



Full wwPDB EM Validation Report ⓘ

Dec 8, 2022 – 12:30 PM JST

PDB ID : 8GWN
EMDB ID : EMD-34317
Title : A mechanism for SARS-CoV-2 RNA capping and its inhibition by nucleotide analogue inhibitors
Authors : Yan, L.M.; Huang, Y.C.; Ge, J.; Liu, Z.Y.; Gao, Y.; Rao, Z.H.; Lou, Z.Y.
Deposited on : 2022-09-17
Resolution : 3.38 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

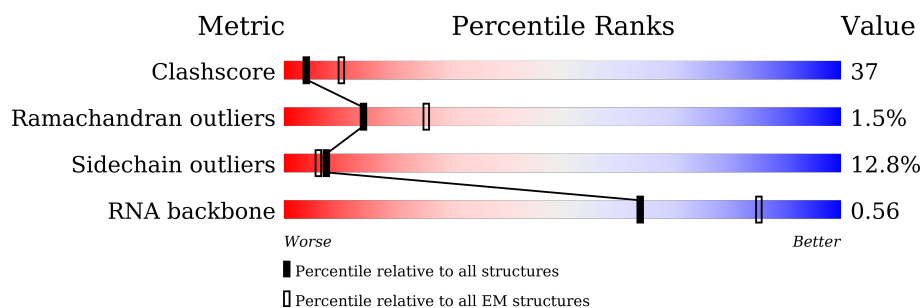
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	932	
2	B	198	
2	D	198	
3	C	83	
4	I	25	
5	J	33	
6	E	601	

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Mol	Chain	Length	Quality of chain
6	F	601	
7	G	113	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GNP	A	1003	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21860 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	926	Total	C	N	O	S	0	0
			7458	4763	1251	1390	54		

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1396	872	240	273	11		
2	D	186	Total	C	N	O	S	0	0
			1414	889	242	272	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	72	Total	C	N	O	S	0	0
			553	349	91	107	6		

- Molecule 4 is a RNA chain called primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	25	Total	C	N	O	P	0	0
			545	242	105	173	25		

- Molecule 5 is a RNA chain called template.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	27	Total	C	N	O	P	0	0
			565	253	94	191	27		

- Molecule 6 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	585	Total	C	N	O	S	1	0
			4508	2875	750	848	35		
6	E	586	Total	C	N	O	S	1	0
			4513	2878	751	849	35		

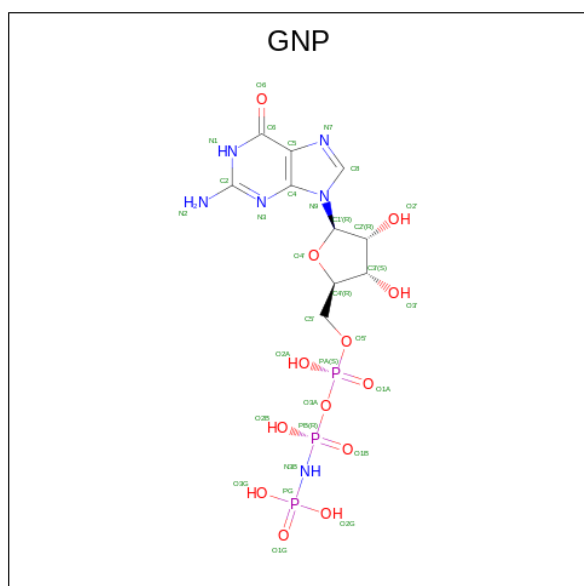
- Molecule 7 is a protein called Non-structural protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	113	Total	C	N	O	S	0	0
			868	549	150	164	5		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Zn	0
			2	2	
8	F	3	Total	Zn	0
			3	3	
8	E	3	Total	Zn	0
			3	3	

- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

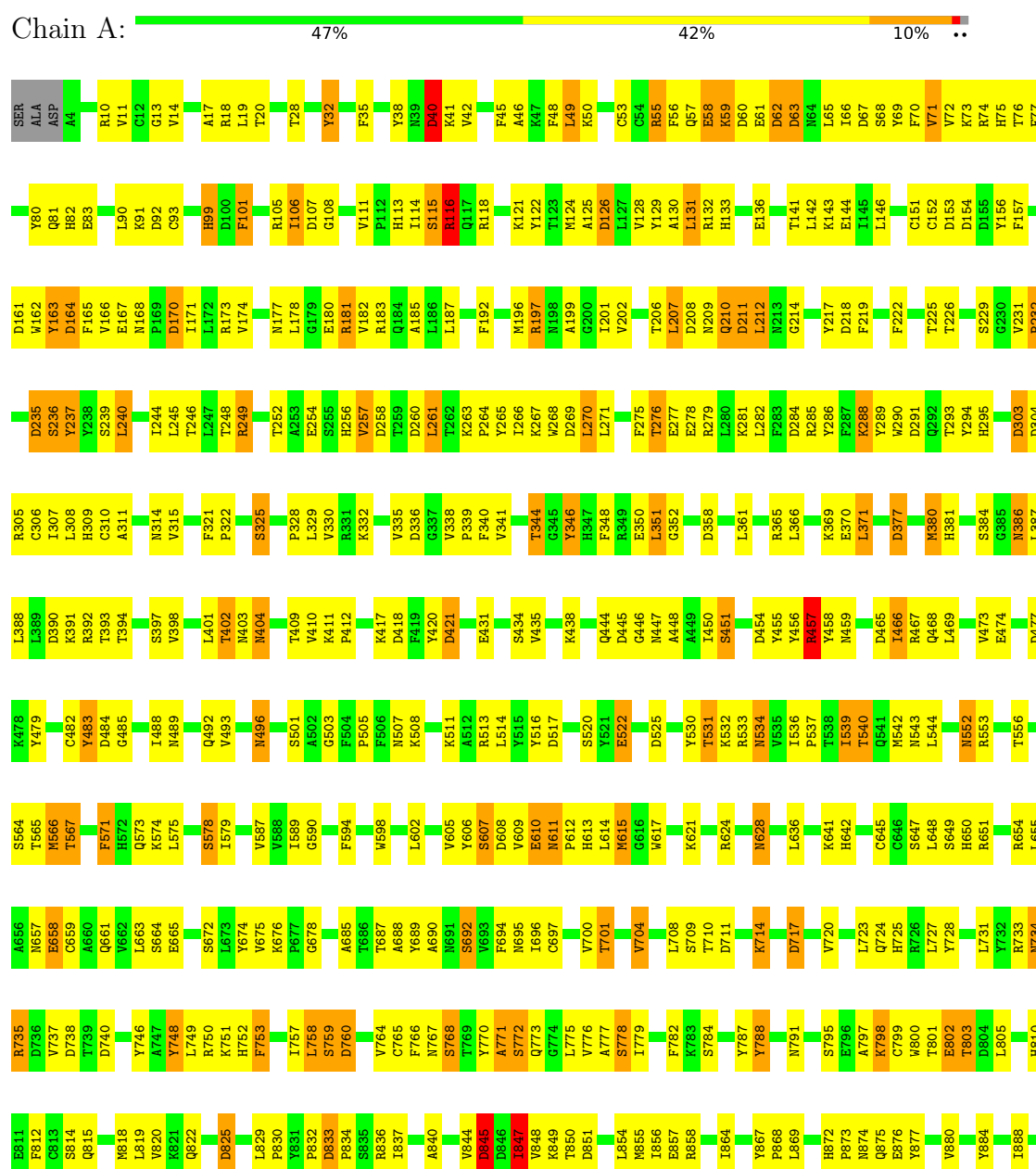


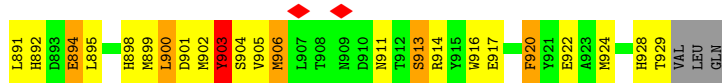
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	32	10	6	13	3	0

3 Residue-property plots

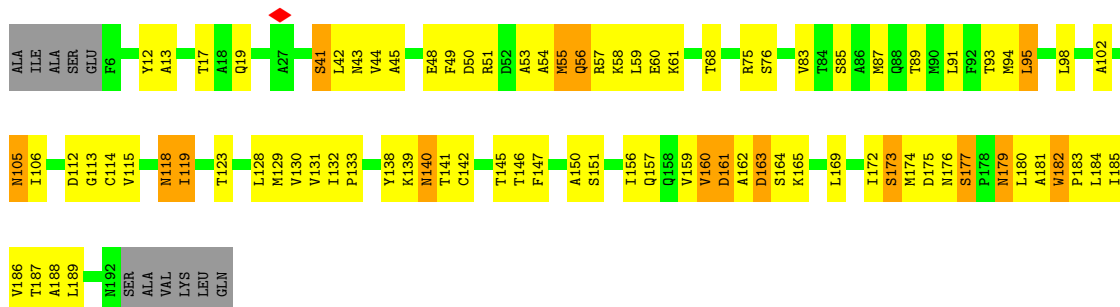
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RNA-directed RNA polymerase

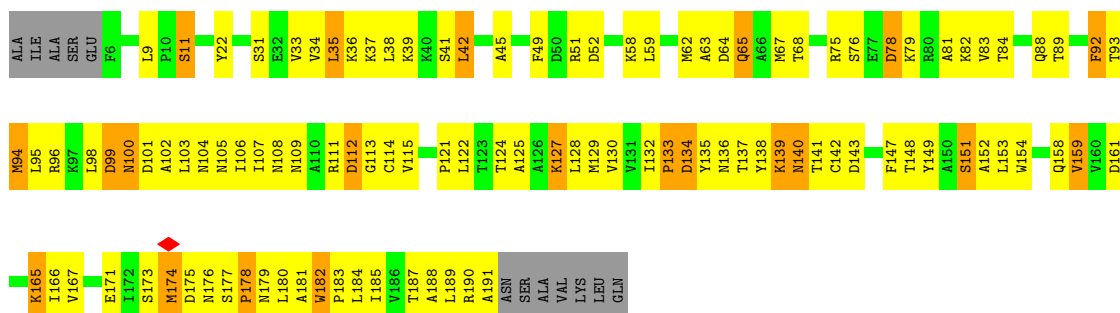




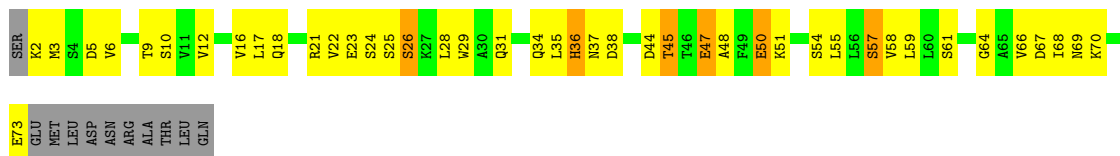
• Molecule 2: Non-structural protein 8



• Molecule 2: Non-structural protein 8



• Molecule 3: Non-structural protein 7



• Molecule 4: primer



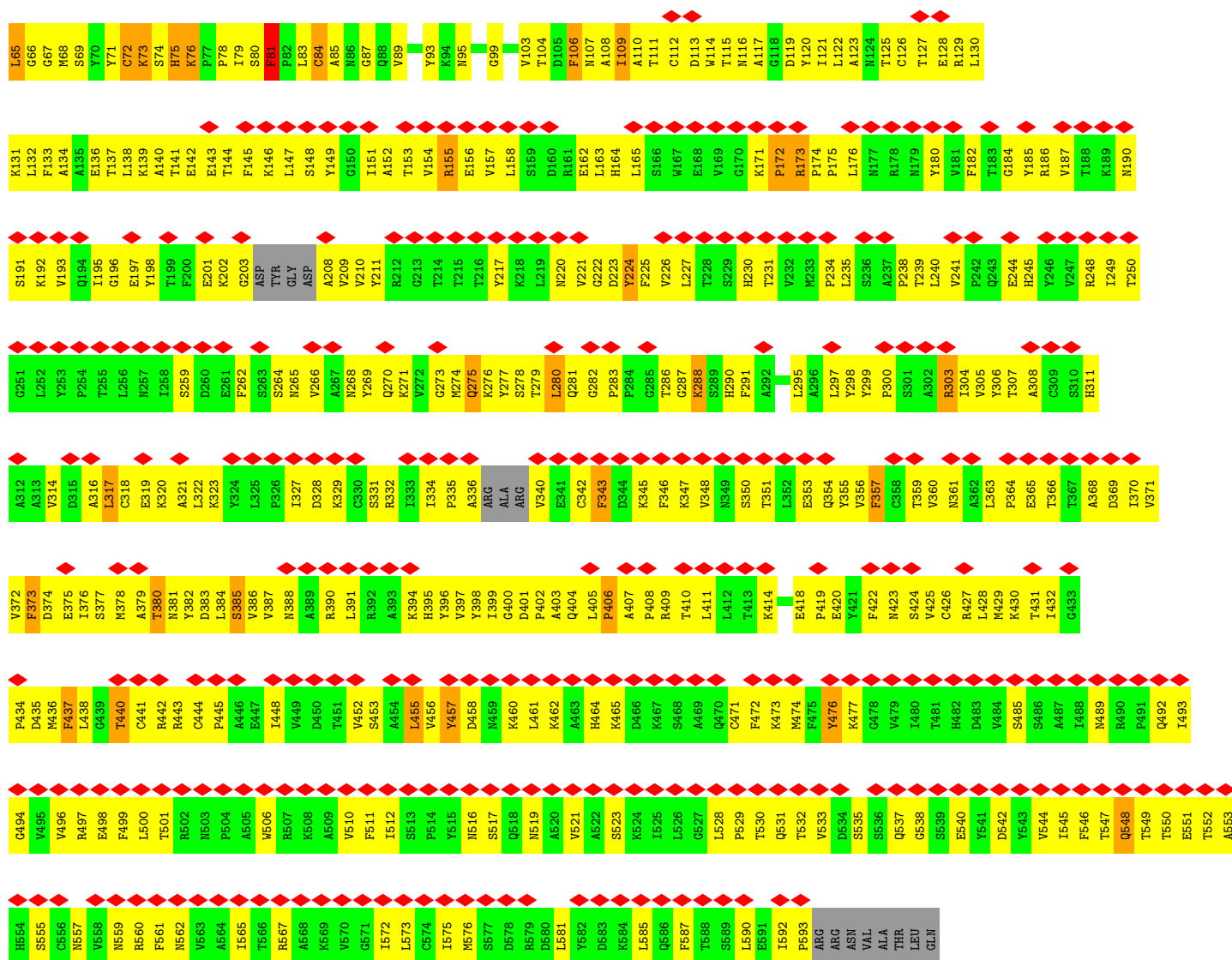
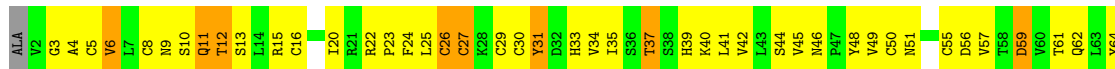
• Molecule 5: template

Chain J: 9% 55% 18% 18%



• Molecule 6: Helicase

Chain F: 32% 53% 59% 6%



• Molecule 6: Helicase

Chain E: 31% 34% 62% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	975171	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.470	Depositor
Minimum map value	-0.640	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	367.36, 367.36, 367.36	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	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, GNP

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	1.05	3/7647 (0.0%)	0.71	3/10379 (0.0%)
2	B	0.68	0/1414	0.64	0/1922
2	D	0.60	0/1433	0.62	0/1944
3	C	0.81	0/556	0.70	0/749
4	I	1.52	7/611 (1.1%)	1.25	2/953 (0.2%)
5	J	1.51	3/628 (0.5%)	1.25	4/974 (0.4%)
6	E	0.41	0/4615	0.57	1/6290 (0.0%)
6	F	0.41	0/4610	0.59	2/6283 (0.0%)
7	G	0.47	0/884	0.62	0/1200
All	All	0.81	13/22398 (0.1%)	0.70	12/30694 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	1
6	F	0	1
7	G	0	1
All	All	0	7

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	32	A	N9-C4	-7.76	1.33	1.37
4	I	32	A	N7-C5	-7.27	1.34	1.39
4	I	29	A	N9-C4	-7.07	1.33	1.37
1	A	217	TYR	CD2-CE2	-6.33	1.29	1.39
4	I	32	A	N3-C4	-6.27	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	29	A	N3-C4	-5.85	1.31	1.34
5	J	30	C	N1-C6	-5.68	1.33	1.37
5	J	31	U	N1-C2	-5.55	1.33	1.38
1	A	130	ALA	CA-C	-5.45	1.38	1.52
1	A	210	GLN	CA-CB	-5.21	1.42	1.53
5	J	36	A	N9-C4	-5.14	1.34	1.37
4	I	31	C	N1-C6	-5.14	1.34	1.37
4	I	32	A	C5-C6	-5.04	1.36	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	172	PRO	C-N-CA	7.36	140.10	121.70
5	J	27	C	C6-N1-C2	6.41	122.86	120.30
5	J	32	C	C6-N1-C2	6.12	122.75	120.30
1	A	116	ARG	NE-CZ-NH1	-6.07	117.27	120.30
6	F	406	PRO	C-N-CA	-5.76	107.30	121.70
1	A	40	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	240	LEU	CB-CG-CD2	-5.23	102.11	111.00
5	J	28	U	C5-C6-N1	-5.22	120.09	122.70
4	I	32	A	C6-C5-N7	-5.16	128.69	132.30
6	E	25	LEU	CA-CB-CG	-5.10	103.57	115.30
4	I	26	G	N3-C4-N9	-5.05	122.97	126.00
5	J	32	C	N3-C4-C5	5.03	123.91	121.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	845	ASP	Peptide
1	A	848	VAL	Peptide
1	A	903	TYR	Peptide
1	A	911	ASN	Peptide
2	B	182	TRP	Peptide
6	F	76	LYS	Peptide
7	G	10	ARG	Peptide

