



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:58 PM UTC

PDB ID : 9CM2 / pdb_00009cm2
EMDB ID : EMD-45737
Title : Cryo-EM model derived from localized reconstruction of human adenovirus 6-hexon-FX complex at 4.3Å resolution
Authors : Reddy, V.S.; Ma, O.X.
Deposited on : 2024-07-12
Resolution : 5.01 Å(reported)
Based on initial model : 6BIT

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

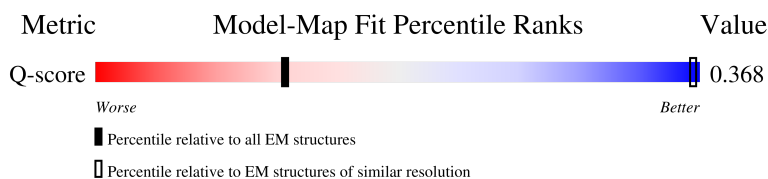
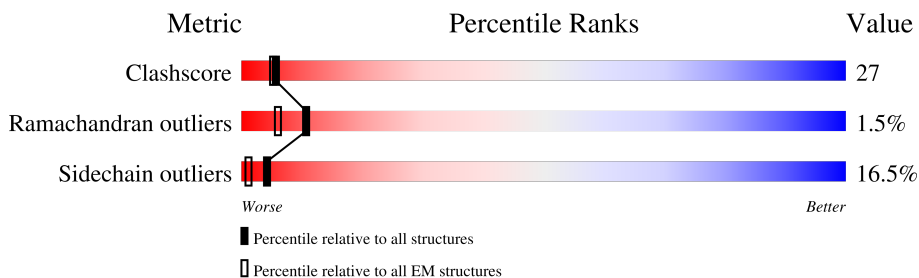
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.01 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	859 (4.51 - 5.51)

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	J	963	
1	K	963	
1	L	963	
2	Z	488	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25229 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	931	Total	C	N	O	S	0	0
			7400	4691	1258	1413	38		
1	K	935	Total	C	N	O	S	0	0
			7426	4707	1262	1419	38		
1	L	930	Total	C	N	O	S	0	0
			7397	4691	1256	1412	38		

- Molecule 2 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	377	Total	C	N	O	S	0	0
			3002	1849	516	606	31		

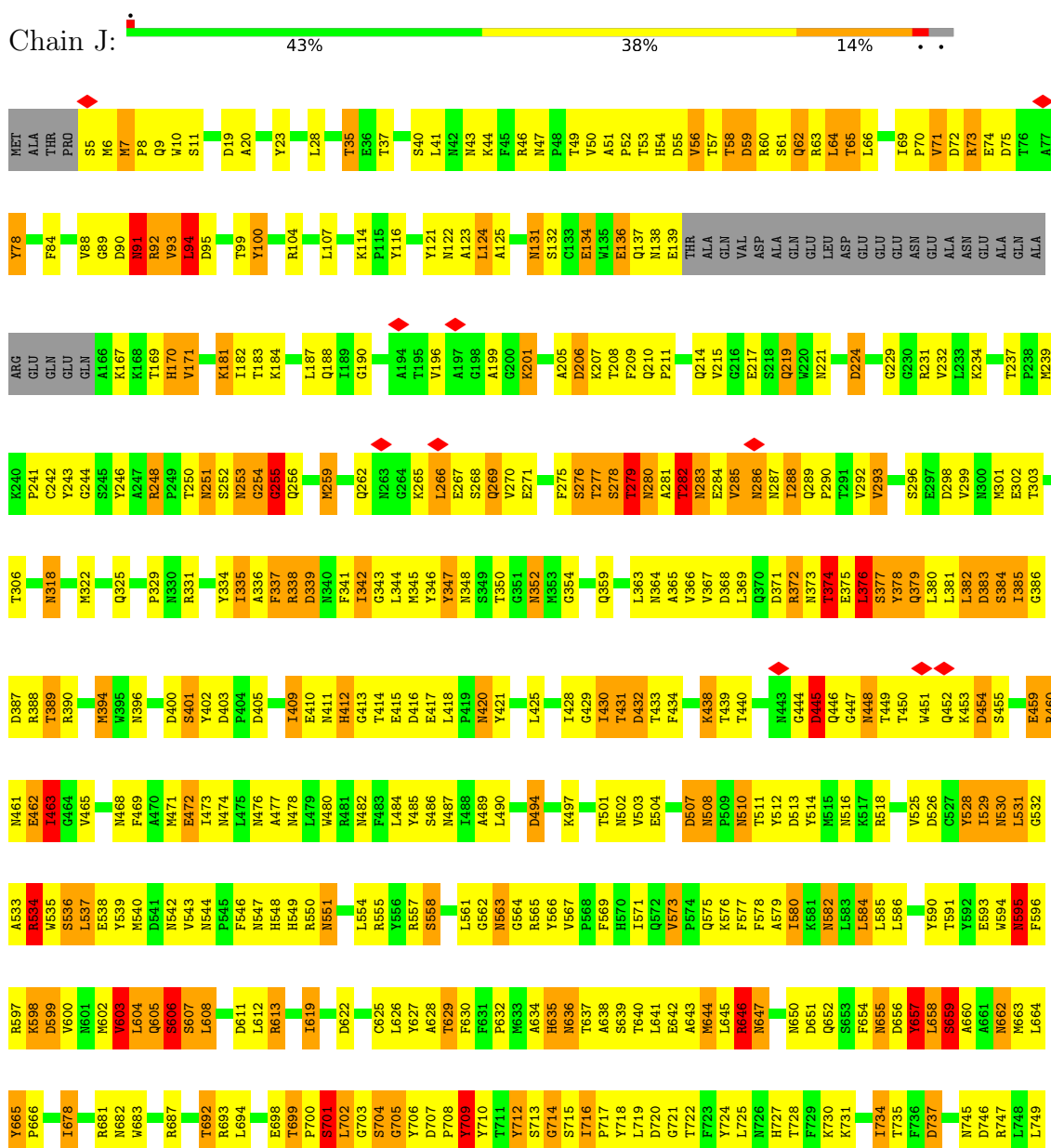
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

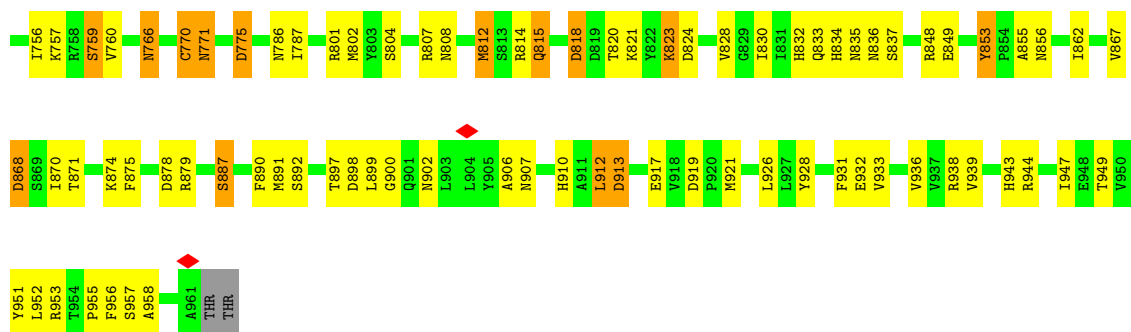
Mol	Chain	Residues	Atoms		AltConf
3	Z	4	Total	Ca	0
			4	4	

3 Residue-property plots

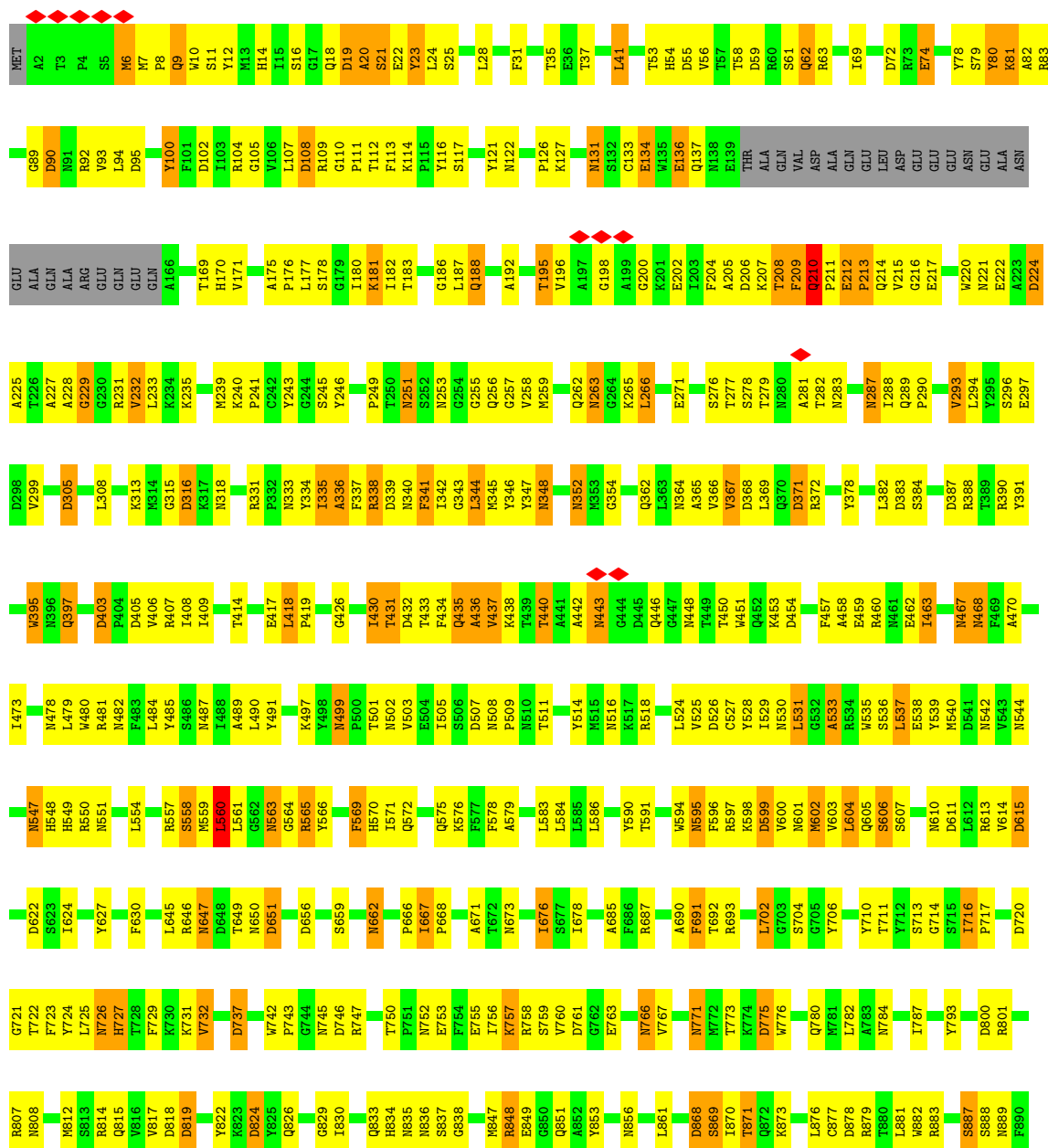
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





• Molecule 1: Hexon protein





Chain Z:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1769	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	81	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	154.112, 191.74399, 118.271996	wwPDB
Map dimensions	107, 66, 86	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.7919999, 1.7919999, 1.7919999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	J	0.56	5/7592 (0.1%)	0.68	18/10326 (0.2%)
1	K	0.39	0/7619	0.53	9/10365 (0.1%)
1	L	0.35	0/7590	0.49	3/10325 (0.0%)
2	Z	0.10	0/2918	0.28	0/3912
All	All	0.42	5/25719 (0.0%)	0.55	30/34928 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	647	ASN	N-CA	6.96	1.55	1.46
1	J	459	GLU	CA-C	-5.65	1.47	1.53
1	J	283	ASN	N-CA	5.58	1.53	1.46
1	J	657	TYR	CA-C	-5.46	1.47	1.52
1	J	59	ASP	CA-C	-5.08	1.46	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	448	ASN	N-CA-C	-12.86	97.26	111.28
1	J	657	TYR	N-CA-C	-11.64	97.44	112.93
1	J	280	ASN	N-CA-C	-8.34	102.15	111.82
1	J	376	LEU	N-CA-C	-7.40	102.72	112.34
1	L	170	HIS	N-CA-C	-7.29	100.70	110.55
1	J	699	THR	CA-C-N	-7.12	111.72	119.98
1	J	699	THR	C-N-CA	-7.12	111.72	119.98
1	K	210	GLN	CA-C-N	-7.01	112.21	120.13
1	K	210	GLN	C-N-CA	-7.01	112.21	120.13
1	J	658	LEU	N-CA-C	-6.82	102.70	111.02
1	J	534	ARG	N-CA-C	-6.69	100.53	110.23
1	J	647	ASN	N-CA-C	6.44	119.37	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	20	ALA	N-CA-C	-6.42	104.55	112.38
1	J	637	THR	N-CA-C	-6.34	104.64	112.38
1	K	229	GLY	N-CA-C	6.24	120.28	111.42
1	J	701	SER	N-CA-C	-6.13	101.23	110.24
1	J	59	ASP	N-CA-C	-6.01	105.86	113.43
1	J	94	LEU	N-CA-C	5.99	118.07	109.14
1	J	378	TYR	N-CA-C	-5.87	104.23	111.75
1	K	436	ALA	N-CA-C	5.84	118.75	109.81
1	J	279	THR	N-CA-C	-5.73	104.64	111.69
1	L	694	LEU	N-CA-C	5.63	117.95	109.23
1	K	212	GLU	CA-C-N	-5.44	113.04	119.84
1	K	212	GLU	C-N-CA	-5.44	113.04	119.84
1	J	595	ASN	N-CA-C	5.29	117.03	108.26
1	K	533	ALA	N-CA-C	5.26	116.64	107.49
1	J	255	GLY	N-CA-C	5.23	125.57	113.18
1	J	283	ASN	N-CA-C	5.16	121.79	110.80
1	L	562	GLY	N-CA-C	5.14	125.36	113.18
1	K	560	LEU	N-CA-C	-5.02	105.08	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	7400	0	7100	554	0
1	K	7426	0	7126	461	0
1	L	7397	0	7100	398	0
2	Z	3002	0	2796	64	0
3	Z	4	0	0	0	0
All	All	25229	0	24122	1349	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 27.

