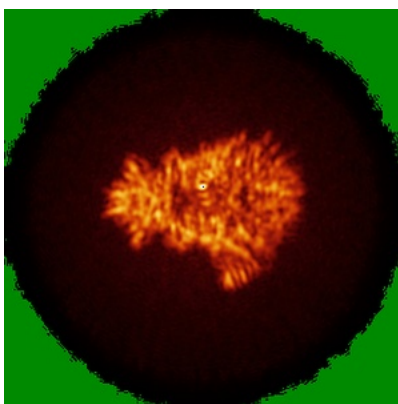
The images above show the largest variance slices of the map in three orthogonal directions.

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

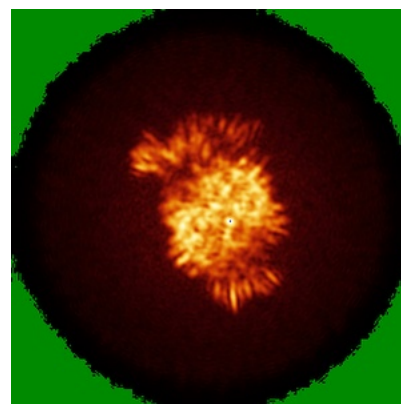
6.4.1 Primary map



X

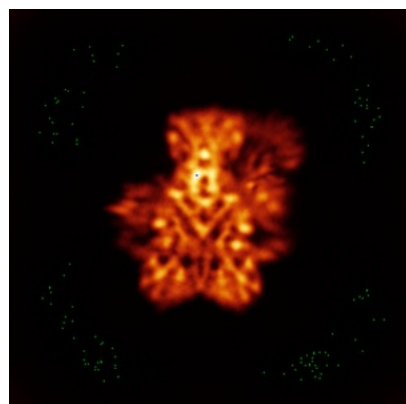


Y

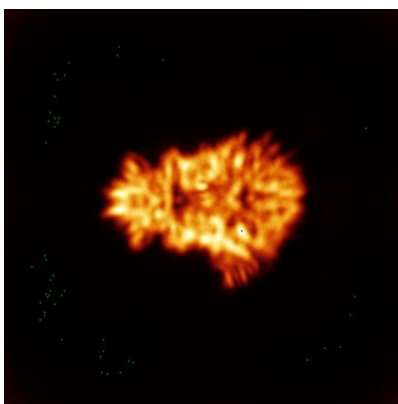