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	7458	0	7191	398	0
2	B	1396	0	1365	66	0
2	D	1414	0	1416	114	0
3	C	553	0	585	36	0
4	I	545	0	272	31	0
5	J	565	0	291	44	0
6	E	4513	0	4431	423	0
6	F	4508	0	4423	422	0
7	G	868	0	880	90	0
8	A	2	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
9	A	32	0	13	9	0
All	All	21860	0	20867	1568	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 (1568) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:16:ALA:HA	7:G:54:ALA:HA	1.42	1.01
6:F:374:ASP:HA	6:F:399:ILE:HB	1.46	0.98
6:E:5:CYS:SG	6:E:26:CYS:HB2	2.02	0.97
1:A:392:ARG:HH11	2:B:131:VAL:HG11	1.31	0.96
1:A:533:ARG:O	1:A:534:ASN:ND2	1.99	0.95
6:F:5:CYS:SG	6:F:8:CYS:HB2	2.08	0.93
6:F:9:ASN:H	6:F:129:ARG:HH12	1.17	0.91
6:F:107:ASN:O	6:F:111:THR:N	2.03	0.91
6:E:264:SER:O	6:E:268:ASN:ND2	2.04	0.91
6:F:62:GLN:HE22	6:F:72:CYS:HB2	1.36	0.91
6:F:151:ILE:HG22	6:F:224:TYR:HB2	1.51	0.90
6:F:26:CYS:O	6:F:30:CYS:N	2.05	0.90
6:E:118:GLY:HA2	6:E:121:ILE:HD12	1.53	0.89
6:E:473:LYS:HE2	6:E:587:PHE:HB2	1.53	0.88
4:I:18:G:N2	5:J:42:C:O2	2.07	0.87
1:A:304:ASP:O	1:A:307:ILE:N	2.07	0.87
7:G:31:TYR:HB2	7:G:43:ALA:HB3	1.57	0.86
7:G:14:CYS:SG	7:G:15:ALA:N	2.45	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:11:G:N1	5:J:49:C:N3	2.23	0.86
6:E:153:THR:HA	6:E:224:TYR:HA	1.58	0.86
6:E:381:ASN:HA	6:E:384:LEU:HD12	1.57	0.85
7:G:74:ARG:HH12	7:G:76:VAL:HG23	1.40	0.85
6:F:6:VAL:HG12	6:F:129:ARG:HB3	1.57	0.84
7:G:32:TYR:HA	7:G:41:VAL:HA	1.58	0.84
6:F:365:GLU:HA	6:F:390:ARG:HB3	1.58	0.84
1:A:40:ASP:O	1:A:725:HIS:NE2	2.10	0.83
2:D:171:GLU:O	2:D:176:ASN:ND2	2.11	0.83
6:E:61:THR:HA	6:E:84:CYS:HB2	1.59	0.83
1:A:610:GLU:OE1	1:A:767:ASN:ND2	2.10	0.83
6:F:65:LEU:HD23	6:F:66:GLY:H	1.44	0.83
6:E:252:LEU:HD11	6:E:370:ILE:HD11	1.61	0.82
2:D:139:LYS:NZ	2:D:140:ASN:OD1	2.12	0.82
6:E:145:PHE:O	6:E:148:SER:OG	1.98	0.82
1:A:50:LYS:NZ	9:A:1003:GNP:O1A	2.13	0.82
1:A:277:GLU:N	1:A:277:GLU:OE1	2.13	0.82
6:F:376:ILE:H	6:F:400:GLY:HA3	1.45	0.82
6:E:576:MET:HE3	6:E:582:TYR:HA	1.63	0.81
6:E:510:VAL:HA	6:E:529:PRO:HD2	1.63	0.81
6:F:152:ALA:HB3	6:F:225:PHE:HB2	1.61	0.81
6:E:304:ILE:HD11	6:E:372:VAL:HG13	1.63	0.81
2:B:55:MET:HA	2:B:58:LYS:HE2	1.63	0.80
6:F:103:VAL:O	6:F:107:ASN:N	2.11	0.80
4:I:11:G:O6	5:J:49:C:N4	2.10	0.80
6:F:420:GLU:HB2	6:F:427:ARG:HA	1.64	0.80
7:G:44:LEU:HD13	7:G:69:LEU:HD11	1.63	0.80
1:A:392:ARG:HH21	1:A:450:ILE:HG21	1.47	0.80
6:F:540:GLU:HB3	6:F:567:ARG:HE	1.45	0.80
1:A:767:ASN:OD1	1:A:768:SER:N	2.15	0.80
7:G:44:LEU:HB3	7:G:89:TYR:HB2	1.64	0.80
6:F:203:GLY:HA2	6:F:210:VAL:HG23	1.62	0.80
4:I:23:C:N3	5:J:37:G:N1	2.30	0.79
4:I:22:G:N1	5:J:38:C:N3	2.28	0.79
6:E:184:GLY:HA3	6:E:225:PHE:HD1	1.47	0.79
1:A:197:ARG:NH1	1:A:289:TYR:OH	2.16	0.79
6:F:371:VAL:O	6:F:397:VAL:N	2.16	0.79
1:A:421:ASP:OD1	1:A:421:ASP:N	2.15	0.79
6:E:157:VAL:HA	6:E:163:LEU:HD22	1.63	0.78
6:F:175:PRO:HA	6:F:485:SER:HB3	1.63	0.78
6:E:421:TYR:HA	6:E:427:ARG:HH12	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:57:PRO:HA	7:G:64:THR:HA	1.65	0.78
1:A:392:ARG:NH1	2:B:131:VAL:HG11	1.99	0.78
7:G:95:ASN:ND2	7:G:98:ASN:OD1	2.15	0.78
4:I:23:C:O2	5:J:37:G:N2	2.16	0.78
6:F:73:LYS:HA	6:F:76:LYS:HD3	1.66	0.77
6:E:12:THR:OG1	6:E:13:SER:N	2.09	0.77
1:A:496:ASN:N	1:A:496:ASN:OD1	2.17	0.77
6:F:269:TYR:OH	6:F:291:PHE:O	2.00	0.77
6:F:320:LYS:HA	6:F:323:LYS:HE2	1.64	0.77
6:E:332:ARG:HB2	6:E:357:PHE:HB2	1.64	0.77
1:A:717:ASP:OD1	1:A:717:ASP:N	2.18	0.77
6:E:451:THR:O	6:E:455:LEU:HB3	1.83	0.77
1:A:514:LEU:HD21	2:B:83:VAL:HG21	1.67	0.77
6:E:423:ASN:HD21	6:E:425:VAL:HG12	1.49	0.76
4:I:20:A:N6	5:J:40:U:O4	2.18	0.76
1:A:305:ARG:NH1	1:A:474:GLU:OE2	2.18	0.76
1:A:505:PRO:O	1:A:508:LYS:NZ	2.19	0.76
2:B:50:ASP:O	2:B:51:ARG:NH1	2.19	0.76
2:D:35:LEU:HA	2:D:38:LEU:HB2	1.66	0.76
6:F:271:LYS:NZ	6:F:435:ASP:O	2.17	0.76
6:E:120:TYR:O	6:E:124:ASN:ND2	2.19	0.75
6:F:445:PRO:HB3	6:F:465:LYS:HG3	1.68	0.75
6:F:128:GLU:HA	6:F:131:LYS:HG2	1.66	0.75
6:F:376:ILE:HG21	6:F:398:TYR:HB3	1.68	0.75
6:F:443:ARG:HG3	6:F:444:CYS:H	1.50	0.75
6:E:318:CYS:HG	6:E:346:PHE:HE1	1.35	0.75
1:A:778:SER:OG	1:A:779:ILE:N	2.18	0.75
1:A:40:ASP:OD1	1:A:41:LYS:N	2.19	0.75
1:A:402:THR:OG1	1:A:403:ASN:N	2.18	0.75
7:G:71:PRO:HD3	7:G:92:LYS:HE3	1.68	0.75
6:F:12:THR:OG1	6:F:13:SER:N	2.18	0.75
6:E:334:ILE:HD12	6:E:342:CYS:HB2	1.69	0.75
1:A:358:ASP:OD2	1:A:533:ARG:NH2	2.20	0.75
1:A:211:ASP:N	1:A:211:ASP:OD1	2.19	0.74
1:A:304:ASP:OD1	1:A:305:ARG:N	2.20	0.74
6:F:83:LEU:O	6:F:85:ALA:N	2.20	0.74
6:E:542:ASP:HB3	6:E:569:LYS:HB2	1.67	0.74
1:A:607:SER:OG	1:A:608:ASP:OD2	2.05	0.74
2:D:104:ASN:O	2:D:108:ASN:ND2	2.20	0.74
7:G:55:ARG:NH1	7:G:64:THR:OG1	2.21	0.74
3:C:70:LYS:HE3	2:D:88:GLN:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:TYR:OH	6:F:84:CYS:SG	2.44	0.74
6:F:268:ASN:HD22	6:F:291:PHE:HE2	1.31	0.74
6:E:148:SER:HA	6:E:171:LYS:HE2	1.69	0.74
6:E:281:GLN:HB3	6:E:437:PHE:HB3	1.69	0.74
6:E:555:SER:HA	6:E:560:ARG:HD2	1.69	0.74
1:A:552:ASN:OD1	1:A:552:ASN:N	2.21	0.74
1:A:207:LEU:O	1:A:209:ASN:N	2.20	0.74
6:F:342:CYS:SG	6:F:343:PHE:N	2.61	0.74
2:D:182:TRP:O	2:D:184:LEU:N	2.21	0.73
6:E:511:PHE:O	6:E:519:ASN:ND2	2.22	0.73
1:A:267:LYS:NZ	1:A:268:TRP:O	2.18	0.73
6:F:268:ASN:HB2	6:F:291:PHE:CZ	2.24	0.73
6:E:59:ASP:HB3	6:E:62:GLN:HB3	1.70	0.73
6:E:235:LEU:HD11	6:E:382:TYR:HD1	1.53	0.73
6:E:495:VAL:HA	6:E:498:GLU:HB3	1.68	0.73
1:A:657:ASN:OD1	1:A:661:GLN:NE2	2.21	0.73
1:A:132:ARG:O	1:A:133:HIS:ND1	2.21	0.73
6:E:330:CYS:O	6:E:347:LYS:NZ	2.21	0.73
3:C:45:THR:O	3:C:45:THR:OG1	2.02	0.72
6:E:453:SER:HB3	6:E:459:ASN:HA	1.71	0.72
6:F:187:VAL:N	6:F:223:ASP:OD1	2.18	0.72
6:F:154:VAL:HG11	6:F:163:LEU:HD22	1.70	0.72
1:A:164:ASP:OD1	1:A:166:VAL:N	2.23	0.72
6:E:318:CYS:HB3	6:E:345:LYS:HE3	1.71	0.72
1:A:57:GLN:NE2	1:A:66:ILE:O	2.22	0.72
6:E:163:LEU:H	6:E:209:VAL:H	1.36	0.72
6:F:67:GLY:O	6:F:69:SER:N	2.23	0.71
6:F:9:ASN:H	6:F:129:ARG:NH1	1.87	0.71
6:F:316:ALA:O	6:F:320:LYS:NZ	2.21	0.71
6:F:455:LEU:HD23	6:F:456:VAL:HG23	1.72	0.71
1:A:676:LYS:NZ	1:A:678:GLY:O	2.23	0.71
6:E:510:VAL:HB	6:E:544:VAL:HG13	1.72	0.71
1:A:802:GLU:OE1	1:A:810:HIS:N	2.23	0.71
5:J:40:U:H2'	5:J:41:G:C8	2.24	0.71
1:A:50:LYS:NZ	9:A:1003:GNP:O1G	2.23	0.70
1:A:483:TYR:HE1	1:A:579:ILE:HG23	1.56	0.70
6:F:559:ASN:OD1	6:F:562:ASN:ND2	2.24	0.70
6:F:55:CYS:SG	6:F:56:ASP:N	2.64	0.70
6:F:286:THR:H	6:F:288:LYS:HZ2	1.38	0.70
6:F:372:VAL:HA	6:F:397:VAL:HB	1.74	0.70
2:D:167:VAL:HG21	2:D:180:LEU:HD23	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:98:ASN:HA	7:G:101:MET:HE2	1.72	0.70
2:B:173:SER:OG	2:B:174:MET:N	2.24	0.70
6:F:581:LEU:HD23	6:F:585:LEU:HB2	1.73	0.70
7:G:33:ASN:N	7:G:40:PHE:O	2.21	0.70
6:F:423:ASN:ND2	6:F:426:CYS:SG	2.64	0.69
1:A:225:THR:OG1	1:A:226:THR:N	2.22	0.69
2:D:134:ASP:OD1	2:D:136:ASN:N	2.22	0.69
6:E:176:LEU:HD21	6:E:516:ASN:HB2	1.74	0.69
6:F:173:ARG:HH12	6:F:176:LEU:HB2	1.57	0.69
6:E:13:SER:O	6:E:13:SER:OG	2.08	0.69
1:A:129:TYR:CZ	1:A:133:HIS:HD2	2.11	0.69
1:A:350:GLU:OE2	1:A:350:GLU:N	2.25	0.69
1:A:533:ARG:C	1:A:534:ASN:HD22	1.93	0.69
2:D:132:ILE:HB	2:D:184:LEU:HD13	1.73	0.69
1:A:876:GLU:N	1:A:876:GLU:OE1	2.26	0.69
4:I:18:G:N1	5:J:42:C:N3	2.33	0.69
6:E:479:VAL:HB	6:E:491:PRO:HG2	1.74	0.69
1:A:66:ILE:HG13	1:A:67:ASP:H	1.56	0.69
2:B:112:ASP:O	2:B:114:CYS:N	2.25	0.69
6:F:244:GLU:O	6:F:276:LYS:NZ	2.23	0.69
6:E:451:THR:O	6:E:455:LEU:CB	2.41	0.69
2:B:173:SER:OG	2:B:175:ASP:OD1	2.10	0.69
6:F:265:ASN:ND2	6:F:269:TYR:OH	2.26	0.69
6:F:268:ASN:HB2	6:F:291:PHE:HZ	1.58	0.69
6:F:331:SER:HB3	6:F:347:LYS:HE3	1.75	0.69
1:A:235:ASP:O	1:A:239:SER:OG	2.10	0.68
6:E:268:ASN:HB2	6:E:291:PHE:HZ	1.58	0.68
2:B:118:ASN:OD1	2:B:118:ASN:N	2.20	0.68
6:F:279:THR:HG21	6:F:425:VAL:HG11	1.75	0.68
1:A:697:CYS:O	1:A:701:THR:HG22	1.93	0.68
6:F:127:THR:O	6:F:131:LYS:N	2.26	0.68
6:E:448:ILE:HA	6:E:451:THR:HB	1.75	0.68
1:A:489:ASN:ND2	1:A:492:GLN:OE1	2.26	0.68
2:B:50:ASP:OD1	2:B:51:ARG:NH1	2.23	0.68
7:G:10:ARG:HH21	7:G:31:TYR:HB3	1.58	0.68
1:A:269:ASP:OD1	1:A:270:LEU:N	2.27	0.68
1:A:226:THR:O	1:A:229:SER:OG	2.11	0.68
3:C:54:SER:O	3:C:57:SER:OG	2.10	0.68
6:F:545:ILE:HD12	6:F:573:LEU:HD23	1.75	0.68
6:F:559:ASN:HA	6:F:562:ASN:HB2	1.75	0.68
6:E:129:ARG:O	6:E:129:ARG:NH2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:ASP:N	1:A:825:ASP:OD1	2.22	0.68
6:E:445:PRO:HG3	6:E:570:VAL:HG22	1.76	0.68
6:E:545:ILE:HG23	6:E:573:LEU:HB3	1.76	0.68
6:F:20:ILE:O	6:F:22:ARG:NH1	2.28	0.67
1:A:244:ILE:O	1:A:246:THR:N	2.27	0.67
1:A:483:TYR:CD1	1:A:579:ILE:HG12	2.29	0.67
6:F:138:LEU:HD23	6:F:139:LYS:HZ1	1.60	0.67
6:F:151:ILE:HG23	6:F:226:VAL:HG13	1.74	0.67
1:A:340:PHE:HE2	2:B:95:LEU:HD22	1.59	0.67
1:A:465:ASP:OD1	1:A:466:ILE:N	2.28	0.67
6:F:376:ILE:N	6:F:400:GLY:HA3	2.08	0.67
1:A:70:PHE:O	1:A:72:VAL:N	2.27	0.67
6:E:331:SER:HB2	6:E:356:VAL:HG12	1.74	0.67
7:G:44:LEU:O	7:G:89:TYR:N	2.28	0.67
1:A:397:SER:OG	1:A:398:VAL:N	2.28	0.67
6:F:360:VAL:HA	6:F:363:LEU:HD22	1.76	0.67
6:E:44:SER:OG	6:E:45:VAL:N	2.21	0.67
1:A:447:ASN:O	1:A:447:ASN:ND2	2.27	0.67
1:A:53:CYS:O	1:A:55:ARG:N	2.28	0.67
2:B:161:ASP:OD1	2:B:161:ASP:N	2.25	0.67
6:F:185:TYR:HB2	6:F:192:LYS:HE2	1.76	0.67
6:F:418:GLU:HG2	6:F:419:PRO:HD2	1.77	0.67
1:A:38:TYR:HE2	1:A:725:HIS:HE1	1.43	0.67
1:A:309:HIS:O	1:A:309:HIS:ND1	2.28	0.67
1:A:565:THR:O	1:A:567:THR:N	2.28	0.67
1:A:647:SER:HB3	1:A:650:HIS:ND1	2.10	0.67
7:G:68:GLU:OE1	7:G:92:LYS:NZ	2.25	0.67
1:A:445:ASP:OD1	1:A:445:ASP:N	2.19	0.66
1:A:770:TYR:O	1:A:772:SER:N	2.28	0.66
1:A:58:GLU:OE2	1:A:118:ARG:NH1	2.29	0.66
1:A:254:GLU:OE1	1:A:286:TYR:OH	2.06	0.66
1:A:539:ILE:HG22	1:A:540:THR:H	1.60	0.66
6:F:270:GLN:OE1	6:F:298:TYR:OH	2.12	0.66
6:E:306:TYR:HA	6:E:372:VAL:HG22	1.77	0.66
6:E:5:CYS:SG	6:E:26:CYS:CB	2.82	0.66
1:A:187:LEU:HD11	1:A:286:TYR:HE1	1.61	0.66
1:A:276:THR:O	1:A:276:THR:OG1	2.12	0.66
2:B:41:SER:OG	2:B:42:LEU:N	2.26	0.66
6:F:33:HIS:HA	6:F:107:ASN:HD21	1.60	0.66
6:F:396:TYR:HB3	6:F:398:TYR:CE1	2.31	0.66
1:A:83:GLU:OE2	1:A:219:PHE:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ASN:HD22	1:A:760:ASP:HA	1.61	0.66
1:A:928:HIS:O	1:A:929:THR:OG1	2.12	0.66
6:F:30:CYS:O	6:F:34:VAL:HG12	1.96	0.66
6:F:72:CYS:O	6:F:76:LYS:N	2.29	0.66
6:F:184:GLY:HA3	6:F:195:ILE:HB	1.79	0.66
6:F:163:LEU:H	6:F:209:VAL:H	1.43	0.65
6:E:281:GLN:H	6:E:437:PHE:HA	1.61	0.65
1:A:202:VAL:HG22	1:A:231:VAL:HG12	1.77	0.65
1:A:209:ASN:ND2	9:A:1003:GNP:O1B	2.28	0.65
6:F:286:THR:HG22	6:F:441:CYS:HA	1.78	0.65
1:A:303:ASP:N	1:A:303:ASP:OD1	2.27	0.65
1:A:647:SER:OG	1:A:648:LEU:N	2.25	0.65
1:A:187:LEU:HD11	1:A:286:TYR:CE1	2.31	0.65
4:I:22:G:H2'	4:I:23:C:H6	1.59	0.65
6:F:176:LEU:HD23	6:F:202:LYS:HD2	1.77	0.65
6:F:537:GLN:HG2	6:F:567:ARG:HH12	1.61	0.65
6:E:266:VAL:HA	6:E:269:TYR:CD2	2.31	0.65
2:B:145:THR:HG23	2:B:146:THR:HG23	1.78	0.65
6:E:263:SER:OG	6:E:264:SER:N	2.28	0.65
1:A:115:SER:O	1:A:115:SER:OG	2.11	0.65
6:E:16:CYS:HB2	6:E:25:LEU:HD12	1.79	0.65
6:E:366:THR:OG1	6:E:367:THR:N	2.24	0.65
1:A:520:SER:OG	1:A:522:GLU:OE2	2.11	0.64
1:A:657:ASN:O	1:A:661:GLN:NE2	2.30	0.64
2:B:131:VAL:HG22	2:B:185:ILE:HG12	1.79	0.64
6:F:403:ALA:HB1	6:F:457:TYR:CE2	2.33	0.64
6:E:380:THR:OG1	6:E:383:ASP:OD1	2.12	0.64
1:A:836:ARG:NH2	1:A:840:ALA:HB2	2.13	0.64
4:I:9:G:N7	4:I:10:C:N4	2.44	0.64
6:F:116:ASN:HB2	6:F:119:ASP:H	1.62	0.64
6:E:159:SER:OG	6:E:160:ASP:N	2.29	0.64
7:G:77:THR:HA	7:G:112:LEU:HA	1.78	0.64
1:A:122:TYR:OH	1:A:144:GLU:OE1	2.14	0.64
6:E:480:ILE:HD11	6:E:551:GLU:HB2	1.79	0.64
1:A:503:GLY:O	1:A:507:ASN:ND2	2.19	0.64
1:A:901:ASP:OD1	1:A:902:MET:N	2.31	0.64
6:F:373:PHE:N	6:F:397:VAL:O	2.31	0.64
6:E:358:CYS:SG	6:E:359:THR:N	2.71	0.64
6:E:314:VAL:HG23	6:E:317:LEU:HD12	1.79	0.64
1:A:727:LEU:O	1:A:731:LEU:HB2	1.98	0.64
6:F:369:ASP:O	6:F:394:LYS:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:152:ALA:O	6:E:225:PHE:N	2.31	0.64
6:F:548:GLN:HE22	6:F:576:MET:HA	1.61	0.63
6:E:184:GLY:HA2	6:E:225:PHE:HA	1.80	0.63
6:F:15:ARG:HG2	6:F:22:ARG:HB3	1.80	0.63
6:E:437:PHE:HB2	6:E:460:LYS:HE3	1.80	0.63
1:A:766:PHE:HD2	1:A:767:ASN:O	1.81	0.63
6:F:42:VAL:HG23	6:F:48:TYR:HD2	1.62	0.63
6:F:116:ASN:ND2	6:F:119:ASP:OD1	2.31	0.63
1:A:116:ARG:HH22	9:A:1003:GNP:C5'	2.10	0.63
1:A:849:LYS:O	1:A:851:ASP:N	2.26	0.63
6:E:202:LYS:O	6:E:210:VAL:N	2.32	0.63
4:I:22:G:O6	5:J:38:C:N4	2.20	0.63
6:E:322:LEU:HG	6:E:327:ILE:HD12	1.81	0.62
7:G:31:TYR:N	7:G:43:ALA:O	2.32	0.62
1:A:903:TYR:HE1	2:D:67:MET:HG2	1.63	0.62
6:E:440:THR:O	6:E:442:ARG:NH2	2.30	0.62
1:A:257:VAL:HA	1:A:266:ILE:HG12	1.80	0.62
1:A:696:ILE:O	1:A:700:VAL:HG23	2.00	0.62
3:C:47:GLU:HG3	3:C:51:LYS:HZ2	1.64	0.62
6:E:276:LYS:HA	6:E:395:HIS:HA	1.81	0.62
6:E:403:ALA:O	6:E:457:TYR:OH	2.11	0.62
6:E:473:LYS:HG2	6:E:574:CYS:HB2	1.81	0.62
7:G:17:GLY:N	7:G:53:TRP:O	2.32	0.62
1:A:165:PHE:HE1	1:A:787:TYR:CE1	2.17	0.62
6:F:351:THR:HG21	6:F:366:THR:HG21	1.82	0.62
6:F:239:THR:HG22	6:F:385:SER:HB3	1.80	0.62
7:G:10:ARG:HA	7:G:10:ARG:CZ	2.29	0.62
1:A:612:PRO:O	1:A:613:HIS:ND1	2.33	0.62
7:G:35:THR:OG1	7:G:38:GLY:O	2.17	0.62
1:A:80:TYR:HE1	1:A:101:PHE:HB3	1.64	0.62
1:A:903:TYR:HB3	1:A:905:VAL:H	1.63	0.62
6:F:383:ASP:O	6:F:386:VAL:HG22	1.99	0.62
6:E:538:GLY:N	6:E:540:GLU:OE1	2.30	0.62
6:E:557:ASN:HD21	6:E:560:ARG:HB2	1.64	0.62
6:E:281:GLN:N	6:E:437:PHE:HA	2.14	0.62
1:A:658:GLU:OE1	1:A:659:CYS:N	2.33	0.62
2:D:34:VAL:O	2:D:38:LEU:N	2.32	0.62
1:A:483:TYR:HD1	1:A:579:ILE:HG12	1.64	0.62
1:A:701:THR:HA	1:A:704:VAL:HG23	1.82	0.62
6:F:44:SER:OG	6:F:45:VAL:N	2.30	0.62
6:E:114:TRP:CE3	6:E:119:ASP:HB3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:SER:O	1:A:664:SER:OG	2.16	0.61
6:F:9:ASN:N	6:F:129:ARG:HH12	1.94	0.61
6:F:37:THR:HG21	6:F:111:THR:HG21	1.82	0.61
6:E:115:THR:N	6:E:119:ASP:OD2	2.22	0.61
6:E:153:THR:N	6:E:166:SER:O	2.29	0.61
6:E:444:CYS:O	6:E:464:HIS:ND1	2.30	0.61
1:A:540:THR:OG1	1:A:665:GLU:OE1	2.18	0.61
2:D:65:GLN:NE2	6:F:68:MET:SD	2.72	0.61
1:A:17:ALA:O	1:A:19:LEU:N	2.30	0.61
6:E:500:LEU:HD11	6:E:507:ARG:HA	1.83	0.61
6:E:331:SER:HG	6:E:353:GLU:HG3	1.64	0.61
2:D:177:SER:O	2:D:179:ASN:N	2.33	0.61
5:J:41:G:H2'	5:J:42:C:C6	2.35	0.61
6:F:304:ILE:HD11	6:F:372:VAL:HG13	1.80	0.61
6:E:541:TYR:HD1	6:E:543:TYR:H	1.48	0.61
2:D:136:ASN:O	2:D:139:LYS:N	2.33	0.61
7:G:111:ARG:NH1	7:G:111:ARG:HA	2.15	0.61
1:A:309:HIS:O	1:A:309:HIS:CG	2.54	0.61
6:E:197:GLU:N	6:E:215:THR:OG1	2.32	0.61
2:B:175:ASP:OD1	2:B:176:ASN:N	2.34	0.61
6:E:531:GLN:NE2	6:E:536:SER:OG	2.32	0.61
1:A:164:ASP:OD1	1:A:165:PHE:N	2.34	0.61
6:F:381:ASN:HD21	6:F:424:SER:HB3	1.66	0.61
6:E:163:LEU:HD11	6:E:219:LEU:HD22	1.83	0.61
6:E:185:TYR:HB2	6:E:224:TYR:CE1	2.35	0.61
6:E:424:SER:HA	6:E:427:ARG:HE	1.66	0.60
7:G:17:GLY:O	7:G:52:LYS:N	2.29	0.60
7:G:70:GLU:HA	7:G:92:LYS:HE3	1.83	0.60
4:I:24:U:H2'	4:I:25:A:C8	2.37	0.60
6:E:401:ASP:HB2	6:E:404:GLN:HE22	1.64	0.60
7:G:72:PRO:HA	7:G:89:TYR:CE2	2.36	0.60
1:A:417:LYS:O	1:A:420:TYR:N	2.34	0.60
2:D:22:TYR:HD1	2:D:38:LEU:HB3	1.66	0.60
6:F:157:VAL:HA	6:F:163:LEU:HD23	1.83	0.60
6:E:81:PHE:HD1	6:E:82:PRO:HD2	1.66	0.60
6:F:39:HIS:O	6:F:40:LYS:HD3	2.01	0.60
6:F:585:LEU:HD11	6:F:587:PHE:CE1	2.36	0.60
6:E:31:TYR:O	6:E:35:ILE:HG12	2.01	0.60
1:A:332:LYS:HD2	1:A:339:PRO:HB2	1.84	0.60
1:A:456:TYR:O	1:A:458:TYR:N	2.34	0.60
4:I:23:C:N4	5:J:37:G:O6	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:386:VAL:O	6:E:390:ARG:HG2	2.00	0.60
6:E:423:ASN:ND2	6:E:425:VAL:HG12	2.17	0.60
6:F:387:VAL:HA	6:F:390:ARG:HD2	1.82	0.60
2:B:182:TRP:CZ3	2:B:184:LEU:HD12	2.36	0.60
6:E:449:VAL:HG12	6:E:461:LEU:HD21	1.83	0.60
7:G:87:TYR:HB3	7:G:89:TYR:HE2	1.67	0.60
1:A:904:SER:N	6:F:95:ASN:OD1	2.35	0.60
6:E:121:ILE:HA	6:E:124:ASN:HD21	1.67	0.60
3:C:18:GLN:O	3:C:18:GLN:NE2	2.34	0.60
6:F:184:GLY:N	6:F:196:GLY:O	2.26	0.60
6:F:196:GLY:HA3	6:F:217:TYR:CE2	2.36	0.60
6:E:21:ARG:HG3	6:E:136:GLU:OE1	2.01	0.59
7:G:29:LEU:HB3	7:G:31:TYR:HE1	1.66	0.59
6:F:114:TRP:HH2	6:F:123:ALA:HB2	1.67	0.59
6:F:545:ILE:HG23	6:F:573:LEU:HD23	1.83	0.59
1:A:531:THR:O	1:A:531:THR:OG1	2.15	0.59
1:A:615:MET:HB2	1:A:766:PHE:HE1	1.67	0.59
6:E:138:LEU:O	6:E:141:THR:OG1	2.15	0.59
6:F:283:PRO:HG2	6:F:461:LEU:HD21	1.84	0.59
6:E:492:GLN:NE2	6:E:548:GLN:HE21	1.99	0.59
6:E:154:VAL:O	6:E:223:ASP:N	2.35	0.59
1:A:38:TYR:CD1	1:A:728:TYR:HE1	2.21	0.59
6:F:62:GLN:NE2	6:F:73:LYS:HG2	2.18	0.59
6:F:279:THR:HG22	6:F:398:TYR:CG	2.37	0.59
6:F:377:SER:OG	6:F:405:LEU:O	2.20	0.59
6:E:536:SER:OG	6:E:567:ARG:NH1	2.36	0.59
1:A:72:VAL:HG22	1:A:72:VAL:O	2.01	0.59
1:A:248:THR:O	1:A:248:THR:OG1	2.10	0.59
2:B:53:ALA:O	2:B:57:ARG:NH2	2.36	0.59
6:E:368:ALA:N	6:E:392:ARG:O	2.27	0.59
1:A:77:PHE:O	1:A:80:TYR:HB3	2.03	0.59
6:E:203:GLY:HA2	6:E:210:VAL:HG23	1.85	0.59
6:E:422:PHE:HB2	6:E:426:CYS:SG	2.43	0.59
6:F:307:THR:HG21	6:F:363:LEU:HD13	1.84	0.58
6:F:492:GLN:O	6:F:496:VAL:HG23	2.03	0.58
4:I:11:G:N2	5:J:49:C:O2	2.24	0.58
6:F:239:THR:HG21	6:F:381:ASN:HB3	1.85	0.58
6:F:266:VAL:HA	6:F:269:TYR:HB2	1.85	0.58
6:F:286:THR:N	6:F:288:LYS:HZ2	2.01	0.58
1:A:126:ASP:OD1	1:A:126:ASP:N	2.35	0.58
1:A:759:SER:O	1:A:759:SER:OG	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:SER:OG	2:D:33:VAL:HG12	2.04	0.58
2:D:113:GLY:O	2:D:115:VAL:N	2.36	0.58
7:G:17:GLY:O	7:G:53:TRP:N	2.24	0.58
6:F:489:ASN:HD22	6:F:492:GLN:HB2	1.69	0.58
6:F:494:GLY:HA2	6:F:497:ARG:HE	1.69	0.58
6:E:331:SER:O	6:E:357:PHE:N	2.37	0.58
1:A:387:LEU:HD12	1:A:388:LEU:H	1.69	0.58
6:E:15:ARG:HD3	6:E:24:PHE:HE1	1.69	0.58
7:G:11:GLN:HA	7:G:31:TYR:HA	1.85	0.58
2:D:101:ASP:OD1	2:D:102:ALA:N	2.37	0.58
6:F:145:PHE:O	6:F:148:SER:OG	2.14	0.58
6:E:254:PRO:HA	6:E:299:TYR:CZ	2.39	0.58
1:A:321:PHE:HB3	1:A:322:PRO:HD2	1.86	0.58
6:F:336:ALA:HA	6:F:340:VAL:HG23	1.85	0.58
6:E:262:PHE:HB2	6:E:265:ASN:HB2	1.85	0.58
6:E:519:ASN:ND2	6:E:529:PRO:O	2.35	0.58
1:A:488:ILE:HD11	1:A:493:VAL:HG12	1.85	0.58
1:A:795:SER:O	1:A:797:ALA:N	2.35	0.58
6:F:163:LEU:O	6:F:208:ALA:N	2.37	0.58
6:F:180:TYR:HA	6:F:227:LEU:HD21	1.85	0.58
6:F:538:GLY:H	6:F:567:ARG:HH22	1.51	0.58
1:A:467:ARG:HH21	1:A:735:ARG:NH1	2.02	0.57
6:F:248:ARG:HD2	6:F:250:THR:HB	1.86	0.57
6:F:264:SER:O	6:F:268:ASN:ND2	2.37	0.57
6:F:440:THR:O	6:F:442:ARG:N	2.37	0.57
6:E:124:ASN:OD1	6:E:125:THR:OG1	2.22	0.57
7:G:6:PRO:O	7:G:7:VAL:HG22	2.04	0.57
2:D:178:PRO:O	2:D:179:ASN:ND2	2.36	0.57
6:E:114:TRP:HD1	6:E:141:THR:HG21	1.69	0.57
1:A:708:LEU:O	1:A:710:THR:N	2.36	0.57
1:A:737:VAL:HG12	1:A:738:ASP:H	1.69	0.57
1:A:759:SER:O	1:A:760:ASP:HB3	2.04	0.57
6:F:240:LEU:HD22	6:F:424:SER:HB2	1.85	0.57
6:F:453:SER:O	6:F:458:ASP:N	2.34	0.57
6:E:154:VAL:N	6:E:223:ASP:O	2.37	0.57
6:E:393:ALA:O	6:E:396:TYR:OH	2.21	0.57
6:E:423:ASN:O	6:E:427:ARG:NH2	2.36	0.57
1:A:451:SER:O	1:A:451:SER:OG	2.23	0.57
6:F:472:PHE:CD1	6:F:590:LEU:HD11	2.39	0.57
1:A:621:LYS:HE2	1:A:624:ARG:HD2	1.87	0.57
1:A:845:ASP:OD1	1:A:845:ASP:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:SER:O	2:D:151:SER:OG	2.20	0.57
6:F:364:PRO:HB2	6:F:366:THR:HG23	1.86	0.57
6:E:295:LEU:HD12	6:E:298:TYR:HB3	1.86	0.57
1:A:770:TYR:O	1:A:773:GLN:N	2.29	0.57
6:F:553:ALA:O	6:F:557:ASN:HB2	2.04	0.57
2:B:164:SER:OG	2:B:164:SER:O	2.18	0.57
6:F:6:VAL:HG23	6:F:106:PHE:HZ	1.70	0.57
1:A:196:MET:HE3	1:A:232:PRO:HB3	1.85	0.57
6:F:457:TYR:O	6:F:460:LYS:HG2	2.04	0.57
6:E:449:VAL:HG21	6:E:464:HIS:H	1.68	0.57
2:D:58:LYS:NZ	6:F:79:ILE:HG21	2.19	0.57
2:D:81:ALA:O	2:D:82:LYS:HD2	2.04	0.57
6:F:50:CYS:HB3	6:F:57:VAL:HG21	1.87	0.57
6:F:173:ARG:NH1	6:F:176:LEU:HB2	2.17	0.57
1:A:284:ASP:OD1	1:A:288:LYS:NZ	2.38	0.56
6:F:314:VAL:HG23	6:F:317:LEU:HD12	1.87	0.56
6:F:400:GLY:HA2	6:F:404:GLN:HE22	1.70	0.56
6:E:445:PRO:HA	6:E:465:LYS:HG2	1.86	0.56
6:E:569:LYS:HG3	6:E:570:VAL:HG23	1.86	0.56
1:A:156:TYR:OH	1:A:170:ASP:OD2	2.17	0.56
1:A:814:SER:O	1:A:814:SER:OG	2.16	0.56
2:D:51:ARG:HH11	2:D:51:ARG:HG2	1.69	0.56
2:D:143:ASP:OD1	2:D:143:ASP:N	2.37	0.56
6:F:311:HIS:NE2	6:F:335:PRO:HD2	2.20	0.56
6:E:26:CYS:SG	6:E:97:CYS:HB2	2.44	0.56
6:E:64:TYR:N	6:E:71:TYR:O	2.23	0.56
6:E:373:PHE:O	6:E:399:ILE:N	2.26	0.56
7:G:48:LEU:HD12	7:G:48:LEU:H	1.69	0.56
1:A:73:LYS:HD3	1:A:116:ARG:HH12	1.69	0.56
1:A:122:TYR:O	1:A:212:LEU:HD12	2.04	0.56
2:D:22:TYR:HB2	2:D:38:LEU:HD12	1.88	0.56
6:F:29:CYS:HB2	6:F:99:GLY:HA2	1.86	0.56
6:F:345:LYS:HE2	6:F:346:PHE:HE1	1.71	0.56
6:F:537:GLN:HG2	6:F:567:ARG:NH1	2.19	0.56
6:E:5:CYS:HB3	6:E:12:THR:HG21	1.88	0.56
6:E:428:LEU:HG	6:E:432:ILE:HD12	1.87	0.56
3:C:70:LYS:CE	2:D:88:GLN:HB3	2.35	0.56
6:E:285:GLY:CA	6:E:288:LYS:HZ1	2.19	0.56
1:A:180:GLU:OE1	1:A:183:ARG:NH1	2.39	0.56
1:A:207:LEU:C	1:A:209:ASN:H	2.08	0.56
1:A:539:ILE:O	1:A:540:THR:OG1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:VAL:HG21	2:D:147:PHE:HE2	1.71	0.56
2:D:134:ASP:CG	2:D:136:ASN:H	2.09	0.56
6:F:276:LYS:O	6:F:396:TYR:N	2.39	0.56
6:F:332:ARG:O	6:F:348:VAL:HG22	2.05	0.56
6:F:550:THR:HG22	6:F:551:GLU:H	1.70	0.56
6:E:118:GLY:O	6:E:122:LEU:HG	2.06	0.56
7:G:19:THR:HG22	7:G:20:GLN:HG2	1.87	0.56
2:B:163:ASP:OD1	2:B:163:ASP:N	2.38	0.56
6:F:287:GLY:O	6:F:291:PHE:HB2	2.06	0.56
6:E:52:ALA:HB3	6:E:55:CYS:HB2	1.86	0.56
6:E:249:ILE:HD13	6:E:299:TYR:OH	2.05	0.56
1:A:810:HIS:O	1:A:810:HIS:ND1	2.39	0.56
2:D:38:LEU:HA	2:D:41:SER:HG	1.69	0.56
6:F:80:SER:O	6:F:81:PHE:HB2	2.06	0.56
6:F:425:VAL:HG13	6:F:428:LEU:HD22	1.88	0.56
6:E:18:ALA:HB3	6:E:39:HIS:ND1	2.21	0.56
6:E:255:THR:OG1	6:E:298:TYR:O	2.11	0.56
5:J:45:C:H2'	5:J:46:U:O4'	2.06	0.56
6:F:496:VAL:O	6:F:500:LEU:HG	2.06	0.56
6:E:448:ILE:O	6:E:452:VAL:HG13	2.06	0.56
6:F:365:GLU:HG3	6:F:390:ARG:HG2	1.88	0.55
6:F:496:VAL:HG13	6:F:545:ILE:HG21	1.87	0.55
6:E:88:GLN:NE2	6:E:94:LYS:O	2.39	0.55
4:I:10:C:H2'	4:I:11:G:C8	2.40	0.55
4:I:22:G:N2	5:J:38:C:O2	2.28	0.55
4:I:23:C:H2'	4:I:24:U:C6	2.41	0.55
4:I:32:A:O5'	4:I:32:A:H8	1.89	0.55
1:A:598:TRP:HE1	1:A:602:LEU:HD11	1.71	0.55
1:A:752:HIS:O	1:A:753:PHE:HB2	2.07	0.55
6:E:5:CYS:SG	6:E:10:SER:OG	2.64	0.55
6:E:71:TYR:HB3	6:E:75:HIS:HB2	1.88	0.55
6:E:199:THR:OG1	6:E:212:ARG:O	2.23	0.55
1:A:161:ASP:O	1:A:168:ASN:ND2	2.38	0.55
2:D:177:SER:C	2:D:179:ASN:H	2.09	0.55
6:F:283:PRO:HD3	6:F:460:LYS:NZ	2.22	0.55
6:F:332:ARG:HG3	6:F:357:PHE:O	2.07	0.55
6:E:276:LYS:O	6:E:396:TYR:N	2.36	0.55
6:F:71:TYR:HB3	6:F:76:LYS:HA	1.88	0.55
4:I:26:G:N2	5:J:35:U:O2	2.40	0.55
2:D:132:ILE:HG21	2:D:138:TYR:HB2	1.89	0.55
6:F:303:ARG:HG2	6:F:354:GLN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:THR:H	7:G:22:ALA:HB3	1.71	0.55
6:F:41:LEU:HD12	6:F:42:VAL:H	1.72	0.55
6:F:50:CYS:HB2	6:F:72:CYS:HB3	1.89	0.55
6:F:329:LYS:HE3	6:F:354:GLN:H	1.72	0.55
6:F:448:ILE:O	6:F:452:VAL:HG23	2.06	0.55
6:E:562:ASN:O	6:E:562:ASN:ND2	2.40	0.55
1:A:311:ALA:HB1	1:A:350:GLU:HB3	1.88	0.55
6:F:378:MET:HB3	6:F:405:LEU:HB2	1.89	0.55
6:F:429:MET:HG2	6:F:434:PRO:HA	1.89	0.55
6:E:243:GLN:HB3	6:E:277:TYR:HD2	1.72	0.55