All (1349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:28:ARG:HD2	2:Z:37:THR:CG2	1.74	1.16
1:J:411:ASN:HB3	1:J:531:LEU:HD23	1.32	1.09
1:K:211:PRO:HB2	1:K:231:ARG:HH12	1.05	1.08
2:Z:23:SER:O	2:Z:24:TYR:CD1	2.06	1.08
2:Z:32:CGU:OE22	2:Z:32:CGU:HA	1.55	1.05
1:J:439:THR:HA	1:J:450:THR:HG22	1.36	1.04
2:Z:50:CYS:SG	2:Z:63:ASP:OD1	2.15	1.04
1:L:134:GLU:HB3	1:L:171:VAL:HG13	1.40	1.03
1:J:94:LEU:HB2	1:J:630:PHE:HE1	1.20	1.03
1:K:211:PRO:HB2	1:K:231:ARG:NH1	1.73	1.03
2:Z:28:ARG:HG2	2:Z:37:THR:OG1	1.59	1.01
1:J:251:ASN:H	1:J:255:GLY:HA3	1.21	0.99
2:Z:28:ARG:HD2	2:Z:37:THR:HG21	1.44	0.98
1:K:74:GLU:HB2	1:K:81:LYS:HE3	1.49	0.94
1:J:712:TYR:CZ	1:J:714:GLY:HA3	2.03	0.94
1:J:430:ILE:HG22	2:Z:9:LYS:HG3	1.48	0.94
2:Z:9:LYS:HG2	2:Z:10:LYS:H	1.32	0.93
2:Z:28:ARG:HH21	2:Z:34:SER:HB3	1.33	0.92
1:J:94:LEU:HB2	1:J:630:PHE:CE1	2.05	0.91
1:J:698:GLU:HG2	1:J:712:TYR:CZ	2.07	0.90
1:K:211:PRO:CB	1:K:231:ARG:HH12	1.85	0.88
2:Z:28:ARG:HD2	2:Z:37:THR:HG23	1.55	0.88
1:J:440:THR:HG23	1:J:450:THR:HA	1.55	0.87
1:J:770:CYS:SG	1:J:771:ASN:N	2.46	0.87
1:J:702:LEU:HD12	1:J:703:GLY:H	1.40	0.86
1:J:78:TYR:CZ	1:J:706:TYR:HB3	2.12	0.85
1:J:251:ASN:N	1:J:255:GLY:HA3	1.91	0.84
1:J:448:ASN:HB3	1:L:289:GLN:HA	1.58	0.84
1:J:461:ASN:HD21	1:L:171:VAL:H	1.22	0.84
2:Z:19:CGU:O	2:Z:19:CGU:OE11	1.97	0.82
1:K:20:ALA:HB2	1:K:23:TYR:CZ	2.15	0.82
1:J:461:ASN:HD21	1:L:171:VAL:N	1.76	0.81
1:J:121:TYR:HB2	1:J:244:GLY:HA2	1.63	0.81
1:L:786:ASN:ND2	1:L:891:MET:SD	2.52	0.81
1:J:373:ASN:HD22	1:J:376:LEU:HD22	1.45	0.81
1:J:411:ASN:HD22	1:J:531:LEU:HA	1.45	0.81
1:J:698:GLU:HG2	1:J:712:TYR:CE2	2.17	0.80
1:L:80:TYR:HB3	1:L:596:PHE:HD1	1.46	0.80
1:L:655:ASN:HB3	1:L:936:VAL:HG12	1.64	0.79
2:Z:28:ARG:NH2	2:Z:34:SER:HB3	1.96	0.79
1:K:565:ARG:HD2	1:K:566:TYR:CZ	2.18	0.78
1:J:562:GLY:HA3	1:L:815:GLN:HE22	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:373:ASN:ND2	1:J:376:LEU:HD22	1.99	0.78
1:K:691:PHE:HE1	1:K:882:TRP:HB2	1.47	0.78
2:Z:28:ARG:CG	2:Z:37:THR:OG1	2.30	0.78
1:K:535:TRP:CE3	1:K:814:ARG:HB3	2.19	0.77
1:L:313:LYS:HG2	1:L:315:GLY:H	1.47	0.77
1:K:206:ASP:H	1:K:210:GLN:HB2	1.48	0.76
1:L:724:TYR:O	1:L:725:LEU:C	2.28	0.76
1:J:643:ALA:O	1:J:646:ARG:HB2	1.86	0.76
1:J:730:LYS:HB3	1:J:917:GLU:HG3	1.67	0.76
1:K:818:ASP:HB2	1:K:869:SER:HA	1.68	0.76
1:J:276:SER:HB3	1:K:435:GLN:HE22	1.51	0.76
1:K:305:ASP:N	1:K:305:ASP:OD1	2.17	0.75
1:L:940:HIS:HB3	1:L:948:GLU:OE1	1.86	0.75
1:J:373:ASN:ND2	1:J:376:LEU:H	1.82	0.75
1:J:280:ASN:O	1:J:284:GLU:HG2	1.86	0.75
1:K:111:PRO:HB3	1:K:565:ARG:HH11	1.51	0.75
1:J:251:ASN:H	1:J:255:GLY:CA	2.00	0.74
1:K:808:ASN:HD22	1:K:879:ARG:HB3	1.52	0.74
1:J:208:THR:O	1:J:231:ARG:NH2	2.21	0.74
1:K:348:ASN:ND2	1:K:372:ARG:O	2.21	0.74
1:J:448:ASN:CB	1:L:290:PRO:HD2	2.18	0.74
1:K:331:ARG:NH2	1:K:490:LEU:O	2.21	0.74
1:L:478:ASN:OD1	1:L:478:ASN:N	2.18	0.74
1:J:369:LEU:H	1:J:372:ARG:HH21	1.36	0.74
1:J:279:THR:HA	1:J:282:THR:HG23	1.70	0.74
1:J:439:THR:CA	1:J:450:THR:HG22	2.16	0.74
1:L:544:ASN:O	1:L:547:ASN:ND2	2.21	0.74
1:J:815:GLN:NE2	1:K:563:ASN:H	1.86	0.73
1:K:211:PRO:HD2	1:K:231:ARG:HH22	1.52	0.73
1:J:214:GLN:HE21	1:L:834:HIS:HB3	1.53	0.73
1:J:114:LYS:NZ	1:J:116:TYR:O	2.22	0.73
1:J:478:ASN:OD1	1:L:420:ASN:ND2	2.21	0.73
1:J:687:ARG:HH11	1:J:932:GLU:HB3	1.54	0.72
1:J:461:ASN:ND2	1:L:171:VAL:H	1.88	0.72
1:L:371:ASP:O	1:L:662:ASN:ND2	2.22	0.72
1:J:707:ASP:O	1:J:708:PRO:C	2.30	0.72
2:Z:9:LYS:HG2	2:Z:10:LYS:N	2.02	0.72
1:K:207:LYS:O	1:K:208:THR:C	2.32	0.72
1:K:771:ASN:OD1	1:K:771:ASN:N	2.22	0.72
1:L:953:ARG:HH21	1:L:956:PHE:HB2	1.53	0.72
1:J:318:ASN:OD1	1:J:318:ASN:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:239:MET:HG3	1:K:318:ASN:HD22	1.55	0.72
1:K:542:ASN:ND2	1:K:921:MET:SD	2.63	0.72
1:J:551:ASN:ND2	1:J:554:LEU:H	1.87	0.71
1:J:563:ASN:ND2	1:L:532:GLY:O	2.24	0.71
1:J:856:ASN:HB2	1:K:249:PRO:HG3	1.71	0.71
1:K:547:ASN:OD1	1:K:547:ASN:N	2.20	0.71
1:L:303:THR:HG1	1:L:306:THR:HG1	1.38	0.71
1:L:331:ARG:NH2	1:L:490:LEU:O	2.22	0.71
2:Z:23:SER:O	2:Z:24:TYR:CG	2.43	0.71
1:J:60:ARG:HD2	1:J:635:HIS:CE1	2.25	0.71
1:J:375:GLU:C	1:J:377:SER:N	2.40	0.71
1:J:828:VAL:O	1:J:833:GLN:NE2	2.24	0.71
2:Z:24:TYR:HE1	2:Z:41:TRP:CZ2	2.07	0.71
1:K:89:GLY:HA3	1:K:92:ARG:HH11	1.55	0.70
1:L:112:THR:O	1:L:333:ASN:ND2	2.23	0.70
1:J:254:GLY:O	1:J:256:GLN:N	2.25	0.70
1:J:529:ILE:O	1:J:530:ASN:C	2.34	0.70
1:J:91:ASN:CB	1:J:635:HIS:HB3	2.22	0.70
1:K:20:ALA:HB2	1:K:23:TYR:CE1	2.26	0.70
1:K:766:ASN:OD1	1:K:766:ASN:N	2.25	0.70
1:J:346:TYR:CE2	1:J:597:ARG:HG3	2.27	0.70
1:J:468:ASN:O	1:K:848:ARG:NH1	2.24	0.70
1:L:613:ARG:NH1	1:L:706:TYR:OH	2.25	0.70
1:J:373:ASN:C	1:J:375:GLU:H	1.97	0.70
1:K:206:ASP:N	1:K:210:GLN:HB2	2.06	0.70
1:J:373:ASN:O	1:J:375:GLU:N	2.25	0.70
1:J:91:ASN:HB3	1:J:635:HIS:HB3	1.74	0.69
1:J:381:LEU:O	1:J:385:ILE:HG23	1.91	0.69
1:J:645:LEU:O	1:J:646:ARG:C	2.36	0.69
1:J:5:SER:OG	1:J:7:MET:SD	2.50	0.69
1:J:384:SER:O	1:J:801:ARG:NH1	2.25	0.69
1:L:78:TYR:O	1:L:598:LYS:HB2	1.92	0.69
1:K:478:ASN:O	1:K:482:ASN:ND2	2.23	0.69
1:K:851:GLN:NE2	1:L:174:GLN:O	2.25	0.69
1:J:275:PHE:CD1	1:K:436:ALA:HB2	2.28	0.69
1:J:277:THR:HG23	1:J:280:ASN:HB2	1.74	0.69
1:J:771:ASN:N	1:J:771:ASN:OD1	2.25	0.69
1:L:536:SER:O	1:L:874:LYS:NZ	2.25	0.69
1:J:766:ASN:OD1	1:J:766:ASN:N	2.22	0.69
1:K:251:ASN:OD1	1:K:255:GLY:N	2.25	0.69
1:K:647:ASN:OD1	1:K:647:ASN:N	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:24:TYR:CE1	2:Z:41:TRP:CZ2	2.81	0.69
1:J:211:PRO:O	1:J:231:ARG:NH1	2.26	0.69
1:J:90:ASP:O	1:J:91:ASN:C	2.32	0.69
1:J:656:ASP:OD2	1:J:658:LEU:HB3	1.93	0.69
1:J:720:ASP:OD1	1:J:721:GLY:N	2.25	0.69
1:K:526:ASP:OD1	1:K:527:CYS:N	2.25	0.69
1:J:376:LEU:O	1:J:379:GLN:HB2	1.94	0.68
1:J:448:ASN:HD22	1:L:289:GLN:HB3	1.58	0.68
1:J:535:TRP:CD1	1:J:536:SER:H	2.12	0.68
1:K:613:ARG:NH2	1:K:710:TYR:O	2.26	0.68
2:Z:1:ALA:N	2:Z:20:CGU:OE11	2.25	0.68
1:J:131:ASN:OD1	1:J:131:ASN:N	2.26	0.68
1:J:196:VAL:HG22	1:J:199:ALA:HB2	1.74	0.68
1:J:507:ASP:OD1	1:J:507:ASP:N	2.24	0.68
1:J:100:TYR:CE1	1:J:627:TYR:HB3	2.29	0.68
1:J:747:ARG:HH12	1:K:62:GLN:H	1.39	0.68
1:J:375:GLU:C	1:J:377:SER:H	1.99	0.68
1:J:747:ARG:NH1	1:K:62:GLN:H	1.91	0.68
1:K:662:ASN:OD1	1:K:662:ASN:N	2.26	0.68
1:L:730:LYS:O	1:L:756:ILE:HG13	1.93	0.68
1:K:217:GLU:O	1:L:467:ASN:ND2	2.26	0.68
1:K:530:ASN:O	1:K:531:LEU:C	2.38	0.67
1:K:856:ASN:HB2	1:L:249:PRO:HG3	1.74	0.67
2:Z:131:PRO:HG2	2:Z:134:LYS:HG3	1.74	0.67
1:L:134:GLU:HB3	1:L:171:VAL:CG1	2.21	0.67
1:J:341:PHE:O	1:J:342:ILE:C	2.37	0.67
1:K:20:ALA:HA	1:K:23:TYR:CG	2.30	0.67
1:K:565:ARG:HB3	1:K:566:TYR:CE2	2.30	0.67
1:L:770:CYS:SG	1:L:771:ASN:N	2.67	0.67
1:K:824:ASP:N	1:K:824:ASP:OD1	2.28	0.67
1:K:20:ALA:O	1:K:21:SER:C	2.36	0.67
1:J:651:ASP:HB2	1:J:938:ARG:HH11	1.60	0.67
1:J:542:ASN:HD22	1:J:921:MET:HE3	1.59	0.67
1:J:582:ASN:OD1	1:J:582:ASN:N	2.26	0.67
1:J:775:ASP:N	1:J:775:ASP:OD1	2.27	0.67
1:J:868:ASP:OD1	1:J:868:ASP:N	2.28	0.67
2:Z:28:ARG:CD	2:Z:37:THR:OG1	2.43	0.67
1:J:373:ASN:C	1:J:375:GLU:N	2.50	0.66
1:K:784:ASN:OD1	1:K:883:ARG:NH1	2.28	0.66
1:L:83:ARG:NE	1:L:593:GLU:OE2	2.28	0.66
1:J:338:ARG:O	1:J:396:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:369:LEU:H	1:J:372:ARG:NH2	1.93	0.66
1:J:438:LYS:NZ	1:J:455:SER:OG	2.29	0.66
1:K:211:PRO:O	1:K:231:ARG:NH1	2.28	0.66
1:K:114:LYS:NZ	1:K:116:TYR:O	2.29	0.66
1:K:529:ILE:HG13	1:K:530:ASN:ND2	2.10	0.66
1:K:345:MET:SD	1:K:347:TYR:OH	2.54	0.66
1:K:316:ASP:N	1:K:316:ASP:OD1	2.28	0.66
1:L:276:SER:HB2	1:L:290:PRO:HA	1.77	0.66
1:J:801:ARG:N	1:J:804:SER:OG	2.28	0.66
1:K:758:ARG:HH22	1:K:763:GLU:H	1.43	0.66
1:J:420:ASN:ND2	1:K:478:ASN:OD1	2.25	0.66
1:K:338:ARG:HG2	1:K:605:GLN:HB2	1.78	0.66
1:K:499:ASN:OD1	1:K:499:ASN:N	2.27	0.66
1:J:259:MET:HG3	1:J:265:LYS:HB3	1.78	0.66
1:J:376:LEU:O	1:J:380:LEU:HD12	1.96	0.66
1:J:411:ASN:ND2	1:J:531:LEU:HA	2.10	0.66
1:L:667:ILE:O	1:L:924:PRO:HA	1.96	0.66
1:J:267:GLU:O	1:J:269:GLN:NE2	2.29	0.65
1:J:598:LYS:O	1:J:599:ASP:C	2.38	0.65
1:K:80:TYR:HE1	1:K:596:PHE:HB2	1.61	0.65
2:Z:271:HIS:HE1	2:Z:273:ARG:HE	1.42	0.65
1:J:338:ARG:NH2	1:J:602:MET:O	2.28	0.65
1:J:373:ASN:OD1	1:J:375:GLU:HB2	1.96	0.65
1:L:364:ASN:OD1	1:L:365:ALA:N	2.29	0.65
1:L:440:THR:HG22	1:L:451:TRP:CE2	2.31	0.65
1:K:537:LEU:HB3	1:K:540:MET:HG2	1.77	0.65
1:J:551:ASN:HD21	1:J:554:LEU:H	1.44	0.65
2:Z:9:LYS:CG	2:Z:10:LYS:H	2.06	0.65
1:J:94:LEU:HG	1:J:95:ASP:N	2.12	0.65
1:J:331:ARG:NH2	1:J:490:LEU:O	2.29	0.65
1:K:437:VAL:HB	1:K:450:THR:HB	1.78	0.65
1:K:601:ASN:OD1	1:K:613:ARG:NE	2.27	0.65
2:Z:267:VAL:HB	2:Z:287:ARG:HB3	1.79	0.65
1:L:171:VAL:HG12	1:L:172:TYR:H	1.62	0.65
1:L:261:GLU:HA	1:L:265:LYS:HA	1.78	0.65
1:L:903:LEU:HA	1:L:906:ALA:HB3	1.79	0.65
1:J:287:ASN:ND2	1:J:289:GLN:OE1	2.30	0.65
1:J:636:ASN:O	1:J:640:THR:HG23	1.97	0.65
1:J:835:ASN:OD1	1:J:836:ASN:ND2	2.29	0.65
1:K:889:ASN:ND2	1:K:891:MET:SD	2.70	0.65
1:K:533:ALA:O	1:K:535:TRP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:615:ASP:N	1:K:615:ASP:OD1	2.30	0.64
1:L:438:LYS:NZ	1:L:455:SER:OG	2.30	0.64
1:K:870:ILE:HG13	1:K:871:THR:H	1.62	0.64
1:J:99:THR:HG22	1:J:628:ALA:HB2	1.79	0.64
1:J:383:ASP:O	1:J:384:SER:C	2.39	0.64
1:J:906:ALA:O	1:J:907:ASN:ND2	2.30	0.64
1:L:5:SER:O	1:L:5:SER:OG	2.13	0.64
1:L:437:VAL:HB	1:L:450:THR:HG21	1.79	0.64
1:J:250:THR:O	1:L:826:GLN:HG3	1.96	0.64
1:J:815:GLN:HE22	1:K:563:ASN:CG	2.05	0.64
1:L:726:ASN:O	1:L:727:HIS:C	2.38	0.64
1:J:535:TRP:CG	1:J:536:SER:H	2.15	0.64
1:L:538:GLU:CD	1:L:538:GLU:H	2.06	0.64
1:L:586:LEU:HG	1:L:941:GLN:HE21	1.62	0.64
1:J:635:HIS:O	1:J:638:ALA:HB3	1.98	0.64
1:L:7:MET:SD	1:L:7:MET:N	2.71	0.64
1:J:604:LEU:HD23	1:J:604:LEU:H	1.62	0.63
1:J:708:PRO:O	1:J:710:TYR:N	2.31	0.63
1:J:439:THR:HA	1:J:450:THR:CG2	2.22	0.63
1:L:183:THR:HG23	1:L:185:GLU:H	1.64	0.63
1:J:138:ASN:HA	1:J:167:LYS:HD3	1.80	0.63
1:J:381:LEU:O	1:J:382:LEU:C	2.42	0.63
1:L:731:LYS:HG2	1:L:917:GLU:HB3	1.80	0.63
1:J:275:PHE:CE1	1:K:436:ALA:HB2	2.33	0.63
1:K:437:VAL:C	1:K:453:LYS:HB2	2.24	0.63
1:L:878:ASP:O	1:L:880:THR:HG22	1.99	0.63
1:J:448:ASN:CG	1:L:290:PRO:HD2	2.24	0.63
1:J:706:TYR:CZ	1:J:708:PRO:HA	2.33	0.63
1:K:108:ASP:OD1	1:K:565:ARG:HD3	1.99	0.63
1:L:485:TYR:O	1:L:489:ALA:HB3	1.98	0.63
1:J:373:ASN:HD21	1:J:376:LEU:H	1.46	0.63
1:J:335:ILE:HG12	1:J:606:SER:HA	1.81	0.62
1:K:387:ASP:OD1	1:K:388:ARG:N	2.32	0.62
1:L:417:GLU:OE1	1:L:417:GLU:N	2.31	0.62
1:J:461:ASN:ND2	1:L:170:HIS:HA	2.15	0.62
1:J:338:ARG:HG3	1:J:342:ILE:HG23	1.80	0.62
1:L:188:GLN:NE2	1:L:190:GLY:O	2.31	0.62
1:L:491:TYR:OH	1:L:549:HIS:ND1	2.27	0.62
1:L:824:ASP:N	1:L:824:ASP:OD1	2.32	0.62
1:J:270:VAL:HA	1:J:296:SER:O	1.99	0.62
1:J:345:MET:HE2	1:J:594:TRP:NE1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:259:MET:O	1:K:265:LYS:NZ	2.24	0.62
1:K:335:ILE:HD12	1:K:335:ILE:H	1.64	0.62
1:L:171:VAL:O	1:L:172:TYR:HB2	1.98	0.62
1:K:602:MET:HE1	1:K:710:TYR:CE2	2.35	0.62
1:K:678:ILE:HB	1:K:912:LEU:HB3	1.81	0.62
1:L:544:ASN:ND2	1:L:547:ASN:OD1	2.33	0.62
1:L:565:ARG:HD3	1:L:566:TYR:CE1	2.34	0.62
1:J:284:GLU:HG3	1:J:288:ILE:HG22	1.82	0.62
1:J:377:SER:O	1:J:378:TYR:C	2.41	0.62
1:J:902:ASN:O	1:J:906:ALA:N	2.32	0.62
1:K:90:ASP:OD1	1:K:92:ARG:NH1	2.33	0.62
1:L:73:ARG:NE	1:L:80:TYR:OH	2.33	0.62
1:J:613:ARG:HH21	1:J:706:TYR:HE1	1.47	0.62
1:K:104:ARG:HG2	1:K:570:HIS:HA	1.82	0.62
1:K:758:ARG:NH1	1:K:761:ASP:O	2.32	0.62
1:L:497:LYS:O	1:L:518:ARG:NH1	2.33	0.62
1:L:880:THR:OG1	1:L:881:LEU:N	2.30	0.62
1:L:346:TYR:CE2	1:L:597:ARG:HG2	2.35	0.61
1:L:388:ARG:NE	1:L:397:GLN:OE1	2.33	0.61
1:J:526:ASP:HB3	1:J:528:TYR:CE1	2.36	0.61
1:J:534:ARG:H	1:K:559:MET:HE2	1.65	0.61
1:J:288:ILE:HD13	1:J:288:ILE:H	1.65	0.61
1:J:478:ASN:O	1:J:482:ASN:ND2	2.31	0.61
1:J:354:GLY:HA3	1:J:594:TRP:CE3	2.35	0.61
1:J:808:ASN:ND2	1:J:878:ASP:O	2.23	0.61
1:K:209:PHE:O	1:K:210:GLN:C	2.43	0.61
1:J:78:TYR:OH	1:J:706:TYR:HB3	1.99	0.61
1:J:514:TYR:OH	1:J:518:ARG:NH2	2.32	0.61
1:K:257:GLY:HA2	1:K:299:VAL:HG12	1.82	0.61
1:L:725:LEU:HA	1:L:727:HIS:NE2	2.15	0.61
1:J:529:ILE:O	1:J:531:LEU:N	2.34	0.61
1:K:606:SER:N	1:K:713:SER:O	2.33	0.61
1:J:532:GLY:O	1:K:563:ASN:HB3	2.01	0.61
1:K:468:ASN:OD1	1:K:468:ASN:N	2.33	0.61
1:K:613:ARG:NH1	1:K:706:TYR:OH	2.33	0.61
1:L:902:ASN:O	1:L:906:ALA:N	2.33	0.61
1:K:501:THR:OG1	1:K:502:ASN:OD1	2.17	0.61
1:J:64:LEU:N	1:L:747:ARG:O	2.34	0.60
1:K:514:TYR:OH	1:K:518:ARG:NH1	2.34	0.60
1:K:109:ARG:NH2	1:K:558:SER:OG	2.34	0.60
1:L:726:ASN:H	1:L:727:HIS:CD2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:344:LEU:H	1:L:344:LEU:HD23	1.65	0.60
1:L:58:THR:OG1	1:L:59:ASP:N	2.35	0.60
1:L:727:HIS:CE1	1:L:876:LEU:HD13	2.37	0.60
1:J:720:ASP:OD1	1:J:722:THR:N	2.28	0.60
1:J:771:ASN:HD21	1:J:874:LYS:HA	1.65	0.60
1:L:114:LYS:NZ	1:L:116:TYR:O	2.33	0.60
1:J:655:ASN:CB	1:J:936:VAL:HG12	2.32	0.60
1:K:771:ASN:ND2	1:K:873:LYS:O	2.25	0.60
1:L:526:ASP:OD1	1:L:527:CYS:N	2.33	0.60
1:J:438:LYS:HB3	1:J:453:LYS:HG3	1.84	0.60
1:L:474:ASN:O	1:L:478:ASN:ND2	2.33	0.60
1:J:662:ASN:N	1:J:662:ASN:OD1	2.35	0.60
1:K:826:GLN:NE2	1:L:250:THR:O	2.34	0.60
2:Z:263:HIS:ND1	2:Z:290:THR:OG1	2.34	0.60
1:J:512:TYR:O	1:J:516:ASN:ND2	2.31	0.60
1:J:237:THR:OG1	1:J:298:ASP:OD1	2.20	0.60
1:K:19:ASP:CG	1:K:21:SER:HB3	2.27	0.60
1:K:262:GLN:NE2	1:K:263:ASN:OD1	2.35	0.60
1:L:180:ILE:HG22	1:L:181:LYS:HG2	1.84	0.60
1:J:385:ILE:HG13	1:J:386:GLY:N	2.14	0.59
1:K:726:ASN:OD1	1:K:726:ASN:N	2.35	0.59
1:J:747:ARG:HH22	1:K:61:SER:HA	1.66	0.59
1:J:832:HIS:CD2	1:K:253:ASN:HB2	2.37	0.59
1:J:338:ARG:HG3	1:J:342:ILE:CG2	2.31	0.59
1:K:818:ASP:CB	1:K:869:SER:HA	2.31	0.59
1:K:847:MET:HE1	1:L:220:TRP:HB3	1.82	0.59
1:J:345:MET:HE3	1:J:596:PHE:CE1	2.37	0.59
1:L:656:ASP:O	1:L:659:SER:OG	2.20	0.59
2:Z:263:HIS:HB2	2:Z:288:LEU:HD13	1.85	0.59
1:J:206:ASP:OD1	1:J:210:GLN:N	2.35	0.59
1:J:425:LEU:HD11	1:K:470:ALA:HB3	1.84	0.59
1:K:131:ASN:OD1	1:K:131:ASN:N	2.35	0.59
1:K:231:ARG:HH11	1:K:231:ARG:HG2	1.68	0.59
1:K:599:ASP:O	1:K:603:VAL:HG13	2.02	0.59
1:L:954:THR:HB	1:L:955:PRO:HD3	1.85	0.59
1:J:411:ASN:HB3	1:J:531:LEU:CD2	2.22	0.59
1:J:657:TYR:O	1:J:658:LEU:C	2.43	0.59
1:K:14:HIS:CE1	1:K:23:TYR:CZ	2.90	0.59
1:L:318:ASN:OD1	1:L:318:ASN:N	2.35	0.59
1:J:7:MET:SD	1:J:7:MET:N	2.76	0.59
1:J:35:THR:O	1:J:35:THR:OG1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:61:SER:HA	1:L:745:ASN:HB2	1.84	0.59
1:K:497:LYS:O	1:K:518:ARG:NH2	2.35	0.59
1:J:78:TYR:CE1	1:J:706:TYR:HB3	2.36	0.59
1:J:88:VAL:HG22	1:J:630:PHE:HZ	1.68	0.59
1:K:646:ARG:NH1	1:K:943:HIS:O	2.36	0.59
1:K:650:ASN:HD21	1:L:25:SER:H	1.50	0.59
1:J:544:ASN:OD1	1:J:547:ASN:N	2.26	0.59
1:K:340:ASN:O	1:K:342:ILE:N	2.36	0.59
1:K:853:TYR:OH	1:L:297:GLU:OE2	2.20	0.59
1:L:575:GLN:OE1	1:L:577:PHE:N	2.24	0.59
2:Z:25:CGU:OE21	2:Z:28:ARG:HD3	2.03	0.59
1:L:938:ARG:O	1:L:949:THR:HA	2.03	0.59
1:K:720:ASP:OD1	1:K:722:THR:N	2.26	0.58
1:L:546:PHE:HE1	1:L:879:ARG:HH21	1.51	0.58
1:J:348:ASN:ND2	1:J:368:ASP:OD2	2.29	0.58
1:J:364:ASN:ND2	1:J:366:VAL:O	2.32	0.58
1:K:24:LEU:HB3	1:K:28:LEU:HD11	1.86	0.58
1:K:432:ASP:O	1:K:433:THR:C	2.45	0.58
2:Z:46:ASP:OD1	2:Z:46:ASP:N	2.36	0.58
1:J:704:SER:O	1:J:705:GLY:C	2.44	0.58
1:K:408:ILE:HG12	1:K:536:SER:HB3	1.85	0.58
2:Z:100:CYS:H	2:Z:308:TRP:CD1	2.21	0.58
1:J:70:PRO:HA	1:J:84:PHE:HB3	1.86	0.58
1:J:473:ILE:HB	1:L:422:CYS:HB3	1.86	0.58
1:K:341:PHE:HD2	1:K:344:LEU:HD12	1.68	0.58
1:K:780:GLN:O	1:K:784:ASN:ND2	2.30	0.58
1:K:364:ASN:OD1	1:K:366:VAL:N	2.36	0.58
1:L:346:TYR:CZ	1:L:597:ARG:HD3	2.38	0.58
1:J:338:ARG:O	1:J:557:ARG:NE	2.35	0.58
1:J:448:ASN:O	1:J:450:THR:HG23	2.04	0.58
1:J:508:ASN:OD1	1:J:511:THR:N	2.37	0.58
1:K:80:TYR:CE1	1:K:596:PHE:HD2	2.21	0.58
1:K:177:LEU:O	1:K:228:ALA:HB1	2.04	0.58
1:J:64:LEU:HB2	1:L:747:ARG:O	2.03	0.58
1:J:611:ASP:OD1	1:J:612:LEU:N	2.36	0.58
1:J:913:ASP:N	1:J:913:ASP:OD1	2.37	0.58
1:K:19:ASP:OD1	1:K:22:GLU:HG3	2.03	0.58
1:K:440:THR:HG22	1:K:451:TRP:CE2	2.38	0.58
1:K:727:HIS:O	1:K:757:LYS:NZ	2.36	0.58
1:K:808:ASN:ND2	1:K:879:ARG:HB3	2.19	0.58
1:K:887:SER:OG	1:K:888:SER:N	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:5:LEU:HD12	2:Z:8:MET:HB3	1.84	0.58
1:J:281:ALA:O	1:J:282:THR:C	2.46	0.58
1:J:708:PRO:C	1:J:710:TYR:H	2.12	0.58
1:K:847:MET:SD	1:K:848:ARG:NH2	2.76	0.58
1:J:368:ASP:OD1	1:J:369:LEU:N	2.37	0.58
1:J:375:GLU:O	1:J:377:SER:N	2.37	0.58
1:J:770:CYS:SG	1:J:875:PHE:HB3	2.44	0.58
1:K:289:GLN:OE1	1:L:448:ASN:ND2	2.36	0.58
1:K:491:TYR:OH	1:K:549:HIS:ND1	2.36	0.58
1:L:369:LEU:H	1:L:372:ARG:HH12	1.50	0.58
1:J:655:ASN:HB2	1:J:936:VAL:HG12	1.86	0.58
2:Z:287:ARG:NH1	2:Z:429:ARG:O	2.37	0.58
1:J:401:SER:OG	1:J:402:TYR:N	2.37	0.57
1:K:180:ILE:HG22	1:K:181:LYS:HG2	1.84	0.57
1:L:93:VAL:HB	1:L:584:LEU:HD11	1.84	0.57
1:J:444:GLY:O	1:J:445:ASP:HB3	2.04	0.57
1:L:192:ALA:HB2	1:L:201:LYS:HB2	1.85	0.57
1:L:438:LYS:HZ1	1:L:453:LYS:HG3	1.69	0.57
1:J:100:TYR:HE1	1:J:627:TYR:HB3	1.68	0.57
1:J:759:SER:OG	1:J:760:VAL:N	2.33	0.57
1:K:407:ARG:HE	1:K:876:LEU:HD21	1.67	0.57
1:J:448:ASN:HA	1:L:290:PRO:HD2	1.85	0.57
1:L:348:ASN:ND2	1:L:372:ARG:O	2.36	0.57
1:L:690:ALA:HA	1:L:882:TRP:O	2.04	0.57
2:Z:48:ASP:OD1	2:Z:49:GLN:N	2.35	0.57
1:J:62:GLN:OE1	1:J:92:ARG:NE	2.38	0.57
1:J:700:PRO:O	1:J:701:SER:C	2.46	0.57
1:K:337:PHE:CZ	1:K:569:PHE:HE2	2.23	0.57
1:L:601:ASN:ND2	1:L:613:ARG:HH21	2.01	0.57
1:L:693:ARG:O	1:L:725:LEU:HD13	2.05	0.57
1:J:84:PHE:HE1	1:J:626:LEU:HD22	1.67	0.57
1:K:136:GLU:HG2	1:K:235:LYS:HZ3	1.68	0.57
1:K:207:LYS:O	1:K:209:PHE:N	2.37	0.57
1:K:335:ILE:O	1:K:558:SER:OG	2.21	0.57
1:K:431:THR:OG1	1:K:463:ILE:N	2.38	0.57
1:L:211:PRO:HD2	1:L:231:ARG:HH12	1.70	0.57
1:L:440:THR:HG21	1:L:449:THR:HG22	1.87	0.57
1:L:770:CYS:SG	1:L:772:MET:N	2.76	0.57
1:K:239:MET:O	1:K:240:LYS:NZ	2.37	0.57
1:K:340:ASN:O	1:K:341:PHE:C	2.48	0.57
1:K:368:ASP:OD1	1:K:372:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:605:GLN:HE21	1:K:714:GLY:HA2	1.69	0.57
1:K:111:PRO:HA	1:K:565:ARG:HE	1.69	0.57
1:L:405:ASP:OD1	1:L:405:ASP:N	2.26	0.57
1:J:700:PRO:HG3	1:J:716:ILE:HD13	1.86	0.57
1:K:551:ASN:OD1	1:K:554:LEU:N	2.29	0.57
1:J:20:ALA:HA	1:J:23:TYR:CZ	2.39	0.57
1:J:57:THR:HG23	1:J:632:PRO:HB2	1.86	0.57
1:J:531:LEU:HD13	1:K:116:TYR:CD2	2.40	0.57
1:K:531:LEU:HD13	1:L:116:TYR:CD2	2.39	0.57
1:L:168:LYS:HZ2	1:L:168:LYS:HB3	1.70	0.57
1:L:724:TYR:CD2	1:L:725:LEU:HG	2.40	0.57
1:K:459:GLU:HG2	1:K:460:ARG:HG3	1.86	0.56
1:K:676:ILE:HG22	1:K:914:MET:HB2	1.85	0.56
1:K:745:ASN:HD22	1:L:61:SER:HA	1.70	0.56
1:L:80:TYR:HB3	1:L:596:PHE:CD1	2.35	0.56
1:J:336:ALA:HB2	1:J:558:SER:HA	1.85	0.56
1:J:345:MET:HE3	1:J:596:PHE:HE1	1.70	0.56
1:J:448:ASN:HD22	1:L:289:GLN:CB	2.18	0.56
1:J:461:ASN:HD21	1:L:170:HIS:CA	2.17	0.56
1:K:20:ALA:C	1:K:22:GLU:N	2.55	0.56
1:J:938:ARG:NH2	1:K:12:TYR:O	2.34	0.56
1:K:6:MET:SD	1:K:7:MET:N	2.70	0.56
1:K:726:ASN:ND2	1:K:877:CYS:O	2.38	0.56
1:L:416:ASP:OD1	1:L:416:ASP:N	2.38	0.56
1:L:551:ASN:HD22	1:L:554:LEU:HD12	1.70	0.56
1:J:20:ALA:H	1:J:47:ASN:HB3	1.69	0.56
1:K:868:ASP:OD1	1:K:868:ASP:N	2.38	0.56
1:L:695:LYS:O	1:L:696:THR:C	2.47	0.56
1:J:134:GLU:HB3	1:J:171:VAL:HG13	1.87	0.56
1:J:339:ASP:O	1:J:342:ILE:HG22	2.04	0.56
1:J:446:GLN:HA	1:J:449:THR:OG1	2.05	0.56
1:K:188:GLN:HG3	1:K:202:GLU:HB3	1.88	0.56
1:K:720:ASP:OD1	1:K:721:GLY:N	2.39	0.56
1:L:250:THR:HG21	1:L:257:GLY:H	1.71	0.56
1:L:341:PHE:HD2	1:L:344:LEU:HD11	1.71	0.56
1:L:646:ARG:HD3	1:L:942:PRO:O	2.05	0.56
1:J:660:ALA:HB1	1:J:931:PHE:O	2.06	0.56
1:K:559:MET:O	1:K:560:LEU:C	2.47	0.56
1:L:766:ASN:HA	1:L:773:THR:HA	1.87	0.56
1:J:440:THR:OG1	1:J:446:GLN:HB3	2.05	0.56