Z

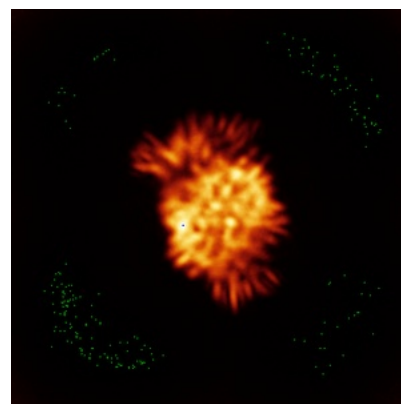
6.4.2 Raw map



X



Y

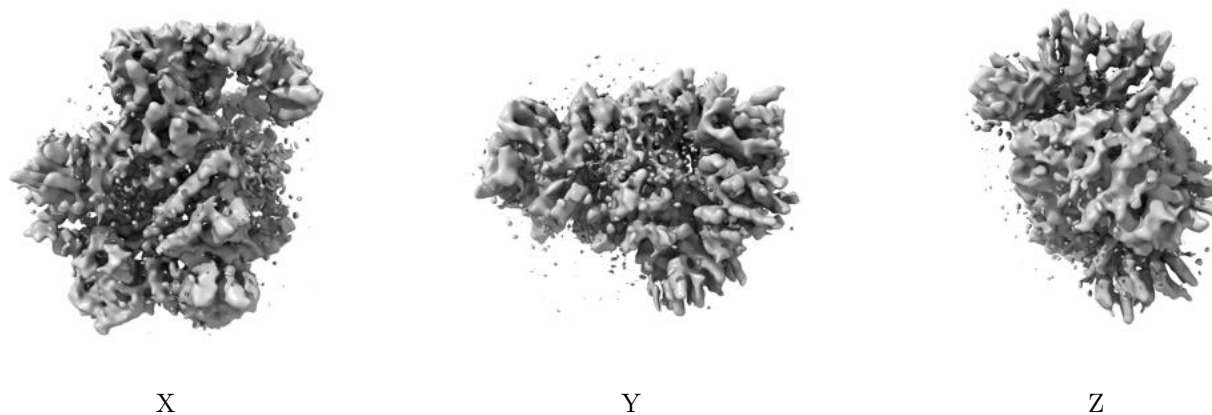


Z

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

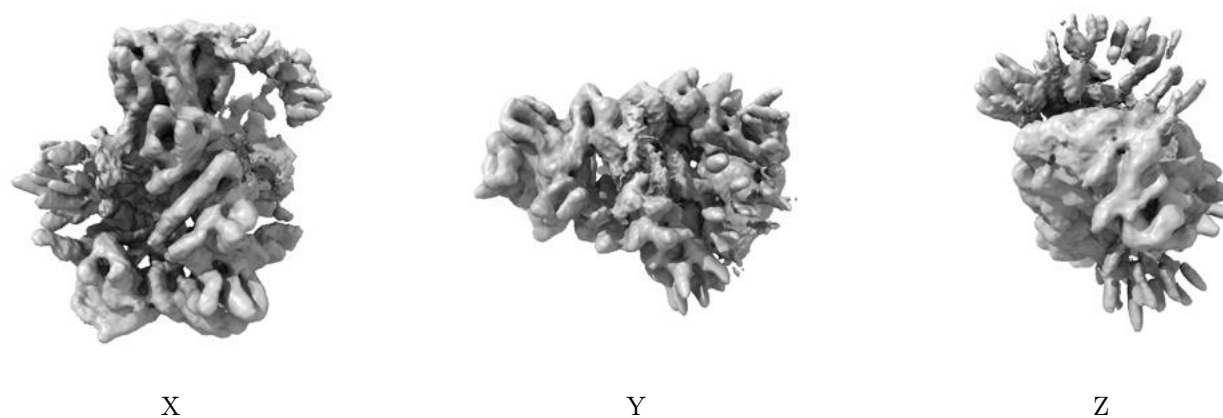
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.109. 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.