6:E:383:ASP:OD1	6:E:383:ASP:N	2.39	0.55
6:E:424:SER:O	6:E:427:ARG:HG2	2.07	0.55
7:G:24:THR:OG1	7:G:27:ASN:ND2	2.40	0.55
6:F:265:ASN:HB3	6:F:269:TYR:CZ	2.41	0.55
6:F:548:GLN:NE2	6:F:575:ILE:O	2.39	0.55
6:E:38:SER:OG	6:E:38:SER:O	2.22	0.55
1:A:758:LEU:HD12	1:A:759:SER:H	1.72	0.54
3:C:25:SER:OG	3:C:25:SER:O	2.24	0.54
6:F:286:THR:HA	6:F:440:THR:O	2.07	0.54
6:E:382:TYR:O	6:E:386:VAL:HG23	2.07	0.54
6:F:471:CYS:HB3	6:F:587:PHE:CZ	2.41	0.54
6:F:496:VAL:HG21	6:F:511:PHE:CZ	2.42	0.54
7:G:53:TRP:CZ3	7:G:66:TYR:HB3	2.42	0.54
7:G:55:ARG:HA	7:G:65:ILE:O	2.07	0.54
7:G:97:LEU:O	7:G:101:MET:HG3	2.08	0.54
1:A:197:ARG:O	1:A:199:ALA:N	2.40	0.54
6:F:197:GLU:N	6:F:197:GLU:OE1	2.40	0.54
6:E:121:ILE:HG12	6:E:421:TYR:HE2	1.72	0.54
1:A:607:SER:OG	1:A:608:ASP:N	2.41	0.54
2:D:89:THR:O	2:D:93:THR:HG23	2.08	0.54
6:E:127:THR:O	6:E:131:LYS:HG2	2.08	0.54
1:A:162:TRP:HA	1:A:168:ASN:ND2	2.22	0.54
6:F:268:ASN:HB3	6:F:436:MET:HG2	1.89	0.54
6:E:147:LEU:HG	6:E:229:SER:HB3	1.90	0.54
6:E:149:TYR:C	6:E:171:LYS:HG2	2.28	0.54
1:A:905:VAL:HG22	1:A:906:MET:H	1.72	0.54
6:F:262:PHE:CZ	6:F:290:HIS:HB3	2.43	0.54
6:F:106:PHE:HA	6:F:130:LEU:HD21	1.90	0.54
6:E:57:VAL:HG11	6:E:62:GLN:NE2	2.22	0.54
1:A:894:GLU:OE1	1:A:895:LEU:N	2.40	0.54
2:D:161:ASP:HB2	2:D:181:ALA:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:165:LEU:HB3	6:F:209:VAL:HG21	1.89	0.54
6:E:367:THR:HA	6:E:392:ARG:H	1.73	0.54
7:G:58:LYS:HD2	7:G:59:SER:H	1.72	0.54
2:D:49:PHE:O	2:D:51:ARG:N	2.40	0.54
2:D:112:ASP:N	2:D:112:ASP:OD1	2.38	0.54
6:F:133:PHE:O	6:F:137:THR:HG23	2.08	0.54
6:F:332:ARG:HB2	6:F:346:PHE:CD2	2.43	0.54
1:A:60:ASP:OD1	1:A:61:GLU:N	2.40	0.53
1:A:517:ASP:N	1:A:517:ASP:OD1	2.41	0.53
5:J:40:U:H2'	5:J:41:G:H8	1.72	0.53
6:F:382:TYR:O	6:F:386:VAL:HG13	2.09	0.53
6:E:151:ILE:HG23	6:E:226:VAL:HG12	1.90	0.53
7:G:12:MET:HB2	7:G:39:ARG:HH22	1.73	0.53
7:G:79:THR:OG1	7:G:81:LYS:HG2	2.07	0.53
1:A:124:MET:O	1:A:124:MET:HG3	2.09	0.53
2:D:33:VAL:O	2:D:37:LYS:HG2	2.09	0.53
2:D:100:ASN:O	2:D:104:ASN:N	2.39	0.53
6:E:310:SER:N	6:E:375:GLU:OE1	2.40	0.53
1:A:903:TYR:CE1	2:D:67:MET:HG2	2.43	0.53
2:D:138:TYR:O	2:D:142:CYS:N	2.21	0.53
6:F:163:LEU:HD11	6:F:211:TYR:CE1	2.44	0.53
6:E:311:HIS:CE1	6:E:359:THR:HB	2.42	0.53
6:E:563:VAL:O	6:E:567:ARG:NE	2.41	0.53
1:A:483:TYR:N	1:A:483:TYR:CD2	2.76	0.53
3:C:6:VAL:HG11	3:C:48:ALA:HB1	1.90	0.53
2:D:140:ASN:OD1	2:D:140:ASN:N	2.41	0.53
6:F:117:ALA:O	6:F:121:ILE:HG12	2.09	0.53
6:F:386:VAL:HB	6:F:390:ARG:HE	1.72	0.53
6:E:427:ARG:HB3	6:E:427:ARG:NH1	2.23	0.53
1:A:82:HIS:NE2	1:A:222:PHE:O	2.39	0.53
1:A:136:GLU:OE1	1:A:136:GLU:N	2.42	0.53
1:A:256:HIS:O	1:A:258:ASP:N	2.41	0.53
2:B:130:VAL:HG13	2:B:186:VAL:HB	1.90	0.53
6:F:311:HIS:ND1	6:F:359:THR:OG1	2.39	0.53
6:E:121:ILE:O	6:E:125:THR:OG1	2.24	0.53
1:A:20:THR:O	1:A:20:THR:OG1	2.19	0.53
6:F:275:GLN:H	6:F:395:HIS:CE1	2.27	0.53
6:E:31:TYR:CE1	6:E:87:GLY:HA2	2.42	0.53
6:E:311:HIS:HE2	6:E:361:ASN:HB2	1.73	0.53
2:B:182:TRP:CH2	2:B:184:LEU:HD12	2.43	0.53
6:F:136:GLU:OE1	6:F:234:PRO:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:156:GLU:HB2	6:F:164:HIS:HB3	1.91	0.53
6:E:34:VAL:HG23	6:E:39:HIS:O	2.08	0.53
1:A:418:ASP:N	1:A:418:ASP:OD2	2.39	0.53
6:F:238:PRO:O	6:F:388:ASN:ND2	2.39	0.53
6:F:288:LYS:HA	6:F:291:PHE:HB2	1.90	0.53
6:F:373:PHE:O	6:F:399:ILE:N	2.42	0.53
2:B:128:LEU:HG	2:B:129:MET:N	2.24	0.53
6:F:275:GLN:NE2	6:F:277:TYR:O	2.42	0.53
6:F:436:MET:HE2	6:F:437:PHE:H	1.74	0.53
6:E:152:ALA:HB3	6:E:225:PHE:HB2	1.91	0.53
7:G:47:ASP:O	7:G:49:GLN:NE2	2.42	0.53
2:B:102:ALA:O	2:B:106:ILE:HG23	2.08	0.52
3:C:70:LYS:HG2	2:D:92:PHE:HD2	1.74	0.52
6:F:34:VAL:HG23	6:F:39:HIS:O	2.09	0.52
6:E:315:ASP:OD2	6:E:316:ALA:N	2.42	0.52
1:A:60:ASP:HB2	1:A:66:ILE:HB	1.91	0.52
1:A:218:ASP:OD2	9:A:1003:GNP:N3B	2.41	0.52
1:A:578:SER:O	1:A:578:SER:OG	2.26	0.52
1:A:711:ASP:O	1:A:714:LYS:HG3	2.08	0.52
2:B:160:VAL:HA	2:B:165:LYS:O	2.09	0.52
2:D:125:ALA:O	2:D:189:LEU:HD22	2.09	0.52
6:F:62:GLN:HE21	6:F:73:LYS:HG2	1.74	0.52
6:E:153:THR:O	6:E:166:SER:OG	2.20	0.52
1:A:431:GLU:OE2	3:C:2:LYS:N	2.43	0.52
6:F:276:LYS:HD3	6:F:395:HIS:HD2	1.73	0.52
6:E:50:CYS:SG	6:E:71:TYR:HA	2.50	0.52
2:B:161:ASP:OD2	2:B:165:LYS:NZ	2.22	0.52
2:B:54:ALA:HA	2:B:57:ARG:HH22	1.74	0.52
3:C:21:ARG:NH2	3:C:23:GLU:OE2	2.42	0.52
6:E:365:GLU:OE2	6:E:390:ARG:HA	2.10	0.52
3:C:17:LEU:HD21	3:C:59:LEU:HB2	1.90	0.52
6:F:279:THR:OG1	6:F:435:ASP:OD2	2.26	0.52
6:F:401:ASP:OD2	6:F:403:ALA:HB3	2.09	0.52
6:E:561:PHE:O	6:E:565:ILE:HG22	2.08	0.52
7:G:9:LEU:HD13	7:G:32:TYR:HE2	1.73	0.52
1:A:260:ASP:HB2	1:A:263:LYS:HD2	1.91	0.52
1:A:834:PRO:HG2	1:A:877:TYR:CE1	2.44	0.52
6:F:113:ASP:HB3	6:F:115:THR:HG23	1.90	0.52
6:E:21:ARG:HD3	6:E:140:ALA:HB2	1.92	0.52
6:E:427:ARG:HB3	6:E:427:ARG:HH11	1.74	0.52
6:E:470:GLN:NE2	6:E:505:ALA:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1003:GNP:N3	9:A:1003:GNP:H2'	2.24	0.52
2:D:62:MET:HE1	6:F:65:LEU:HD22	1.92	0.52
6:F:278:SER:OG	6:F:397:VAL:HA	2.10	0.52
6:E:252:LEU:HB3	6:E:299:TYR:CD1	2.44	0.52
6:E:382:TYR:O	6:E:385:SER:OG	2.14	0.52
6:E:455:LEU:HD23	6:E:456:VAL:HG23	1.92	0.52
2:D:182:TRP:CZ3	2:D:184:LEU:HD11	2.44	0.52
6:F:370:ILE:HD12	6:F:395:HIS:HB2	1.90	0.52
1:A:770:TYR:C	1:A:772:SER:H	2.13	0.52
2:B:54:ALA:HA	2:B:57:ARG:NH2	2.25	0.52
3:C:35:LEU:O	3:C:38:ASP:N	2.43	0.52
6:E:252:LEU:HB3	6:E:299:TYR:HD1	1.75	0.52
6:E:269:TYR:CE1	6:E:295:LEU:HB2	2.45	0.52
1:A:884:TYR:O	1:A:888:ILE:HG13	2.10	0.51
6:F:540:GLU:HB3	6:F:567:ARG:NE	2.20	0.51
6:E:280:LEU:HA	6:E:436:MET:HB2	1.92	0.51
6:E:548:GLN:O	6:E:550:THR:N	2.39	0.51
6:F:142:GLU:O	6:F:146:LYS:HG3	2.10	0.51
6:F:320:LYS:H	6:F:320:LYS:HZ3	1.57	0.51
6:F:407:ALA:HB3	6:F:409:ARG:NH1	2.26	0.51
6:E:243:GLN:HA	6:E:276:LYS:HD3	1.92	0.51
6:E:246:TYR:N	6:E:274:MET:O	2.36	0.51
6:E:248:ARG:HD3	6:E:249:ILE:N	2.25	0.51
6:E:419:PRO:HA	6:E:422:PHE:CE1	2.45	0.51
3:C:73:GLU:H	2:D:96:ARG:HH12	1.58	0.51
6:F:343:PHE:HD2	6:F:345:LYS:HG2	1.76	0.51
6:F:424:SER:HA	6:F:427:ARG:NE	2.25	0.51
1:A:608:ASP:OD2	1:A:608:ASP:N	2.44	0.51
6:F:493:ILE:O	6:F:497:ARG:HG2	2.11	0.51
6:E:31:TYR:O	6:E:34:VAL:HG12	2.10	0.51
6:E:378:MET:SD	6:E:378:MET:N	2.83	0.51
2:D:108:ASN:HA	2:D:111:ARG:HH12	1.75	0.51
2:D:174:MET:SD	2:D:174:MET:N	2.82	0.51
6:F:544:VAL:HB	6:F:572:ILE:HG13	1.93	0.51
6:E:61:THR:HA	6:E:84:CYS:CB	2.36	0.51
6:E:544:VAL:HG12	6:E:545:ILE:H	1.76	0.51
1:A:751:LYS:C	1:A:752:HIS:HD1	2.14	0.51
2:B:55:MET:HA	2:B:58:LYS:CE	2.39	0.51
2:D:132:ILE:HD11	2:D:147:PHE:CZ	2.46	0.51
6:E:238:PRO:O	6:E:385:SER:HA	2.11	0.51
7:G:11:GLN:NE2	7:G:12:MET:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:VAL:O	2:B:115:VAL:HG23	2.11	0.51
2:D:108:ASN:HA	2:D:111:ARG:NH1	2.26	0.51
6:F:288:LYS:HG2	6:F:438:LEU:HD23	1.92	0.51
6:F:304:ILE:HG13	6:F:370:ILE:O	2.11	0.51
6:E:140:ALA:O	6:E:143:GLU:HG2	2.10	0.51
7:G:54:ALA:O	7:G:66:TYR:HD1	1.94	0.51
1:A:38:TYR:HE2	1:A:725:HIS:CE1	2.26	0.51
1:A:38:TYR:CG	1:A:38:TYR:O	2.63	0.51
3:C:3:MET:O	3:C:6:VAL:N	2.43	0.51
6:F:380:THR:HG22	6:F:381:ASN:H	1.76	0.51
1:A:571:PHE:HE1	1:A:642:HIS:NE2	2.09	0.51
2:B:105:ASN:OD1	2:B:105:ASN:N	2.43	0.51
6:F:140:ALA:O	6:F:144:THR:HG23	2.11	0.51
6:F:152:ALA:O	6:F:225:PHE:HD2	1.94	0.51
6:F:182:PHE:O	6:F:198:TYR:HB2	2.11	0.51
6:F:249:ILE:HD12	6:F:273:GLY:HA3	1.93	0.51
6:F:311:HIS:HB3	6:F:342:CYS:SG	2.51	0.51
6:E:269:TYR:HB3	6:E:295:LEU:HD13	1.92	0.51
6:E:306:TYR:HA	6:E:372:VAL:CG2	2.40	0.51
1:A:687:THR:O	1:A:689:TYR:N	2.44	0.51
6:F:25:LEU:HB3	6:F:30:CYS:HB2	1.93	0.51
6:F:51:ASN:HD21	6:F:69:SER:HB3	1.75	0.51
6:F:306:TYR:HB2	6:F:357:PHE:CG	2.46	0.51
6:E:248:ARG:HD2	6:E:250:THR:HG23	1.93	0.51
6:E:519:ASN:O	6:E:523:SER:OG	2.22	0.51
1:A:76:THR:OG1	1:A:77:PHE:N	2.44	0.50
6:F:305:VAL:HG23	6:F:356:VAL:HG13	1.93	0.50
6:E:245:HIS:CD2	6:E:275:GLN:HB2	2.46	0.50
6:E:511:PHE:HB3	6:E:519:ASN:ND2	2.26	0.50
2:B:162:ALA:HB3	2:B:181:ALA:HB1	1.93	0.50
3:C:28:LEU:HA	3:C:31:GLN:OE1	2.11	0.50
6:F:422:PHE:HB2	6:F:426:CYS:SG	2.50	0.50
6:F:537:GLN:HA	6:F:567:ARG:HH12	1.76	0.50
6:E:154:VAL:HA	6:E:165:LEU:HA	1.93	0.50
1:A:32:TYR:CE1	1:A:49:LEU:HD12	2.46	0.50
1:A:344:THR:O	1:A:344:THR:OG1	2.21	0.50
1:A:566:MET:O	1:A:566:MET:HG2	2.10	0.50
2:D:159:VAL:HG23	2:D:184:LEU:HD23	1.92	0.50
4:I:22:G:C6	5:J:39:A:C6	3.00	0.50
6:F:173:ARG:HH11	6:F:174:PRO:HD2	1.76	0.50
6:E:332:ARG:HD3	6:E:334:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:544:VAL:O	6:E:572:ILE:HA	2.11	0.50
6:E:37:THR:HG22	6:E:38:SER:H	1.77	0.50
6:E:235:LEU:HD11	6:E:382:TYR:CD1	2.40	0.50
6:E:489:ASN:HD22	6:E:549:THR:HA	1.75	0.50
1:A:800:TRP:O	1:A:801:THR:OG1	2.28	0.50
3:C:2:LYS:NZ	2:D:98:LEU:HD12	2.27	0.50
6:F:127:THR:OG1	6:F:128:GLU:OE1	2.24	0.50
6:F:171:LYS:HG3	6:F:172:PRO:HD2	1.93	0.50
6:E:370:ILE:HD12	6:E:395:HIS:HB2	1.92	0.50
6:F:55:CYS:SG	6:F:57:VAL:HG13	2.52	0.50
6:F:262:PHE:CE1	6:F:290:HIS:HB3	2.46	0.50
6:F:287:GLY:O	6:F:438:LEU:HD21	2.12	0.50
6:F:399:ILE:HD12	6:F:399:ILE:H	1.77	0.50
6:E:163:LEU:HG	6:E:211:TYR:CE2	2.47	0.50
1:A:163:TYR:HD1	1:A:164:ASP:N	2.10	0.50
1:A:314:ASN:ND2	1:A:350:GLU:O	2.30	0.50
1:A:899:MET:O	1:A:903:TYR:HB2	2.11	0.50
2:D:101:ASP:O	2:D:105:ASN:HB3	2.11	0.50
2:D:176:ASN:OD1	2:D:176:ASN:N	2.42	0.50
5:J:39:A:C6	5:J:40:U:C4	2.99	0.50
6:E:6:VAL:O	6:E:7:LEU:HD23	2.11	0.50
6:F:357:PHE:N	6:F:357:PHE:HD1	2.10	0.50
6:F:472:PHE:HD1	6:F:590:LEU:HD11	1.76	0.50
6:E:286:THR:H	6:E:288:LYS:NZ	2.08	0.50
2:D:38:LEU:HA	2:D:41:SER:OG	2.12	0.50
6:F:16:CYS:HB2	6:F:25:LEU:HD12	1.94	0.50
6:F:238:PRO:HB2	6:F:240:LEU:O	2.12	0.50
6:F:496:VAL:HG21	6:F:511:PHE:CE1	2.47	0.50
6:E:184:GLY:HA3	6:E:225:PHE:CD1	2.37	0.50
3:C:2:LYS:NZ	2:D:98:LEU:O	2.42	0.49
6:F:372:VAL:HB	6:F:399:ILE:HD11	1.94	0.49
6:F:420:GLU:O	6:F:427:ARG:N	2.45	0.49
6:E:283:PRO:HD2	6:E:286:THR:HG21	1.94	0.49
6:E:420:GLU:O	6:E:427:ARG:NH1	2.45	0.49
6:E:479:VAL:H	6:E:491:PRO:HB2	1.77	0.49
1:A:32:TYR:HE1	1:A:49:LEU:HD12	1.77	0.49
1:A:329:LEU:O	1:A:330:VAL:HG13	2.13	0.49
1:A:795:SER:HG	1:A:798:LYS:HZ3	1.54	0.49
6:F:173:ARG:HH22	6:F:176:LEU:HD22	1.76	0.49
6:E:163:LEU:HG	6:E:211:TYR:HE2	1.75	0.49
6:E:506:TRP:O	6:E:545:ILE:HD11	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ARG:HH21	1:A:735:ARG:HH11	1.60	0.49
2:B:55:MET:HE3	2:B:56:GLN:N	2.27	0.49
6:F:115:THR:OG1	6:F:116:ASN:OD1	2.29	0.49
6:F:281:GLN:O	6:F:460:LYS:NZ	2.45	0.49
6:E:151:ILE:O	6:E:167:TRP:HA	2.12	0.49
1:A:388:LEU:HD23	1:A:397:SER:OG	2.13	0.49
1:A:409:THR:OG1	1:A:410:VAL:N	2.45	0.49
5:J:38:C:H2'	5:J:39:A:H8	1.76	0.49
6:E:51:ASN:OD1	6:E:51:ASN:N	2.42	0.49
6:E:167:TRP:CZ2	6:E:173:ARG:HG3	2.47	0.49
1:A:308:LEU:O	1:A:310:CYS:N	2.45	0.49
6:F:112:CYS:SG	6:F:122:LEU:HD12	2.52	0.49
6:F:510:VAL:HG11	6:F:531:GLN:HG3	1.94	0.49
6:E:278:SER:N	6:E:396:TYR:O	2.45	0.49
1:A:456:TYR:C	1:A:458:TYR:H	2.15	0.49
1:A:795:SER:OG	1:A:798:LYS:NZ	2.24	0.49
3:C:64:GLY:O	3:C:66:VAL:N	2.46	0.49
4:I:20:A:C6	5:J:41:G:C6	3.01	0.49
6:F:138:LEU:HD23	6:F:139:LYS:NZ	2.27	0.49
6:E:126:CYS:SG	6:E:127:THR:N	2.86	0.49
6:E:126:CYS:SG	6:E:131:LYS:N	2.86	0.49
6:E:489:ASN:ND2	6:E:492:GLN:OE1	2.45	0.49
6:E:547:THR:HA	6:E:575:ILE:CG2	2.43	0.49
2:B:45:ALA:O	2:B:48:GLU:HB2	2.12	0.49
2:B:159:VAL:HG22	2:B:186:VAL:HG22	1.94	0.49
5:J:39:A:H2'	5:J:40:U:C6	2.47	0.49
6:F:11:GLN:HB2	6:F:93:TYR:CZ	2.48	0.49
6:F:149:TYR:CE1	6:F:174:PRO:HA	2.46	0.49
7:G:70:GLU:HB3	7:G:90:PHE:O	2.12	0.49
1:A:829:LEU:HD23	1:A:868:PRO:HB3	1.95	0.49
2:B:177:SER:HA	2:B:180:LEU:HD12	1.95	0.49
3:C:44:ASP:OD1	3:C:47:GLU:HB3	2.13	0.49
2:D:49:PHE:C	2:D:51:ARG:H	2.16	0.49
2:D:187:THR:HG22	2:D:188:ALA:N	2.28	0.49
6:F:269:TYR:CD1	6:F:295:LEU:HD13	2.47	0.49
6:F:321:ALA:HB2	6:F:357:PHE:CE2	2.47	0.49
6:F:552:THR:N	6:F:555:SER:OG	2.46	0.49
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.77	0.49
1:A:271:LEU:H	1:A:271:LEU:HD12	1.77	0.49
1:A:411:LYS:H	1:A:411:LYS:HZ3	1.61	0.49
6:F:26:CYS:O	6:F:27:CYS:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:328:ASP:OD2	6:F:329:LYS:HD2	2.13	0.49
6:F:443:ARG:HG3	6:F:444:CYS:N	2.25	0.49
6:E:162:GLU:HG3	6:E:210:VAL:HG22	1.94	0.49
6:E:495:VAL:HG13	6:E:498:GLU:OE1	2.12	0.49
1:A:63:ASP:OD1	1:A:63:ASP:N	2.46	0.49
1:A:346:TYR:HE1	1:A:537:PRO:HB3	1.78	0.49
1:A:505:PRO:HB2	1:A:508:LYS:HZ1	1.78	0.49
6:F:131:LYS:HG3	6:F:132:LEU:N	2.28	0.49
6:E:108:ALA:O	6:E:112:CYS:N	2.32	0.49
6:E:235:LEU:HD21	6:E:382:TYR:CE1	2.48	0.49
6:E:442:ARG:HA	6:E:464:HIS:CE1	2.48	0.49
7:G:75:PHE:CZ	7:G:88:LEU:HB2	2.48	0.49
6:F:62:GLN:NE2	6:F:73:LYS:H	2.11	0.48
6:F:220:ASN:HB2	6:F:223:ASP:OD2	2.13	0.48
6:F:277:TYR:HB2	6:F:398:TYR:CE1	2.47	0.48
6:F:347:LYS:CE	6:F:350:SER:HB3	2.43	0.48
6:F:548:GLN:NE2	6:F:576:MET:HA	2.28	0.48
6:E:499:PHE:CE1	6:E:573:LEU:HD13	2.47	0.48
1:A:257:VAL:HG12	1:A:263:LYS:HB3	1.96	0.48
1:A:565:THR:HG22	1:A:685:ALA:HB2	1.96	0.48
2:D:173:SER:O	2:D:177:SER:OG	2.26	0.48
6:F:153:THR:HA	6:F:224:TYR:HB3	1.95	0.48
6:E:307:THR:HG22	6:E:372:VAL:O	2.13	0.48
1:A:56:PHE:HE1	1:A:72:VAL:HG11	1.77	0.48
1:A:348:PHE:HD2	1:A:351:LEU:HB2	1.78	0.48
1:A:920:PHE:C	1:A:920:PHE:CD1	2.86	0.48
6:F:158:LEU:HB2	6:F:163:LEU:HA	1.95	0.48
6:F:265:ASN:ND2	6:F:291:PHE:HA	2.28	0.48
6:F:269:TYR:CG	6:F:295:LEU:HD13	2.48	0.48
6:F:448:ILE:HB	6:F:587:PHE:HZ	1.78	0.48
1:A:72:VAL:HA	1:A:115:SER:HA	1.95	0.48
6:E:8:CYS:HB3	6:E:98:VAL:HG22	1.95	0.48
6:E:31:TYR:CD1	6:E:87:GLY:HA2	2.48	0.48
6:E:145:PHE:CE2	6:E:410:THR:HG21	2.47	0.48
6:E:296:ALA:O	6:E:355:TYR:OH	2.28	0.48
6:E:493:ILE:HA	6:E:496:VAL:HG23	1.94	0.48
7:G:12:MET:HG3	7:G:13:SER:H	1.77	0.48
1:A:55:ARG:NH2	9:A:1003:GNP:O6	2.37	0.48
1:A:83:GLU:OE2	1:A:83:GLU:HA	2.14	0.48
1:A:275:PHE:O	1:A:279:ARG:HG3	2.14	0.48
1:A:636:LEU:HD11	1:A:655:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ARG:HG2	2:B:75:ARG:HH21	1.78	0.48
6:F:198:TYR:CD1	6:F:225:PHE:HE1	2.30	0.48
6:E:309:CYS:HB3	6:E:375:GLU:CD	2.34	0.48
6:E:371:VAL:O	6:E:397:VAL:N	2.43	0.48
6:E:510:VAL:C	6:E:528:LEU:HD23	2.33	0.48
1:A:55:ARG:HH22	1:A:121:LYS:HZ3	1.62	0.48
6:F:155:ARG:HA	6:F:222:GLY:H	1.79	0.48
6:E:13:SER:O	6:E:14:LEU:HD23	2.14	0.48
1:A:19:LEU:HD23	1:A:58:GLU:HA	1.95	0.48
1:A:444:GLN:NE2	1:A:552:ASN:O	2.29	0.48
2:D:130:VAL:HG21	2:D:147:PHE:CE2	2.49	0.48
6:F:61:THR:HA	6:F:84:CYS:HB3	1.95	0.48
6:F:107:ASN:O	6:F:110:ALA:N	2.47	0.48
6:F:116:ASN:HB3	6:F:414:LYS:NZ	2.28	0.48
6:F:442:ARG:HA	6:F:464:HIS:CE1	2.49	0.48
6:E:152:ALA:HB1	6:E:165:LEU:HD21	1.96	0.48
6:E:163:LEU:O	6:E:209:VAL:N	2.47	0.48
6:E:308:ALA:HB2	6:E:374:ASP:HB3	1.95	0.48
1:A:111:VAL:O	1:A:113:HIS:ND1	2.47	0.48
1:A:171:ILE:HD12	1:A:174:VAL:HB	1.96	0.48
2:D:100:ASN:N	2:D:104:ASN:OD1	2.46	0.48
2:D:161:ASP:OD2	2:D:165:LYS:HE2	2.14	0.48
6:E:34:VAL:HG21	6:E:60:VAL:CG1	2.44	0.48
6:E:132:LEU:HD11	6:E:235:LEU:O	2.14	0.48
6:E:163:LEU:N	6:E:209:VAL:H	2.09	0.48
6:E:489:ASN:O	6:E:493:ILE:HG13	2.14	0.48
6:F:440:THR:HA	6:F:462:LYS:NZ	2.29	0.48
6:F:500:LEU:HD22	6:F:506:TRP:HB3	1.96	0.48
6:E:32:ASP:HB3	6:E:103:VAL:HG11	1.96	0.48
7:G:5:SER:OG	7:G:101:MET:HG2	2.14	0.48
7:G:56:PHE:HD1	7:G:57:PRO:HD2	1.78	0.48
7:G:76:VAL:HG22	7:G:85:VAL:HG22	1.95	0.48
1:A:75:HIS:ND1	1:A:76:THR:HG22	2.29	0.48
1:A:771:ALA:HB2	1:A:776:VAL:HG23	1.94	0.48
1:A:876:GLU:CD	1:A:876:GLU:H	2.10	0.48
1:A:900:LEU:HA	1:A:905:VAL:O	2.14	0.48
6:F:331:SER:O	6:F:357:PHE:N	2.43	0.48
6:F:334:ILE:HG13	6:F:343:PHE:O	2.13	0.48
6:E:138:LEU:O	6:E:142:GLU:HG2	2.14	0.48
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.62	0.47
1:A:454:ASP:OD2	1:A:457:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:LEU:O	1:A:615:MET:HB2	2.14	0.47
1:A:740:ASP:OD1	1:A:740:ASP:C	2.51	0.47
1:A:875:GLN:O	1:A:877:TYR:N	2.47	0.47
3:C:73:GLU:HG2	2:D:96:ARG:NH1	2.29	0.47
6:F:31:TYR:O	6:F:35:ILE:HG23	2.14	0.47
6:E:203:GLY:HA2	6:E:210:VAL:H	1.77	0.47
6:E:299:TYR:O	6:E:301:SER:N	2.38	0.47
6:E:544:VAL:HB	6:E:572:ILE:HD12	1.96	0.47
1:A:18:ARG:HB3	1:A:59:LYS:HZ3	1.79	0.47
1:A:628:ASN:N	1:A:628:ASN:OD1	2.45	0.47
1:A:833:ASP:O	1:A:836:ARG:N	2.44	0.47
3:C:47:GLU:O	3:C:50:GLU:HG2	2.14	0.47
6:F:186:ARG:HA	6:F:223:ASP:HB3	1.96	0.47
6:F:245:HIS:HA	6:F:275:GLN:HA	1.96	0.47
6:F:311:HIS:NE2	6:F:334:ILE:HG23	2.29	0.47
6:F:357:PHE:N	6:F:357:PHE:CD1	2.81	0.47
6:E:15:ARG:O	6:E:17:GLY:N	2.47	0.47
6:E:25:LEU:HD23	6:E:25:LEU:HA	1.63	0.47
6:E:258:ILE:HD13	6:E:298:TYR:HA	1.96	0.47
6:E:271:LYS:HE3	6:E:436:MET:SD	2.54	0.47
2:B:188:ALA:O	2:B:189:LEU:HD12	2.14	0.47
2:D:132:ILE:HD11	2:D:147:PHE:HZ	1.80	0.47
5:J:25:G:O5'	5:J:25:G:H8	1.96	0.47
6:E:394:LYS:HG2	6:E:395:HIS:CE1	2.49	0.47
6:E:551:GLU:HG3	6:E:578:ASP:HA	1.95	0.47
7:G:69:LEU:O	7:G:92:LYS:HG3	2.13	0.47
1:A:733:ARG:NH2	7:G:3:GLU:O	2.46	0.47
6:F:203:GLY:HA3	6:F:208:ALA:O	2.14	0.47
6:F:471:CYS:HB3	6:F:587:PHE:CE2	2.50	0.47
6:E:198:TYR:HB2	6:E:200:PHE:HE1	1.79	0.47
6:E:371:VAL:HB	6:E:396:TYR:HA	1.97	0.47
3:C:47:GLU:HA	3:C:50:GLU:OE2	2.15	0.47
2:D:39:LYS:HE2	2:D:39:LYS:HB3	1.76	0.47
2:D:109:ASN:HA	2:D:112:ASP:OD2	2.15	0.47
2:D:173:SER:N	2:D:177:SER:OG	2.47	0.47
6:F:25:LEU:HD22	6:F:30:CYS:HA	1.96	0.47
6:F:283:PRO:HD3	6:F:460:LYS:HZ2	1.77	0.47
6:F:473:LYS:HG2	6:F:587:PHE:HB2	1.96	0.47
6:F:519:ASN:O	6:F:523:SER:OG	2.28	0.47
6:E:161:ARG:C	6:E:210:VAL:HA	2.35	0.47
6:E:470:GLN:HG2	6:E:571:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:SER:O	1:A:237:TYR:C	2.53	0.47
2:B:95:LEU:HA	2:B:98:LEU:HD13	1.96	0.47
6:F:370:ILE:HG22	6:F:371:VAL:H	1.79	0.47
6:E:75:HIS:N	6:E:75:HIS:CD2	2.82	0.47
6:E:181:VAL:O	6:E:181:VAL:HG23	2.14	0.47
1:A:404:ASN:N	1:A:404:ASN:OD1	2.47	0.47
1:A:913:SER:O	1:A:913:SER:OG	2.32	0.47
2:B:59:LEU:HA	2:B:59:LEU:HD23	1.69	0.47
3:C:2:LYS:HZ2	2:D:98:LEU:HD12	1.79	0.47
3:C:24:SER:O	3:C:24:SER:OG	2.26	0.47
2:D:115:VAL:HG23	2:D:115:VAL:O	2.14	0.47
4:I:10:C:H2'	4:I:11:G:H8	1.80	0.47
6:F:190:ASN:OD1	6:F:191:SER:N	2.48	0.47
6:F:329:LYS:HB3	6:F:354:GLN:HB2	1.97	0.47
6:F:498:GLU:O	6:F:593:PRO:HG2	2.15	0.47
6:F:547:THR:HG22	6:F:549:THR:H	1.79	0.47
6:E:158:LEU:HD21	6:E:164:HIS:CE1	2.50	0.47
6:E:307:THR:HG23	6:E:373:PHE:CD1	2.49	0.47
6:E:417:LEU:HD11	6:E:421:TYR:HB3	1.96	0.47
1:A:278:GLU:O	1:A:282:LEU:HG	2.15	0.47
1:A:612:PRO:HB2	1:A:805:LEU:HD21	1.95	0.47
2:D:109:ASN:O	2:D:112:ASP:N	2.47	0.47
6:E:322:LEU:HG	6:E:327:ILE:HG23	1.97	0.47
7:G:55:ARG:O	7:G:64:THR:OG1	2.33	0.47
1:A:483:TYR:N	1:A:483:TYR:HD2	2.13	0.47
1:A:770:TYR:C	1:A:772:SER:N	2.67	0.47
2:D:121:PRO:HG3	2:D:127:LYS:O	2.14	0.47
6:F:319:GLU:O	6:F:323:LYS:HG3	2.13	0.47
6:E:11:GLN:OE1	6:E:12:THR:N	2.48	0.47
6:E:109:ILE:HD13	6:E:134:ALA:HB2	1.96	0.47
6:E:143:GLU:HA	6:E:146:LYS:NZ	2.30	0.47
6:E:449:VAL:HG23	6:E:450:ASP:H	1.80	0.47
1:A:252:THR:C	1:A:254:GLU:H	2.18	0.47
1:A:377:ASP:O	1:A:381:HIS:ND1	2.48	0.47
1:A:605:VAL:O	1:A:607:SER:N	2.41	0.47
2:B:172:ILE:HD12	2:B:172:ILE:N	2.29	0.47
6:F:275:GLN:OE1	6:F:278:SER:HB3	2.14	0.47
6:F:331:SER:HA	6:F:347:LYS:H	1.80	0.47
6:F:472:PHE:HA	6:F:587:PHE:HB3	1.97	0.47
6:F:535:SER:OG	6:F:535:SER:O	2.32	0.47
6:E:443:ARG:C	6:E:465:LYS:HZ1	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:449:VAL:HG11	6:E:464:HIS:HB2	1.97	0.47
6:E:485:SER:O	6:E:485:SER:OG	2.32	0.47
6:E:500:LEU:HD12	6:E:506:TRP:HB3	1.95	0.47
7:G:96:ASN:O	7:G:99:ARG:N	2.48	0.47
1:A:210:GLN:O	1:A:210:GLN:HG2	2.13	0.46
1:A:370:GLU:O	1:A:371:LEU:C	2.52	0.46
1:A:454:ASP:O	1:A:456:TYR:N	2.48	0.46
1:A:594:PHE:CD2	5:J:31:U:H4'	2.50	0.46
1:A:615:MET:HB2	1:A:766:PHE:CE1	2.50	0.46
1:A:624:ARG:HG2	1:A:624:ARG:HH11	1.79	0.46
6:F:184:GLY:C	6:F:195:ILE:H	2.18	0.46
6:E:7:LEU:CD2	6:E:130:LEU:HD21	2.45	0.46
6:E:62:GLN:HG2	6:E:73:LYS:NZ	2.30	0.46
6:E:350:SER:O	6:E:350:SER:OG	2.31	0.46
6:E:369:ASP:C	6:E:393:ALA:HB1	2.35	0.46
6:E:423:ASN:C	6:E:427:ARG:HH21	2.17	0.46
6:E:444:CYS:O	6:E:465:LYS:HE2	2.15	0.46
1:A:164:ASP:OD1	1:A:164:ASP:C	2.53	0.46
1:A:335:VAL:HG13	1:A:336:ASP:OD1	2.15	0.46
6:F:408:PRO:HA	6:F:560:ARG:HH22	1.80	0.46
6:F:458:ASP:O	6:F:460:LYS:N	2.48	0.46
6:F:561:PHE:O	6:F:565:ILE:HG12	2.15	0.46
6:E:268:ASN:HB2	6:E:291:PHE:CZ	2.46	0.46
6:E:285:GLY:HA2	6:E:288:LYS:HZ1	1.79	0.46
6:E:288:LYS:HA	6:E:291:PHE:HB2	1.97	0.46
6:E:489:ASN:CG	6:E:492:GLN:HB2	2.35	0.46
1:A:380:MET:HB3	2:B:94:MET:HE1	1.98	0.46
1:A:611:ASN:N	1:A:611:ASN:OD1	2.47	0.46
1:A:764:VAL:O	1:A:764:VAL:HG12	2.14	0.46
2:B:42:LEU:O	2:B:44:VAL:N	2.48	0.46
6:F:153:THR:CA	6:F:224:TYR:HB3	2.44	0.46
6:E:278:SER:O	6:E:397:VAL:HA	2.15	0.46
6:E:328:ASP:OD2	6:E:328:ASP:N	2.34	0.46
6:E:487:ALA:HB3	6:E:515:TYR:CD2	2.50	0.46
2:B:140:ASN:OD1	2:B:140:ASN:N	2.47	0.46
2:D:58:LYS:HZ3	6:F:79:ILE:HG21	1.78	0.46
6:F:12:THR:OG1	6:F:25:LEU:O	2.22	0.46
6:F:61:THR:OG1	6:F:62:GLN:N	2.48	0.46
6:F:173:ARG:NH1	6:F:174:PRO:O	2.48	0.46
6:F:317:LEU:HD11	6:F:374:ASP:HB2	1.97	0.46
6:F:382:TYR:O	6:F:385:SER:OG	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:76:LYS:HE3	6:E:80:SER:CB	2.46	0.46
6:E:155:ARG:HD3	6:E:222:GLY:HA2	1.97	0.46
6:E:394:LYS:HG2	6:E:395:HIS:NE2	2.30	0.46
7:G:77:THR:HB	7:G:86:LYS:HE3	1.97	0.46
1:A:456:TYR:C	1:A:458:TYR:N	2.69	0.46
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.64	0.46
3:C:5:ASP:O	3:C:9:THR:HG22	2.16	0.46
2:D:36:LYS:HA	2:D:36:LYS:HD3	1.56	0.46
4:I:28:G:N2	5:J:33:C:C2	2.83	0.46
6:F:241:VAL:HG22	6:F:277:TYR:HB3	1.98	0.46
6:F:279:THR:HA	6:F:398:TYR:HB2	1.98	0.46
6:E:161:ARG:O	6:E:210:VAL:HA	2.16	0.46
6:E:340:VAL:HG13	6:E:342:CYS:SG	2.55	0.46
6:E:427:ARG:O	6:E:431:THR:OG1	2.34	0.46
6:E:509:ALA:O	6:E:528:LEU:HG	2.16	0.46
7:G:14:CYS:HG	7:G:56:PHE:HA	1.81	0.46
1:A:182:VAL:O	1:A:185:ALA:N	2.48	0.46
2:D:149:TYR:O	2:D:152:ALA:N	2.45	0.46
5:J:41:G:C6	5:J:42:C:C4	3.03	0.46
5:J:49:C:H2'	5:J:50:G:C8	2.51	0.46
6:E:385:SER:OG	6:E:386:VAL:N	2.49	0.46
2:D:92:PHE:CD1	2:D:95:LEU:HD12	2.51	0.46
2:D:127:LYS:HB3	2:D:127:LYS:HE2	1.50	0.46
2:D:136:ASN:HA	2:D:139:LYS:HD3	1.98	0.46
2:D:139:LYS:HG2	2:D:140:ASN:OD1	2.15	0.46
6:F:245:HIS:NE2	6:F:275:GLN:HG3	2.31	0.46
6:E:145:PHE:CG	6:E:411:LEU:HD21	2.51	0.46
6:E:570:VAL:O	6:E:570:VAL:HG12	2.16	0.46
7:G:34:THR:HA	7:G:39:ARG:HA	1.97	0.46
7:G:35:THR:OG1	7:G:40:PHE:HB2	2.15	0.46
1:A:125:ALA:O	1:A:128:VAL:N	2.49	0.46
1:A:263:LYS:HB3	1:A:264:PRO:HD2	1.98	0.46
1:A:485:GLY:HA2	1:A:574:LYS:HD2	1.98	0.46
6:F:78:PRO:O	6:F:80:SER:N	2.48	0.46
6:F:332:ARG:HG2	6:F:334:ILE:HD11	1.97	0.46
6:E:108:ALA:O	6:E:111:THR:N	2.49	0.46
6:E:180:TYR:C	6:E:227:LEU:HD21	2.36	0.46
6:E:334:ILE:HG21	6:E:342:CYS:H	1.80	0.46
1:A:256:HIS:CD2	1:A:261:LEU:HD23	2.51	0.46
1:A:687:THR:O	1:A:690:ALA:N	2.49	0.46
1:A:874:ASN:OD1	1:A:875:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:SER:HB3	2:D:174:MET:SD	2.56	0.46
4:I:11:G:C6	5:J:50:G:C6	3.04	0.46
6:F:303:ARG:HH22	6:F:356:VAL:HG12	1.81	0.46
6:E:143:GLU:HA	6:E:146:LYS:HZ3	1.81	0.46
6:E:475:PHE:HD2	6:E:475:PHE:O	1.99	0.46
1:A:672:SER:O	1:A:672:SER:OG	2.32	0.46