1:K:746:ASP:OD2	1:L:63:ARG:NE	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:870:ILE:HG23	1:K:871:THR:N	2.21	0.56
2:Z:20:CGU:N	2:Z:44:TYR:OH	2.39	0.56
1:J:375:GLU:O	1:J:376:LEU:C	2.43	0.56
1:J:411:ASN:HD22	1:J:531:LEU:CA	2.17	0.56
1:K:729:PHE:HA	1:K:918:VAL:HG12	1.88	0.56
1:K:775:ASP:OD1	1:K:775:ASP:N	2.38	0.56
2:Z:17:CYS:SG	2:Z:26:CGU:HB3	2.46	0.56
1:J:94:LEU:O	1:J:584:LEU:HD13	2.06	0.56
1:J:494:ASP:HA	1:J:497:LYS:HE2	1.87	0.56
1:J:538:GLU:OE1	1:J:538:GLU:N	2.38	0.56
1:L:825:TYR:O	1:L:826:GLN:NE2	2.36	0.56
1:J:461:ASN:HD21	1:L:170:HIS:HA	1.70	0.55
1:K:136:GLU:OE1	1:K:137:GLN:N	2.39	0.55
1:K:206:ASP:O	1:K:207:LYS:C	2.47	0.55
1:K:253:ASN:O	1:K:253:ASN:ND2	2.39	0.55
1:K:346:TYR:CE2	1:K:597:ARG:HG2	2.40	0.55
1:L:586:LEU:HG	1:L:941:GLN:NE2	2.21	0.55
1:J:219:GLN:OE1	1:J:221:ASN:ND2	2.39	0.55
1:J:440:THR:OG1	1:J:446:GLN:O	2.24	0.55
1:J:643:ALA:O	1:J:644:MET:C	2.49	0.55
1:K:178:SER:HB2	1:K:225:ALA:HB3	1.89	0.55
1:K:431:THR:HG21	1:K:462:GLU:HB3	1.87	0.55
1:K:437:VAL:O	1:K:453:LYS:HB2	2.06	0.55
1:K:960:ASN:CG	1:K:962:THR:H	2.14	0.55
1:K:335:ILE:HA	1:K:606:SER:HA	1.88	0.55
1:L:134:GLU:CB	1:L:171:VAL:HG13	2.26	0.55
1:L:409:ILE:HD13	1:L:409:ILE:H	1.71	0.55
1:L:755:GLU:OE2	1:L:756:ILE:N	2.38	0.55
1:K:750:THR:HG22	1:K:752:ASN:H	1.71	0.55
1:J:9:GLN:OE1	1:J:10:TRP:N	2.39	0.55
1:L:78:TYR:C	1:L:598:LYS:HB2	2.30	0.55
1:L:392:PHE:H	1:L:397:GLN:HB3	1.71	0.55
1:J:472:GLU:HG2	1:K:126:PRO:HB3	1.88	0.55
1:J:700:PRO:HA	1:J:710:TYR:CE1	2.42	0.55
1:K:137:GLN:OE1	1:K:170:HIS:NE2	2.39	0.55
1:K:537:LEU:HD13	1:K:539:TYR:H	1.71	0.55
1:J:88:VAL:HG22	1:J:630:PHE:CZ	2.41	0.55
1:J:849:GLU:OE1	1:K:216:GLY:N	2.40	0.55
1:L:307:HIS:ND1	1:L:328:MET:O	2.37	0.55
1:J:367:VAL:HB	1:J:951:TYR:HE2	1.72	0.55
1:J:626:LEU:HD12	1:J:627:TYR:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:808:ASN:ND2	1:J:879:ARG:HB3	2.22	0.55
1:K:352:ASN:OD1	1:K:352:ASN:N	2.40	0.55
1:L:39:PHE:HD2	1:L:41:LEU:HD21	1.72	0.55
1:L:692:THR:HG22	1:L:693:ARG:H	1.71	0.55
1:J:122:ASN:ND2	1:J:242:CYS:SG	2.80	0.54
1:J:248:ARG:O	1:J:248:ARG:HG3	2.02	0.54
1:J:644:MET:SD	1:K:28:LEU:HB3	2.46	0.54
1:J:646:ARG:HH12	1:J:943:HIS:C	2.15	0.54
1:L:344:LEU:HD23	1:L:344:LEU:N	2.21	0.54
1:K:338:ARG:NE	1:K:602:MET:O	2.32	0.54
1:L:138:ASN:OD1	1:L:167:LYS:NZ	2.40	0.54
1:L:757:LYS:HA	1:L:772:MET:HA	1.89	0.54
1:K:62:GLN:HE22	1:K:92:ARG:HE	1.55	0.54
1:K:528:TYR:HB3	1:L:120:ALA:HB1	1.89	0.54
1:K:745:ASN:HD21	1:K:747:ARG:HH22	1.55	0.54
1:L:341:PHE:O	1:L:344:LEU:HG	2.06	0.54
1:L:433:THR:HA	1:L:461:ASN:O	2.07	0.54
1:L:869:SER:OG	1:L:870:ILE:N	2.39	0.54
1:K:717:PRO:HA	1:K:720:ASP:OD1	2.08	0.54
1:L:81:LYS:HG3	1:L:595:ASN:OD1	2.08	0.54
1:K:241:PRO:O	1:K:245:SER:OG	2.26	0.54
1:J:403:ASP:OD1	1:J:405:ASP:N	2.40	0.54
1:J:746:ASP:OD2	1:K:63:ARG:NE	2.40	0.54
1:J:757:LYS:NZ	1:J:919:ASP:OD2	2.41	0.54
1:K:233:LEU:HB2	1:K:297:GLU:O	2.08	0.54
1:J:280:ASN:O	1:J:281:ALA:C	2.51	0.54
1:J:656:ASP:CG	1:J:659:SER:H	2.15	0.54
1:K:211:PRO:C	1:K:231:ARG:HH12	2.16	0.54
1:K:651:ASP:OD1	1:K:651:ASP:N	2.37	0.54
2:Z:358:ILE:HG23	2:Z:362:MET:HB2	1.89	0.54
1:J:682:ASN:OD1	1:J:683:TRP:N	2.41	0.54
1:J:834:HIS:O	1:J:834:HIS:ND1	2.41	0.54
1:L:647:ASN:CG	1:L:649:THR:HG22	2.32	0.54
1:J:660:ALA:HA	1:J:933:VAL:HG22	1.89	0.54
1:J:692:THR:HG22	1:J:693:ARG:H	1.72	0.54
1:K:20:ALA:HA	1:K:23:TYR:CD2	2.43	0.54
1:L:729:PHE:HA	1:L:918:VAL:HG12	1.90	0.54
1:J:454:ASP:OD1	1:J:454:ASP:N	2.41	0.53
1:J:485:TYR:O	1:J:489:ALA:HB3	2.08	0.53
1:J:815:GLN:NE2	1:K:563:ASN:N	2.56	0.53
1:K:20:ALA:HB1	1:K:24:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:LEU:HB2	1:K:630:PHE:HE1	1.72	0.53
1:J:217:GLU:OE2	1:J:219:GLN:NE2	2.31	0.53
1:J:278:SER:O	1:J:282:THR:HG23	2.08	0.53
1:K:22:GLU:O	1:K:24:LEU:N	2.41	0.53
1:K:181:LYS:NZ	1:K:182:ILE:O	2.41	0.53
1:K:673:ASN:ND2	1:K:917:GLU:OE1	2.41	0.53
1:L:575:GLN:OE1	1:L:576:LYS:N	2.41	0.53
1:J:431:THR:HG21	1:J:462:GLU:HG3	1.90	0.53
1:L:445:ASP:OD1	1:L:445:ASP:N	2.41	0.53
1:J:600:VAL:HG13	1:J:604:LEU:HD11	1.91	0.53
1:J:678:ILE:HB	1:J:912:LEU:HD23	1.90	0.53
1:J:953:ARG:NE	1:J:956:PHE:O	2.36	0.53
1:L:542:ASN:HD22	1:L:921:MET:HE3	1.74	0.53
1:J:64:LEU:HG	1:L:747:ARG:HB3	1.90	0.53
1:J:341:PHE:O	1:J:343:GLY:N	2.42	0.53
1:J:544:ASN:HD21	1:J:546:PHE:HB2	1.72	0.53
1:L:6:MET:HA	1:L:9:GLN:HE22	1.73	0.53
1:J:440:THR:HG21	1:J:449:THR:HG22	1.91	0.53
1:K:737:ASP:OD1	1:K:737:ASP:N	2.41	0.53
1:L:736:PHE:HE2	1:L:742:TRP:HD1	1.56	0.53
1:L:693:ARG:HH22	1:L:921:MET:HG3	1.74	0.53
1:J:656:ASP:OD1	1:J:657:TYR:N	2.37	0.53
1:J:666:PRO:HA	1:J:926:LEU:HD23	1.91	0.53
1:K:371:ASP:OD1	1:K:371:ASP:N	2.41	0.53
1:J:446:GLN:CA	1:J:449:THR:HB	2.39	0.53
1:K:508:ASN:OD1	1:K:511:THR:N	2.39	0.53
2:Z:25:CGU:O	2:Z:29:CGU:N	2.41	0.53
1:J:306:THR:HG22	1:J:329:PRO:HA	1.91	0.53
1:J:448:ASN:CA	1:L:290:PRO:HD2	2.38	0.53
1:J:279:THR:HA	1:J:282:THR:CG2	2.38	0.52
1:J:416:ASP:HB3	1:J:476:ASN:HD21	1.74	0.52
1:K:430:ILE:HG21	2:Z:3:SER:HB2	1.89	0.52
1:K:835:ASN:OD1	1:K:836:ASN:N	2.42	0.52
1:K:869:SER:OG	1:K:870:ILE:N	2.40	0.52
1:L:695:LYS:O	1:L:697:LYS:N	2.42	0.52
1:J:123:ALA:H	1:L:836:ASN:HD21	1.57	0.52
1:J:468:ASN:HB2	1:L:174:GLN:HE22	1.73	0.52
1:K:815:GLN:HB2	1:L:563:ASN:O	2.09	0.52
1:K:948:GLU:OE1	1:K:949:THR:N	2.43	0.52
1:J:377:SER:C	1:J:379:GLN:N	2.63	0.52
1:J:411:ASN:HD22	1:J:530:ASN:C	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:411:ASN:ND2	1:J:530:ASN:O	2.42	0.52
1:J:440:THR:HG23	1:J:450:THR:CA	2.32	0.52
1:L:438:LYS:C	1:L:450:THR:HG23	2.34	0.52
1:L:685:ALA:HB3	1:L:954:THR:HG21	1.91	0.52
1:L:726:ASN:O	1:L:728:THR:N	2.42	0.52
1:L:727:HIS:HE1	1:L:876:LEU:HD13	1.72	0.52
1:J:206:ASP:OD1	1:J:209:PHE:N	2.40	0.52
1:J:290:PRO:HD2	1:K:448:ASN:CG	2.34	0.52
1:J:369:LEU:N	1:J:372:ARG:HH21	2.05	0.52
1:K:175:ALA:HB1	1:K:229:GLY:O	2.09	0.52
1:J:279:THR:CA	1:J:282:THR:HG23	2.38	0.52
1:J:837:SER:HB2	1:K:213:PRO:O	2.10	0.52
1:L:100:TYR:CE1	1:L:627:TYR:HB2	2.45	0.52
1:L:276:SER:OG	1:L:280:ASN:ND2	2.39	0.52
1:L:494:ASP:HA	1:L:497:LYS:HE2	1.91	0.52
2:Z:28:ARG:CD	2:Z:37:THR:CG2	2.67	0.52
1:J:378:TYR:CD2	1:J:576:LYS:HG2	2.44	0.52
1:J:431:THR:HB	1:J:462:GLU:OE1	2.10	0.52
1:K:335:ILE:O	1:K:336:ALA:HB2	2.10	0.52
1:J:280:ASN:O	1:J:284:GLU:CG	2.58	0.52
1:K:369:LEU:HD12	1:K:372:ARG:HH22	1.74	0.52
1:L:606:SER:OG	1:L:609:GLY:N	2.41	0.52
1:L:646:ARG:NH1	1:L:941:GLN:O	2.43	0.52
1:J:334:TYR:O	1:J:607:SER:HB3	2.10	0.52
1:J:531:LEU:O	1:J:532:GLY:C	2.53	0.52
1:J:535:TRP:CG	1:J:536:SER:N	2.78	0.52
1:K:188:GLN:HA	1:K:204:PHE:HA	1.92	0.52
1:J:730:LYS:HD2	1:J:757:LYS:HE2	1.92	0.52
2:Z:97:ASP:OD2	2:Z:124:CYS:N	2.42	0.52
1:J:5:SER:HB3	1:L:905:TYR:HE1	1.75	0.51
1:J:59:ASP:O	1:J:60:ARG:C	2.52	0.51
1:J:364:ASN:OD1	1:J:365:ALA:N	2.44	0.51
1:J:486:SER:OG	1:J:487:ASN:N	2.43	0.51
1:J:99:THR:HG22	1:J:628:ALA:CB	2.40	0.51
1:J:434:PHE:HA	1:L:278:SER:H	1.75	0.51
1:J:639:SER:O	1:J:640:THR:C	2.52	0.51
1:K:19:ASP:C	1:K:21:SER:N	2.64	0.51
1:K:656:ASP:OD2	1:K:659:SER:N	2.30	0.51
1:L:195:THR:OG1	1:L:199:ALA:N	2.44	0.51
1:L:342:ILE:HG22	1:L:343:GLY:N	2.25	0.51
2:Z:316:GLN:HG3	2:Z:385:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:181:LYS:NZ	1:J:182:ILE:H	2.08	0.51
1:J:336:ALA:HB2	1:J:558:SER:CA	2.40	0.51
1:J:440:THR:HA	1:J:451:TRP:CE2	2.45	0.51
1:J:471:MET:HE2	1:L:471:MET:HG3	1.92	0.51
1:J:528:TYR:HD2	1:J:835:ASN:HD22	1.58	0.51
1:J:731:LYS:HG2	1:J:917:GLU:HG2	1.93	0.51
1:K:24:LEU:HD22	1:K:28:LEU:HD11	1.93	0.51
1:K:313:LYS:HG3	1:K:315:GLY:H	1.75	0.51
1:K:745:ASN:OD1	1:K:745:ASN:N	2.44	0.51
1:L:601:ASN:OD1	1:L:613:ARG:NE	2.40	0.51
1:J:214:GLN:OE1	1:J:214:GLN:N	2.44	0.51
1:J:345:MET:HG2	1:J:596:PHE:HD1	1.75	0.51
1:J:411:ASN:ND2	1:J:529:ILE:O	2.44	0.51
1:J:657:TYR:CD1	1:J:657:TYR:C	2.89	0.51
1:J:699:THR:O	1:J:700:PRO:C	2.45	0.51
1:J:820:THR:O	1:J:823:LYS:NZ	2.44	0.51
1:J:472:GLU:OE1	1:J:473:ILE:N	2.43	0.51
1:K:544:ASN:CG	1:K:724:TYR:HE2	2.18	0.51
1:L:345:MET:HE3	1:L:594:TRP:CD1	2.46	0.51
1:L:459:GLU:OE1	1:L:459:GLU:N	2.43	0.51
1:L:652:GLN:O	1:L:938:ARG:HA	2.10	0.51
1:L:693:ARG:NH1	1:L:728:THR:OG1	2.44	0.51
1:L:942:PRO:HD2	1:L:946:VAL:HG12	1.93	0.51
2:Z:24:TYR:HE1	2:Z:41:TRP:CE2	2.28	0.51
1:J:342:ILE:HD11	1:J:719:LEU:HB3	1.92	0.51
1:K:212:GLU:HB3	1:K:213:PRO:CD	2.40	0.51
1:K:335:ILE:H	1:K:335:ILE:CD1	2.21	0.51
1:L:615:ASP:OD1	1:L:615:ASP:N	2.41	0.51
1:L:848:ARG:O	1:L:848:ARG:NE	2.44	0.51
1:J:832:HIS:HD2	1:K:253:ASN:HB2	1.76	0.51
1:K:89:GLY:HA3	1:K:92:ARG:HD2	1.92	0.51
1:K:258:VAL:HG23	1:K:299:VAL:HA	1.93	0.51
1:K:535:TRP:CE2	1:K:814:ARG:HD3	2.46	0.51
1:L:898:ASP:OD1	1:L:898:ASP:N	2.41	0.51
1:L:957:SER:O	1:L:957:SER:OG	2.26	0.51
1:J:635:HIS:HA	1:J:638:ALA:HB2	1.93	0.51
1:K:338:ARG:CZ	1:K:716:ILE:HD11	2.41	0.51
1:J:605:GLN:HG3	1:J:606:SER:N	2.25	0.51
1:L:262:GLN:NE2	1:L:263:ASN:OD1	2.43	0.51
1:J:121:TYR:CE1	1:L:858:PRO:HG2	2.46	0.51
1:J:377:SER:OG	1:J:378:TYR:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:448:ASN:HA	1:L:290:PRO:CD	2.41	0.51
1:J:644:MET:O	1:J:645:LEU:C	2.52	0.51
1:K:337:PHE:HZ	1:K:569:PHE:HE2	1.57	0.51
1:J:448:ASN:HB3	1:L:290:PRO:CD	2.41	0.50
1:K:346:TYR:CZ	1:K:597:ARG:HG2	2.45	0.50
1:L:696:THR:H	1:L:925:THR:HA	1.76	0.50
1:L:878:ASP:O	1:L:879:ARG:C	2.53	0.50
1:J:347:TYR:OH	1:J:575:GLN:OE1	2.20	0.50
1:J:383:ASP:OD2	1:J:802:MET:HB3	2.11	0.50
1:J:575:GLN:OE1	1:J:576:LYS:N	2.44	0.50
1:K:8:PRO:O	1:K:11:SER:OG	2.21	0.50
1:K:133:CYS:HA	1:K:232:VAL:CG2	2.41	0.50
1:K:887:SER:OG	1:K:889:ASN:OD1	2.27	0.50
1:L:695:LYS:O	1:L:698:GLU:N	2.37	0.50
1:L:853:TYR:CG	1:L:854:PRO:HD2	2.46	0.50
1:J:72:ASP:OD1	1:J:73:ARG:N	2.44	0.50
1:J:603:VAL:O	1:J:604:LEU:C	2.55	0.50
1:K:232:VAL:O	1:K:296:SER:HA	2.10	0.50
1:K:339:ASP:O	1:K:340:ASN:C	2.50	0.50
1:L:546:PHE:CE2	1:L:722:THR:HB	2.47	0.50
1:L:612:LEU:O	1:L:616:GLY:N	2.44	0.50
2:Z:98:GLN:HG2	2:Z:392:PHE:HZ	1.76	0.50
1:J:278:SER:O	1:J:281:ALA:HB3	2.10	0.50
1:J:656:ASP:CG	1:J:657:TYR:N	2.70	0.50
1:K:78:TYR:C	1:K:598:LYS:HD3	2.37	0.50
1:K:537:LEU:HD22	1:K:538:GLU:H	1.77	0.50
1:J:251:ASN:OD1	1:J:254:GLY:N	2.44	0.50
1:J:440:THR:HG22	1:J:451:TRP:CD1	2.47	0.50
1:J:549:HIS:CE1	1:J:550:ARG:HG2	2.47	0.50
1:J:641:LEU:O	1:J:644:MET:HB2	2.11	0.50
1:K:922:ASP:OD1	1:K:922:ASP:N	2.45	0.50
1:J:510:ASN:OD1	1:J:510:ASN:N	2.44	0.50
1:J:635:HIS:HA	1:J:638:ALA:CB	2.41	0.50
1:K:531:LEU:HD22	1:L:116:TYR:HB3	1.93	0.50
1:L:334:TYR:OH	1:L:555:ARG:NH2	2.44	0.50
1:L:942:PRO:HG2	1:L:943:HIS:H	1.75	0.50
1:J:747:ARG:NH1	1:K:62:GLN:O	2.45	0.50
1:K:419:PRO:HG3	1:L:127:LYS:HG3	1.93	0.50
1:K:835:ASN:OD1	1:K:836:ASN:ND2	2.44	0.50
1:L:91:ASN:N	1:L:91:ASN:OD1	2.43	0.50
1:L:224:ASP:OD1	1:L:224:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:651:ASP:CG	1:L:938:ARG:HD3	2.37	0.50
1:L:922:ASP:OD1	1:L:923:GLU:N	2.44	0.50
2:Z:329:GLU:HG2	2:Z:330:LYS:HG3	1.94	0.50
1:J:411:ASN:HA	1:J:480:TRP:HH2	1.76	0.50
1:K:287:ASN:OD1	1:K:289:GLN:NE2	2.43	0.50
1:K:731:LYS:HB2	1:K:753:GLU:CD	2.37	0.50
1:J:63:ARG:HG3	1:J:63:ARG:HH11	1.76	0.50
1:J:448:ASN:CB	1:L:290:PRO:CD	2.90	0.50
1:J:702:LEU:HD12	1:J:703:GLY:N	2.17	0.50
1:K:100:TYR:CE1	1:K:627:TYR:HB2	2.47	0.50
1:K:9:GLN:OE1	1:K:9:GLN:N	2.45	0.49
1:K:345:MET:HB2	1:K:347:TYR:CE2	2.47	0.49
1:L:442:ALA:HA	1:L:446:GLN:HB2	1.93	0.49
1:L:501:THR:OG1	1:L:502:ASN:OD1	2.29	0.49
1:L:726:ASN:C	1:L:728:THR:N	2.69	0.49
1:J:382:LEU:O	1:J:383:ASP:C	2.53	0.49
1:K:731:LYS:HG2	1:K:917:GLU:HB3	1.93	0.49
1:L:114:LYS:H	1:L:333:ASN:HB3	1.78	0.49
1:L:415:GLU:OE1	1:L:415:GLU:N	2.45	0.49
1:L:606:SER:HG	1:L:608:LEU:H	1.61	0.49
1:J:652:GLN:HB2	1:J:939:VAL:HB	1.94	0.49
1:K:80:TYR:CE1	1:K:596:PHE:HB2	2.45	0.49
1:L:67:ARG:NH2	1:L:625:CYS:SG	2.85	0.49
1:L:80:TYR:O	1:L:595:ASN:HA	2.12	0.49
1:L:419:PRO:HB2	1:L:421:TYR:CE1	2.48	0.49
1:J:712:TYR:OH	1:J:714:GLY:HA3	2.12	0.49
1:K:481:ARG:NE	1:K:526:ASP:OD2	2.33	0.49
1:J:94:LEU:CG	1:J:95:ASP:N	2.75	0.49
1:J:414:THR:OG1	1:J:415:GLU:N	2.45	0.49
1:J:878:ASP:N	1:J:878:ASP:OD1	2.44	0.49
1:L:599:ASP:OD2	1:L:602:MET:N	2.44	0.49
1:J:50:VAL:HG22	1:L:896:LEU:HB3	1.95	0.49
1:J:410:GLU:HG2	1:J:534:ARG:HG3	1.94	0.49
1:J:421:TYR:CE1	1:J:472:GLU:HB2	2.47	0.49
1:J:438:LYS:O	1:J:450:THR:HB	2.13	0.49
1:L:137:GLN:HB3	1:L:170:HIS:CE1	2.47	0.49
1:J:46:ARG:HG2	1:L:653:SER:HB2	1.95	0.49
1:K:183:THR:HG21	1:K:204:PHE:CE1	2.48	0.49
1:K:693:ARG:HG2	1:K:725:LEU:HD13	1.95	0.49
1:L:170:HIS:ND1	1:L:170:HIS:N	2.59	0.49
1:L:853:TYR:CD1	1:L:854:PRO:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:TYR:HE2	1:J:394:MET:HE1	1.77	0.49
1:J:383:ASP:O	1:J:386:GLY:O	2.31	0.49
1:J:645:LEU:O	1:J:647:ASN:N	2.46	0.49
1:J:656:ASP:CG	1:J:657:TYR:H	2.21	0.49
1:J:737:ASP:OD1	1:J:737:ASP:N	2.45	0.49
1:K:279:THR:O	1:K:282:THR:OG1	2.27	0.49
1:L:415:GLU:O	1:L:476:ASN:ND2	2.35	0.49
1:L:431:THR:OG1	1:L:463:ILE:N	2.45	0.49
1:J:276:SER:OG	1:J:277:THR:N	2.44	0.48
1:J:887:SER:OG	1:J:890:PHE:N	2.46	0.48
1:J:46:ARG:HD2	1:J:46:ARG:HA	1.72	0.48
1:J:250:THR:N	1:J:255:GLY:O	2.46	0.48
1:J:604:LEU:HD23	1:J:604:LEU:N	2.27	0.48
1:K:240:LYS:HD3	1:K:241:PRO:HD2	1.94	0.48
1:K:731:LYS:HB2	1:K:753:GLU:OE2	2.13	0.48
1:L:346:TYR:O	1:L:347:TYR:CG	2.67	0.48
1:J:438:LYS:HZ1	1:J:453:LYS:HA	1.78	0.48
1:K:611:ASP:OD2	1:K:614:VAL:N	2.45	0.48
1:K:766:ASN:HD22	1:K:771:ASN:HA	1.76	0.48
1:L:392:PHE:CZ	1:L:394:MET:HB3	2.48	0.48
1:L:400:ASP:N	1:L:400:ASP:OD1	2.42	0.48
1:L:724:TYR:CD1	1:L:724:TYR:N	2.81	0.48
1:J:277:THR:HA	1:K:434:PHE:HD1	1.79	0.48
1:K:105:GLY:HA2	1:K:622:ASP:CG	2.39	0.48
1:K:111:PRO:CA	1:K:565:ARG:HE	2.26	0.48
1:K:610:ASN:OD1	1:K:610:ASN:N	2.46	0.48
1:L:548:HIS:CG	1:L:549:HIS:H	2.32	0.48
1:L:644:MET:O	1:L:650:ASN:ND2	2.47	0.48
1:J:181:LYS:HZ2	1:J:182:ILE:H	1.60	0.48
1:J:201:LYS:O	1:J:201:LYS:NZ	2.42	0.48
1:K:815:GLN:N	1:K:815:GLN:OE1	2.47	0.48
1:L:9:GLN:HE21	1:L:10:TRP:CD1	2.31	0.48
1:L:691:PHE:N	1:L:691:PHE:CD1	2.80	0.48
1:J:418:LEU:HD12	1:K:482:ASN:HA	1.95	0.48
1:J:643:ALA:C	1:J:646:ARG:HB2	2.39	0.48
1:K:590:TYR:HE1	1:K:945:GLY:HA2	1.78	0.48
1:L:307:HIS:HD1	1:L:307:HIS:H	1.61	0.48
1:J:611:ASP:OD1	1:J:613:ARG:N	2.46	0.48
1:K:724:TYR:O	1:K:727:HIS:NE2	2.47	0.48
2:Z:55:CYS:HB3	2:Z:81:CYS:SG	2.53	0.48
1:J:531:LEU:HD13	1:K:116:TYR:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:343:GLY:O	1:K:597:ARG:NH1	2.46	0.48
1:K:586:LEU:HB2	1:K:941:GLN:OE1	2.13	0.48
1:L:691:PHE:CZ	1:L:882:TRP:HB3	2.49	0.48
2:Z:23:SER:C	2:Z:24:TYR:CG	2.91	0.48
1:J:345:MET:HG2	1:J:596:PHE:CD1	2.48	0.48
1:J:409:ILE:HD13	1:J:409:ILE:H	1.79	0.48
1:K:227:ALA:O	1:K:228:ALA:HB2	2.14	0.48
1:K:685:ALA:HB2	1:L:10:TRP:HZ2	1.77	0.48
1:L:771:ASN:N	1:L:771:ASN:OD1	2.38	0.48
1:J:815:GLN:HB3	1:J:871:THR:OG1	2.14	0.48
1:K:58:THR:OG1	1:K:59:ASP:N	2.47	0.48
1:K:334:TYR:HB2	1:K:607:SER:HB3	1.96	0.48
1:K:530:ASN:O	1:L:563:ASN:ND2	2.47	0.48
1:K:575:GLN:OE1	1:K:576:LYS:N	2.47	0.48
1:J:84:PHE:CE1	1:J:626:LEU:HD22	2.48	0.47
1:J:446:GLN:HA	1:J:449:THR:CB	2.43	0.47
1:J:734:ILE:O	1:J:735:THR:OG1	2.29	0.47
1:L:207:LYS:NZ	1:L:270:VAL:O	2.37	0.47
1:L:435:GLN:NE2	1:L:454:ASP:OD1	2.46	0.47
1:J:289:GLN:CD	1:K:448:ASN:HD22	2.22	0.47
1:J:476:ASN:OD1	1:J:477:ALA:N	2.46	0.47
1:J:497:LYS:O	1:J:518:ARG:NH1	2.46	0.47
1:K:723:PHE:O	1:K:878:ASP:HB2	2.14	0.47
1:K:870:ILE:HG13	1:K:871:THR:N	2.28	0.47
1:K:113:PHE:HA	1:K:335:ILE:HD11	1.96	0.47
1:L:887:SER:OG	1:L:890:PHE:N	2.48	0.47
1:L:606:SER:HG	1:L:609:GLY:H	1.62	0.47
1:K:134:GLU:OE2	1:K:235:LYS:N	2.47	0.47
1:K:224:ASP:OD1	1:K:224:ASP:N	2.47	0.47
1:K:480:TRP:CZ2	1:K:484:LEU:HD21	2.49	0.47
1:K:569:PHE:CD1	1:K:569:PHE:N	2.82	0.47
1:K:690:ALA:HB3	1:K:930:LEU:HB2	1.96	0.47
1:J:535:TRP:CE3	1:J:814:ARG:HB3	2.50	0.47
1:J:715:SER:O	1:J:717:PRO:HD3	2.13	0.47
1:J:897:THR:HG23	1:J:900:GLY:H	1.78	0.47
1:J:65:THR:OG1	1:J:629:THR:HG23	2.15	0.47
1:J:224:ASP:N	1:J:224:ASP:OD1	2.45	0.47
1:J:282:THR:OG1	1:J:283:ASN:N	2.48	0.47
1:J:338:ARG:NH1	1:J:716:ILE:HG13	2.30	0.47
1:J:639:SER:OG	1:J:640:THR:N	2.48	0.47
1:J:664:LEU:HD23	1:J:928:TYR:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:14:HIS:CE1	1:K:23:TYR:CE1	3.02	0.47
1:K:340:ASN:C	1:K:342:ILE:N	2.72	0.47
1:K:384:SER:O	1:K:801:ARG:NH2	2.47	0.47
1:K:565:ARG:HB3	1:K:566:TYR:CD2	2.50	0.47
1:K:578:PHE:CG	1:K:579:ALA:N	2.82	0.47
1:K:822:TYR:CZ	1:K:824:ASP:HB2	2.49	0.47
1:J:378:TYR:CE1	1:J:382:LEU:HD12	2.50	0.47
1:J:461:ASN:HD21	1:L:170:HIS:C	2.22	0.47
1:J:508:ASN:ND2	1:J:510:ASN:OD1	2.47	0.47
1:J:577:PHE:HB3	1:J:580:ILE:HG12	1.96	0.47
1:J:600:VAL:HG13	1:J:604:LEU:CD1	2.44	0.47
1:K:19:ASP:HB2	1:K:21:SER:HB3	1.97	0.47
1:K:169:THR:HB	1:L:457:PHE:CD1	2.50	0.47
1:L:772:MET:HE1	1:L:809:PHE:CE2	2.50	0.47
1:J:211:PRO:HD2	1:J:231:ARG:NH2	2.30	0.47
1:J:271:GLU:N	1:J:271:GLU:OE1	2.48	0.47
1:J:338:ARG:HH11	1:J:716:ILE:HG13	1.80	0.47
1:J:373:ASN:O	1:J:374:THR:C	2.58	0.47
1:J:412:HIS:O	1:K:117:SER:N	2.45	0.47
1:K:22:GLU:C	1:K:24:LEU:H	2.21	0.47
1:K:90:ASP:O	1:K:92:ARG:HG3	2.15	0.47
1:K:727:HIS:HE1	1:K:876:LEU:HD13	1.78	0.47
1:L:78:TYR:O	1:L:598:LYS:N	2.48	0.47
1:L:489:ALA:HA	1:L:492:LEU:HD23	1.97	0.47
1:J:56:VAL:O	1:J:634:ALA:N	2.43	0.47
1:J:338:ARG:CG	1:J:342:ILE:HG23	2.43	0.47
1:K:271:GLU:OE1	1:K:271:GLU:N	2.48	0.47
1:K:481:ARG:HE	1:K:526:ASP:CG	2.19	0.47
1:L:369:LEU:H	1:L:372:ARG:NH1	2.12	0.47
1:L:538:GLU:OE1	1:L:538:GLU:N	2.35	0.47
1:L:908:SER:OG	1:L:910:HIS:NE2	2.30	0.47
2:Z:25:CGU:OE21	2:Z:28:ARG:NH1	2.48	0.47
1:J:196:VAL:H	1:J:199:ALA:HB2	1.81	0.46
1:J:374:THR:O	1:J:377:SER:HB3	2.15	0.46
1:K:134:GLU:HB3	1:K:171:VAL:HG22	1.97	0.46
1:K:808:ASN:O	1:K:877:CYS:HA	2.15	0.46
1:L:761:ASP:OD2	1:L:764:GLY:N	2.45	0.46
1:J:61:SER:OG	1:L:746:ASP:N	2.49	0.46
1:J:345:MET:SD	1:J:573:VAL:HG11	2.55	0.46
1:J:413:GLY:HA3	1:K:117:SER:O	2.15	0.46
1:J:716:ILE:O	1:J:720:ASP:CG	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:287:ASN:O	1:K:289:GLN:NE2	2.38	0.46
1:K:599:ASP:OD2	1:K:602:MET:HE2	2.15	0.46
1:L:692:THR:HG21	1:L:723:PHE:CD2	2.50	0.46
1:J:636:ASN:OD1	1:J:636:ASN:N	2.47	0.46
1:J:699:THR:O	1:J:701:SER:N	2.49	0.46
1:K:100:TYR:HE1	1:K:627:TYR:HB2	1.80	0.46
1:K:431:THR:OG1	1:K:432:ASP:N	2.46	0.46
1:K:667:ILE:HG13	1:K:925:THR:C	2.40	0.46
1:L:20:ALA:HA	1:L:23:TYR:CE2	2.50	0.46
1:J:58:THR:OG1	1:J:59:ASP:N	2.49	0.46
1:J:92:ARG:O	1:J:93:VAL:HG13	2.15	0.46
1:J:201:LYS:H	1:J:201:LYS:HD3	1.80	0.46
1:K:403:ASP:OD1	1:K:406:VAL:N	2.38	0.46
1:K:554:LEU:HD23	1:K:554:LEU:HA	1.67	0.46
1:L:175:ALA:HB1	1:L:229:GLY:C	2.40	0.46
1:L:578:PHE:CG	1:L:579:ALA:N	2.83	0.46
1:L:766:ASN:OD1	1:L:766:ASN:N	2.49	0.46
1:L:904:LEU:O	1:L:907:ASN:HB2	2.16	0.46
1:J:531:LEU:HD22	1:K:116:TYR:HB3	1.97	0.46
1:K:290:PRO:HD2	1:L:448:ASN:CG	2.41	0.46
1:K:572:GLN:N	1:K:572:GLN:OE1	2.49	0.46
1:L:24:LEU:HD12	1:L:24:LEU:H	1.80	0.46
1:L:239:MET:O	1:L:325:GLN:NE2	2.48	0.46
2:Z:245:LYS:HE2	2:Z:264:GLU:HG2	1.98	0.46
1:J:250:THR:OG1	1:J:255:GLY:O	2.32	0.46
1:K:217:GLU:HG2	1:K:222:GLU:HB3	1.98	0.46
1:K:565:ARG:HD2	1:K:566:TYR:CE1	2.51	0.46
1:K:817:VAL:HG12	1:K:818:ASP:O	2.16	0.46
1:J:432:ASP:O	1:J:433:THR:C	2.56	0.46
1:J:438:LYS:NZ	1:J:453:LYS:HA	2.31	0.46
1:K:830:ILE:HA	1:K:833:GLN:CD	2.41	0.46
1:K:899:LEU:HA	1:K:899:LEU:HD23	1.68	0.46
1:L:307:HIS:HB2	1:L:517:LYS:NZ	2.30	0.46
1:L:834:HIS:O	1:L:834:HIS:ND1	2.48	0.46
1:J:61:SER:CB	1:L:745:ASN:HB2	2.45	0.46
1:J:533:ALA:HB2	1:K:563:ASN:CG	2.41	0.46
1:J:706:TYR:CE2	1:J:708:PRO:HA	2.51	0.46
1:K:829:GLY:O	1:K:833:GLN:HG3	2.16	0.46
1:K:928:TYR:CZ	1:K:930:LEU:HD21	2.50	0.46
1:L:188:GLN:NE2	1:L:203:ILE:O	2.49	0.46
1:J:657:TYR:C	1:J:657:TYR:HD1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:717:PRO:HA	1:J:720:ASP:OD1	2.16	0.46
1:K:23:TYR:HD1	1:K:23:TYR:O	1.98	0.46