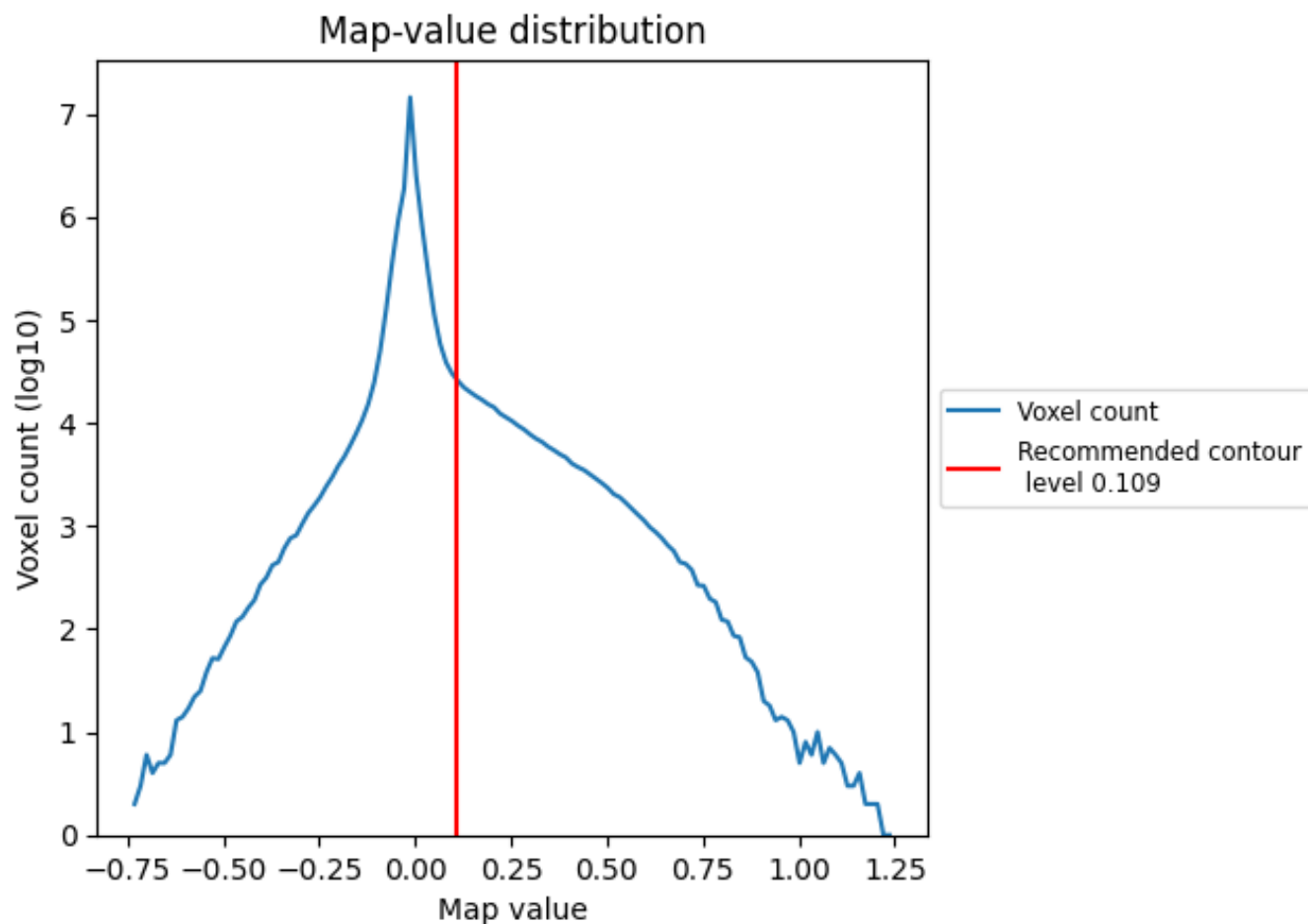
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