6:F:359:THR:HG22	6:F:361:ASN:H	1.81	0.46
6:E:64:TYR:CD2	6:E:82:PRO:HA	2.51	0.46
1:A:153:ASP:OD1	1:A:154:ASP:N	2.49	0.45
1:A:822:GLN:NE2	1:A:922:GLU:OE2	2.50	0.45
2:D:58:LYS:NZ	6:F:79:ILE:HD13	2.32	0.45
5:J:41:G:H2'	5:J:42:C:H6	1.80	0.45
6:F:62:GLN:HE21	6:F:73:LYS:H	1.64	0.45
6:F:279:THR:HG22	6:F:398:TYR:CD1	2.50	0.45
6:F:376:ILE:HG13	6:F:400:GLY:C	2.36	0.45
6:E:2:VAL:HG12	6:E:11:GLN:OE1	2.16	0.45
6:E:393:ALA:HB3	6:E:396:TYR:CE1	2.50	0.45
6:E:468:SER:H	6:E:570:VAL:HG11	1.79	0.45
6:E:511:PHE:HB2	6:E:528:LEU:HB3	1.98	0.45
1:A:59:LYS:HA	1:A:66:ILE:HG22	1.97	0.45
1:A:325:SER:O	1:A:325:SER:OG	2.25	0.45
1:A:810:HIS:HD1	1:A:810:HIS:C	2.18	0.45
6:F:265:ASN:HB3	6:F:269:TYR:CE2	2.51	0.45
6:F:427:ARG:O	6:F:431:THR:HG23	2.16	0.45
6:E:289:SER:C	6:E:293:ILE:HD13	2.37	0.45
6:E:490:ARG:HB3	6:E:491:PRO:HD3	1.98	0.45
1:A:18:ARG:HH12	1:A:63:ASP:CG	2.19	0.45
1:A:173:ARG:O	1:A:173:ARG:HG2	2.15	0.45
1:A:575:LEU:HD22	1:A:641:LYS:HG3	1.98	0.45
1:A:748:TYR:CD2	1:A:748:TYR:C	2.90	0.45
3:C:34:GLN:NE2	3:C:34:GLN:O	2.50	0.45
6:F:138:LEU:O	6:F:142:GLU:HG3	2.17	0.45
6:E:114:TRP:CH2	6:E:123:ALA:HB2	2.51	0.45
6:E:269:TYR:CG	6:E:295:LEU:HD13	2.51	0.45
7:G:10:ARG:NH2	7:G:31:TYR:HB3	2.28	0.45
6:F:142:GLU:HB3	6:F:146:LYS:HZ3	1.80	0.45
6:F:424:SER:HA	6:F:427:ARG:HE	1.81	0.45
6:E:5:CYS:HB2	6:E:26:CYS:H	1.82	0.45
7:G:10:ARG:HA	7:G:10:ARG:NE	2.30	0.45
1:A:116:ARG:NH2	9:A:1003:GNP:H5'2	2.32	0.45
1:A:565:THR:C	1:A:567:THR:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:LEU:HD12	1:A:749:LEU:HA	1.68	0.45
2:D:175:ASP:OD1	2:D:176:ASN:N	2.42	0.45
6:F:295:LEU:O	6:F:299:TYR:N	2.37	0.45
6:F:347:LYS:HE3	6:F:347:LYS:HB3	1.75	0.45
6:F:581:LEU:O	6:F:585:LEU:N	2.47	0.45
6:E:439:GLY:O	6:E:441:CYS:N	2.50	0.45
7:G:27:ASN:O	7:G:51:LEU:HD21	2.17	0.45
1:A:844:VAL:HG11	1:A:849:LYS:CB	2.47	0.45
6:F:3:GLY:N	6:F:24:PHE:CE2	2.84	0.45
6:F:355:TYR:HB3	6:F:357:PHE:HE1	1.82	0.45
6:F:489:ASN:ND2	6:F:492:GLN:OE1	2.49	0.45
6:E:276:LYS:HB3	6:E:396:TYR:CE2	2.52	0.45
1:A:361:LEU:HA	1:A:361:LEU:HD13	1.66	0.45
1:A:543:ASN:O	1:A:556:THR:HG23	2.16	0.45
1:A:864:ILE:HD13	1:A:924:MET:SD	2.57	0.45
2:D:130:VAL:HG11	2:D:147:PHE:CZ	2.51	0.45
4:I:33:G:H1	5:J:27:C:H42	1.64	0.45
6:E:65:LEU:HB3	6:E:81:PHE:HB3	1.99	0.45
6:E:139:LYS:HD3	6:E:139:LYS:HA	1.71	0.45
6:E:232:VAL:HG23	6:E:382:TYR:CE1	2.52	0.45
6:E:287:GLY:HA3	6:E:442:ARG:NH1	2.32	0.45
6:E:384:LEU:HD11	6:E:423:ASN:HB2	1.97	0.45
7:G:87:TYR:HB3	7:G:89:TYR:CE2	2.48	0.45
1:A:18:ARG:O	1:A:59:LYS:N	2.47	0.45
1:A:105:ARG:NH1	1:A:107:ASP:O	2.44	0.45
1:A:587:VAL:HG12	1:A:589:ILE:H	1.82	0.45
1:A:617:TRP:CD1	1:A:617:TRP:C	2.89	0.45
1:A:752:HIS:CD2	1:A:770:TYR:CE1	3.04	0.45
3:C:36:HIS:O	3:C:36:HIS:CG	2.69	0.45
2:D:175:ASP:C	2:D:178:PRO:HD2	2.38	0.45
6:F:15:ARG:HH11	6:F:15:ARG:HG3	1.82	0.45
6:E:31:TYR:CD1	6:E:35:ILE:HD11	2.51	0.45
6:E:40:LYS:HD2	6:E:59:ASP:OD2	2.17	0.45
6:E:448:ILE:HD12	6:E:451:THR:HB	1.98	0.45
7:G:44:LEU:HD22	7:G:89:TYR:HB2	1.99	0.45
1:A:62:ASP:OD1	1:A:62:ASP:N	2.48	0.45
1:A:384:SER:HB2	2:B:98:LEU:HD12	1.99	0.45
1:A:390:ASP:OD2	1:A:674:TYR:OH	2.21	0.45
1:A:850:THR:HG22	2:D:79:LYS:HZ1	1.82	0.45
6:F:49:VAL:HG23	6:F:57:VAL:O	2.17	0.45
7:G:18:THR:HA	7:G:52:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HG3	1:A:74:ARG:N	2.32	0.45
1:A:164:ASP:OD2	1:A:167:GLU:HB3	2.17	0.45
1:A:278:GLU:CD	1:A:278:GLU:H	2.18	0.45
1:A:571:PHE:HE1	1:A:642:HIS:CE1	2.35	0.45
1:A:855:MET:C	1:A:857:GLU:H	2.20	0.45
2:D:124:THR:HA	2:D:190:ARG:HG2	1.99	0.45
6:F:44:SER:OG	6:F:46:ASN:O	2.29	0.45
6:F:62:GLN:NE2	6:F:62:GLN:O	2.50	0.45
6:F:195:ILE:HD11	6:F:223:ASP:C	2.37	0.45
6:F:276:LYS:HZ2	6:F:395:HIS:CD2	2.35	0.45
6:F:318:CYS:HA	6:F:346:PHE:HZ	1.82	0.45
6:F:332:ARG:HA	6:F:357:PHE:O	2.17	0.45
6:F:546:PHE:HB2	6:F:572:ILE:HD11	1.99	0.45
6:E:277:TYR:HA	6:E:396:TYR:HB2	1.99	0.45
1:A:91:LYS:HB2	1:A:91:LYS:HE2	1.73	0.44
1:A:143:LYS:HG2	1:A:157:PHE:CE2	2.53	0.44
1:A:350:GLU:O	1:A:352:GLY:N	2.49	0.44
1:A:484:ASP:OD1	1:A:484:ASP:N	2.50	0.44
2:B:160:VAL:HG12	2:B:165:LYS:O	2.17	0.44
5:J:38:C:H2'	5:J:39:A:C8	2.50	0.44
6:F:174:PRO:HB2	6:F:180:TYR:CD2	2.53	0.44
6:F:331:SER:HA	6:F:346:PHE:HB3	2.00	0.44
6:E:425:VAL:HA	6:E:428:LEU:HB2	1.98	0.44
6:E:440:THR:OG1	6:E:442:ARG:NH2	2.49	0.44
6:E:473:LYS:HD2	6:E:576:MET:SD	2.56	0.44
7:G:16:ALA:O	7:G:23:CYS:HA	2.17	0.44
2:B:42:LEU:HD23	2:B:43:ASN:N	2.33	0.44
2:B:91:LEU:HD23	2:B:91:LEU:HA	1.74	0.44
6:F:62:GLN:HG2	6:F:73:LYS:NZ	2.33	0.44
6:E:14:LEU:HB2	6:E:25:LEU:O	2.17	0.44
6:E:135:ALA:O	6:E:138:LEU:HB3	2.17	0.44
6:E:167:TRP:HE1	6:E:173:ARG:HE	1.64	0.44
6:E:329:LYS:HE2	6:E:355:TYR:CZ	2.52	0.44
1:A:99:HIS:N	1:A:99:HIS:HD1	2.15	0.44
1:A:181:ARG:HE	1:A:181:ARG:HB3	1.51	0.44
1:A:386:ASN:OD1	1:A:386:ASN:N	2.50	0.44
1:A:687:THR:OG1	1:A:688:ALA:N	2.50	0.44
1:A:757:ILE:HG22	1:A:758:LEU:O	2.17	0.44
2:D:92:PHE:O	2:D:96:ARG:HG3	2.17	0.44
6:E:117:ALA:HB2	6:E:415:GLY:O	2.18	0.44
6:E:152:ALA:HB2	6:E:167:TRP:CH2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:243:GLN:NE2	6:E:275:GLN:HG3	2.32	0.44
6:E:589:SER:O	6:E:589:SER:OG	2.30	0.44
7:G:14:CYS:SG	7:G:56:PHE:HA	2.57	0.44
7:G:69:LEU:HD12	7:G:89:TYR:HD1	1.82	0.44
6:F:329:LYS:HE3	6:F:329:LYS:HA	1.98	0.44
6:F:540:GLU:OE1	6:F:567:ARG:NH2	2.50	0.44
6:E:92:LEU:HB3	6:E:93:TYR:CD2	2.52	0.44
6:E:184:GLY:O	6:E:195:ILE:HB	2.18	0.44
6:E:239:THR:OG1	6:E:240:LEU:HD23	2.17	0.44
6:E:347:LYS:HE2	6:E:353:GLU:HG3	1.98	0.44
6:E:515:TYR:OH	6:E:550:THR:HG21	2.18	0.44
1:A:20:THR:HG21	1:A:59:LYS:HD3	2.00	0.44
1:A:83:GLU:OE1	1:A:219:PHE:N	2.38	0.44
6:F:62:GLN:HE22	6:F:72:CYS:CB	2.18	0.44
6:F:174:PRO:HB2	6:F:180:TYR:CE2	2.53	0.44
6:E:528:LEU:CD2	6:E:545:ILE:HD12	2.47	0.44
6:E:585:LEU:HD12	6:E:586:GLN:H	1.82	0.44
1:A:66:ILE:CG1	1:A:67:ASP:H	2.28	0.44
1:A:187:LEU:N	1:A:187:LEU:HD12	2.33	0.44
1:A:256:HIS:CE1	1:A:265:TYR:HE2	2.36	0.44
1:A:456:TYR:O	1:A:459:ASN:N	2.44	0.44
1:A:788:TYR:C	1:A:788:TYR:CD2	2.90	0.44
2:B:138:TYR:CD1	2:B:138:TYR:C	2.90	0.44
3:C:37:ASN:OD1	3:C:37:ASN:N	2.49	0.44
2:D:94:MET:HE2	2:D:94:MET:HB2	1.57	0.44
6:F:249:ILE:HB	6:F:274:MET:HG2	2.00	0.44
6:F:280:LEU:HB3	6:F:436:MET:HB3	1.99	0.44
6:E:41:LEU:HD13	6:E:58:THR:HG23	1.99	0.44
6:E:258:ILE:HG12	6:E:266:VAL:HG11	2.00	0.44
6:E:331:SER:O	6:E:357:PHE:HD2	2.00	0.44
6:E:443:ARG:H	6:E:464:HIS:CE1	2.36	0.44
1:A:81:GLN:OE1	1:A:81:GLN:N	2.51	0.44
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.74	0.44
1:A:457:ARG:NH2	1:A:458:TYR:OH	2.50	0.44
1:A:709:SER:O	1:A:709:SER:OG	2.31	0.44
6:F:379:ALA:HB1	6:F:383:ASP:OD1	2.18	0.44
6:E:280:LEU:HA	6:E:436:MET:C	2.38	0.44
1:A:438:LYS:HZ1	1:A:438:LYS:HB3	1.83	0.44
3:C:28:LEU:HA	3:C:28:LEU:HD12	1.73	0.44
6:F:31:TYR:CE2	6:F:87:GLY:HA2	2.52	0.44
6:F:403:ALA:HB1	6:F:457:TYR:HE2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:33:HIS:CD2	6:E:106:PHE:HE1	2.36	0.44
6:E:40:LYS:HA	6:E:40:LYS:HD3	1.81	0.44
6:E:276:LYS:HB3	6:E:396:TYR:HE2	1.82	0.44
6:E:332:ARG:HB3	6:E:346:PHE:HD1	1.82	0.44
6:E:471:CYS:HB2	6:E:587:PHE:CZ	2.52	0.44
6:E:528:LEU:HD21	6:E:545:ILE:HD12	2.00	0.44
2:B:179:ASN:N	2:B:179:ASN:OD1	2.51	0.44
5:J:42:C:H2'	5:J:43:U:C6	2.53	0.44
6:F:40:LYS:O	6:F:59:ASP:HA	2.18	0.44
6:F:139:LYS:HA	6:F:142:GLU:OE2	2.18	0.44
6:E:307:THR:HG23	6:E:373:PHE:HD1	1.83	0.44
6:E:510:VAL:HG22	6:E:529:PRO:HG2	2.00	0.44
1:A:116:ARG:NH2	9:A:1003:GNP:C5'	2.80	0.43
1:A:590:GLY:HA2	5:J:29:G:O2'	2.18	0.43
6:F:65:LEU:CD2	6:F:66:GLY:H	2.21	0.43
6:F:431:THR:OG1	6:F:432:ILE:N	2.51	0.43
6:F:473:LYS:HE2	6:F:587:PHE:O	2.18	0.43
1:A:248:THR:O	1:A:249:ARG:C	2.57	0.43
2:B:139:LYS:HA	2:B:139:LYS:HD2	1.57	0.43
2:D:154:TRP:CE3	2:D:190:ARG:HA	2.53	0.43
6:F:65:LEU:HD12	6:F:83:LEU:HD21	1.98	0.43
6:F:126:CYS:HB2	6:F:130:LEU:HD23	1.99	0.43
6:F:510:VAL:HG13	6:F:512:ILE:HG13	2.00	0.43
6:E:499:PHE:HE1	6:E:506:TRP:NE1	2.16	0.43
7:G:55:ARG:HB2	7:G:66:TYR:CE1	2.53	0.43
1:A:648:LEU:O	1:A:651:ARG:N	2.51	0.43
1:A:753:PHE:CZ	1:A:764:VAL:HG11	2.52	0.43
3:C:26:SER:O	3:C:29:TRP:N	2.51	0.43
2:D:136:ASN:O	2:D:137:THR:C	2.57	0.43
2:D:147:PHE:N	2:D:154:TRP:O	2.44	0.43
6:F:4:ALA:HA	6:F:10:SER:O	2.19	0.43
6:F:74:SER:OG	6:F:75:HIS:NE2	2.51	0.43
6:F:276:LYS:HA	6:F:395:HIS:CD2	2.54	0.43
6:F:476:TYR:C	6:F:477:LYS:HD2	2.38	0.43
7:G:54:ALA:HB3	7:G:67:THR:OG1	2.18	0.43
1:A:281:LYS:NZ	1:A:285:ARG:HH21	2.16	0.43
1:A:503:GLY:C	1:A:507:ASN:HD22	2.11	0.43
2:B:61:LYS:HE3	2:B:61:LYS:HB2	1.70	0.43
2:D:187:THR:HG22	2:D:188:ALA:H	1.82	0.43
6:F:444:CYS:SG	6:F:445:PRO:HD2	2.58	0.43
6:E:6:VAL:HG11	6:E:23:PRO:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:157:VAL:HG21	6:E:219:LEU:C	2.39	0.43
6:E:223:ASP:HB3	6:E:225:PHE:CZ	2.54	0.43
7:G:88:LEU:HD12	7:G:88:LEU:HA	1.83	0.43
1:A:71:VAL:O	1:A:73:LYS:N	2.52	0.43
1:A:370:GLU:OE2	1:A:370:GLU:HA	2.19	0.43
1:A:571:PHE:HE2	1:A:654:ARG:HB3	1.84	0.43
3:C:12:VAL:O	3:C:16:VAL:HG12	2.17	0.43
6:E:34:VAL:HG21	6:E:60:VAL:HG11	1.99	0.43
7:G:70:GLU:OE2	7:G:89:TYR:HA	2.18	0.43
1:A:10:ARG:HD2	1:A:10:ARG:HA	1.70	0.43
1:A:610:GLU:H	1:A:610:GLU:HG3	1.45	0.43
2:B:161:ASP:HB3	2:B:184:LEU:HD23	2.00	0.43
2:D:42:LEU:O	2:D:45:ALA:N	2.51	0.43
6:F:80:SER:HB3	6:F:81:PHE:H	1.69	0.43
6:F:420:GLU:OE1	6:F:430:LYS:HB2	2.19	0.43
6:F:497:ARG:O	6:F:501:THR:HG22	2.18	0.43
6:E:18:ALA:HB3	6:E:39:HIS:CG	2.54	0.43
6:E:77:PRO:HB2	6:E:78:PRO:HD2	2.01	0.43
1:A:276:THR:N	1:A:277:GLU:OE1	2.51	0.43
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.70	0.43
1:A:847:ILE:HD11	2:D:79:LYS:HB3	2.00	0.43
1:A:857:GLU:OE2	1:A:857:GLU:HA	2.19	0.43
1:A:899:MET:HE3	1:A:899:MET:HB3	1.80	0.43
3:C:70:LYS:HD3	2:D:92:PHE:CE2	2.54	0.43
6:F:15:ARG:HH22	6:F:24:PHE:HE1	1.65	0.43
6:F:381:ASN:HA	6:F:384:LEU:HD12	2.01	0.43
6:F:532:THR:OG1	6:F:533:VAL:N	2.51	0.43
6:E:441:CYS:SG	6:E:461:LEU:HD13	2.59	0.43
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.57	0.43
1:A:571:PHE:CE1	1:A:642:HIS:CE1	3.07	0.43
2:B:150:ALA:O	2:B:151:SER:OG	2.35	0.43
4:I:15:G:N2	5:J:46:U:O2	2.52	0.43
6:F:235:LEU:HD11	6:F:382:TYR:HD1	1.84	0.43
6:F:259:SER:OG	6:F:297:LEU:HD13	2.19	0.43
6:F:311:HIS:CE1	6:F:359:THR:HG1	2.37	0.43
1:A:532:LYS:HB2	1:A:532:LYS:HE2	1.74	0.43
6:E:281:GLN:HA	6:E:401:ASP:OD1	2.18	0.43
6:E:323:LYS:HZ2	6:E:324:TYR:N	2.16	0.43
6:E:370:ILE:CD1	6:E:395:HIS:HB2	2.49	0.43
6:E:413:THR:OG1	6:E:414:LYS:HE2	2.19	0.43
6:E:443:ARG:NH2	6:E:540:GLU:OE2	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:O	1:A:13:GLY:N	2.52	0.43
1:A:46:ALA:O	1:A:48:PHE:CD1	2.72	0.43
1:A:151:CYS:SG	1:A:177:ASN:HB2	2.59	0.43
1:A:152:CYS:SG	1:A:153:ASP:N	2.91	0.43
1:A:335:VAL:O	1:A:338:VAL:N	2.40	0.43
1:A:854:LEU:H	1:A:854:LEU:HG	1.65	0.43
1:A:891:LEU:HD23	1:A:891:LEU:HA	1.57	0.43
2:B:119:ILE:O	2:B:123:THR:HG23	2.18	0.43
5:J:44:A:O2'	5:J:45:C:H5'	2.19	0.43
6:F:16:CYS:HB3	6:F:23:PRO:HD2	2.01	0.43
6:F:155:ARG:O	6:F:221:VAL:HG22	2.19	0.43
6:F:230:HIS:HB2	6:F:231:THR:H	1.71	0.43
6:E:114:TRP:HH2	6:E:123:ALA:HB2	1.84	0.43
6:E:475:PHE:O	6:E:475:PHE:CD2	2.71	0.43
7:G:45:LEU:HD21	7:G:86:LYS:HE2	2.00	0.43
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.74	0.42
1:A:244:ILE:C	1:A:246:THR:H	2.22	0.42
2:B:19:GLN:OE1	2:B:42:LEU:HD12	2.18	0.42
2:B:112:ASP:C	2:B:114:CYS:H	2.22	0.42
2:D:109:ASN:HB3	2:D:114:CYS:HB2	2.01	0.42
6:F:322:LEU:HD22	6:F:327:ILE:HG23	2.01	0.42
6:F:369:ASP:OD2	6:F:370:ILE:HG12	2.19	0.42
6:E:49:VAL:O	6:E:51:ASN:N	2.52	0.42
7:G:85:VAL:HG12	7:G:87:TYR:CE2	2.54	0.42
1:A:181:ARG:H	1:A:181:ARG:HG2	1.45	0.42
1:A:256:HIS:CE1	1:A:265:TYR:CE2	3.07	0.42
1:A:530:TYR:C	1:A:532:LYS:H	2.22	0.42
1:A:855:MET:O	1:A:858:ARG:HG3	2.19	0.42
2:B:177:SER:O	2:B:179:ASN:N	2.52	0.42
2:D:58:LYS:HZ1	6:F:79:ILE:HD13	1.84	0.42
6:F:114:TRP:HD1	6:F:141:THR:HG21	1.84	0.42
6:F:304:ILE:CD1	6:F:372:VAL:HG13	2.46	0.42
6:F:424:SER:O	6:F:427:ARG:HG2	2.19	0.42
6:F:473:LYS:HB3	6:F:585:LEU:HD23	2.02	0.42
6:E:76:LYS:H	6:E:76:LYS:HG2	1.57	0.42
7:G:43:ALA:HB1	7:G:88:LEU:HD11	2.01	0.42
1:A:281:LYS:HB3	1:A:281:LYS:HE3	1.87	0.42
1:A:530:TYR:CZ	1:A:534:ASN:OD1	2.71	0.42
1:A:849:LYS:C	1:A:851:ASP:N	2.72	0.42
1:A:850:THR:HG22	2:D:79:LYS:NZ	2.34	0.42
2:D:128:LEU:C	2:D:129:MET:HG2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:162:GLU:O	6:F:163:LEU:HG	2.19	0.42
6:F:286:THR:HB	6:F:440:THR:H	1.85	0.42
6:E:37:THR:O	6:E:40:LYS:NZ	2.29	0.42
6:E:195:ILE:HA	6:E:217:TYR:CD2	2.54	0.42
6:E:453:SER:OG	6:E:461:LEU:O	2.34	0.42
7:G:68:GLU:OE2	7:G:92:LYS:HB2	2.19	0.42
1:A:41:LYS:HB3	1:A:41:LYS:HE3	1.79	0.42
1:A:330:VAL:HB	1:A:341:VAL:HG12	2.00	0.42
1:A:803:THR:O	1:A:803:THR:OG1	2.34	0.42
1:A:903:TYR:OH	2:D:67:MET:HB3	2.19	0.42
1:A:905:VAL:HG22	1:A:906:MET:N	2.34	0.42
2:D:139:LYS:HG2	2:D:140:ASN:N	2.34	0.42
6:F:64:TYR:CD2	6:F:80:SER:HB3	2.54	0.42
6:F:104:THR:O	6:F:108:ALA:HB2	2.19	0.42
6:F:201:GLU:HG2	6:F:210:VAL:HB	2.00	0.42
6:E:162:GLU:O	6:E:163:LEU:HD23	2.19	0.42
6:E:363:LEU:HD12	6:E:364:PRO:O	2.20	0.42
6:E:420:GLU:HA	6:E:426:CYS:HB3	2.01	0.42
1:A:328:PRO:O	1:A:329:LEU:HD23	2.20	0.42
1:A:814:SER:O	1:A:815:GLN:HG3	2.19	0.42
2:D:158:GLN:HG3	2:D:159:VAL:H	1.85	0.42
2:D:177:SER:C	2:D:179:ASN:N	2.72	0.42
6:F:68:MET:O	6:F:69:SER:OG	2.36	0.42
6:F:269:TYR:OH	6:F:295:LEU:N	2.53	0.42
6:F:494:GLY:O	6:F:498:GLU:HG2	2.19	0.42
6:E:15:ARG:O	6:E:43:LEU:HD12	2.20	0.42
6:E:426:CYS:O	6:E:430:LYS:NZ	2.44	0.42
7:G:20:GLN:HB2	7:G:21:THR:H	1.67	0.42
7:G:29:LEU:HB2	7:G:45:LEU:O	2.19	0.42
1:A:617:TRP:CZ3	1:A:764:VAL:HG21	2.54	0.42
2:D:78:ASP:O	2:D:81:ALA:N	2.51	0.42
6:F:540:GLU:HB3	6:F:567:ARG:HH21	1.84	0.42
6:E:10:SER:OG	6:E:26:CYS:HB2	2.20	0.42
6:E:493:ILE:HD11	6:E:518:GLN:HG2	2.01	0.42
6:E:556:CYS:SG	6:E:578:ASP:HB2	2.59	0.42
7:G:95:ASN:O	7:G:99:ARG:HG3	2.20	0.42
2:D:11:SER:OG	2:D:49:PHE:HA	2.20	0.42
2:D:104:ASN:HA	2:D:107:ILE:HD12	2.01	0.42
6:F:173:ARG:HH22	6:F:176:LEU:CD2	2.33	0.42
6:F:308:ALA:HB2	6:F:374:ASP:HB3	2.01	0.42
6:F:436:MET:HE2	6:F:437:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:155:ARG:HG2	6:E:166:SER:OG	2.19	0.42
6:E:455:LEU:HD23	6:E:456:VAL:N	2.35	0.42
6:E:480:ILE:CD1	6:E:551:GLU:H	2.33	0.42
6:E:500:LEU:HG	6:E:507:ARG:HG2	2.01	0.42
7:G:44:LEU:HB3	7:G:89:TYR:CB	2.41	0.42
7:G:75:PHE:HD2	7:G:112:LEU:HD22	1.84	0.42
7:G:76:VAL:HG13	7:G:84:LYS:H	1.84	0.42
7:G:84:LYS:O	7:G:86:LYS:HG3	2.20	0.42
1:A:445:ASP:HB2	1:A:446:GLY:H	1.59	0.42
1:A:818:MET:HG3	1:A:820:VAL:HG13	2.01	0.42
2:D:135:TYR:O	2:D:138:TYR:HB3	2.19	0.42
2:D:149:TYR:HB3	2:D:154:TRP:CD1	2.55	0.42
6:F:50:CYS:SG	6:F:71:TYR:HA	2.60	0.42
6:F:192:LYS:HE3	6:F:224:TYR:CE1	2.55	0.42
6:F:368:ALA:HB3	6:F:391:LEU:HD21	2.00	0.42
6:F:403:ALA:HB1	6:F:457:TYR:CD2	2.54	0.42
6:E:438:LEU:HD23	6:E:438:LEU:HA	1.85	0.42
6:E:544:VAL:HG12	6:E:545:ILE:N	2.34	0.42
7:G:85:VAL:HG12	7:G:87:TYR:HE2	1.84	0.42
1:A:129:TYR:O	1:A:131:LEU:N	2.53	0.42
1:A:685:ALA:HA	5:J:27:C:O2'	2.19	0.42
1:A:867:TYR:O	1:A:869:LEU:N	2.53	0.42
4:I:21:U:H2'	4:I:22:G:C8	2.54	0.42
6:F:109:ILE:HG23	6:F:134:ALA:HB2	2.01	0.42
6:E:246:TYR:N	6:E:246:TYR:CD2	2.88	0.42
6:E:332:ARG:HB3	6:E:346:PHE:CD1	2.55	0.42
7:G:74:ARG:NH1	7:G:76:VAL:HG23	2.21	0.42
1:A:348:PHE:CD2	1:A:351:LEU:HB2	2.55	0.42
1:A:609:VAL:O	1:A:612:PRO:HD3	2.20	0.42
1:A:612:PRO:HB3	1:A:765:CYS:SG	2.60	0.42
6:F:50:CYS:CB	6:F:72:CYS:HB3	2.47	0.42
6:F:143:GLU:O	6:F:147:LEU:HG	2.20	0.42
6:F:282:GLY:HA2	6:F:283:PRO:HD3	1.90	0.42
6:F:329:LYS:NZ	6:F:353:GLU:HA	2.34	0.42
6:F:347:LYS:HE2	6:F:350:SER:HB3	2.01	0.42
6:F:400:GLY:HA2	6:F:404:GLN:NE2	2.34	0.42
6:F:406:PRO:HG2	6:F:560:ARG:NH1	2.35	0.42
6:E:209:VAL:O	6:E:209:VAL:HG23	2.20	0.42
6:E:334:ILE:HD11	6:E:343:PHE:O	2.20	0.42
7:G:111:ARG:HA	7:G:111:ARG:HH11	1.84	0.42
1:A:201:ILE:HD12	1:A:201:ILE:HG23	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:TYR:O	1:A:532:LYS:N	2.53	0.41
4:I:22:G:HO2'	4:I:23:C:P	2.42	0.41
6:F:235:LEU:HD11	6:F:382:TYR:CD1	2.54	0.41
6:E:167:TRP:CH2	6:E:174:PRO:HD2	2.55	0.41
6:E:420:GLU:HB2	6:E:427:ARG:HA	2.01	0.41
1:A:40:ASP:OD1	1:A:40:ASP:C	2.58	0.41
1:A:692:SER:O	1:A:696:ILE:HG13	2.20	0.41
1:A:877:TYR:O	1:A:880:VAL:N	2.45	0.41
5:J:40:U:H2'	5:J:41:G:O4'	2.19	0.41
5:J:40:U:C2	5:J:41:G:C8	3.08	0.41
6:E:50:CYS:C	6:E:52:ALA:H	2.23	0.41
6:E:411:LEU:O	6:E:413:THR:HG23	2.20	0.41
6:E:419:PRO:HA	6:E:422:PHE:CZ	2.55	0.41
6:E:449:VAL:O	6:E:452:VAL:HG22	2.20	0.41
1:A:446:GLY:O	1:A:448:ALA:N	2.50	0.41
1:A:485:GLY:HA2	1:A:574:LYS:CD	2.50	0.41
2:B:12:TYR:CD1	2:B:49:PHE:HZ	2.38	0.41
4:I:22:G:O2'	4:I:23:C:OP1	2.32	0.41
6:F:73:LYS:HA	6:F:76:LYS:CD	2.42	0.41
6:F:283:PRO:HG2	6:F:461:LEU:HD11	2.02	0.41
6:F:428:LEU:HG	6:F:432:ILE:HB	2.02	0.41
6:E:65:LEU:HD23	6:E:66:GLY:N	2.34	0.41
6:E:277:TYR:OH	6:E:428:LEU:HD23	2.20	0.41
6:E:289:SER:HB2	6:E:320:LYS:HE3	2.02	0.41
6:E:311:HIS:CD2	6:E:361:ASN:HD22	2.38	0.41
1:A:466:ILE:HD12	1:A:466:ILE:HA	1.57	0.41
1:A:777:ALA:HB1	1:A:782:PHE:HE1	1.85	0.41
5:J:42:C:C4	5:J:43:U:C4	3.08	0.41
6:F:15:ARG:NH2	6:F:24:PHE:HE1	2.17	0.41
6:F:275:GLN:NE2	6:F:278:SER:HA	2.35	0.41
6:F:297:LEU:O	6:F:300:PRO:HD3	2.20	0.41
6:F:347:LYS:HE2	6:F:353:GLU:HB2	2.02	0.41
6:E:504:PRO:C	6:E:506:TRP:H	2.24	0.41
7:G:11:GLN:HB2	7:G:31:TYR:CG	2.55	0.41
1:A:68:SER:C	1:A:69:TYR:CD1	2.93	0.41
1:A:171:ILE:HD12	1:A:171:ILE:HA	1.76	0.41
1:A:304:ASP:OD1	1:A:305:ARG:HG3	2.21	0.41
1:A:872:HIS:CG	1:A:873:PRO:HD2	2.55	0.41
4:I:22:G:H2'	4:I:23:C:C6	2.47	0.41
6:F:271:LYS:HD3	6:F:436:MET:SD	2.60	0.41
6:E:187:VAL:HG13	6:E:224:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASP:HB2	1:A:304:ASP:H	1.68	0.41
1:A:511:LYS:O	1:A:513:ARG:N	2.53	0.41
1:A:674:TYR:HB3	1:A:675:VAL:H	1.65	0.41
1:A:904:SER:OG	6:F:95:ASN:HB2	2.20	0.41
3:C:22:VAL:HG12	3:C:22:VAL:O	2.20	0.41
3:C:70:LYS:HD3	2:D:92:PHE:HE2	1.85	0.41
2:D:130:VAL:O	2:D:185:ILE:HA	2.21	0.41
2:D:133:PRO:HG2	2:D:134:ASP:H	1.86	0.41
6:F:120:TYR:HE2	6:F:409:ARG:CZ	2.33	0.41
6:F:474[A]:MET:HG2	6:F:592:ILE:HD11	2.03	0.41
6:E:378:MET:HB3	6:E:378:MET:HE3	1.85	0.41
6:E:421:TYR:HD1	6:E:427:ARG:HH12	1.68	0.41
1:A:290:TRP:HA	1:A:290:TRP:CE3	2.56	0.41
1:A:293:THR:O	1:A:309:HIS:HE1	2.03	0.41
1:A:810:HIS:ND1	1:A:810:HIS:C	2.73	0.41
1:A:837:ILE:HD13	1:A:837:ILE:HA	1.74	0.41
6:F:277:TYR:OH	6:F:428:LEU:HD11	2.20	0.41
6:F:441:CYS:O	6:F:464:HIS:ND1	2.53	0.41
6:F:528:LEU:HA	6:F:529:PRO:HD3	1.91	0.41
6:E:16:CYS:O	6:E:18:ALA:N	2.53	0.41
6:E:37:THR:HG22	6:E:38:SER:N	2.35	0.41
6:E:93:TYR:HB3	6:E:96:THR:OG1	2.21	0.41
6:E:156:GLU:OE2	6:E:158:LEU:HD23	2.21	0.41
6:E:195:ILE:HG12	6:E:217:TYR:CE2	2.56	0.41
6:E:488:ILE:HG23	6:E:493:ILE:HD11	2.02	0.41
1:A:107:ASP:OD1	1:A:108:GLY:N	2.54	0.41
1:A:624:ARG:HG2	1:A:624:ARG:NH1	2.36	0.41
2:B:147:PHE:CD1	2:B:147:PHE:N	2.89	0.41
6:F:139:LYS:HA	6:F:142:GLU:CD	2.41	0.41
6:E:157:VAL:HG21	6:E:219:LEU:O	2.20	0.41
6:E:473:LYS:CE	6:E:587:PHE:HB2	2.38	0.41
6:E:552:THR:O	6:E:556:CYS:N	2.33	0.41
1:A:365:ARG:NE	1:A:365:ARG:HA	2.35	0.41
1:A:411:LYS:HB3	1:A:412:PRO:HD2	2.03	0.41
1:A:847:ILE:C	1:A:849:LYS:N	2.74	0.41
2:B:13:ALA:O	2:B:17:THR:HG22	2.20	0.41
3:C:55:LEU:O	3:C:58:VAL:HB	2.21	0.41
5:J:41:G:O2'	5:J:42:C:H5'	2.21	0.41
5:J:44:A:C6	5:J:45:C:C4	3.08	0.41
6:F:240:LEU:HB3	6:F:425:VAL:CG2	2.51	0.41
6:F:266:VAL:HA	6:F:269:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:374:ASP:OD2	6:F:375:GLU:N	2.54	0.41
6:F:386:VAL:O	6:F:390:ARG:HG3	2.20	0.41
6:F:477:LYS:O	6:F:492:GLN:NE2	2.53	0.41
6:F:517:SER:O	6:F:521:VAL:HG13	2.20	0.41
6:E:98:VAL:HG23	6:E:99:GLY:O	2.20	0.41
6:E:163:LEU:O	6:E:209:VAL:HG22	2.21	0.41
1:A:802:GLU:OE2	1:A:810:HIS:HB2	2.21	0.41
1:A:856:ILE:O	1:A:856:ILE:HG22	2.21	0.41
1:A:916:TRP:O	1:A:916:TRP:CD1	2.74	0.41
2:B:187:THR:HG23	2:B:187:THR:O	2.20	0.41
6:F:73:LYS:CA	6:F:76:LYS:HD3	2.45	0.41
6:F:440:THR:HA	6:F:462:LYS:HZ2	1.86	0.41
6:E:76:LYS:HB2	6:E:80:SER:OG	2.21	0.41
5:J:38:C:C2	5:J:39:A:C8	3.09	0.40
6:F:120:TYR:OH	6:F:409:ARG:HD2	2.22	0.40
6:F:121:ILE:O	6:F:125:THR:OG1	2.28	0.40
6:F:283:PRO:HG3	6:F:460:LYS:HE3	2.03	0.40
6:F:314:VAL:HG22	6:F:318:CYS:HG	1.85	0.40
6:F:383:ASP:HA	6:F:386:VAL:HG13	2.03	0.40
6:F:384:LEU:H	6:F:384:LEU:HG	1.67	0.40
6:F:410:THR:HB	6:F:411:LEU:HD12	2.02	0.40
6:F:499:PHE:CZ	6:F:590:LEU:HD13	2.56	0.40
6:E:184:GLY:C	6:E:195:ILE:HB	2.42	0.40
6:E:245:HIS:NE2	6:E:275:GLN:HB2	2.36	0.40
6:E:492:GLN:O	6:E:496:VAL:HG23	2.21	0.40
1:A:455:TYR:HD1	1:A:455:TYR:HA	1.74	0.40
1:A:723:LEU:HD12	1:A:723:LEU:HA	1.66	0.40
1:A:733:ARG:O	1:A:734:ASN:ND2	2.45	0.40
1:A:768:SER:O	1:A:770:TYR:N	2.54	0.40
1:A:836:ARG:HH21	1:A:840:ALA:HB2	1.85	0.40
2:D:63:ALA:HB2	6:F:81:PHE:CE2	2.56	0.40
4:I:18:G:O6	5:J:42:C:N4	2.51	0.40
6:E:183:THR:HA	6:E:197:GLU:HA	2.03	0.40
6:E:575:ILE:HG23	6:E:575:ILE:O	2.22	0.40
7:G:81:LYS:HD2	7:G:84:LYS:HB3	2.03	0.40
1:A:38:TYR:CD1	1:A:728:TYR:CE1	3.06	0.40
2:D:134:ASP:OD1	2:D:135:TYR:N	2.54	0.40
2:D:153:LEU:O	2:D:191:ALA:HB2	2.21	0.40
6:F:50:CYS:H	6:F:57:VAL:CG2	2.34	0.40
6:E:116:ASN:HB3	6:E:414:LYS:NZ	2.36	0.40
6:E:150:GLY:C	6:E:167:TRP:HE3	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:216:THR:OG1	6:E:217:TYR:N	2.51	0.40
6:E:267:ALA:O	6:E:271:LYS:HE2	2.20	0.40
6:E:287:GLY:O	6:E:291:PHE:N	2.55	0.40
6:E:303:ARG:HE	6:E:354:GLN:HA	1.85	0.40
6:E:363:LEU:O	6:E:390:ARG:NH2	2.52	0.40
6:E:372:VAL:HA	6:E:397:VAL:O	2.21	0.40
6:E:476:TYR:CG	6:E:477:LYS:N	2.89	0.40
7:G:34:THR:HA	7:G:39:ARG:HG2	2.03	0.40
1:A:371:LEU:HD22	2:B:87:MET:HB3	2.03	0.40
1:A:479:TYR:CD2	1:A:746:TYR:HE1	2.40	0.40
1:A:663:LEU:HG	1:A:663:LEU:O	2.22	0.40
2:B:156:ILE:HG21	2:B:169:LEU:HD11	2.04	0.40
2:B:160:VAL:O	2:B:184:LEU:HD23	2.20	0.40
2:D:22:TYR:CD1	2:D:38:LEU:HB3	2.52	0.40
2:D:35:LEU:H	2:D:35:LEU:HG	1.64	0.40
6:F:193:VAL:O	6:F:193:VAL:HG13	2.22	0.40
6:E:7:LEU:HD23	6:E:130:LEU:HD21	2.03	0.40
6:E:83:LEU:HA	6:E:83:LEU:HD23	1.73	0.40
6:E:120:TYR:CD2	6:E:120:TYR:N	2.89	0.40
6:E:248:ARG:HD3	6:E:249:ILE:H	1.86	0.40
6:E:369:ASP:O	6:E:370:ILE:HD13	2.21	0.40
1:A:35:PHE:O	1:A:45:PHE:CD1	2.74	0.40
1:A:59:LYS:HB2	1:A:65:LEU:HD23	2.03	0.40
1:A:201:ILE:HD13	1:A:201:ILE:HA	1.81	0.40
1:A:543:ASN:O	1:A:556:THR:HA	2.22	0.40
2:B:160:VAL:HG23	2:B:185:ILE:HB	2.03	0.40
5:J:41:G:C2	5:J:42:C:C2	3.09	0.40
6:F:401:ASP:OD1	6:F:402:PRO:HD2	2.21	0.40
6:E:158:LEU:HB2	6:E:162:GLU:O	2.21	0.40
6:E:178:ARG:C	6:E:180:TYR:H	2.24	0.40
6:E:323:LYS:HZ2	6:E:324:TYR:H	1.70	0.40
7:G:69:LEU:CD1	7:G:89:TYR:HB3	2.52	0.40
7:G:73:CYS:HB3	7:G:88:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	924/932 (99%)	668 (72%)	235 (25%)	21 (2%)	6	31
2	B	185/198 (93%)	143 (77%)	37 (20%)	5 (3%)	5	27
2	D	184/198 (93%)	134 (73%)	46 (25%)	4 (2%)	6	32
3	C	70/83 (84%)	57 (81%)	13 (19%)	0	100	100
6	E	581/601 (97%)	437 (75%)	140 (24%)	4 (1%)	22	56
6	F	580/601 (96%)	456 (79%)	121 (21%)	3 (0%)	29	63
7	G	111/113 (98%)	80 (72%)	28 (25%)	3 (3%)	5	27
All	All	2635/2726 (97%)	1975 (75%)	620 (24%)	40 (2%)	14	39