1:K:724:TYR:CD1	1:K:725:LEU:HG	2.51	0.46
1:K:849:GLU:OE1	1:L:216:GLY:N	2.48	0.46
1:L:341:PHE:HB3	1:L:344:LEU:CD1	2.46	0.46
1:L:730:LYS:HZ3	1:L:757:LYS:HD3	1.81	0.46
1:L:759:SER:OG	1:L:760:VAL:N	2.49	0.46
1:J:269:GLN:NE2	1:J:269:GLN:H	2.14	0.46
1:J:431:THR:C	1:J:432:ASP:CG	2.83	0.46
1:J:655:ASN:HB3	1:J:936:VAL:HG12	1.98	0.46
1:J:786:ASN:HD21	1:J:892:SER:HB3	1.81	0.46
1:K:338:ARG:HA	1:K:557:ARG:HH21	1.80	0.46
1:K:954:THR:HB	1:K:955:PRO:HD3	1.98	0.46
2:Z:23:SER:O	2:Z:24:TYR:CE1	2.66	0.46
1:J:205:ALA:HB1	1:J:210:GLN:HB3	1.98	0.45
1:J:665:TYR:HD1	1:J:665:TYR:HA	1.67	0.45
1:K:24:LEU:O	1:K:25:SER:C	2.58	0.45
1:K:220:TRP:NE1	1:K:221:ASN:OD1	2.50	0.45
1:L:306:THR:HG22	1:L:329:PRO:HA	1.97	0.45
1:L:753:GLU:N	1:L:753:GLU:OE1	2.49	0.45
2:Z:28:ARG:HG2	2:Z:37:THR:HG1	1.76	0.45
1:J:400:ASP:N	1:J:400:ASP:OD1	2.48	0.45
1:J:681:ARG:NH1	1:J:955:PRO:O	2.49	0.45
1:K:53:THR:OG1	1:K:54:HIS:N	2.50	0.45
1:K:55:ASP:OD1	1:K:55:ASP:N	2.50	0.45
1:K:600:VAL:HA	1:K:603:VAL:HG22	1.97	0.45
1:L:876:LEU:HD12	1:L:877:CYS:N	2.31	0.45
1:J:447:GLY:O	1:J:450:THR:HG23	2.16	0.45
1:J:535:TRP:CE2	1:J:814:ARG:HD3	2.52	0.45
1:K:78:TYR:O	1:K:598:LYS:HB2	2.17	0.45
1:K:288:ILE:HD12	1:L:437:VAL:HG12	1.99	0.45
1:K:776:TRP:O	1:K:780:GLN:HG2	2.17	0.45
1:L:341:PHE:HB3	1:L:344:LEU:HD11	1.97	0.45
1:J:63:ARG:HG3	1:J:63:ARG:NH1	2.32	0.45
1:J:92:ARG:HB2	1:J:92:ARG:HH11	1.82	0.45
1:J:132:SER:HB3	1:J:232:VAL:HG23	1.98	0.45
1:J:452:GLN:HB3	1:J:454:ASP:OD1	2.16	0.45
1:J:643:ALA:HA	1:J:646:ARG:HB2	1.98	0.45
1:K:41:LEU:HD13	1:K:41:LEU:HA	1.74	0.45
1:K:94:LEU:HB2	1:K:630:PHE:CE1	2.50	0.45
1:K:732:VAL:HA	1:K:915:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:GLN:OE1	1:L:92:ARG:NE	2.47	0.45
2:Z:402:GLY:HA3	2:Z:405:ARG:HD2	1.97	0.45
1:J:8:PRO:O	1:J:11:SER:OG	2.31	0.45
1:J:341:PHE:CZ	1:J:396:ASN:HB2	2.51	0.45
1:J:342:ILE:HG23	1:J:342:ILE:O	2.17	0.45
1:J:354:GLY:HA3	1:J:594:TRP:CZ3	2.52	0.45
1:J:474:ASN:ND2	1:J:476:ASN:OD1	2.43	0.45
1:K:490:LEU:HA	1:K:490:LEU:HD23	1.70	0.45
1:K:745:ASN:ND2	1:L:60:ARG:O	2.50	0.45
1:K:818:ASP:CG	1:K:819:ASP:N	2.74	0.45
1:K:955:PRO:HD2	1:K:956:PHE:HD1	1.81	0.45
1:L:109:ARG:HD3	1:L:113:PHE:CG	2.52	0.45
1:L:341:PHE:CD2	1:L:344:LEU:HD11	2.52	0.45
2:Z:3:SER:OG	2:Z:6:CGU:N	2.50	0.45
2:Z:62:LYS:HB3	2:Z:69:THR:HB	1.99	0.45
1:J:239:MET:O	1:J:325:GLN:NE2	2.41	0.45
1:J:440:THR:HG22	1:J:451:TRP:NE1	2.31	0.45
1:J:712:TYR:CZ	1:J:714:GLY:CA	2.89	0.45
1:K:175:ALA:HB1	1:K:229:GLY:C	2.42	0.45
1:K:691:PHE:CE1	1:K:882:TRP:HB2	2.38	0.45
1:K:960:ASN:ND2	1:K:962:THR:H	2.14	0.45
1:L:205:ALA:HA	1:L:210:GLN:HG2	1.98	0.45
1:K:198:GLY:O	1:K:200:GLY:N	2.48	0.45
1:K:211:PRO:C	1:K:231:ARG:NH1	2.74	0.45
1:K:437:VAL:HA	1:K:453:LYS:H	1.81	0.45
1:L:178:SER:OG	1:L:179:GLY:N	2.50	0.45
1:L:647:ASN:OD1	1:L:649:THR:HG22	2.16	0.45
1:L:771:ASN:ND2	1:L:874:LYS:HA	2.32	0.45
1:J:269:GLN:H	1:J:269:GLN:HE21	1.65	0.45
1:J:331:ARG:HG2	1:J:490:LEU:HD13	1.99	0.45
1:J:745:ASN:O	1:J:747:ARG:N	2.48	0.45
1:K:691:PHE:CD1	1:K:691:PHE:N	2.83	0.45
1:L:270:VAL:HG22	1:L:297:GLU:HB3	1.98	0.45
1:L:356:LEU:O	1:L:365:ALA:HB3	2.16	0.45
1:L:373:ASN:H	1:L:662:ASN:ND2	2.15	0.45
1:L:403:ASP:OD2	1:L:406:VAL:N	2.42	0.45
1:L:649:THR:HG23	1:L:650:ASN:OD1	2.17	0.45
1:L:830:ILE:HD12	1:L:830:ILE:H	1.82	0.45
1:J:104:ARG:NH1	1:L:762:GLY:O	2.38	0.45
1:J:207:LYS:HG2	1:J:270:VAL:HB	1.99	0.45
1:J:812:MET:HB2	1:J:812:MET:HE3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:111:PRO:CB	1:K:565:ARG:HH11	2.25	0.45
1:K:232:VAL:CG2	1:K:233:LEU:N	2.80	0.45
1:K:276:SER:HB2	1:K:290:PRO:HA	1.99	0.45
1:L:808:ASN:ND2	1:L:879:ARG:HB3	2.32	0.45
1:L:939:VAL:HG13	1:L:949:THR:HG22	1.98	0.45
1:J:434:PHE:CE1	1:L:277:THR:HG23	2.52	0.45
1:K:23:TYR:O	1:K:23:TYR:CD1	2.70	0.45
1:L:454:ASP:OD1	1:L:454:ASP:N	2.50	0.45
1:L:473:ILE:HG12	1:L:474:ASN:O	2.17	0.45
1:L:654:PHE:O	1:L:936:VAL:HA	2.17	0.45
1:L:695:LYS:HA	1:L:925:THR:HG22	1.99	0.45
1:L:882:TRP:HA	1:L:882:TRP:CE3	2.53	0.45
1:J:20:ALA:HA	1:J:23:TYR:CE2	2.51	0.44
1:J:205:ALA:HA	1:J:210:GLN:HG2	1.99	0.44
1:K:121:TYR:CD1	1:K:246:TYR:HB2	2.52	0.44
1:K:176:PRO:HD2	1:K:229:GLY:O	2.16	0.44
1:K:239:MET:SD	1:K:318:ASN:HB2	2.57	0.44
1:L:486:SER:OG	1:L:487:ASN:N	2.49	0.44
1:L:820:THR:C	1:L:821:LYS:HZ3	2.25	0.44
1:J:250:THR:HG23	1:J:255:GLY:O	2.16	0.44
1:K:485:TYR:O	1:K:489:ALA:HB3	2.17	0.44
1:L:259:MET:SD	1:L:268:SER:HB3	2.57	0.44
1:L:723:PHE:O	1:L:879:ARG:N	2.44	0.44
1:J:124:LEU:N	1:L:836:ASN:OD1	2.40	0.44
1:J:387:ASP:CG	1:J:389:THR:H	2.26	0.44
1:J:444:GLY:O	1:J:445:ASP:CB	2.64	0.44
1:J:535:TRP:CH2	1:J:814:ARG:HG2	2.52	0.44
1:J:824:ASP:OD1	1:J:824:ASP:N	2.51	0.44
1:K:72:ASP:HB3	1:K:83:ARG:HB3	2.00	0.44
1:K:345:MET:HE3	1:K:596:PHE:HE1	1.83	0.44
1:K:602:MET:HE1	1:K:710:TYR:CD2	2.52	0.44
1:K:613:ARG:HH22	1:K:710:TYR:HB3	1.82	0.44
1:L:270:VAL:HA	1:L:296:SER:O	2.17	0.44
1:L:346:TYR:CD2	1:L:597:ARG:HG2	2.51	0.44
1:L:407:ARG:NH1	1:L:545:PRO:HG3	2.32	0.44
1:L:730:LYS:CB	1:L:917:GLU:O	2.66	0.44
1:L:878:ASP:OD1	1:L:878:ASP:N	2.50	0.44
1:J:396:ASN:OD1	1:J:557:ARG:HD2	2.18	0.44
1:J:421:TYR:HE1	1:J:472:GLU:HB2	1.81	0.44
1:J:836:ASN:CG	1:K:122:ASN:HA	2.42	0.44
1:K:294:LEU:HD23	1:K:294:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:259:MET:HB3	1:L:265:LYS:HG2	1.99	0.44
1:L:581:LYS:HE2	1:L:581:LYS:HB3	1.81	0.44
1:L:940:HIS:CE1	1:L:942:PRO:HD3	2.51	0.44
1:J:122:ASN:HB3	1:J:125:ALA:HB2	1.99	0.44
1:L:763:GLU:HB3	1:L:765:TYR:CE1	2.52	0.44
1:J:43:ASN:C	1:J:44:LYS:HZ2	2.26	0.44
1:J:89:GLY:HA3	1:J:92:ARG:NH1	2.33	0.44
1:J:352:ASN:N	1:J:352:ASN:OD1	2.50	0.44
1:J:786:ASN:OD1	1:J:891:MET:HB3	2.18	0.44
1:J:898:ASP:OD1	1:J:899:LEU:N	2.44	0.44
1:L:7:MET:HB2	1:L:8:PRO:HD3	2.00	0.44
1:L:288:ILE:HD13	1:L:288:ILE:H	1.83	0.44
1:L:314:MET:HE3	1:L:314:MET:HB2	1.86	0.44
1:L:822:TYR:CZ	1:L:824:ASP:HB2	2.53	0.44
1:J:534:ARG:O	1:J:535:TRP:HB2	2.18	0.44
1:J:636:ASN:C	1:J:638:ALA:N	2.71	0.44
1:K:110:GLY:O	1:K:565:ARG:HG2	2.18	0.44
1:K:529:ILE:C	1:K:531:LEU:N	2.75	0.44
1:K:586:LEU:HD23	1:K:586:LEU:HA	1.82	0.44
2:Z:87:LYS:HB3	2:Z:107:VAL:HG23	2.00	0.44
1:J:170:HIS:CE1	1:K:458:ALA:HB2	2.52	0.44
1:J:600:VAL:HG22	1:J:619:ILE:HG22	2.00	0.44
1:J:646:ARG:HH22	1:J:944:ARG:HA	1.82	0.44
1:K:836:ASN:N	1:L:122:ASN:OD1	2.39	0.44
1:L:19:ASP:CG	1:L:21:SER:H	2.24	0.44
1:L:338:ARG:NH1	1:L:716:ILE:HD11	2.33	0.44
1:L:666:PRO:HA	1:L:926:LEU:HD23	1.99	0.44
1:L:786:ASN:HD21	1:L:892:SER:H	1.66	0.44
2:Z:118:ALA:HB2	2:Z:125:ILE:HG13	1.99	0.44
2:Z:365:ALA:HB3	2:Z:412:TYR:CE1	2.53	0.44
1:J:136:GLU:OE1	1:J:137:GLN:N	2.49	0.44
1:J:253:ASN:O	1:L:832:HIS:CD2	2.71	0.44
1:J:268:SER:O	1:J:270:VAL:HG23	2.17	0.44
1:J:338:ARG:HD2	1:J:338:ARG:HA	1.87	0.44
1:J:378:TYR:HE1	1:J:382:LEU:HD12	1.83	0.44
1:J:463:ILE:HD12	1:L:173:ALA:O	2.18	0.44
1:K:812:MET:HE3	1:K:812:MET:HB2	1.89	0.44
1:L:697:LYS:HB3	1:L:697:LYS:HE3	1.61	0.44
1:L:727:HIS:O	1:L:729:PHE:N	2.51	0.44
2:Z:235:ALA:N	2:Z:282:ASP:OD1	2.49	0.44
1:J:298:ASP:OD1	1:J:299:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:957:SER:OG	1:J:958:ALA:N	2.51	0.43
1:K:137:GLN:HB3	1:K:170:HIS:CE1	2.53	0.43
1:K:344:LEU:HD23	1:K:344:LEU:HA	1.85	0.43
1:L:136:GLU:OE1	1:L:137:GLN:N	2.51	0.43
1:J:771:ASN:ND2	1:J:874:LYS:HA	2.33	0.43
1:K:571:ILE:H	1:K:571:ILE:HG13	1.69	0.43
1:J:438:LYS:HE3	1:J:453:LYS:HG3	1.99	0.43
1:J:462:GLU:O	1:J:463:ILE:HD13	2.19	0.43
1:J:952:LEU:HD12	1:J:952:LEU:HA	1.68	0.43
1:K:281:ALA:HA	1:K:288:ILE:HG22	2.00	0.43
1:K:666:PRO:HA	1:K:926:LEU:HD23	2.00	0.43
1:K:870:ILE:CG1	1:K:871:THR:H	2.25	0.43
1:L:14:HIS:CD2	1:L:23:TYR:HH	2.27	0.43
1:L:667:ILE:HD12	1:L:693:ARG:HE	1.83	0.43
1:J:7:MET:HB2	1:J:10:TRP:CZ3	2.53	0.43
1:J:234:LYS:HD3	1:J:234:LYS:HA	1.89	0.43
1:J:939:VAL:HG22	1:J:949:THR:HG22	2.00	0.43
1:K:263:ASN:OD1	1:K:263:ASN:N	2.51	0.43
1:K:526:ASP:HB3	1:K:528:TYR:CE2	2.53	0.43
1:K:569:PHE:N	1:K:569:PHE:HD1	2.17	0.43
1:J:61:SER:CA	1:L:745:ASN:HB2	2.48	0.43
1:J:280:ASN:C	1:J:284:GLU:HG2	2.43	0.43
1:J:368:ASP:OD1	1:J:372:ARG:NH2	2.51	0.43
1:J:694:LEU:HD11	1:J:718:TYR:HB2	2.01	0.43
1:K:338:ARG:NH1	1:K:601:ASN:O	2.51	0.43
1:K:354:GLY:HA3	1:K:594:TRP:CE3	2.52	0.43
1:K:435:GLN:CD	1:K:435:GLN:C	2.86	0.43
1:L:359:GLN:H	1:L:590:TYR:HA	1.84	0.43
1:L:507:ASP:OD1	1:L:507:ASP:N	2.49	0.43
1:L:586:LEU:HD12	1:L:941:GLN:HB2	1.99	0.43
1:L:681:ARG:HD3	1:L:682:ASN:H	1.82	0.43
1:L:701:SER:OG	1:L:707:ASP:OD2	2.24	0.43
1:J:40:SER:C	1:J:41:LEU:HD22	2.44	0.43
1:J:373:ASN:CG	1:J:375:GLU:HB2	2.43	0.43
1:J:501:THR:OG1	1:J:502:ASN:OD1	2.29	0.43
1:K:251:ASN:ND2	1:K:253:ASN:OD1	2.44	0.43
1:K:603:VAL:HG23	1:K:604:LEU:HD23	2.00	0.43
1:K:861:LEU:HD23	1:K:861:LEU:HA	1.84	0.43
1:L:112:THR:O	1:L:112:THR:OG1	2.27	0.43
1:J:206:ASP:OD2	1:J:208:THR:OG1	2.30	0.43
1:J:337:PHE:HE1	1:J:603:VAL:HB	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:730:LYS:HB3	1:J:917:GLU:O	2.19	0.43
1:K:20:ALA:CB	1:K:23:TYR:CE1	3.00	0.43
1:K:251:ASN:HD21	1:K:253:ASN:CG	2.27	0.43
1:K:365:ALA:O	1:K:951:TYR:OH	2.31	0.43
1:L:338:ARG:NH2	1:L:714:GLY:O	2.44	0.43
1:L:682:ASN:HD21	1:L:904:LEU:HD21	1.83	0.43
1:L:690:ALA:HB3	1:L:930:LEU:HB2	2.00	0.43
1:L:831:ILE:HD13	1:L:831:ILE:HA	1.85	0.43
2:Z:12:HIS:NE2	2:Z:14:CGU:OE12	2.51	0.43
1:J:90:ASP:OD1	1:J:90:ASP:N	2.50	0.43
1:J:275:PHE:HA	1:K:435:GLN:O	2.19	0.43
1:K:687:ARG:HD3	1:K:932:GLU:HG2	2.01	0.43
1:K:702:LEU:HD22	1:K:702:LEU:H	1.84	0.43
1:K:800:ASP:OD1	1:K:801:ARG:N	2.51	0.43
1:L:113:PHE:CD2	1:L:115:PRO:HD3	2.54	0.43
1:L:508:ASN:OD1	1:L:511:THR:N	2.52	0.43
1:J:137:GLN:OE1	1:J:170:HIS:NE2	2.52	0.43
1:J:285:VAL:C	1:J:286:ASN:O	2.62	0.43
1:J:535:TRP:CD1	1:J:536:SER:N	2.83	0.43
1:J:586:LEU:O	1:J:590:TYR:OH	2.29	0.43
1:K:78:TYR:O	1:K:598:LYS:N	2.52	0.43
1:K:388:ARG:HH21	1:K:397:GLN:HG2	1.84	0.43
1:K:453:LYS:HD3	1:K:453:LYS:O	2.19	0.43
1:K:724:TYR:HD1	1:K:725:LEU:HG	1.82	0.43
1:K:942:PRO:HB2	1:K:943:HIS:ND1	2.34	0.43
1:L:188:GLN:HE21	1:L:203:ILE:N	2.17	0.43
1:L:305:ASP:OD1	1:L:305:ASP:N	2.50	0.43
1:L:531:LEU:HA	1:L:531:LEU:HD23	1.80	0.43
1:L:596:PHE:CD1	1:L:596:PHE:N	2.77	0.43
1:K:352:ASN:HB3	1:K:595:ASN:ND2	2.34	0.43
1:K:563:ASN:N	1:K:563:ASN:OD1	2.52	0.43
1:K:702:LEU:O	1:K:704:SER:N	2.50	0.43
1:L:594:TRP:CD1	1:L:595:ASN:H	2.37	0.43
1:L:652:GLN:HB2	1:L:939:VAL:HB	2.00	0.43
1:L:724:TYR:CG	1:L:725:LEU:HG	2.53	0.43
1:J:43:ASN:O	1:J:43:ASN:ND2	2.52	0.42
1:J:346:TYR:HA	1:J:597:ARG:HH12	1.84	0.42
1:J:384:SER:OG	1:J:385:ILE:N	2.52	0.42
1:J:534:ARG:N	1:K:559:MET:CE	2.81	0.42
1:J:641:LEU:HA	1:J:644:MET:HB2	2.00	0.42
1:K:266:LEU:H	1:K:266:LEU:HG	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:ALA:HA	1:L:23:TYR:CZ	2.53	0.42
1:L:96:MET:O	1:L:99:THR:OG1	2.29	0.42
1:L:606:SER:OG	1:L:608:LEU:N	2.41	0.42
1:J:91:ASN:HB2	1:J:635:HIS:HB3	2.00	0.42
1:J:241:PRO:HD3	1:J:325:GLN:HG3	2.01	0.42
1:J:418:LEU:HD11	1:K:485:TYR:HB3	2.00	0.42
1:J:659:SER:O	1:J:660:ALA:HB2	2.19	0.42
1:J:700:PRO:HB3	1:J:710:TYR:CE2	2.55	0.42
1:K:183:THR:OG1	1:K:186:GLY:O	2.35	0.42
1:K:405:ASP:OD1	1:K:405:ASP:N	2.51	0.42
1:K:732:VAL:N	1:K:753:GLU:OE1	2.50	0.42
1:L:586:LEU:O	1:L:590:TYR:OH	2.38	0.42
2:Z:70:CYS:SG	2:Z:80:ASN:HA	2.59	0.42
1:J:448:ASN:CA	1:L:290:PRO:CD	2.97	0.42
1:J:463:ILE:HD12	1:J:463:ILE:HA	1.73	0.42
1:J:544:ASN:HB2	1:J:724:TYR:CZ	2.54	0.42
1:J:590:TYR:CD2	1:J:947:ILE:HD11	2.55	0.42
1:K:231:ARG:NH1	1:K:231:ARG:HG2	2.34	0.42
1:K:467:ASN:OD1	1:K:467:ASN:N	2.51	0.42
1:L:185:GLU:C	1:L:272:MET:HE1	2.44	0.42
1:L:472:GLU:HG2	1:L:473:ILE:N	2.33	0.42
1:J:534:ARG:N	1:K:559:MET:HE2	2.31	0.42
1:J:534:ARG:HB3	1:J:534:ARG:HH11	1.83	0.42
1:J:555:ARG:HD3	1:L:412:HIS:CE1	2.54	0.42
1:J:638:ALA:O	1:J:639:SER:C	2.60	0.42
1:K:113:PHE:CE2	1:K:564:GLY:O	2.73	0.42
1:K:133:CYS:HA	1:K:232:VAL:HG21	2.02	0.42
1:K:442:ALA:HA	1:K:446:GLN:HB2	2.01	0.42
1:K:467:ASN:HD22	1:L:848:ARG:HH21	1.67	0.42
1:K:782:LEU:HD23	1:K:787:ILE:O	2.20	0.42
1:L:646:ARG:NH1	1:L:942:PRO:C	2.78	0.42
1:L:652:GLN:O	1:L:938:ARG:HG2	2.20	0.42
1:L:868:ASP:OD1	1:L:868:ASP:N	2.42	0.42
1:J:71:VAL:H	1:J:84:PHE:HB3	1.84	0.42
1:K:81:LYS:NZ	1:K:82:ALA:HA	2.34	0.42
1:K:507:ASP:OD1	1:K:507:ASP:N	2.45	0.42
1:L:942:PRO:HB2	1:L:943:HIS:ND1	2.34	0.42
1:J:347:TYR:HH	1:J:576:LYS:H	1.65	0.42
1:J:594:TRP:CD1	1:J:595:ASN:H	2.37	0.42
1:J:678:ILE:HD13	1:J:678:ILE:HA	1.94	0.42
1:K:487:ASN:HD21	1:K:550:ARG:HH21	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:551:ASN:ND2	1:L:554:LEU:H	2.18	0.42
1:J:70:PRO:HD3	1:J:625:CYS:HA	2.00	0.42
1:J:344:LEU:HD11	1:J:571:ILE:HD11	2.00	0.42
1:J:530:ASN:HD21	1:J:814:ARG:NH2	2.17	0.42
1:J:608:LEU:HD13	1:J:608:LEU:HA	1.71	0.42
1:J:808:ASN:HD21	1:J:879:ARG:HB3	1.84	0.42
1:K:72:ASP:C	1:K:81:LYS:HZ1	2.27	0.42
1:K:338:ARG:NH1	1:K:716:ILE:HD11	2.34	0.42
1:K:787:ILE:HD13	1:K:793:TYR:CE1	2.54	0.42
1:K:848:ARG:H	1:K:848:ARG:HG3	1.59	0.42
1:L:231:ARG:NE	1:L:297:GLU:OE2	2.50	0.42
1:L:693:ARG:NH2	1:L:925:THR:OG1	2.50	0.42
1:L:757:LYS:HE2	1:L:757:LYS:HB2	1.77	0.42
1:J:51:ALA:HB1	1:L:893:MET:HG3	2.01	0.42
1:J:266:LEU:H	1:J:266:LEU:HG	1.62	0.42
1:J:375:GLU:OE1	1:J:375:GLU:HA	2.19	0.42
1:J:855:ALA:O	1:K:256:GLN:NE2	2.53	0.42
1:K:759:SER:OG	1:K:760:VAL:N	2.51	0.42
1:L:349:SER:OG	1:L:352:ASN:O	2.38	0.42
1:L:368:ASP:OD1	1:L:372:ARG:NH1	2.53	0.42
1:L:393:SER:OG	1:L:394:MET:N	2.53	0.42
1:L:678:ILE:HB	1:L:912:LEU:HD23	2.01	0.42
1:L:730:LYS:HD3	1:L:730:LYS:HA	1.27	0.42
1:J:657:TYR:O	1:J:657:TYR:HD1	2.03	0.42
1:K:209:PHE:HD2	1:K:212:GLU:OE2	2.03	0.42
1:K:367:VAL:HB	1:K:951:TYR:HE2	1.85	0.42
1:L:440:THR:HG23	1:L:450:THR:CA	2.50	0.42
1:J:446:GLN:C	1:J:449:THR:HB	2.44	0.42
1:J:480:TRP:HE1	1:J:484:LEU:HD21	1.85	0.42
1:J:713:SER:O	1:J:714:GLY:O	2.38	0.42
1:K:187:LEU:HB2	1:K:293:VAL:HG11	2.01	0.42
1:K:220:TRP:CZ3	1:K:426:GLY:HA3	2.55	0.42
1:K:395:TRP:CD1	1:K:395:TRP:N	2.86	0.42
1:K:565:ARG:C	1:K:566:TYR:CG	2.97	0.42
1:K:717:PRO:HA	1:K:720:ASP:CG	2.45	0.42
1:L:251:ASN:OD1	1:L:255:GLY:N	2.37	0.42
2:Z:343:PRO:HD3	2:Z:367:TYR:CZ	2.54	0.42
1:J:599:ASP:OD2	1:J:602:MET:N	2.53	0.41
1:K:20:ALA:O	1:K:24:LEU:HB2	2.20	0.41
1:K:108:ASP:CG	1:K:110:GLY:H	2.28	0.41
1:K:127:LYS:HE2	1:K:243:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:192:ALA:HB3	1:K:200:GLY:HA2	2.01	0.41
1:K:548:HIS:CG	1:K:549:HIS:H	2.38	0.41
1:K:685:ALA:HB2	1:L:10:TRP:CZ2	2.54	0.41
1:K:727:HIS:CE1	1:K:876:LEU:HD13	2.54	0.41
1:K:807:ARG:HH21	1:L:390:ARG:CZ	2.33	0.41
1:K:830:ILE:H	1:K:830:ILE:HD12	1.86	0.41
1:L:328:MET:HG3	1:L:329:PRO:HD2	2.02	0.41
1:L:438:LYS:O	1:L:450:THR:HG23	2.20	0.41
1:J:116:TYR:CG	1:L:531:LEU:HD13	2.55	0.41
1:J:468:ASN:OD1	1:J:469:PHE:N	2.53	0.41
1:J:635:HIS:C	1:J:638:ALA:HB3	2.46	0.41
1:J:818:ASP:OD2	1:J:820:THR:N	2.54	0.41
1:K:113:PHE:HB2	1:K:335:ILE:HD13	2.02	0.41
1:K:438:LYS:O	1:K:450:THR:HG22	2.20	0.41
1:K:508:ASN:HA	1:K:509:PRO:HD3	1.90	0.41
1:J:432:ASP:O	1:J:434:PHE:HD1	2.03	0.41
1:K:551:ASN:HB3	1:K:554:LEU:HB2	2.02	0.41
1:K:668:PRO:HG2	1:K:671:ALA:HB2	2.02	0.41
1:L:428:ILE:HA	1:L:468:ASN:OD1	2.20	0.41
1:L:676:ILE:HG21	1:L:914:MET:HE2	2.01	0.41
1:J:289:GLN:NE2	1:K:448:ASN:HD22	2.19	0.41
1:J:390:ARG:CZ	1:L:807:ARG:HH21	2.34	0.41
1:K:747:ARG:HA	1:L:64:LEU:HG	2.02	0.41
1:K:898:ASP:OD1	1:K:899:LEU:N	2.53	0.41
1:L:889:ASN:OD1	1:L:891:MET:HB2	2.21	0.41
1:J:379:GLN:C	1:J:381:LEU:N	2.77	0.41
1:J:388:ARG:HA	1:J:388:ARG:HD2	1.69	0.41
1:K:479:LEU:HD12	1:K:479:LEU:HA	1.88	0.41
1:K:569:PHE:HD1	1:K:569:PHE:H	1.68	0.41
1:K:758:ARG:NH2	1:K:763:GLU:H	2.13	0.41
1:L:651:ASP:OD2	1:L:938:ARG:NH1	2.54	0.41
1:L:899:LEU:HA	1:L:899:LEU:HD23	1.80	0.41
1:J:58:THR:HB	1:J:635:HIS:CE1	2.56	0.41
1:J:646:ARG:O	1:J:647:ASN:C	2.64	0.41
1:J:749:LEU:HD22	1:J:749:LEU:H	1.85	0.41
1:J:807:ARG:HH21	1:K:390:ARG:NH1	2.18	0.41
1:J:856:ASN:OD1	1:J:856:ASN:N	2.52	0.41
1:K:443:ASN:OD1	1:K:443:ASN:N	2.53	0.41
1:K:742:TRP:HB3	1:K:743:PRO:HD3	2.02	0.41
1:K:755:GLU:O	1:K:773:THR:OG1	2.23	0.41
1:J:51:ALA:HB1	1:J:52:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:461:ASN:CG	1:L:171:VAL:H	2.28	0.41
1:J:642:GLU:CD	1:J:646:ARG:HE	2.28	0.41
1:K:251:ASN:ND2	1:K:253:ASN:H	2.18	0.41
1:K:339:ASP:O	1:K:342:ILE:HG13	2.20	0.41
1:K:417:GLU:O	1:K:418:LEU:C	2.64	0.41
1:K:717:PRO:HB3	1:K:722:THR:O	2.21	0.41
1:K:834:HIS:HB3	1:L:214:GLN:NE2	2.35	0.41
1:L:342:ILE:O	1:L:344:LEU:HD23	2.20	0.41
1:L:563:ASN:OD1	1:L:563:ASN:N	2.50	0.41
2:Z:397:VAL:HG22	2:Z:412:TYR:CE2	2.56	0.41
2:Z:416:THR:HA	2:Z:419:LEU:HG	2.03	0.41
1:J:440:THR:OG1	1:J:449:THR:O	2.39	0.41
1:J:529:ILE:C	1:J:531:LEU:N	2.79	0.41
1:L:577:PHE:O	1:L:581:LYS:HB2	2.21	0.41
1:L:901:GLN:H	1:L:901:GLN:HG3	1.48	0.41
1:J:169:THR:HB	1:K:457:PHE:CE1	2.56	0.41
1:J:252:SER:O	1:J:253:ASN:HB3	2.20	0.41
1:J:301:MET:HE1	1:L:854:PRO:HG3	2.02	0.41
1:J:605:GLN:OE1	1:J:714:GLY:O	2.39	0.41
1:K:79:SER:N	1:K:598:LYS:HD3	2.36	0.41
1:K:195:THR:HG22	1:K:196:VAL:H	1.85	0.41
1:K:290:PRO:HD2	1:L:448:ASN:OD1	2.21	0.41
1:K:354:GLY:HA3	1:K:594:TRP:CZ3	2.56	0.41
1:K:818:ASP:CG	1:K:819:ASP:H	2.29	0.41
1:L:234:LYS:HD3	1:L:296:SER:HB2	2.02	0.41
1:L:481:ARG:HH12	1:L:840:VAL:HG21	1.85	0.41
1:L:678:ILE:HD13	1:L:678:ILE:HA	1.84	0.41
1:L:702:LEU:H	1:L:702:LEU:HG	1.65	0.41
1:J:188:GLN:OE1	1:J:190:GLY:N	2.54	0.41
1:J:529:ILE:HD12	1:J:529:ILE:HA	1.74	0.41
1:J:579:ALA:HB3	1:J:580:ILE:HD13	2.03	0.41
1:K:206:ASP:H	1:K:210:GLN:CB	2.25	0.41
1:K:318:ASN:OD1	1:K:318:ASN:N	2.52	0.41
1:K:454:ASP:HA	1:K:457:PHE:HB2	2.03	0.41
1:L:340:ASN:HD21	1:L:397:GLN:HA	1.86	0.41
1:L:346:TYR:C	1:L:347:TYR:CG	2.98	0.41
2:Z:28:ARG:NH2	2:Z:34:SER:CB	2.79	0.41
2:Z:82:GLU:OE1	2:Z:83:LEU:N	2.54	0.41
1:J:433:THR:HB	1:J:460:ARG:HH12	1.87	0.40
1:J:709:TYR:N	1:J:709:TYR:CD1	2.89	0.40
1:K:31:PHE:CZ	1:K:35:THR:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:529:ILE:O	1:K:529:ILE:HG23	2.20	0.40
1:L:693:ARG:HH22	1:L:921:MET:CG	2.34	0.40
2:Z:235:ALA:HA	2:Z:284:ALA:HB2	2.03	0.40
1:J:853:TYR:OH	1:K:231:ARG:HD3	2.21	0.40
1:K:19:ASP:CB	1:K:21:SER:HB3	2.51	0.40
1:K:756:ILE:H	1:K:756:ILE:HG13	1.68	0.40
1:K:853:TYR:HE2	1:L:231:ARG:HB3	1.86	0.40
1:L:247:ALA:HB3	1:L:256:GLN:OE1	2.21	0.40
1:L:266:LEU:H	1:L:266:LEU:HG	1.58	0.40
1:L:692:THR:HG21	1:L:723:PHE:HD2	1.86	0.40
1:J:100:TYR:CE2	1:J:394:MET:HE1	2.56	0.40
1:J:229:GLY:HA2	1:J:293:VAL:O	2.22	0.40
1:J:578:PHE:CE2	1:J:655:ASN:HA	2.56	0.40
1:J:818:ASP:OD1	1:J:821:LYS:N	2.54	0.40
1:K:133:CYS:HA	1:K:232:VAL:HG23	2.03	0.40
1:K:378:TYR:CZ	1:K:382:LEU:HD12	2.57	0.40
1:K:603:VAL:O	1:K:604:LEU:HD23	2.22	0.40
1:J:502:ASN:OD1	1:J:502:ASN:N	2.54	0.40
1:J:605:GLN:NE2	1:J:714:GLY:O	2.54	0.40
1:K:656:ASP:O	1:K:659:SER:OG	2.37	0.40
1:L:235:LYS:HB2	1:L:235:LYS:HE2	1.78	0.40
1:L:695:LYS:C	1:L:697:LYS:N	2.79	0.40
1:J:94:LEU:HD23	1:J:585:LEU:HB3	2.03	0.40
1:J:387:ASP:OD2	1:J:389:THR:HG22	2.21	0.40
1:J:537:LEU:HA	1:J:537:LEU:HD13	1.75	0.40
1:J:564:GLY:N	1:L:815:GLN:OE1	2.48	0.40
1:J:565:ARG:HD3	1:J:566:TYR:CZ	2.57	0.40
1:J:725:LEU:O	1:J:728:THR:OG1	2.31	0.40
1:K:24:LEU:HA	1:K:24:LEU:HD23	1.86	0.40
1:K:278:SER:O	1:K:282:THR:HG23	2.21	0.40
1:K:433:THR:HG22	1:K:460:ARG:O	2.21	0.40
1:K:837:SER:OG	1:K:838:GLY:N	2.53	0.40
1:L:611:ASP:OD2	1:L:614:VAL:HG23	2.20	0.40
1:L:651:ASP:C	1:L:652:GLN:HG2	2.46	0.40
1:L:940:HIS:HD1	1:L:948:GLU:HB3	1.86	0.40
2:Z:95:ASP:OD1	2:Z:95:ASP:N	2.55	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	J	927/963 (96%)	763 (82%)	135 (15%)	29 (3%)	3	21
1	K	931/963 (97%)	784 (84%)	139 (15%)	8 (1%)	14	50
1	L	926/963 (96%)	814 (88%)	102 (11%)	10 (1%)	11	45
2	Z	362/488 (74%)	343 (95%)	18 (5%)	1 (0%)	36	72
All	All	3146/3377 (93%)	2704 (86%)	394 (12%)	48 (2%)	11	38