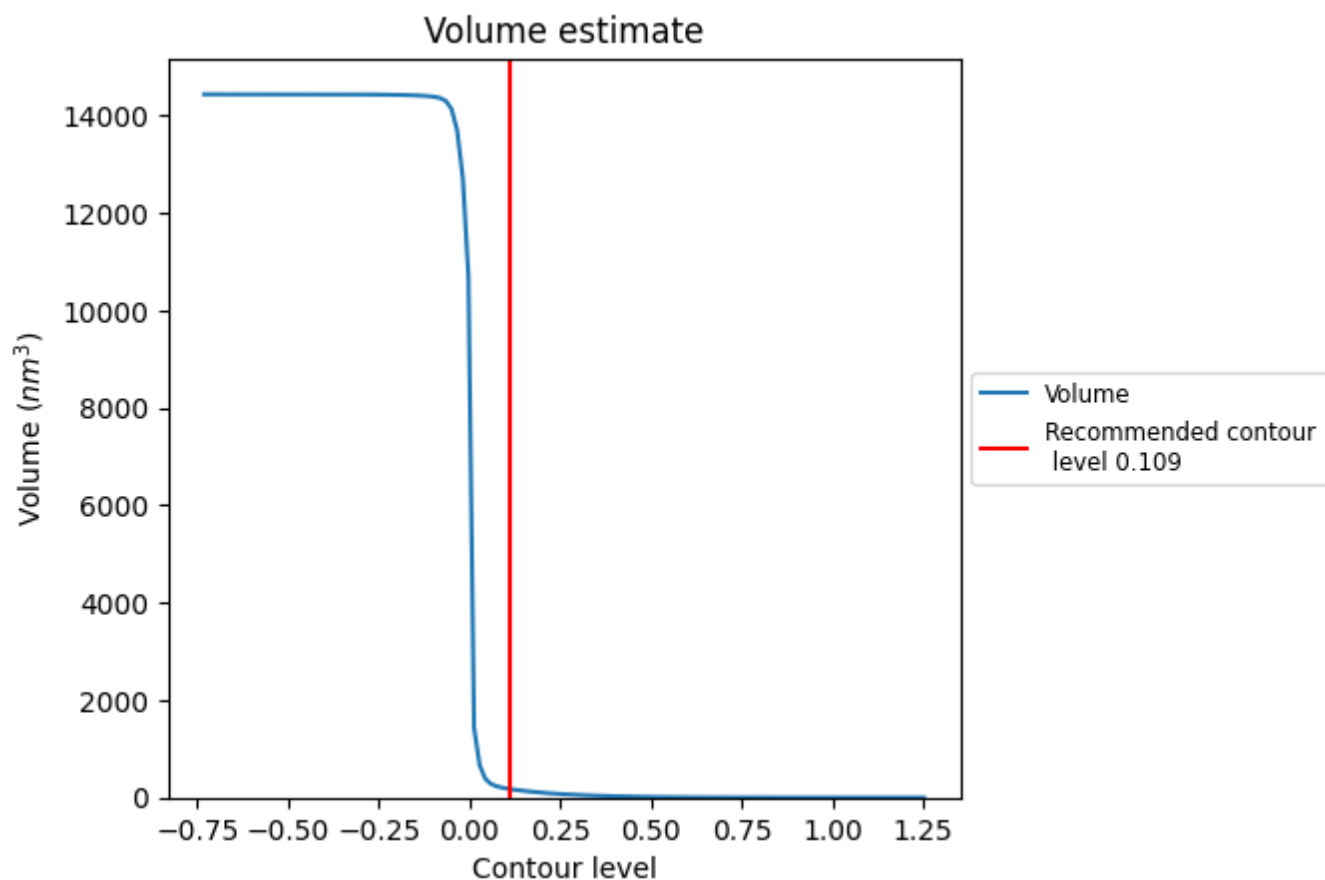
This section contains the results of statistical analysis of the map.

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.