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	A	232	PRO
1	A	237	TYR
1	A	245	LEU
1	A	249	ARG
1	A	457	ARG
1	A	566	MET
1	A	753	PHE
1	A	760	ASP
1	A	832	PRO
1	A	903	TYR
2	B	183	PRO
2	D	133	PRO
6	F	27	CYS
6	F	81	PHE
6	F	84	CYS
6	E	175	PRO
6	E	358	CYS

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Mol	Chain	Res	Type
7	G	7	VAL
1	A	540	THR
1	A	615	MET
1	A	771	ALA
1	A	830	PRO
2	B	113	GLY
6	E	445	PRO
7	G	52	LYS
7	G	91	ILE
1	A	847	ILE
2	D	178	PRO
2	D	183	PRO
1	A	71	VAL
1	A	28	THR
2	B	141	THR
2	D	99	ASP
1	A	539	ILE
2	B	133	PRO
1	A	14	VAL
1	A	214	GLY
2	B	160	VAL
6	E	527	GLY

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	817/823 (99%)	680 (83%)	137 (17%)	2	9
2	B	144/167 (86%)	122 (85%)	22 (15%)	2	12
2	D	149/167 (89%)	115 (77%)	34 (23%)	1	3
3	C	67/77 (87%)	56 (84%)	11 (16%)	2	10
6	E	498/523 (95%)	459 (92%)	39 (8%)	12	40
6	F	498/523 (95%)	461 (93%)	37 (7%)	13	42
7	G	94/94 (100%)	85 (90%)	9 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2267/2374 (96%)	1978 (87%)	289 (13%)	7 18