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	255	GLY
1	J	286	ASN
1	J	530	ASN
1	J	603	VAL
1	J	646	ARG
1	J	91	ASN
1	J	253	ASN
1	J	383	ASP
1	J	429	GLY
1	J	599	ASP
1	J	607	SER
1	J	659	SER
1	J	705	GLY
1	J	709	TYR
1	K	23	TYR
1	L	725	LEU
1	J	338	ARG
1	J	374	THR
1	J	714	GLY
1	K	208	THR
1	K	209	PHE
1	L	172	TYR

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Mol	Chain	Res	Type
1	L	696	THR
1	L	727	HIS
1	L	728	THR
1	J	384	SER
1	J	712	TYR
1	K	205	ALA
1	K	213	PRO
1	L	562	GLY
1	L	879	ARG
2	Z	18	MET
1	J	282	THR
1	J	379	GLN
1	J	445	ASP
1	J	606	SER
1	J	644	MET
1	K	336	ALA
1	K	341	PHE
1	L	173	ALA
1	L	651	ASP
1	J	285	VAL
1	J	463	ILE
1	J	254	GLY
1	J	342	ILE
1	L	942	PRO
1	J	716	ILE
1	K	437	VAL

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	J	800/826 (97%)	618 (77%)	182 (23%)	1	6
1	K	803/826 (97%)	673 (84%)	130 (16%)	2	12
1	L	801/826 (97%)	675 (84%)	126 (16%)	2	12
2	Z	313/408 (77%)	302 (96%)	11 (4%)	32	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2717/2886 (94%)	2268 (84%)	449 (16%)	4 11