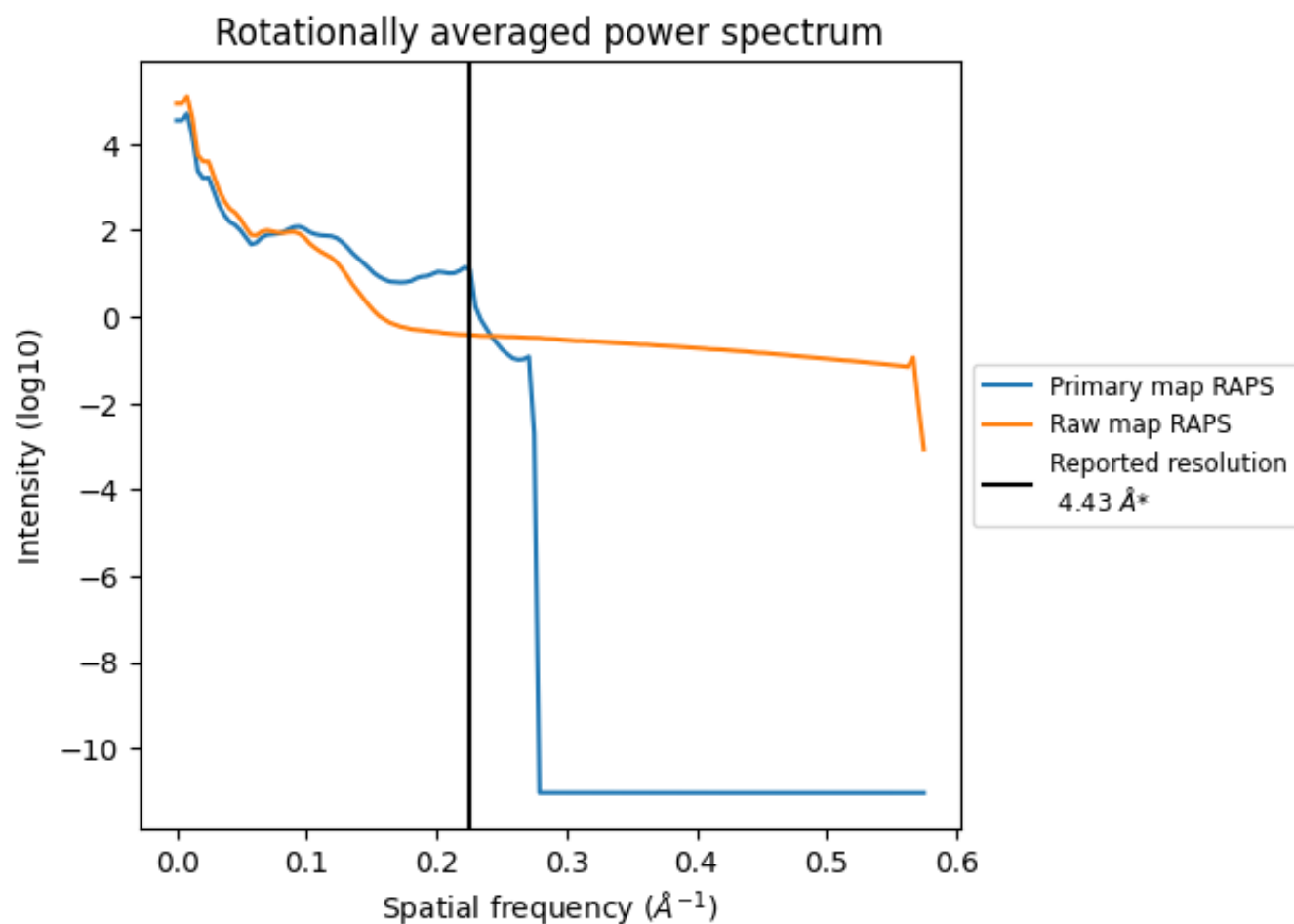
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm³; this corresponds to an approximate mass of 160 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 ⓘ