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	40	ASP
1	A	42	VAL
1	A	49	LEU
1	A	55	ARG
1	A	58	GLU
1	A	59	LYS
1	A	62	ASP
1	A	63	ASP
1	A	90	LEU
1	A	92	ASP
1	A	93	CYS
1	A	99	HIS
1	A	101	PHE
1	A	106	ILE
1	A	114	ILE
1	A	115	SER
1	A	116	ARG
1	A	126	ASP
1	A	131	LEU
1	A	141	THR
1	A	163	TYR
1	A	164	ASP
1	A	170	ASP
1	A	178	LEU
1	A	181	ARG
1	A	192	PHE
1	A	197	ARG
1	A	206	THR
1	A	207	LEU
1	A	211	ASP
1	A	212	LEU
1	A	235	ASP
1	A	236	SER
1	A	257	VAL
1	A	261	LEU
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	276	THR
1	A	288	LYS
1	A	291	ASP
1	A	294	TYR
1	A	295	HIS
1	A	303	ASP
1	A	306	CYS
1	A	315	VAL
1	A	325	SER
1	A	344	THR
1	A	346	TYR
1	A	351	LEU
1	A	366	LEU
1	A	369	LYS
1	A	371	LEU
1	A	377	ASP
1	A	380	MET
1	A	386	ASN
1	A	391	LYS
1	A	393	THR
1	A	394	THR
1	A	401	LEU
1	A	402	THR
1	A	404	ASN
1	A	421	ASP
1	A	434	SER
1	A	435	VAL
1	A	451	SER
1	A	457	ARG
1	A	466	ILE
1	A	468	GLN
1	A	473	VAL
1	A	477	ASP
1	A	482	CYS
1	A	483	TYR
1	A	496	ASN
1	A	501	SER
1	A	516	TYR
1	A	522	GLU
1	A	525	ASP
1	A	531	THR
1	A	534	ASN