All (449) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	6	MET
1	J	7	MET
1	J	19	ASP
1	J	28	LEU
1	J	35	THR
1	J	37	THR
1	J	49	THR
1	J	53	THR
1	J	54	HIS
1	J	55	ASP
1	J	56	VAL
1	J	58	THR
1	J	62	GLN
1	J	64	LEU
1	J	65	THR
1	J	66	LEU
1	J	69	ILE
1	J	71	VAL
1	J	73	ARG
1	J	74	GLU
1	J	75	ASP
1	J	78	TYR
1	J	91	ASN
1	J	92	ARG
1	J	93	VAL
1	J	94	LEU
1	J	100	TYR
1	J	107	LEU
1	J	124	LEU
1	J	131	ASN
1	J	134	GLU
1	J	136	GLU
1	J	139	GLU
1	J	170	HIS
1	J	171	VAL
1	J	181	LYS
1	J	183	THR

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Mol	Chain	Res	Type
1	J	184	LYS
1	J	187	LEU
1	J	201	LYS
1	J	206	ASP
1	J	215	VAL
1	J	219	GLN
1	J	224	ASP
1	J	243	TYR
1	J	246	TYR
1	J	248	ARG
1	J	251	ASN
1	J	259	MET
1	J	262	GLN
1	J	266	LEU
1	J	269	GLN
1	J	276	SER
1	J	277	THR
1	J	278	SER
1	J	279	THR
1	J	282	THR
1	J	288	ILE
1	J	292	VAL
1	J	293	VAL
1	J	302	GLU
1	J	303	THR
1	J	318	ASN
1	J	322	MET
1	J	335	ILE
1	J	337	PHE
1	J	339	ASP
1	J	347	TYR
1	J	350	THR
1	J	352	ASN
1	J	359	GLN
1	J	363	LEU
1	J	371	ASP
1	J	372	ARG
1	J	374	THR
1	J	376	LEU
1	J	377	SER
1	J	382	LEU
1	J	385	ILE

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Mol	Chain	Res	Type
1	J	389	THR
1	J	394	MET
1	J	401	SER
1	J	409	ILE
1	J	412	HIS
1	J	417	GLU
1	J	420	ASN
1	J	428	ILE
1	J	430	ILE
1	J	431	THR
1	J	432	ASP
1	J	438	LYS
1	J	445	ASP
1	J	454	ASP
1	J	459	GLU
1	J	460	ARG
1	J	462	GLU
1	J	463	ILE
1	J	465	VAL
1	J	472	GLU
1	J	494	ASP
1	J	503	VAL
1	J	504	GLU
1	J	507	ASP
1	J	508	ASN
1	J	510	ASN
1	J	513	ASP
1	J	525	VAL
1	J	528	TYR
1	J	529	ILE
1	J	531	LEU
1	J	534	ARG
1	J	536	SER
1	J	537	LEU
1	J	539	TYR
1	J	540	MET
1	J	543	VAL
1	J	548	HIS
1	J	551	ASN
1	J	558	SER
1	J	561	LEU
1	J	563	ASN

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Mol	Chain	Res	Type
1	J	567	VAL
1	J	569	PHE
1	J	573	VAL
1	J	580	ILE
1	J	582	ASN
1	J	584	LEU
1	J	591	THR
1	J	593	GLU
1	J	595	ASN
1	J	598	LYS
1	J	603	VAL
1	J	604	LEU
1	J	605	GLN
1	J	606	SER
1	J	608	LEU
1	J	613	ARG
1	J	619	ILE
1	J	622	ASP
1	J	629	THR
1	J	635	HIS
1	J	636	ASN
1	J	646	ARG
1	J	650	ASN
1	J	654	PHE
1	J	655	ASN
1	J	657	TYR
1	J	659	SER
1	J	662	ASN
1	J	663	MET
1	J	665	TYR
1	J	678	ILE
1	J	692	THR
1	J	701	SER
1	J	702	LEU
1	J	704	SER
1	J	709	TYR
1	J	727	HIS
1	J	734	ILE
1	J	737	ASP
1	J	756	ILE
1	J	759	SER
1	J	766	ASN

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Mol	Chain	Res	Type
1	J	770	CYS
1	J	771	ASN
1	J	775	ASP
1	J	787	ILE
1	J	812	MET
1	J	815	GLN
1	J	818	ASP
1	J	823	LYS
1	J	830	ILE
1	J	848	ARG
1	J	853	TYR
1	J	862	ILE
1	J	867	VAL
1	J	868	ASP
1	J	870	ILE
1	J	887	SER
1	J	910	HIS
1	J	912	LEU
1	J	913	ASP
1	K	6	MET
1	K	9	GLN
1	K	10	TRP
1	K	16	SER
1	K	18	GLN
1	K	19	ASP
1	K	21	SER
1	K	37	THR
1	K	41	LEU
1	K	56	VAL
1	K	62	GLN
1	K	69	ILE
1	K	74	GLU
1	K	80	TYR
1	K	81	LYS
1	K	90	ASP
1	K	93	VAL
1	K	95	ASP
1	K	100	TYR
1	K	102	ASP
1	K	107	LEU
1	K	108	ASP
1	K	112	THR

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Mol	Chain	Res	Type
1	K	131	ASN
1	K	134	GLU
1	K	136	GLU
1	K	181	LYS
1	K	188	GLN
1	K	195	THR
1	K	210	GLN
1	K	214	GLN
1	K	215	VAL
1	K	224	ASP
1	K	232	VAL
1	K	251	ASN
1	K	263	ASN
1	K	266	LEU
1	K	277	THR
1	K	283	ASN
1	K	287	ASN
1	K	293	VAL
1	K	305	ASP
1	K	308	LEU
1	K	316	ASP
1	K	333	ASN
1	K	335	ILE
1	K	338	ARG
1	K	344	LEU
1	K	348	ASN
1	K	352	ASN
1	K	362	GLN
1	K	367	VAL
1	K	371	ASP
1	K	383	ASP
1	K	391	TYR
1	K	395	TRP
1	K	397	GLN
1	K	403	ASP
1	K	409	ILE
1	K	414	THR
1	K	418	LEU
1	K	430	ILE
1	K	431	THR
1	K	435	GLN
1	K	440	THR

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Mol	Chain	Res	Type
1	K	443	ASN
1	K	463	ILE
1	K	467	ASN
1	K	468	ASN
1	K	473	ILE
1	K	499	ASN
1	K	503	VAL
1	K	505	ILE
1	K	516	ASN
1	K	524	LEU
1	K	525	VAL
1	K	531	LEU
1	K	537	LEU
1	K	547	ASN
1	K	558	SER
1	K	560	LEU
1	K	561	LEU
1	K	563	ASN
1	K	565	ARG
1	K	569	PHE
1	K	583	LEU
1	K	584	LEU
1	K	591	THR
1	K	595	ASN
1	K	599	ASP
1	K	602	MET
1	K	604	LEU
1	K	606	SER
1	K	615	ASP
1	K	624	ILE
1	K	645	LEU
1	K	647	ASN
1	K	649	THR
1	K	651	ASP
1	K	662	ASN
1	K	667	ILE
1	K	676	ILE
1	K	691	PHE
1	K	692	THR
1	K	702	LEU
1	K	711	THR
1	K	716	ILE

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Mol	Chain	Res	Type
1	K	726	ASN
1	K	727	HIS
1	K	732	VAL
1	K	737	ASP
1	K	757	LYS
1	K	766	ASN
1	K	767	VAL
1	K	771	ASN
1	K	775	ASP
1	K	819	ASP
1	K	824	ASP
1	K	848	ARG
1	K	868	ASP
1	K	869	SER
1	K	871	THR
1	K	881	LEU
1	K	887	SER
1	K	897	THR
1	K	933	VAL
1	K	935	ASP
1	K	936	VAL
1	K	938	ARG
1	K	940	HIS
1	L	3	THR
1	L	5	SER
1	L	6	MET
1	L	19	ASP
1	L	31	PHE
1	L	38	TYR
1	L	50	VAL
1	L	54	HIS
1	L	55	ASP
1	L	56	VAL
1	L	58	THR
1	L	75	ASP
1	L	91	ASN
1	L	100	TYR
1	L	112	THR
1	L	116	TYR
1	L	139	GLU
1	L	167	LYS
1	L	168	LYS