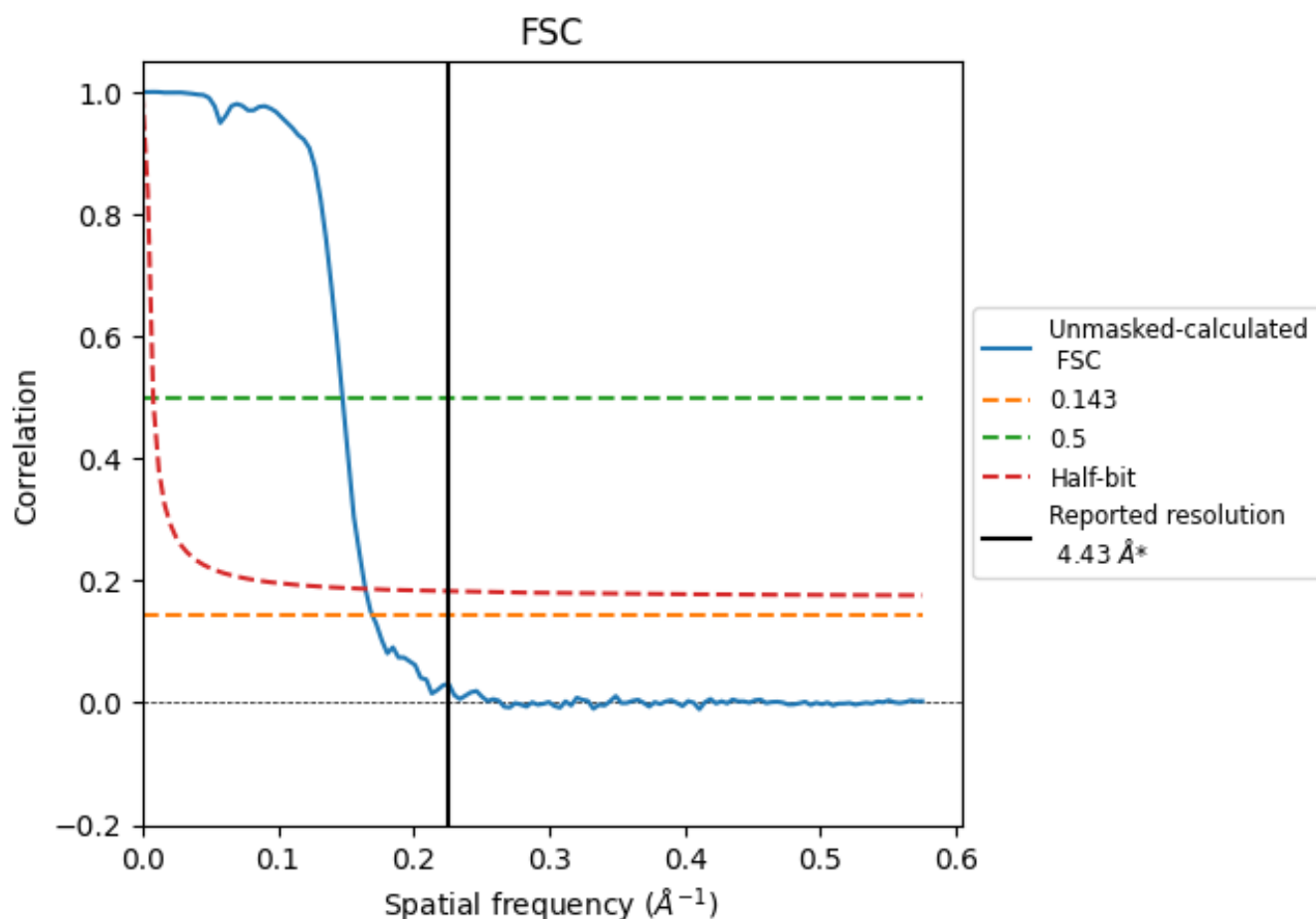


*Reported resolution corresponds to spatial frequency of 0.226 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.226 Å⁻¹

8.2 Resolution estimates [i](#)

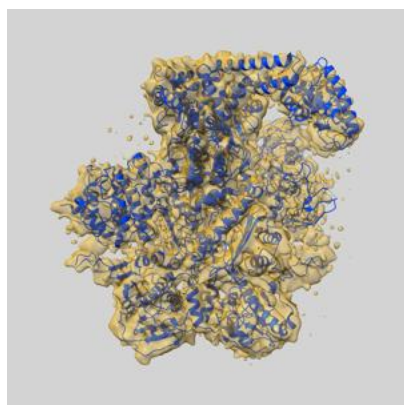
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.43	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.90	6.78	6.08

*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 5.90 differs from the reported value 4.43 by more than 10 %

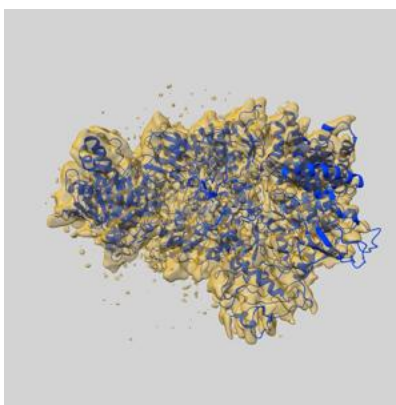
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62482 and PDB model 9KOX. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

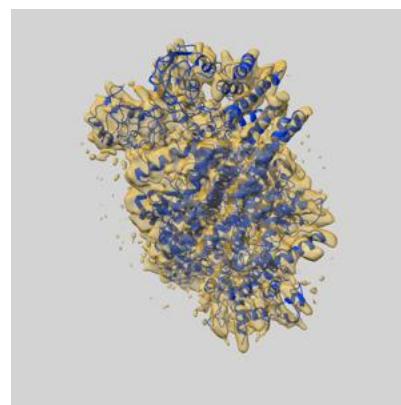
9.1 Map-model overlay [i](#)