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Mol	Chain	Res	Type
1	A	536	ILE
1	A	542	MET
1	A	544	LEU
1	A	552	ASN
1	A	553	ARG
1	A	564	SER
1	A	567	THR
1	A	571	PHE
1	A	573	GLN
1	A	578	SER
1	A	606	TYR
1	A	607	SER
1	A	610	GLU
1	A	611	ASN
1	A	628	ASN
1	A	645	CYS
1	A	649	SER
1	A	658	GLU
1	A	692	SER
1	A	694	PHE
1	A	701	THR
1	A	704	VAL
1	A	714	LYS
1	A	717	ASP
1	A	720	VAL
1	A	724	GLN
1	A	734	ASN
1	A	735	ARG
1	A	748	TYR
1	A	750	ARG
1	A	758	LEU
1	A	759	SER
1	A	768	SER
1	A	772	SER
1	A	778	SER
1	A	784	SER
1	A	788	TYR
1	A	791	ASN
1	A	798	LYS
1	A	799	CYS
1	A	802	GLU
1	A	803	THR

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Mol	Chain	Res	Type
1	A	812	PHE
1	A	819	LEU
1	A	825	ASP
1	A	833	ASP
1	A	845	ASP
1	A	847	ILE
1	A	892	HIS
1	A	894	GLU
1	A	898	HIS
1	A	900	LEU
1	A	903	TYR
1	A	906	MET
1	A	913	SER
1	A	914	ARG
1	A	917	GLU
1	A	920	PHE
2	B	41	SER
2	B	55	MET
2	B	56	GLN
2	B	60	GLU
2	B	68	THR
2	B	76	SER
2	B	85	SER
2	B	89	THR
2	B	93	THR
2	B	95	LEU
2	B	105	ASN
2	B	118	ASN
2	B	119	ILE
2	B	132	ILE
2	B	140	ASN
2	B	142	CYS
2	B	157	GLN
2	B	161	ASP
2	B	163	ASP
2	B	173	SER
2	B	177	SER
2	B	179	ASN
3	C	10	SER
3	C	26	SER
3	C	36	HIS
3	C	45	THR

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Mol	Chain	Res	Type
3	C	47	GLU
3	C	50	GLU
3	C	57	SER
3	C	61	SER
3	C	67	ASP
3	C	68	ILE
3	C	69	ASN
2	D	9	LEU
2	D	11	SER
2	D	35	LEU
2	D	42	LEU
2	D	52	ASP
2	D	59	LEU
2	D	64	ASP
2	D	65	GLN
2	D	68	THR
2	D	75	ARG
2	D	76	SER
2	D	78	ASP
2	D	83	VAL
2	D	84	THR
2	D	92	PHE
2	D	94	MET
2	D	99	ASP
2	D	100	ASN
2	D	103	LEU
2	D	106	ILE
2	D	112	ASP
2	D	122	LEU
2	D	127	LYS
2	D	134	ASP
2	D	139	LYS
2	D	140	ASN
2	D	141	THR
2	D	148	THR
2	D	151	SER
2	D	159	VAL
2	D	165	LYS
2	D	166	ILE
2	D	174	MET
2	D	182	TRP
6	F	6	VAL

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Mol	Chain	Res	Type
6	F	11	GLN
6	F	12	THR
6	F	26	CYS
6	F	31	TYR
6	F	37	THR
6	F	59	ASP
6	F	65	LEU
6	F	72	CYS
6	F	73	LYS
6	F	75	HIS
6	F	81	PHE
6	F	89	VAL
6	F	106	PHE
6	F	109	ILE
6	F	155	ARG
6	F	173	ARG
6	F	224	TYR
6	F	275	GLN
6	F	280	LEU
6	F	288	LYS
6	F	303	ARG
6	F	317	LEU
6	F	343	PHE
6	F	357	PHE
6	F	373	PHE
6	F	380	THR
6	F	385	SER
6	F	437	PHE
6	F	440	THR
6	F	455	LEU
6	F	457	TYR
6	F	476	TYR
6	F	516	ASN
6	F	530	THR
6	F	542	ASP
6	F	548	GLN
6	E	12	THR
6	E	22	ARG
6	E	27	CYS
6	E	31	TYR
6	E	43	LEU
6	E	51	ASN

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Mol	Chain	Res	Type
6	E	69	SER
6	E	72	CYS
6	E	75	HIS
6	E	79	ILE
6	E	81	PHE
6	E	86	ASN
6	E	95	ASN
6	E	97	CYS
6	E	130	LEU
6	E	131	LYS
6	E	133	PHE
6	E	145	PHE
6	E	164	HIS
6	E	188	THR
6	E	240	LEU
6	E	245	HIS
6	E	255	THR
6	E	260	ASP
6	E	277	TYR
6	E	356	VAL
6	E	357	PHE
6	E	378	MET
6	E	380	THR
6	E	383	ASP
6	E	388	ASN
6	E	427	ARG
6	E	455	LEU
6	E	477	LYS
6	E	482	HIS
6	E	492	GLN
6	E	532	THR
6	E	562	ASN
6	E	587	PHE
7	G	10	ARG
7	G	14	CYS
7	G	36	LYS
7	G	40	PHE
7	G	70	GLU
7	G	74	ARG
7	G	79	THR
7	G	97	LEU
7	G	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	A	295	HIS
1	A	695	ASN
2	B	176	ASN
2	D	108	ASN
2	D	179	ASN
6	F	62	GLN
6	F	107	ASN
6	F	268	ASN
6	F	404	GLN
6	F	423	ASN
6	F	489	ASN
6	F	492	GLN
6	E	75	HIS
6	E	361	ASN
6	E	423	ASN
6	E	470	GLN
6	E	531	GLN
6	E	537	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	I	24/25 (96%)	3 (12%)	1 (4%)
5	J	26/33 (78%)	6 (23%)	0
All	All	50/58 (86%)	9 (18%)	1 (2%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	I	10	C
4	I	17	A
4	I	23	C
5	J	26	A
5	J	35	U
5	J	40	U
5	J	42	C
5	J	44	A
5	J	47	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	I	22	G

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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
9	GNP	A	1003	-	29,34,34	1.60	9 (31%)	33,54,54	2.23	8 (24%)

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
9	GNP	A	1003	-	-	7/14/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1003	GNP	PB-O3A	3.56	1.63	1.59
9	A	1003	GNP	PG-N3B	3.09	1.71	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1003	GNP	PB-O2B	-2.57	1.49	1.56
9	A	1003	GNP	PA-O2A	-2.54	1.43	1.55
9	A	1003	GNP	PB-O1B	2.46	1.50	1.46
9	A	1003	GNP	PG-O1G	2.38	1.49	1.46
9	A	1003	GNP	C5-C4	-2.36	1.34	1.40
9	A	1003	GNP	C6-N1	2.29	1.37	1.33
9	A	1003	GNP	C8-N7	-2.16	1.30	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1003	GNP	C5-C6-N1	-8.34	112.02	123.43
9	A	1003	GNP	C2-N1-C6	5.53	124.72	115.93
9	A	1003	GNP	O3G-PG-O1G	-3.10	105.65	113.45
9	A	1003	GNP	PB-O3A-PA	-3.08	121.76	132.62
9	A	1003	GNP	N3-C2-N1	-2.79	123.50	127.22
9	A	1003	GNP	C1'-N9-C4	2.55	131.13	126.64
9	A	1003	GNP	O1B-PB-N3B	-2.33	108.34	111.77
9	A	1003	GNP	C4-C5-C6	-2.07	118.82	120.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1003	GNP	PB-N3B-PG-O1G
9	A	1003	GNP	O4'-C4'-C5'-O5'
9	A	1003	GNP	C3'-C4'-C5'-O5'
9	A	1003	GNP	PG-N3B-PB-O3A
9	A	1003	GNP	PB-O3A-PA-O2A
9	A	1003	GNP	C5'-O5'-PA-O3A
9	A	1003	GNP	C4'-C5'-O5'-PA

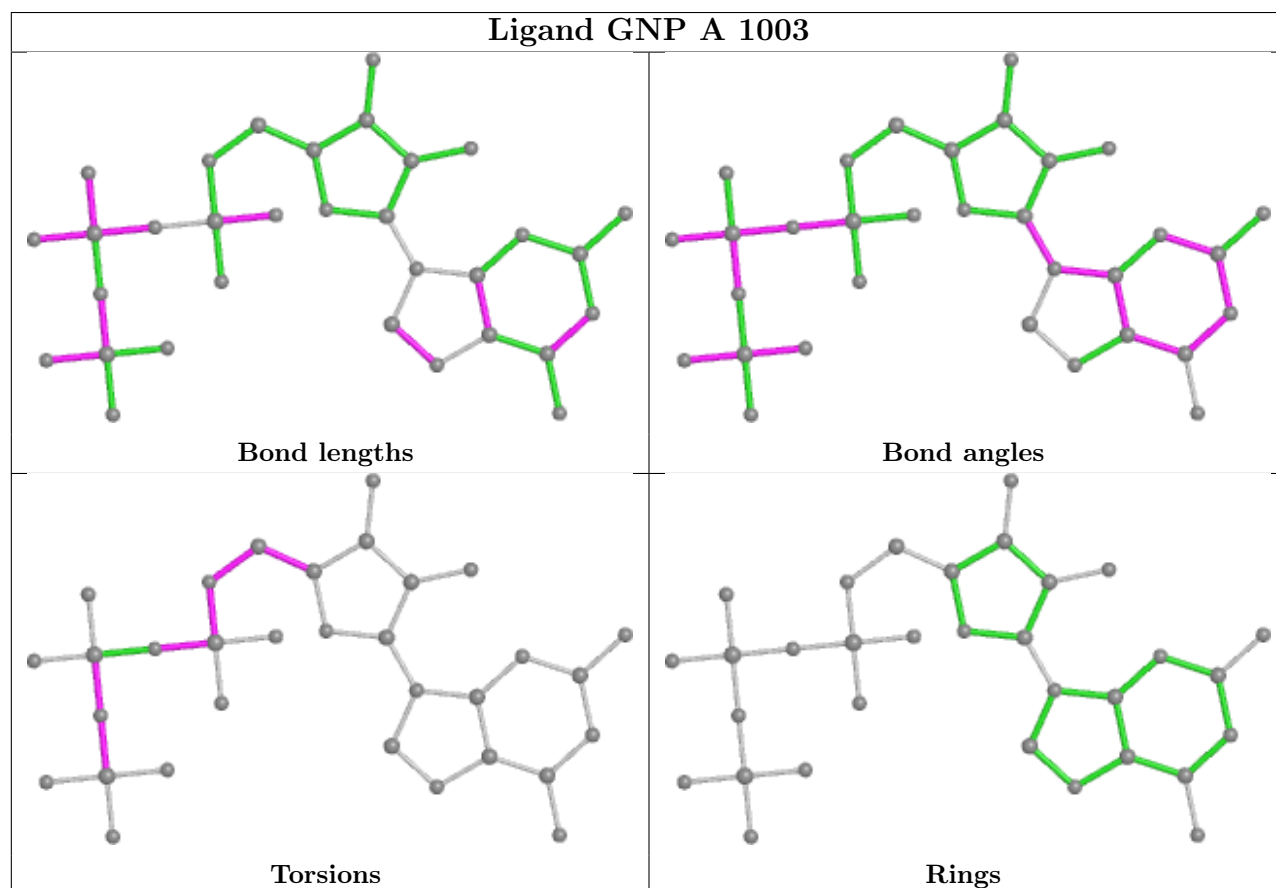
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1003	GNP	9	0

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 [i](#)

There are no chain breaks in this entry.

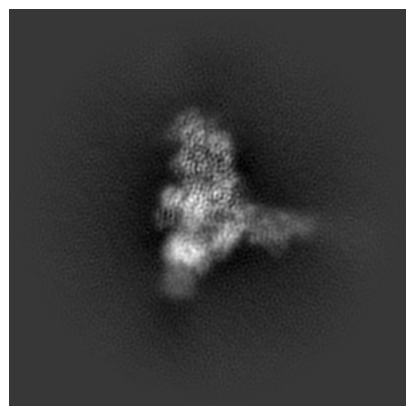
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34317. These allow visual inspection of the internal detail of the map and identification of artifacts.

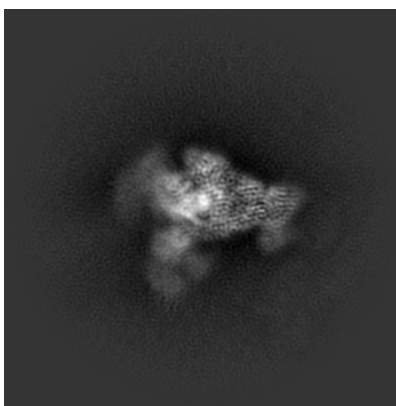
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

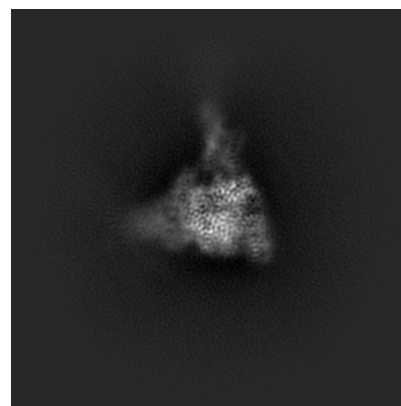
6.1.1 Primary map



X

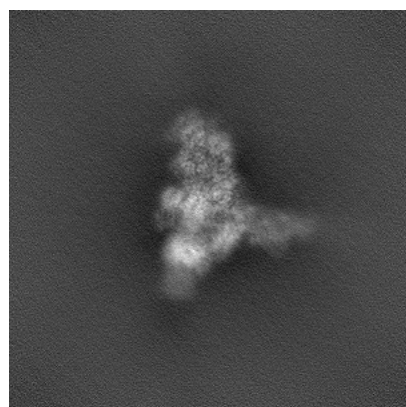


Y

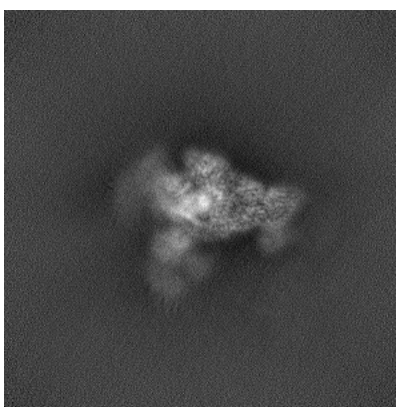


Z

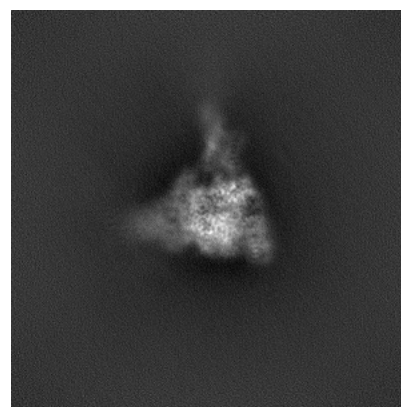
6.1.2 Raw map



X



Y

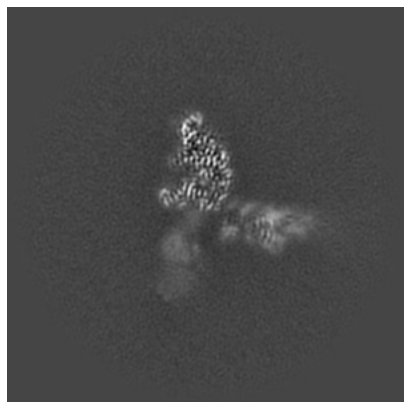


Z

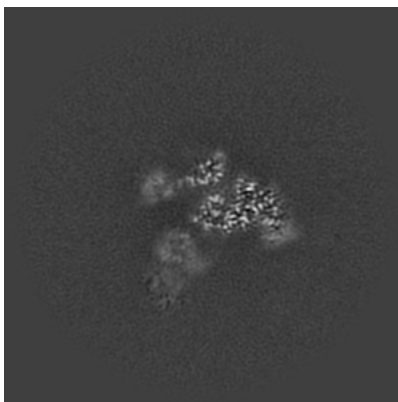
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

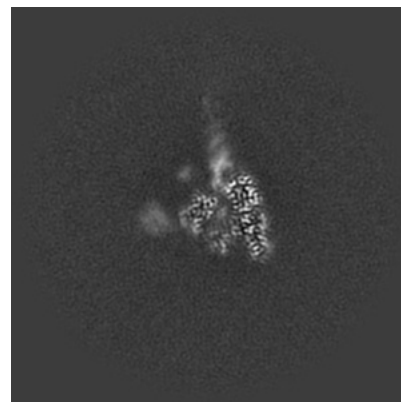
6.2.1 Primary map



X Index: 224

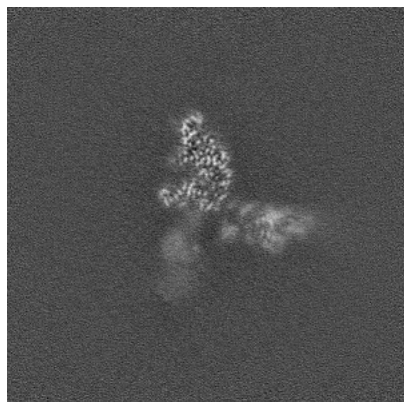


Y Index: 224

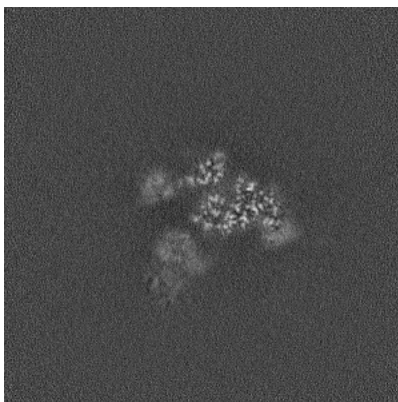


Z Index: 224

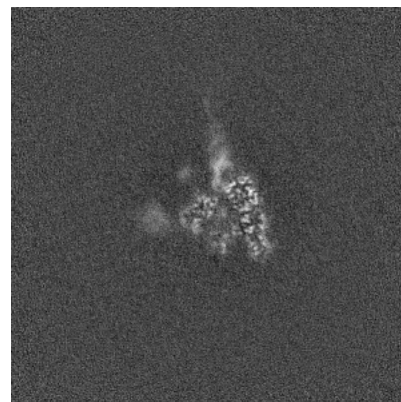
6.2.2 Raw map



X Index: 224



Y Index: 224

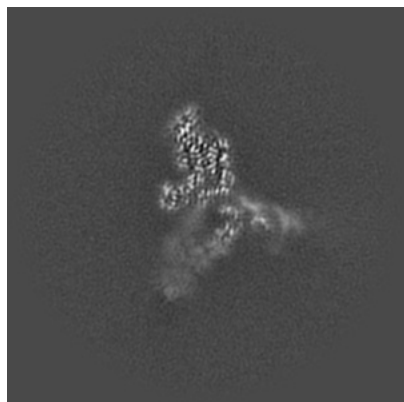


Z Index: 224

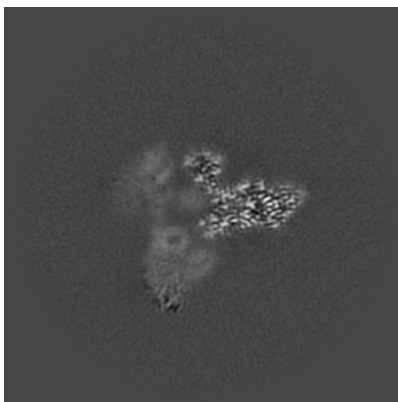
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

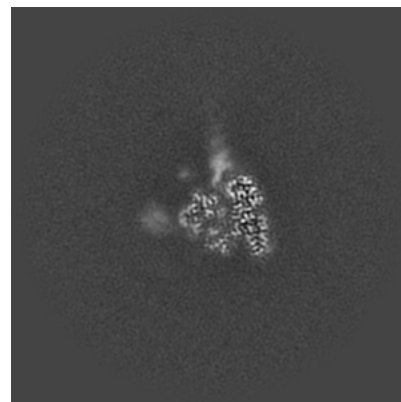
6.3.1 Primary map



X Index: 236

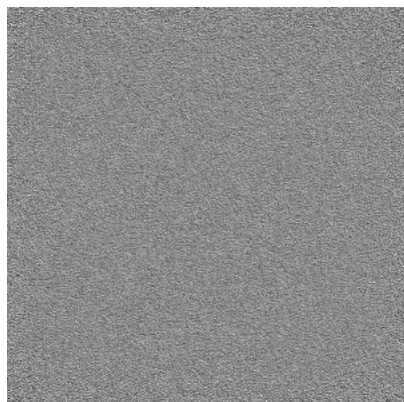


Y Index: 206

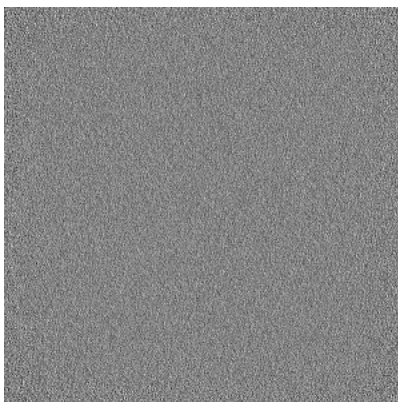


Z Index: 226

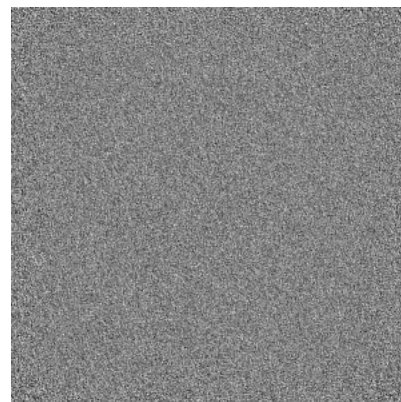
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

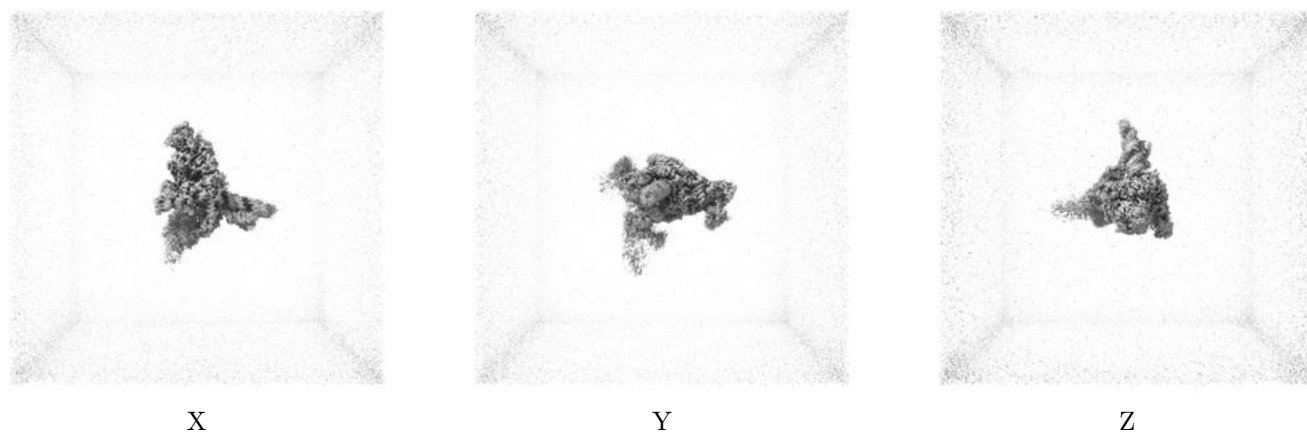
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