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Mol	Chain	Res	Type
1	L	169	THR
1	L	170	HIS
1	L	171	VAL
1	L	181	LYS
1	L	224	ASP
1	L	232	VAL
1	L	235	LYS
1	L	237	THR
1	L	248	ARG
1	L	250	THR
1	L	262	GLN
1	L	266	LEU
1	L	269	GLN
1	L	272	MET
1	L	277	THR
1	L	288	ILE
1	L	293	VAL
1	L	300	ASN
1	L	302	GLU
1	L	303	THR
1	L	313	LYS
1	L	334	TYR
1	L	335	ILE
1	L	337	PHE
1	L	342	ILE
1	L	344	LEU
1	L	345	MET
1	L	356	LEU
1	L	369	LEU
1	L	405	ASP
1	L	409	ILE
1	L	416	ASP
1	L	431	THR
1	L	432	ASP
1	L	445	ASP
1	L	454	ASP
1	L	478	ASN
1	L	501	THR
1	L	503	VAL
1	L	505	ILE
1	L	520	VAL
1	L	525	VAL

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Mol	Chain	Res	Type
1	L	537	LEU
1	L	547	ASN
1	L	563	ASN
1	L	565	ARG
1	L	580	ILE
1	L	585	LEU
1	L	590	TYR
1	L	596	PHE
1	L	598	LYS
1	L	606	SER
1	L	610	ASN
1	L	615	ASP
1	L	619	ILE
1	L	624	ILE
1	L	656	ASP
1	L	663	MET
1	L	664	LEU
1	L	672	THR
1	L	676	ILE
1	L	681	ARG
1	L	692	THR
1	L	702	LEU
1	L	724	TYR
1	L	725	LEU
1	L	727	HIS
1	L	728	THR
1	L	730	LYS
1	L	745	ASN
1	L	749	LEU
1	L	755	GLU
1	L	756	ILE
1	L	757	LYS
1	L	761	ASP
1	L	770	CYS
1	L	771	ASN
1	L	772	MET
1	L	777	PHE
1	L	778	LEU
1	L	779	VAL
1	L	787	ILE
1	L	796	GLU
1	L	800	ASP

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Mol	Chain	Res	Type
1	L	803	TYR
1	L	821	LYS
1	L	824	ASP
1	L	848	ARG
1	L	853	TYR
1	L	861	LEU
1	L	862	ILE
1	L	876	LEU
1	L	878	ASP
1	L	880	THR
1	L	887	SER
1	L	891	MET
1	L	897	THR
1	L	901	GLN
1	L	903	LEU
1	L	904	LEU
1	L	912	LEU
1	L	923	GLU
1	L	929	VAL
1	L	933	VAL
1	L	938	ARG
1	L	940	HIS
1	L	953	ARG
2	Z	17	CYS
2	Z	37	THR
2	Z	41	TRP
2	Z	55	CYS
2	Z	72	CYS
2	Z	82	GLU
2	Z	83	LEU
2	Z	95	ASP
2	Z	102	GLU
2	Z	111	CYS
2	Z	120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	47	ASN
1	J	210	GLN
1	J	269	GLN
1	J	287	ASN

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Mol	Chain	Res	Type
1	J	359	GLN
1	J	370	GLN
1	J	373	ASN
1	J	411	ASN
1	J	448	ASN
1	J	461	ASN
1	J	487	ASN
1	J	605	GLN
1	J	815	GLN
1	K	62	GLN
1	K	256	GLN
1	K	262	GLN
1	K	300	ASN
1	K	318	ASN
1	K	448	ASN
1	K	530	ASN
1	K	595	ASN
1	K	605	GLN
1	K	655	ASN
1	K	769	GLN
1	K	780	GLN
1	L	188	GLN
1	L	262	GLN
1	L	340	ASN
1	L	420	ASN
1	L	468	ASN
1	L	662	ASN
1	L	832	HIS
1	L	907	ASN
2	Z	120	ASN
2	Z	135	GLN
2	Z	199	GLN
2	Z	271	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CGU	Z	25	2	9,11,12	1.40	0	10,14,16	0.90	0
2	CGU	Z	14	2	9,11,12	1.57	2 (22%)	10,14,16	0.86	0
2	CGU	Z	19	2	9,11,12	1.45	1 (11%)	10,14,16	0.97	0
2	CGU	Z	6	2,3	9,11,12	1.81	2 (22%)	10,14,16	0.84	0
2	CGU	Z	26	2,3	9,11,12	1.36	0	10,14,16	0.78	0
2	CGU	Z	32	2	9,11,12	1.55	1 (11%)	10,14,16	0.86	0
2	CGU	Z	29	2,3	9,11,12	1.53	1 (11%)	10,14,16	0.98	0
2	CGU	Z	39	2	9,11,12	1.46	1 (11%)	10,14,16	0.93	0
2	CGU	Z	20	2	9,11,12	1.41	0	10,14,16	0.84	0
2	CGU	Z	16	2,3	9,11,12	1.44	1 (11%)	10,14,16	0.82	0
2	CGU	Z	7	2,3	9,11,12	1.53	1 (11%)	10,14,16	0.83	0

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
2	CGU	Z	25	2	-	5/13/14/16	-
2	CGU	Z	14	2	-	6/13/14/16	-
2	CGU	Z	19	2	-	7/13/14/16	-
2	CGU	Z	6	2,3	-	5/13/14/16	-
2	CGU	Z	26	2,3	-	7/13/14/16	-
2	CGU	Z	32	2	-	7/13/14/16	-
2	CGU	Z	29	2,3	-	6/13/14/16	-
2	CGU	Z	39	2	-	8/13/14/16	-
2	CGU	Z	20	2	-	3/13/14/16	-
2	CGU	Z	16	2,3	-	4/13/14/16	-
2	CGU	Z	7	2,3	-	8/13/14/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	6	CGU	CG-CD2	3.03	1.56	1.52
2	Z	6	CGU	CG-CD1	2.77	1.55	1.52
2	Z	32	CGU	CG-CD2	2.69	1.55	1.52
2	Z	7	CGU	CG-CD2	2.43	1.55	1.52
2	Z	14	CGU	CG-CD2	2.31	1.55	1.52
2	Z	14	CGU	CG-CD1	2.23	1.55	1.52
2	Z	29	CGU	CG-CD2	2.19	1.54	1.52
2	Z	16	CGU	CG-CD2	2.17	1.54	1.52
2	Z	39	CGU	CG-CD1	2.17	1.54	1.52
2	Z	19	CGU	CG-CD2	2.01	1.54	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Z	6	CGU	N-CA-CB-CG
2	Z	6	CGU	C-CA-CB-CG
2	Z	7	CGU	C-CA-CB-CG
2	Z	19	CGU	O-C-CA-CB
2	Z	20	CGU	O-C-CA-CB
2	Z	20	CGU	OE12-CD1-CG-CD2
2	Z	25	CGU	N-CA-CB-CG
2	Z	25	CGU	C-CA-CB-CG
2	Z	25	CGU	CA-CB-CG-CD2
2	Z	25	CGU	OE12-CD1-CG-CB
2	Z	26	CGU	N-CA-CB-CG
2	Z	26	CGU	CA-CB-CG-CD1
2	Z	26	CGU	CA-CB-CG-CD2
2	Z	32	CGU	CA-CB-CG-CD2
2	Z	39	CGU	O-C-CA-CB
2	Z	39	CGU	CA-CB-CG-CD1
2	Z	39	CGU	CA-CB-CG-CD2
2	Z	7	CGU	N-CA-CB-CG
2	Z	32	CGU	N-CA-CB-CG
2	Z	6	CGU	OE21-CD2-CG-CB
2	Z	6	CGU	OE22-CD2-CG-CB
2	Z	7	CGU	OE11-CD1-CG-CB
2	Z	7	CGU	OE12-CD1-CG-CB
2	Z	7	CGU	OE21-CD2-CG-CB
2	Z	14	CGU	OE21-CD2-CG-CB
2	Z	16	CGU	OE11-CD1-CG-CB

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Mol	Chain	Res	Type	Atoms
2	Z	16	CGU	OE12-CD1-CG-CB
2	Z	19	CGU	OE21-CD2-CG-CB
2	Z	19	CGU	OE22-CD2-CG-CB
2	Z	25	CGU	OE11-CD1-CG-CB
2	Z	26	CGU	OE11-CD1-CG-CB
2	Z	26	CGU	OE12-CD1-CG-CB
2	Z	14	CGU	OE21-CD2-CG-CD1
2	Z	14	CGU	OE22-CD2-CG-CD1
2	Z	20	CGU	OE11-CD1-CG-CD2
2	Z	26	CGU	OE11-CD1-CG-CD2
2	Z	26	CGU	OE12-CD1-CG-CD2
2	Z	32	CGU	OE21-CD2-CG-CD1
2	Z	32	CGU	OE22-CD2-CG-CD1
2	Z	39	CGU	OE21-CD2-CG-CD1
2	Z	39	CGU	OE22-CD2-CG-CD1
2	Z	14	CGU	CA-CB-CG-CD1
2	Z	14	CGU	CA-CB-CG-CD2
2	Z	16	CGU	CA-CB-CG-CD1
2	Z	16	CGU	CA-CB-CG-CD2
2	Z	19	CGU	CA-CB-CG-CD1
2	Z	19	CGU	N-CA-CB-CG
2	Z	7	CGU	OE22-CD2-CG-CB
2	Z	14	CGU	OE22-CD2-CG-CB
2	Z	19	CGU	OE11-CD1-CG-CB
2	Z	19	CGU	OE12-CD1-CG-CB
2	Z	29	CGU	OE11-CD1-CG-CB
2	Z	29	CGU	OE12-CD1-CG-CB
2	Z	29	CGU	OE21-CD2-CG-CB
2	Z	29	CGU	OE22-CD2-CG-CB
2	Z	32	CGU	OE11-CD1-CG-CB
2	Z	32	CGU	OE12-CD1-CG-CB
2	Z	39	CGU	OE11-CD1-CG-CB
2	Z	39	CGU	OE12-CD1-CG-CB
2	Z	6	CGU	OE22-CD2-CG-CD1
2	Z	7	CGU	OE21-CD2-CG-CD1
2	Z	7	CGU	OE22-CD2-CG-CD1
2	Z	29	CGU	OE21-CD2-CG-CD1
2	Z	29	CGU	OE22-CD2-CG-CD1
2	Z	32	CGU	OE11-CD1-CG-CD2
2	Z	39	CGU	OE11-CD1-CG-CD2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	25	CGU	3	0
2	Z	14	CGU	1	0
2	Z	19	CGU	1	0
2	Z	6	CGU	1	0
2	Z	26	CGU	1	0
2	Z	32	CGU	1	0
2	Z	29	CGU	1	0
2	Z	20	CGU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

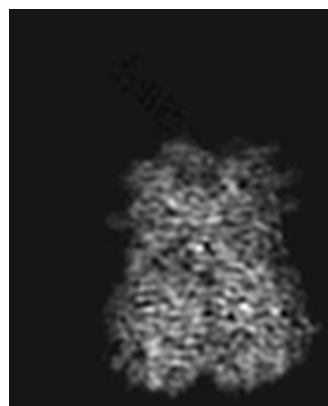
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45737. These allow visual inspection of the internal detail of the map and identification of artifacts.

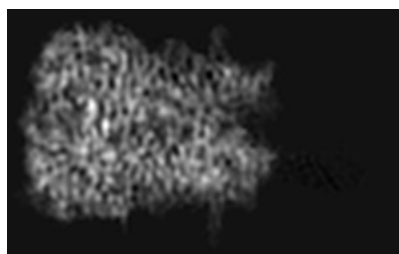
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

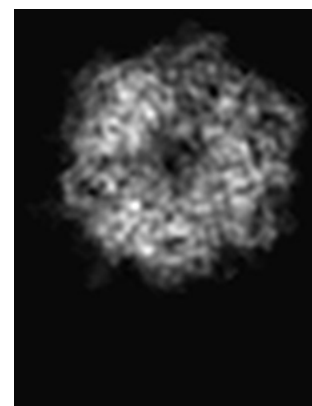
6.1.1 Primary map



X

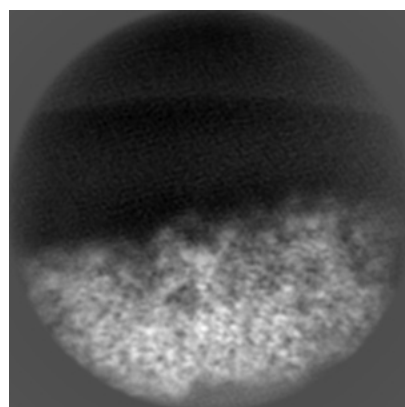


Y

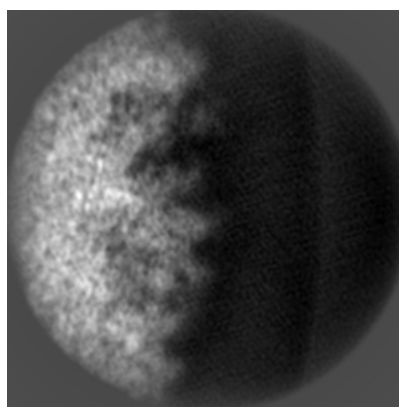


Z

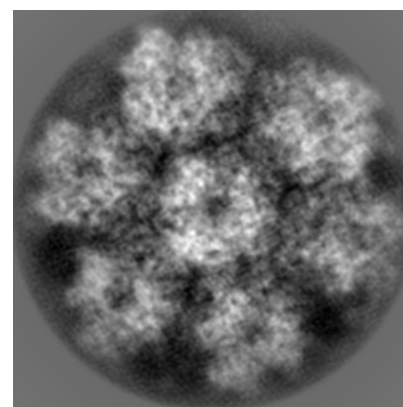
6.1.2 Raw map



X



Y



Z

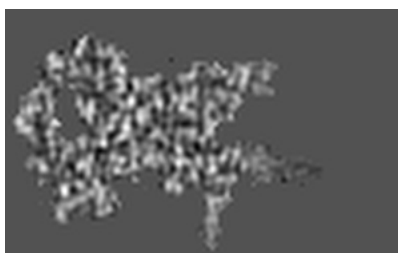
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 33

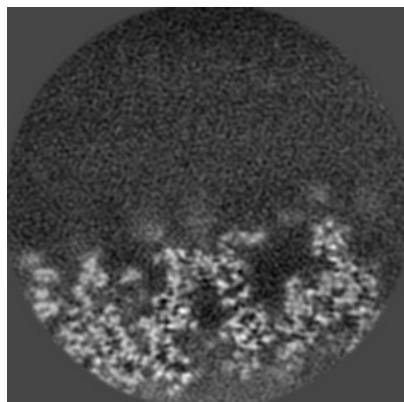


Y Index: 43

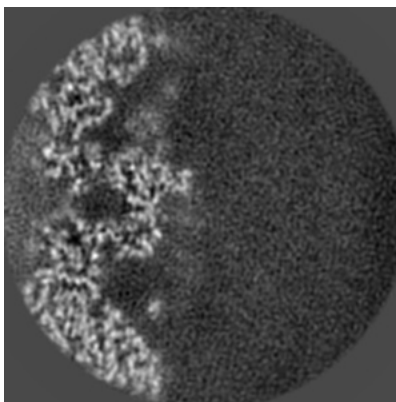


Z Index: 53

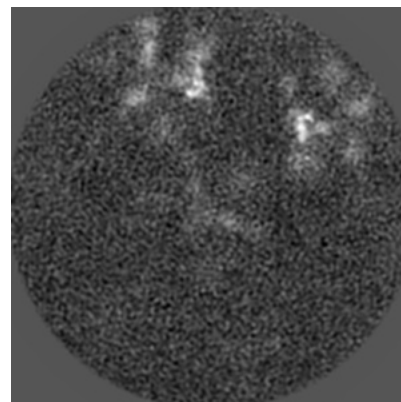
6.2.2 Raw map



X Index: 80



Y Index: 80

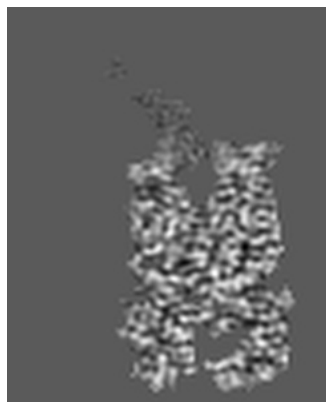


Z Index: 80

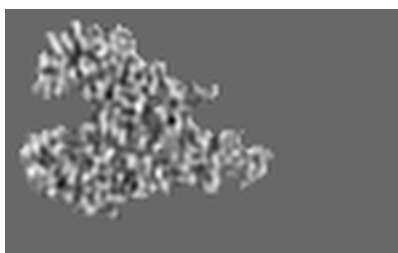
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

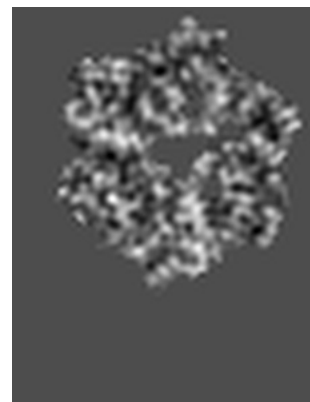
6.3.1 Primary map



X Index: 25

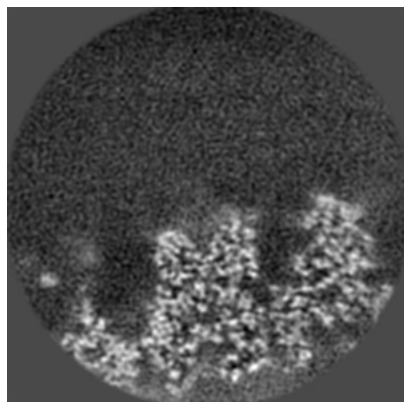


Y Index: 64

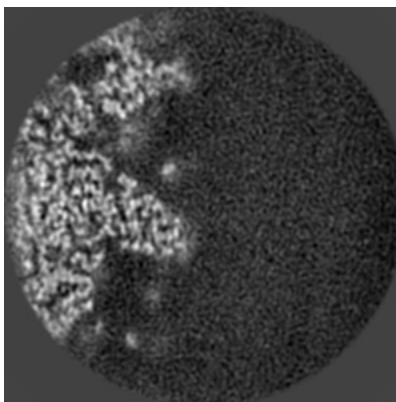


Z Index: 22

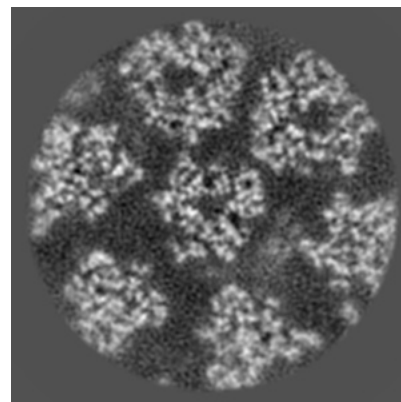
6.3.2 Raw map



X Index: 74



Y Index: 65



Z Index: 46

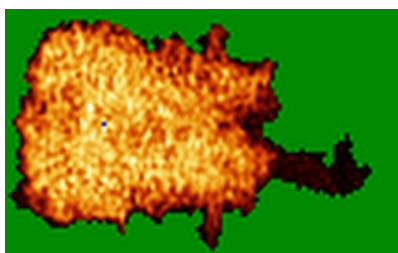
The images above show the largest variance slices of the map in three orthogonal directions.

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

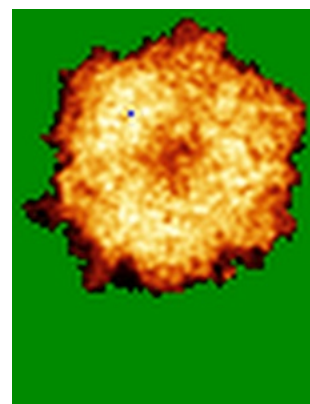
6.4.1 Primary map



X

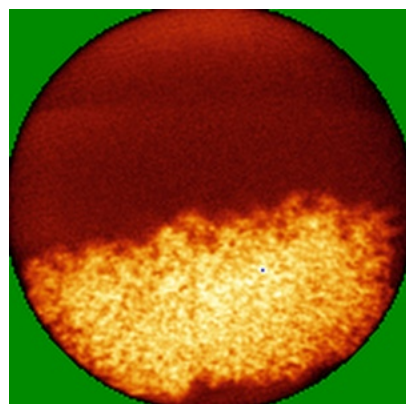


Y

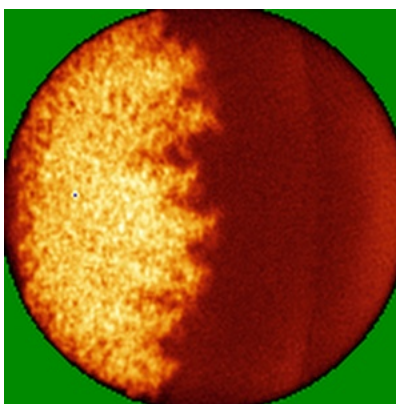


Z

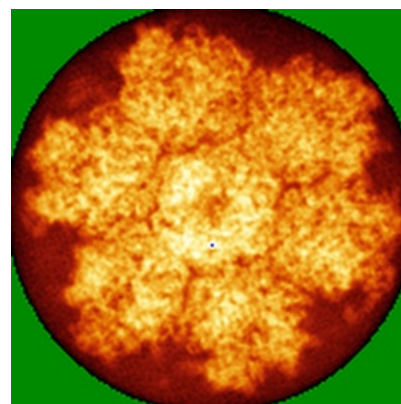
6.4.2 Raw map



X



Y

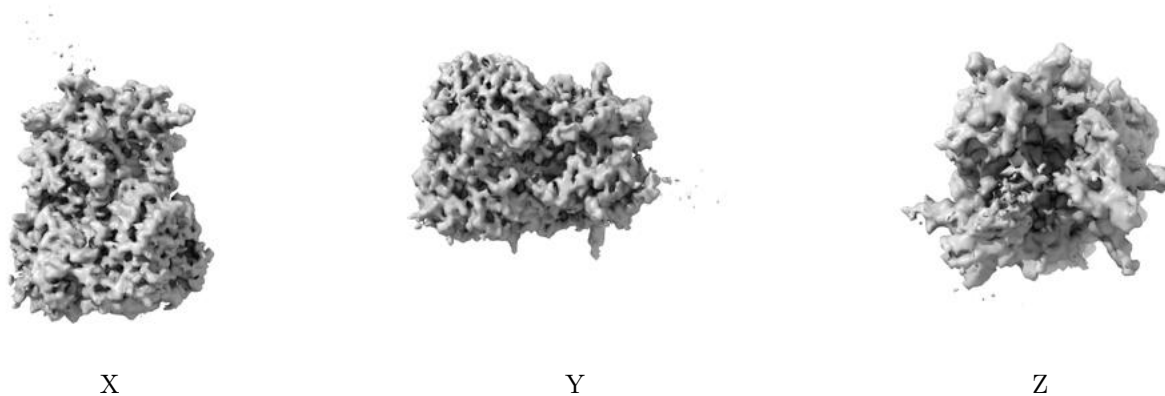


Z

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

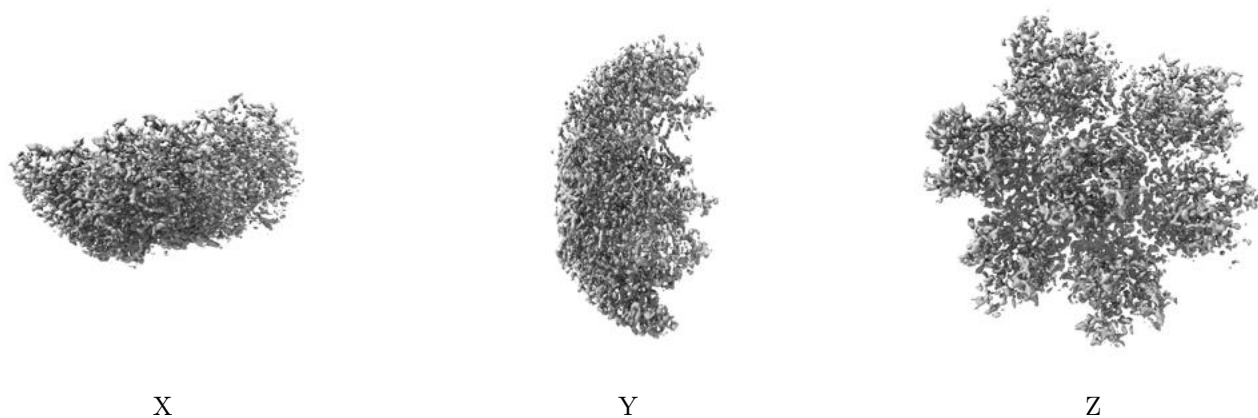
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