X



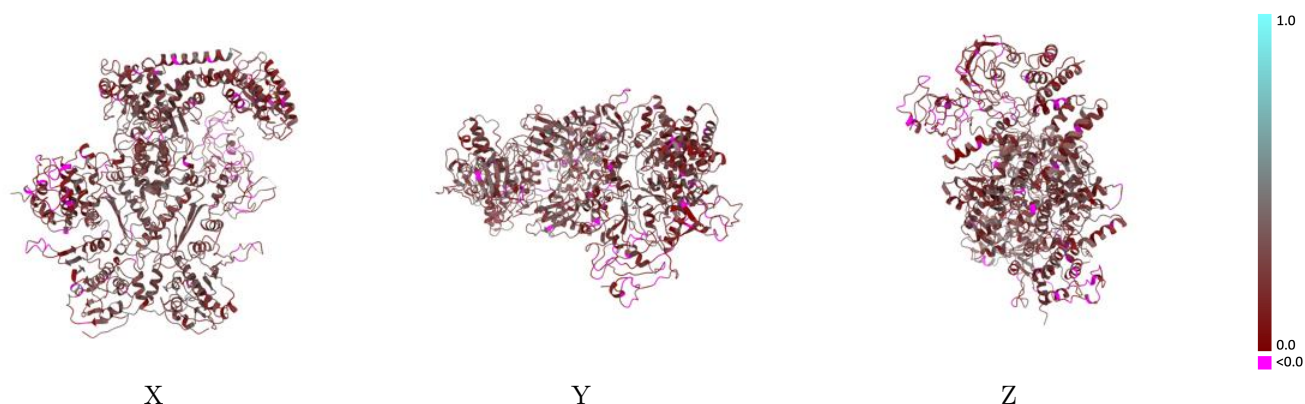
Y



Z

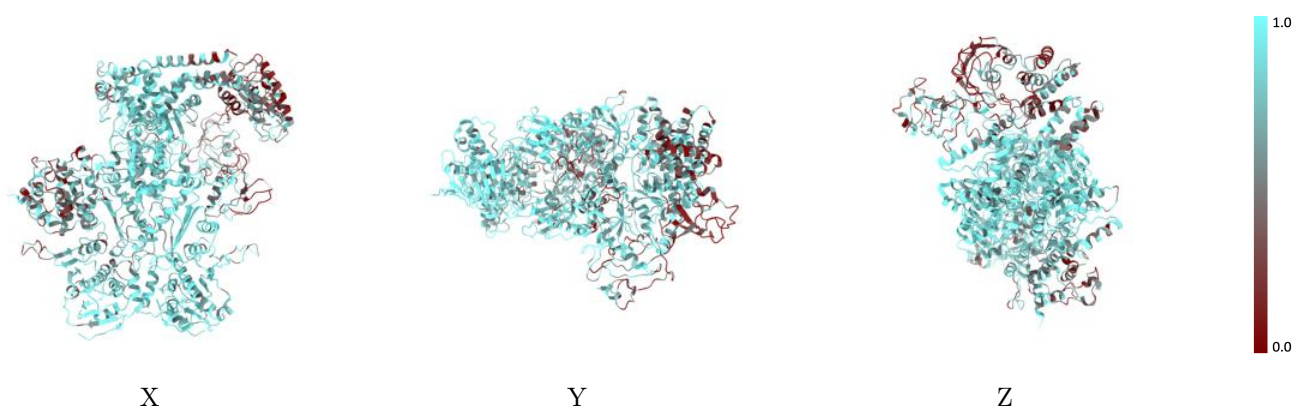
The images above show the 3D surface view of the map at the recommended contour level 0.109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