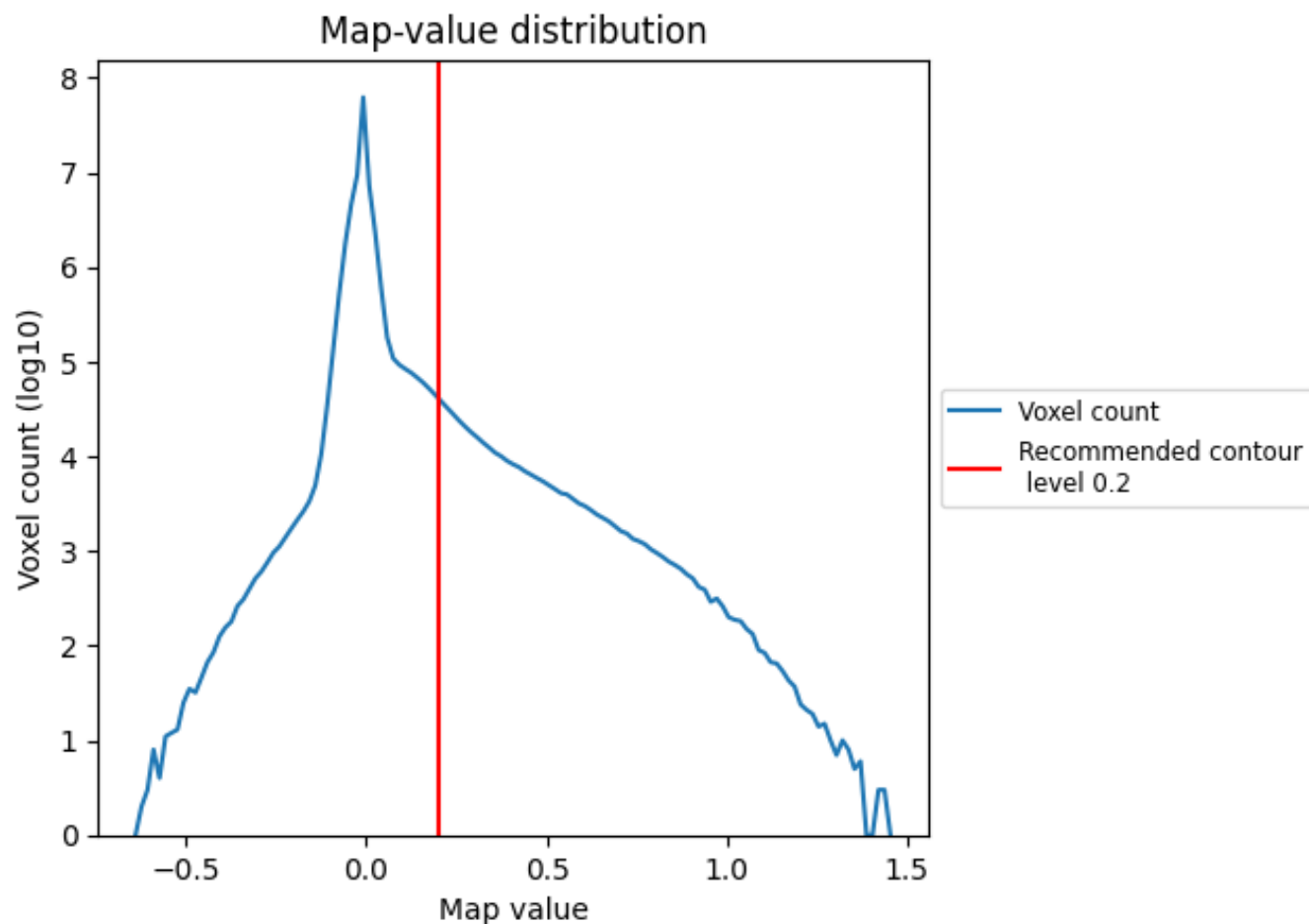
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

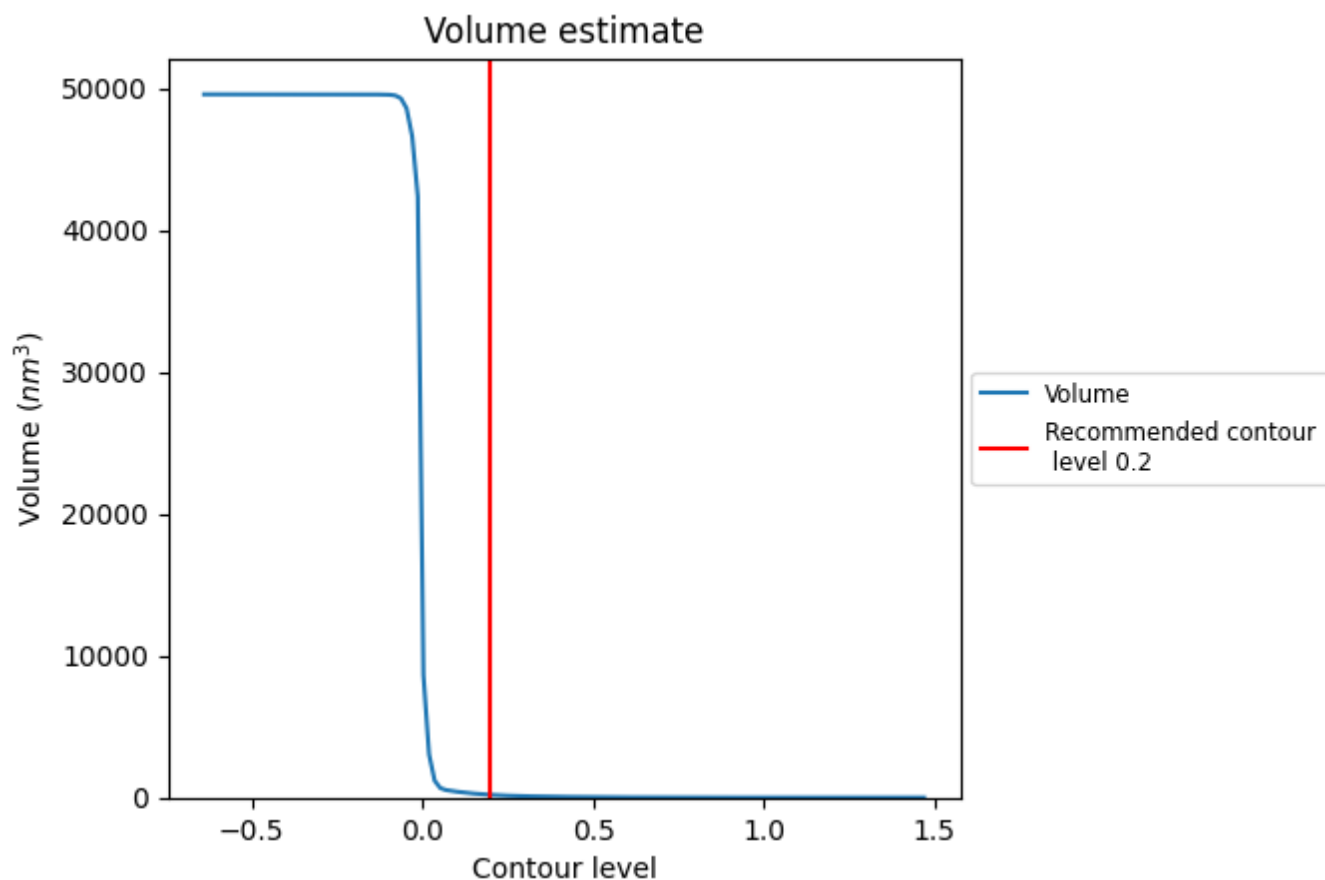
This section contains the results of statistical analysis of the map.

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.

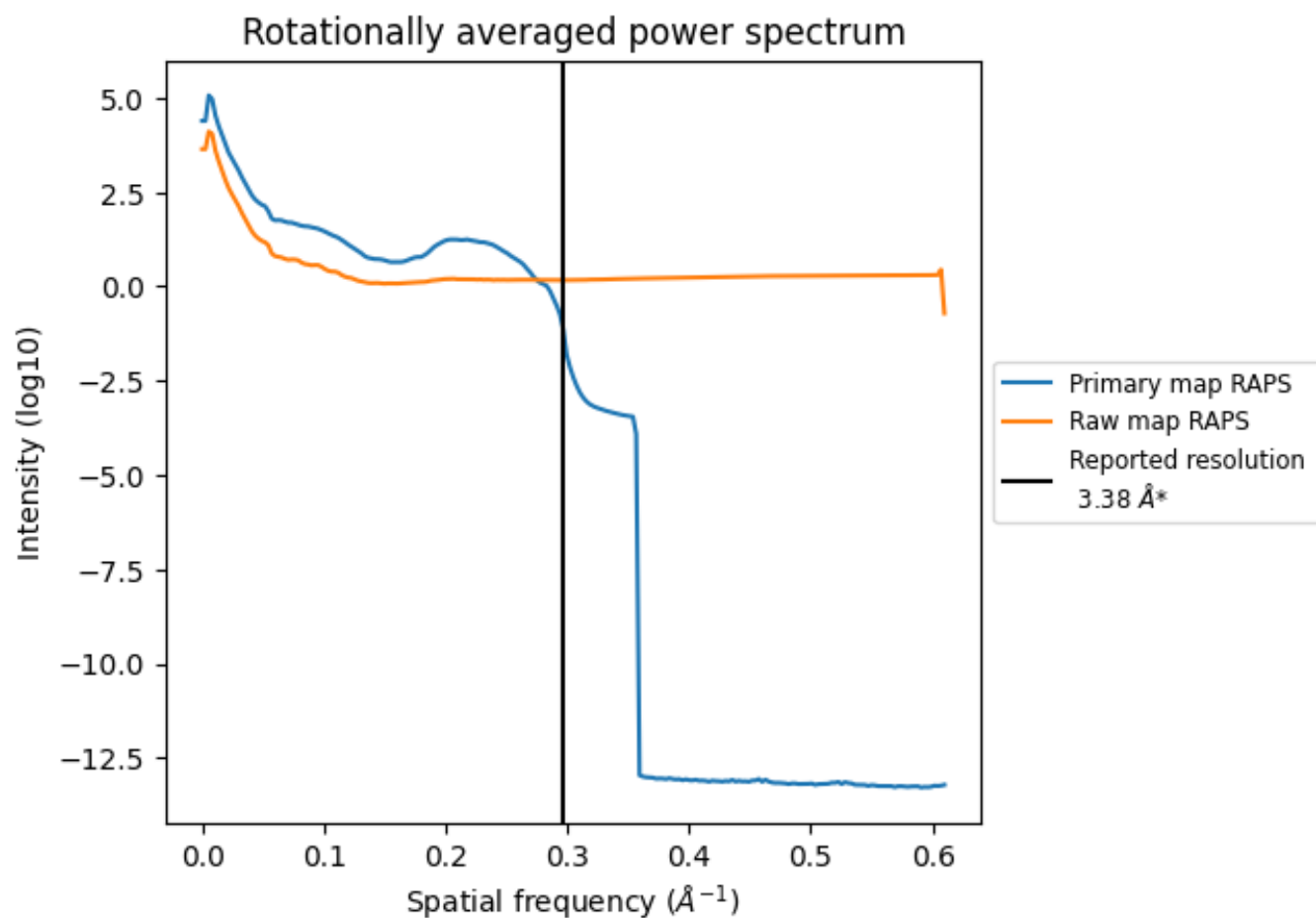
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 173 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 ⓘ

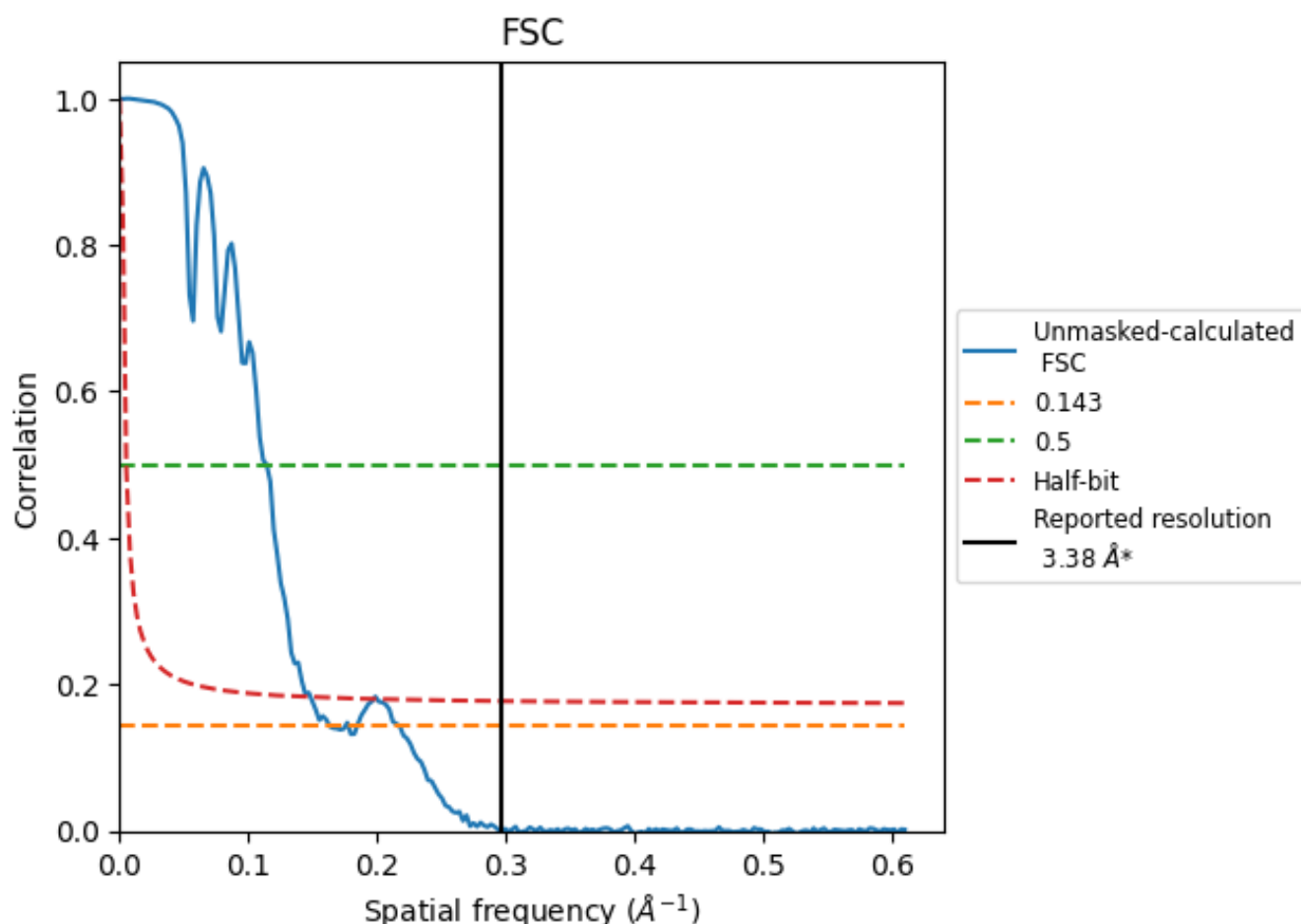


*Reported resolution corresponds to spatial frequency of 0.296 Å⁻¹

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 0.296 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.13	8.76	6.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.13 differs from the reported value 3.38 by more than 10 %

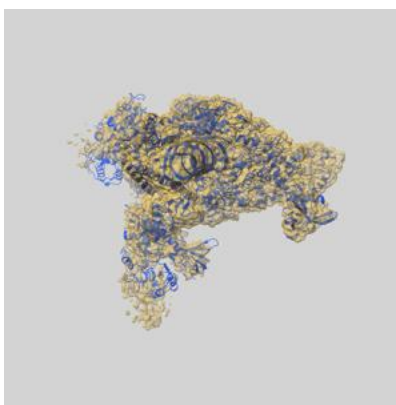
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34317 and PDB model 8GWN. Per-residue inclusion information can be found in section 3 on page 7.

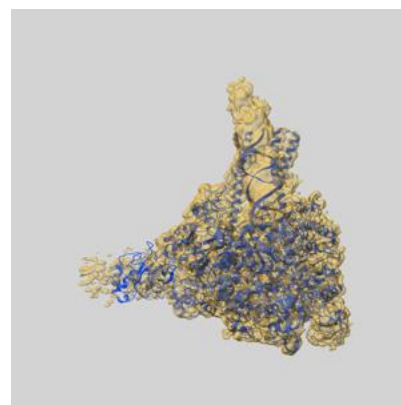
9.1 Map-model overlay [i](#)



X



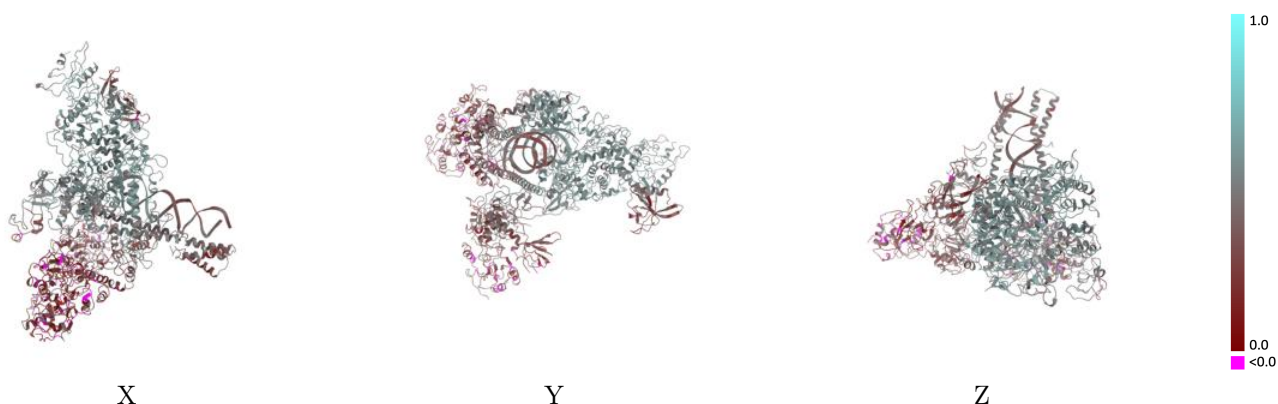
Y



Z

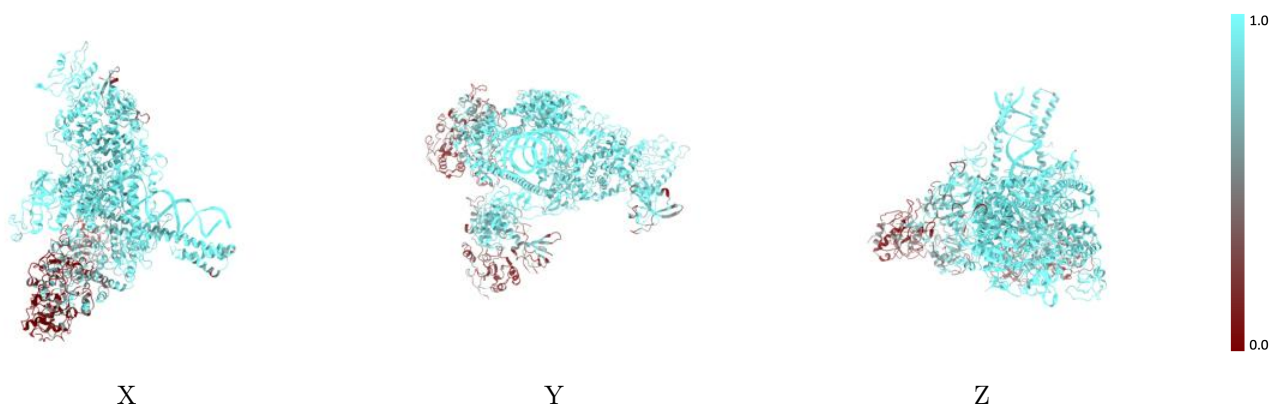
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



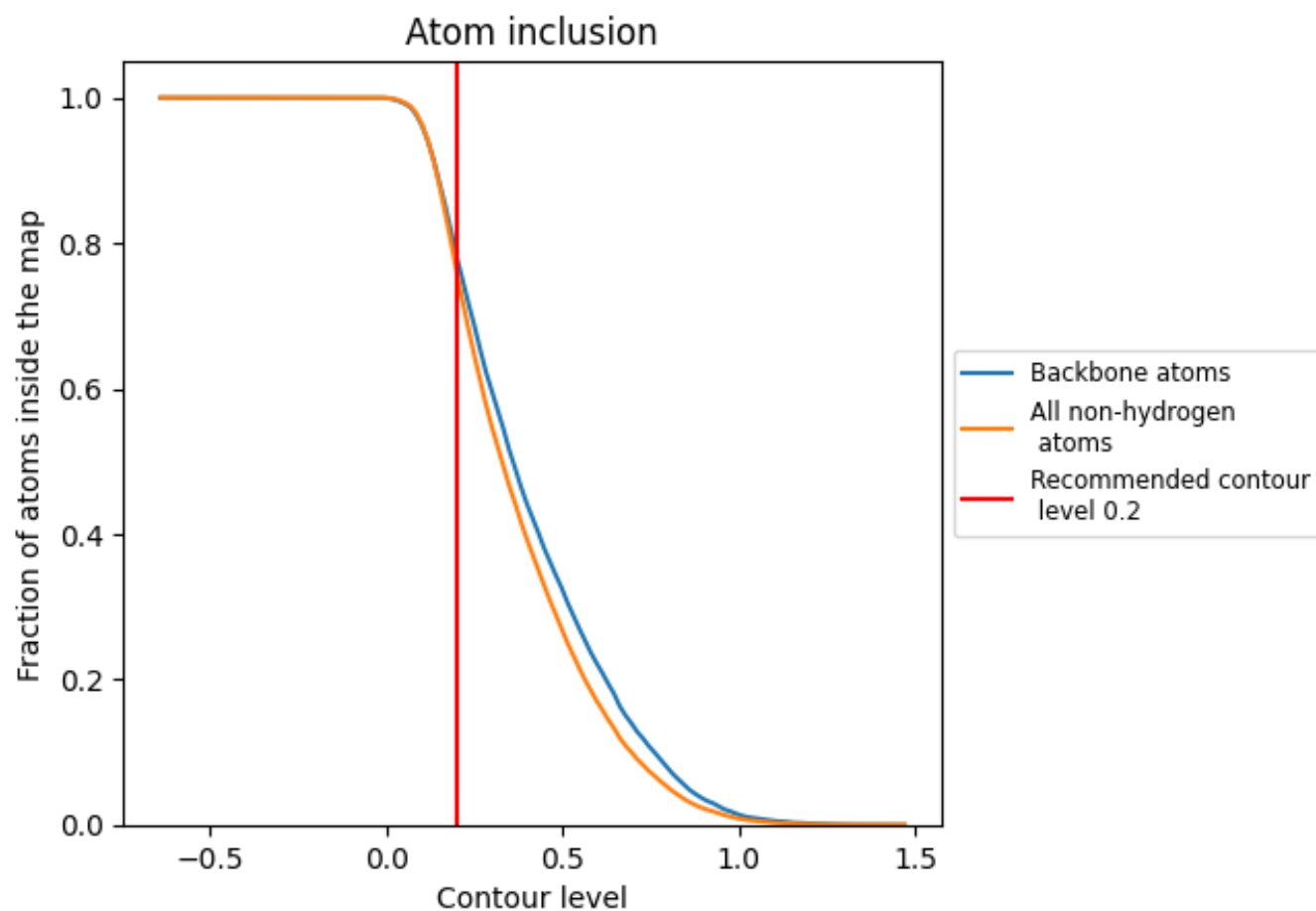
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7609	<div></div> 0.4070
A	<div></div> 0.9684	<div></div> 0.5420
B	<div></div> 0.9484	<div></div> 0.4720
C	<div></div> 0.9545	<div></div> 0.5130
D	<div></div> 0.9461	<div></div> 0.4530
E	<div></div> 0.5727	<div></div> 0.2920
F	<div></div> 0.4124	<div></div> 0.2560
G	<div></div> 0.7259	<div></div> 0.3450
I	<div></div> 0.9963	<div></div> 0.4300
J	<div></div> 0.9965	<div></div> 0.4530

1.0

0.0

<0.0