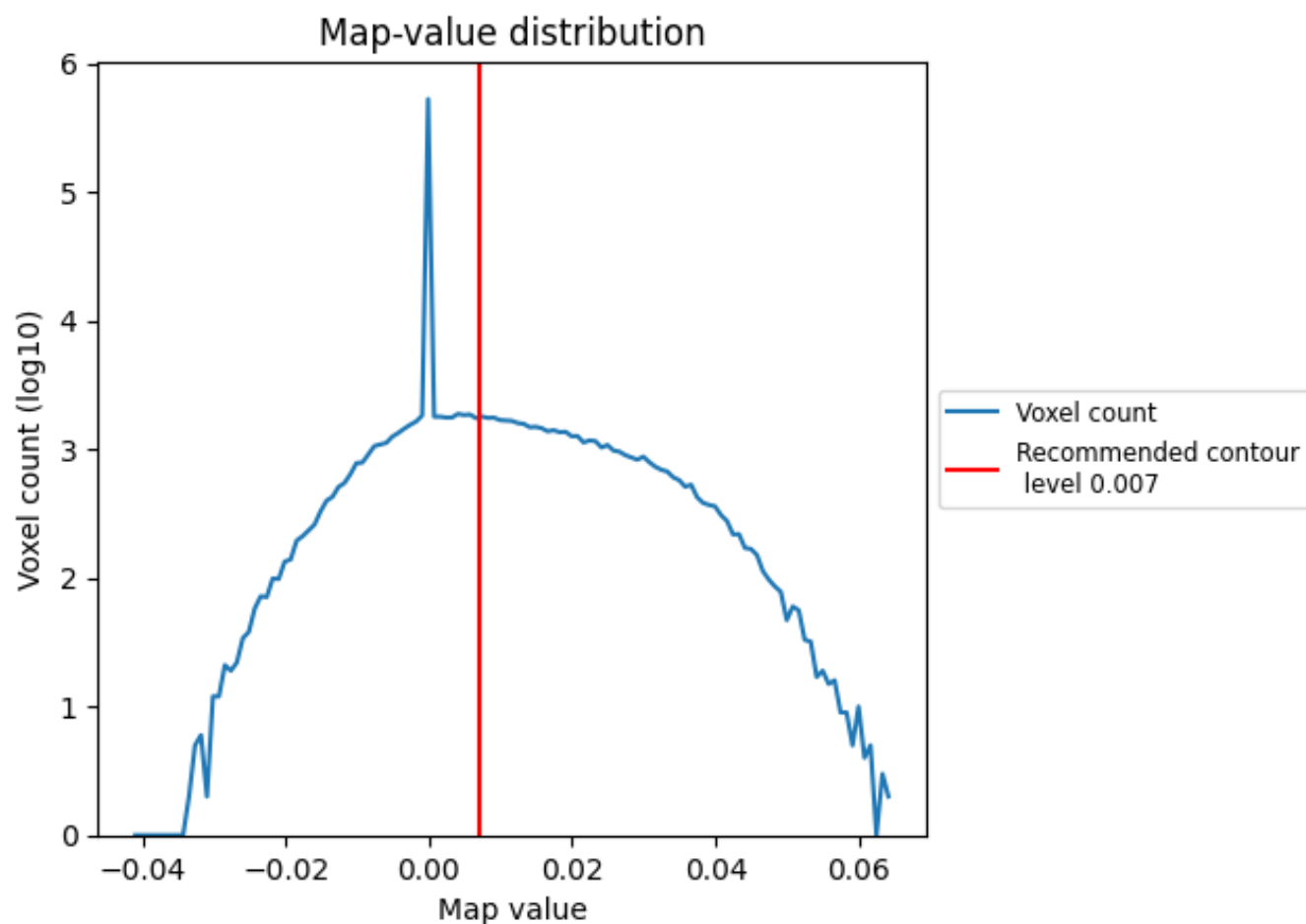
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

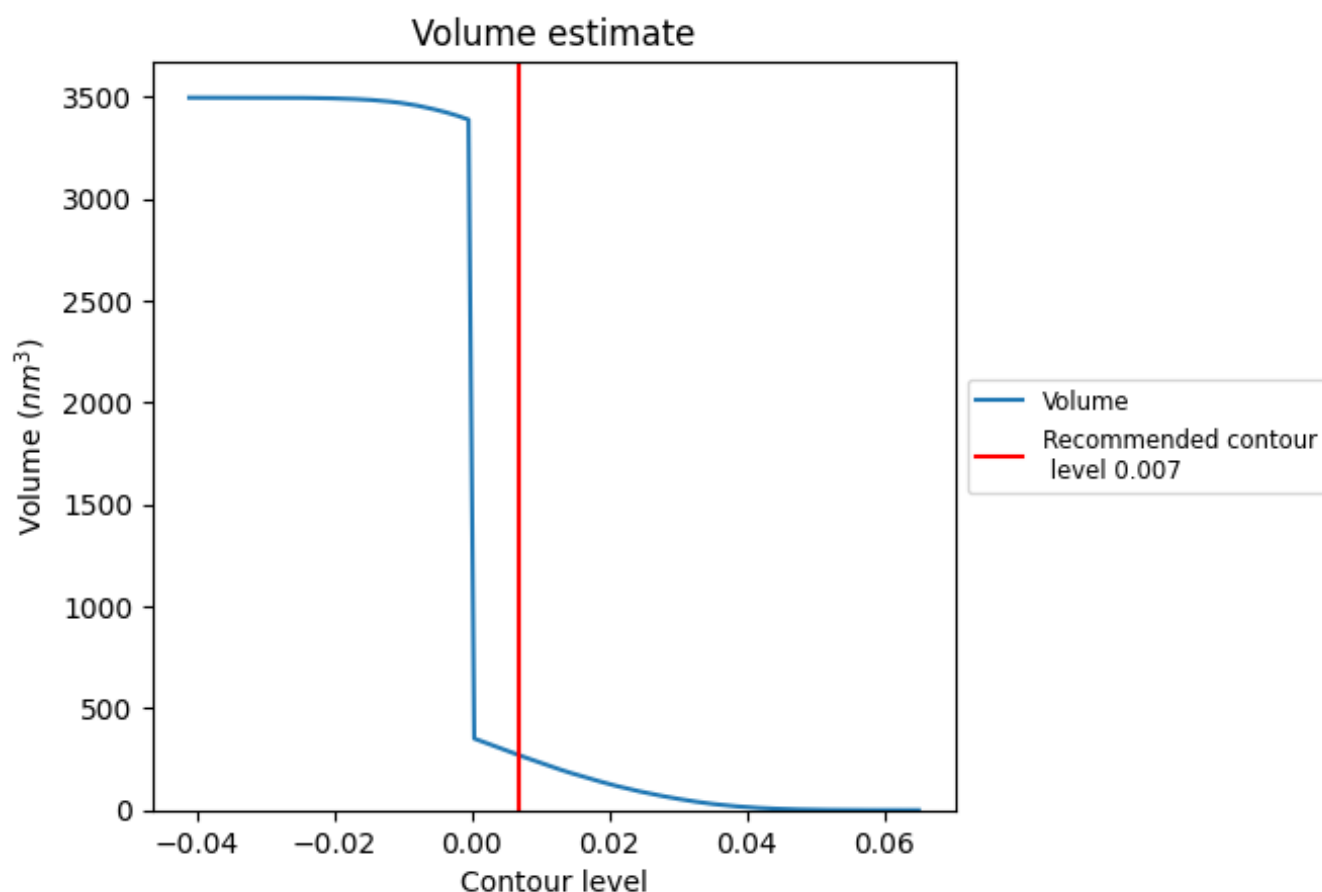
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

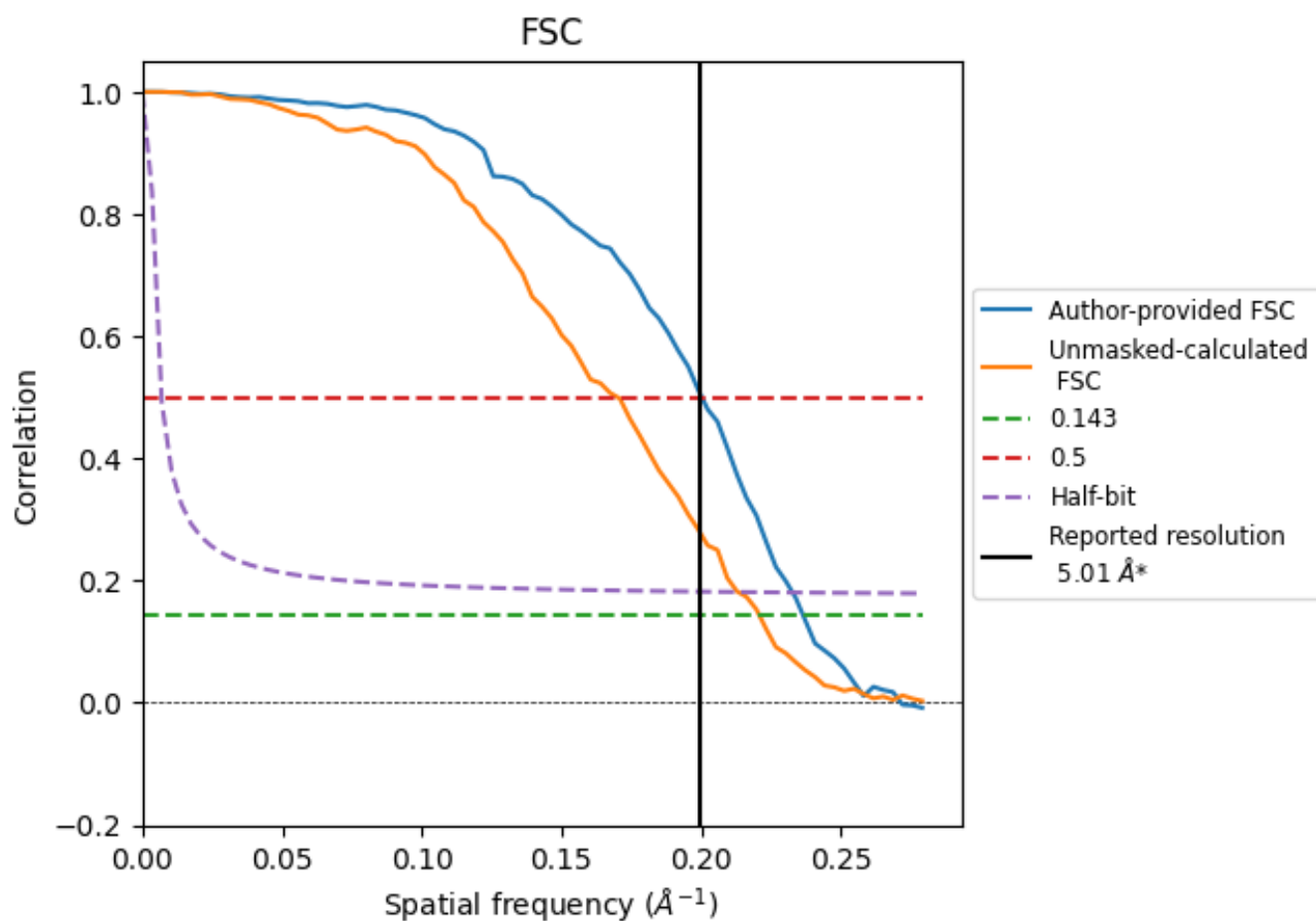
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.200 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

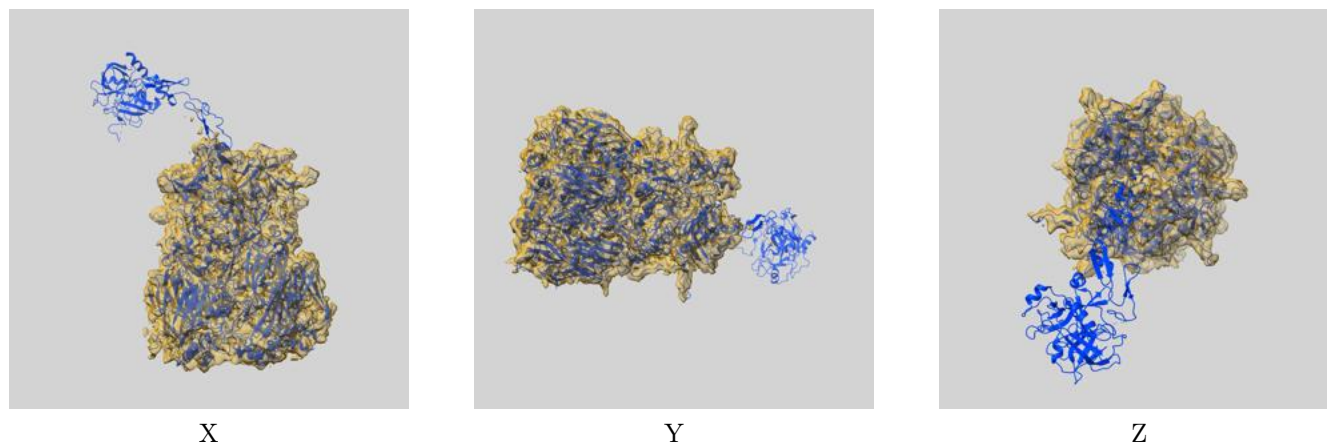
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.01	-	-
Author-provided FSC curve	4.23	5.00	4.30
Unmasked-calculated*	4.53	5.88	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.23 differs from the reported value 5.01 by more than 10 %

9 Map-model fit [i](#)

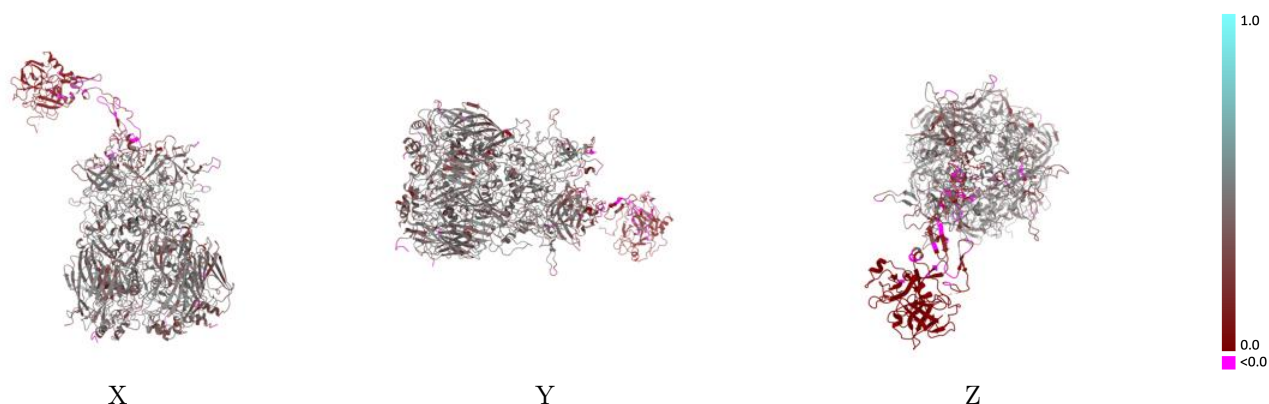
This section contains information regarding the fit between EMDB map EMD-45737 and PDB model 9CM2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



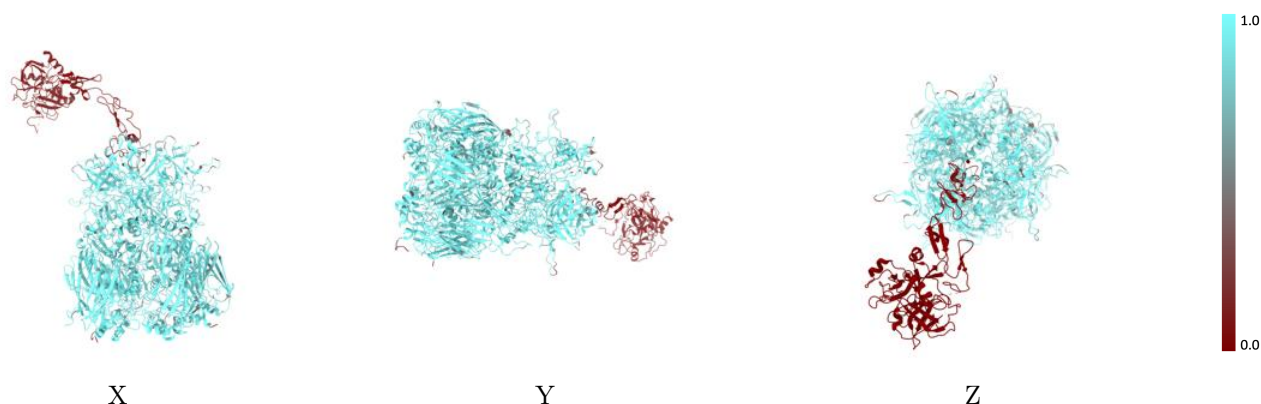
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



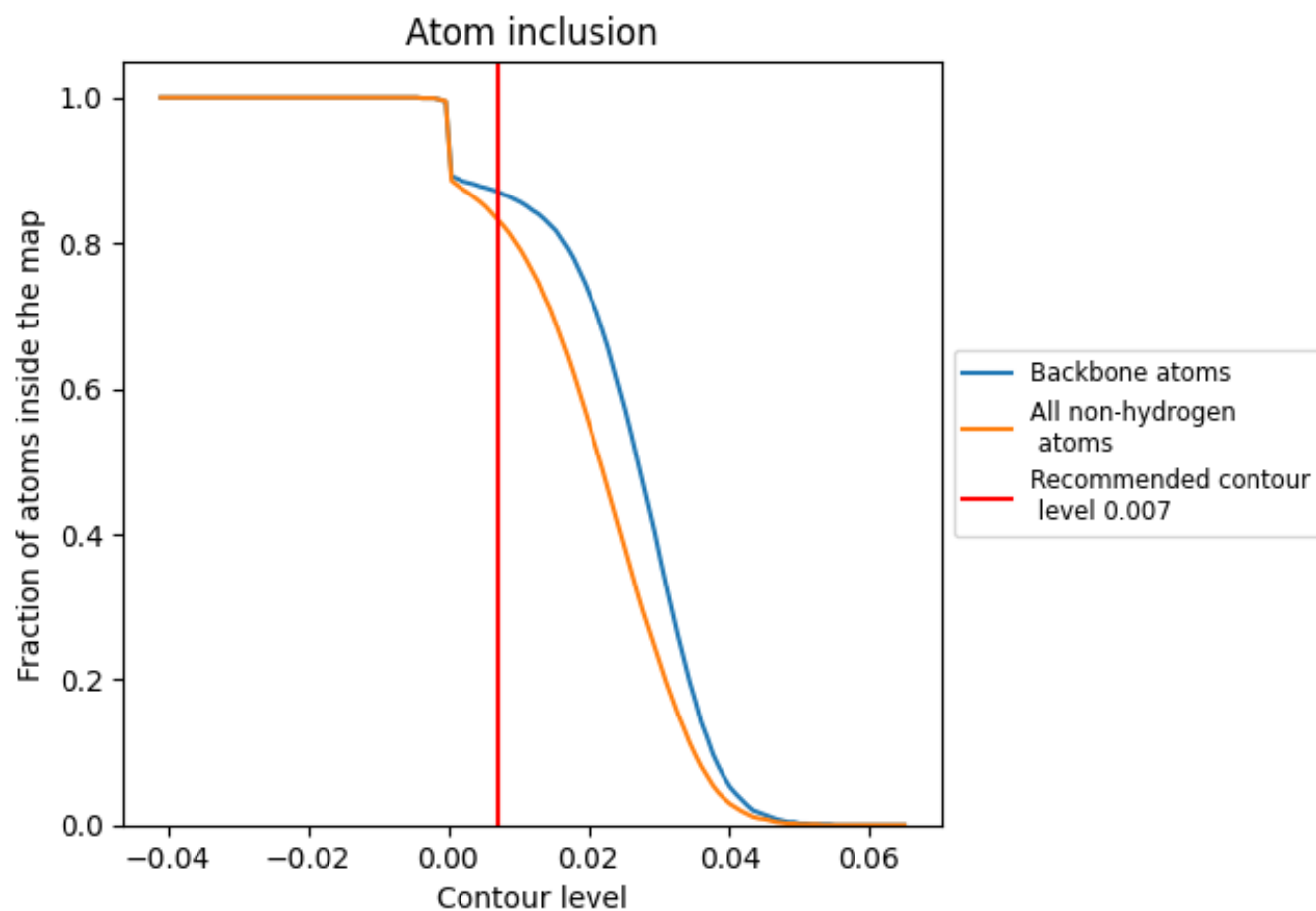
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.3680
J	0.9430	0.4140
K	0.9500	0.4170
L	0.9280	0.4030
Z	0.0430	0.0470