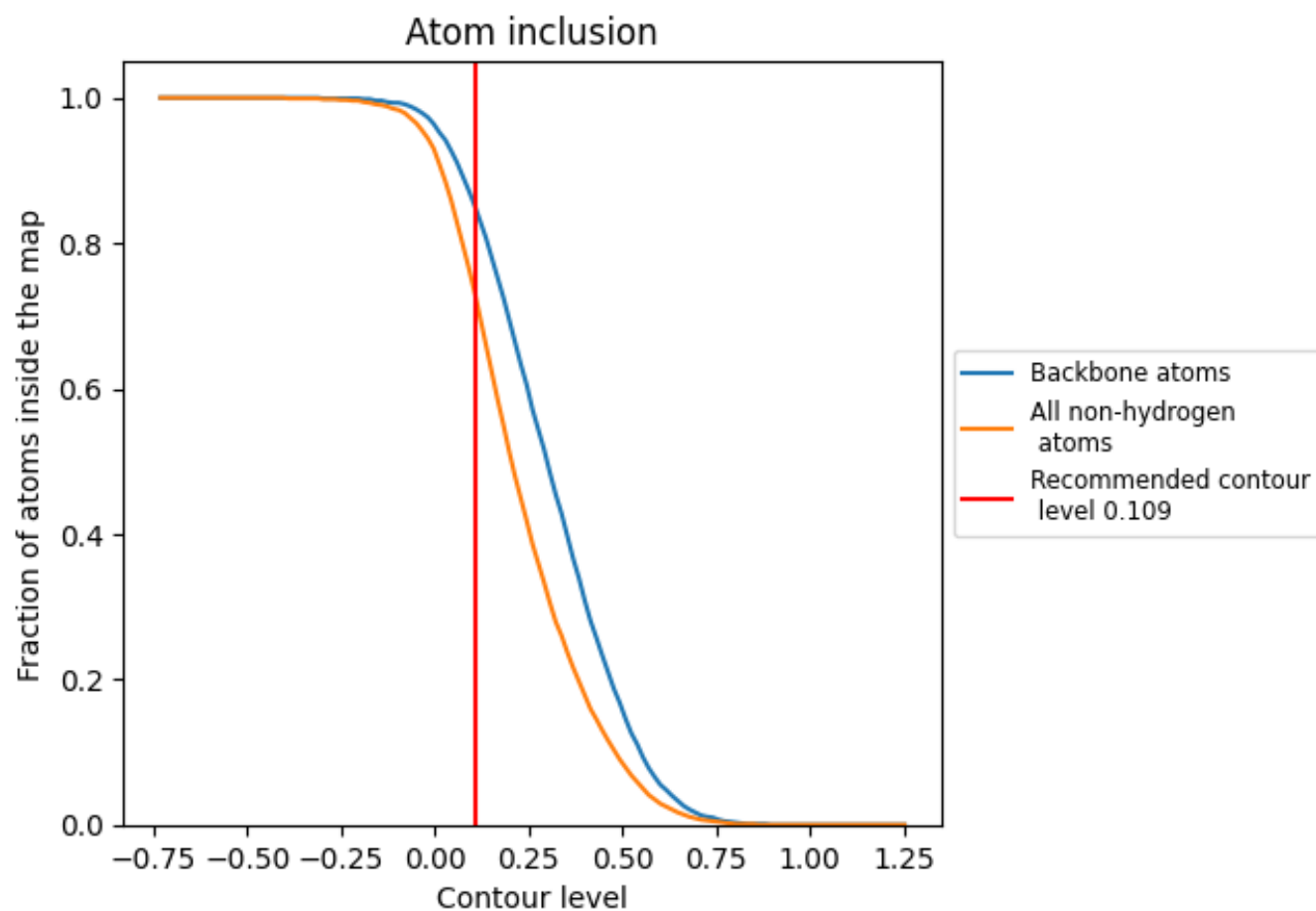
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.109).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 73% 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 (0.109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.2380
A	0.8250	0.2570
B	0.8450	0.2740
C	0.5800	0.2010
D	0.4930	0.1790

