



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 06:13 PM UTC

PDB ID : 9CM9 / pdb_00009cm9
EMDB ID : EMD-45744
Title : Cryo-EM model derived from localized reconstruction of Ad657-hexon-FX complex at 3.86Å resolution
Authors : Reddy, V.S.; Ma, O.X.
Deposited on : 2024-07-13
Resolution : 4.00 Å(reported)
Based on initial model : 6B1T

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

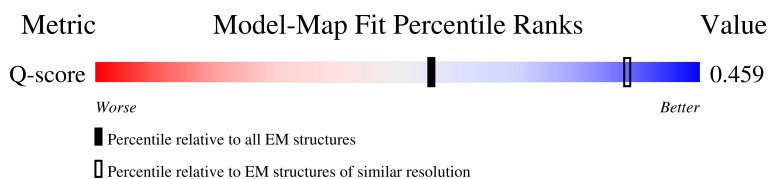
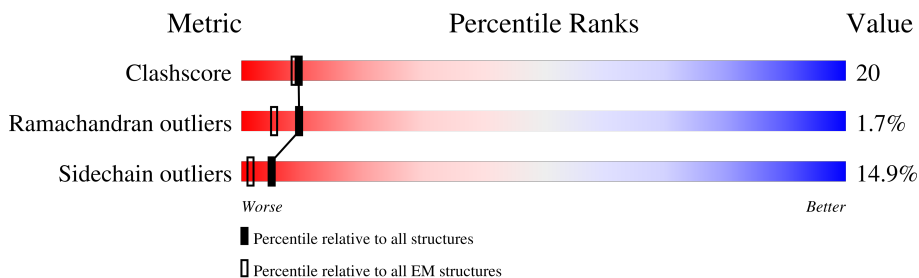
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	959	
1	K	959	
1	L	959	
2	Z	488	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25178 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
			7402	4685	1259	1420	38		
1	K	929	Total	C	N	O	S	0	0
			7393	4680	1258	1417	38		
1	L	927	Total	C	N	O	S	0	0
			7374	4670	1252	1414	38		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	291	LEU	VAL	conflict	UNP A0A348FV85
J	827	ILE	LEU	conflict	UNP A0A348FV85
J	853	VAL	PHE	conflict	UNP A0A348FV85
K	291	LEU	VAL	conflict	UNP A0A348FV85
K	827	ILE	LEU	conflict	UNP A0A348FV85
K	853	VAL	PHE	conflict	UNP A0A348FV85
L	291	LEU	VAL	conflict	UNP A0A348FV85
L	827	ILE	LEU	conflict	UNP A0A348FV85
L	853	VAL	PHE	conflict	UNP A0A348FV85

- 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		

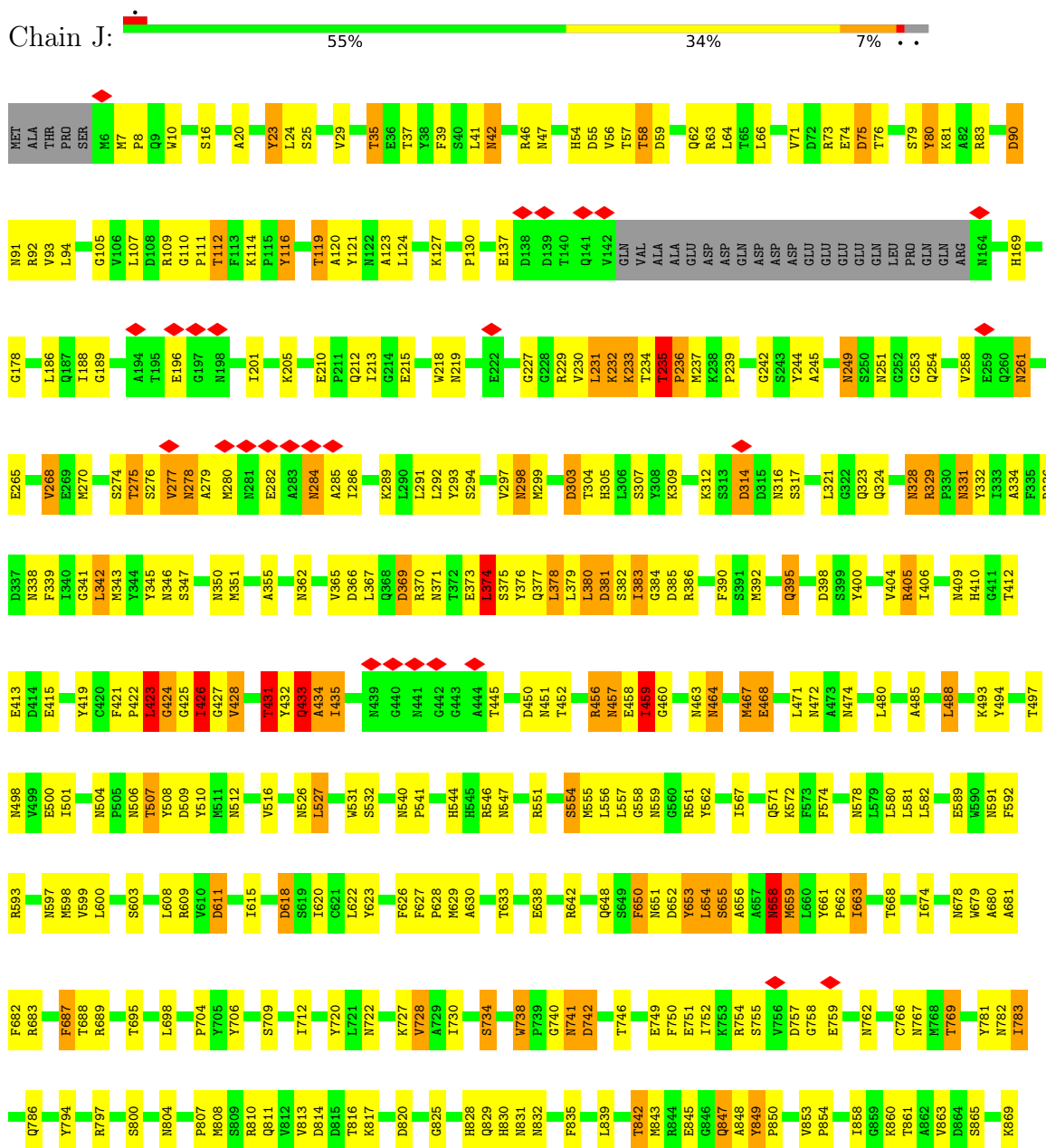
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

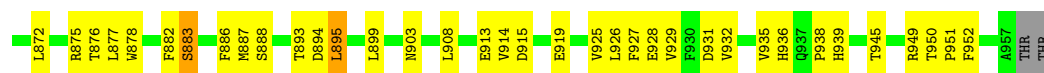
Mol	Chain	Residues	Atoms		AltConf
3	Z	7	Total	Ca	0
			7	7	

3 Residue-property plots

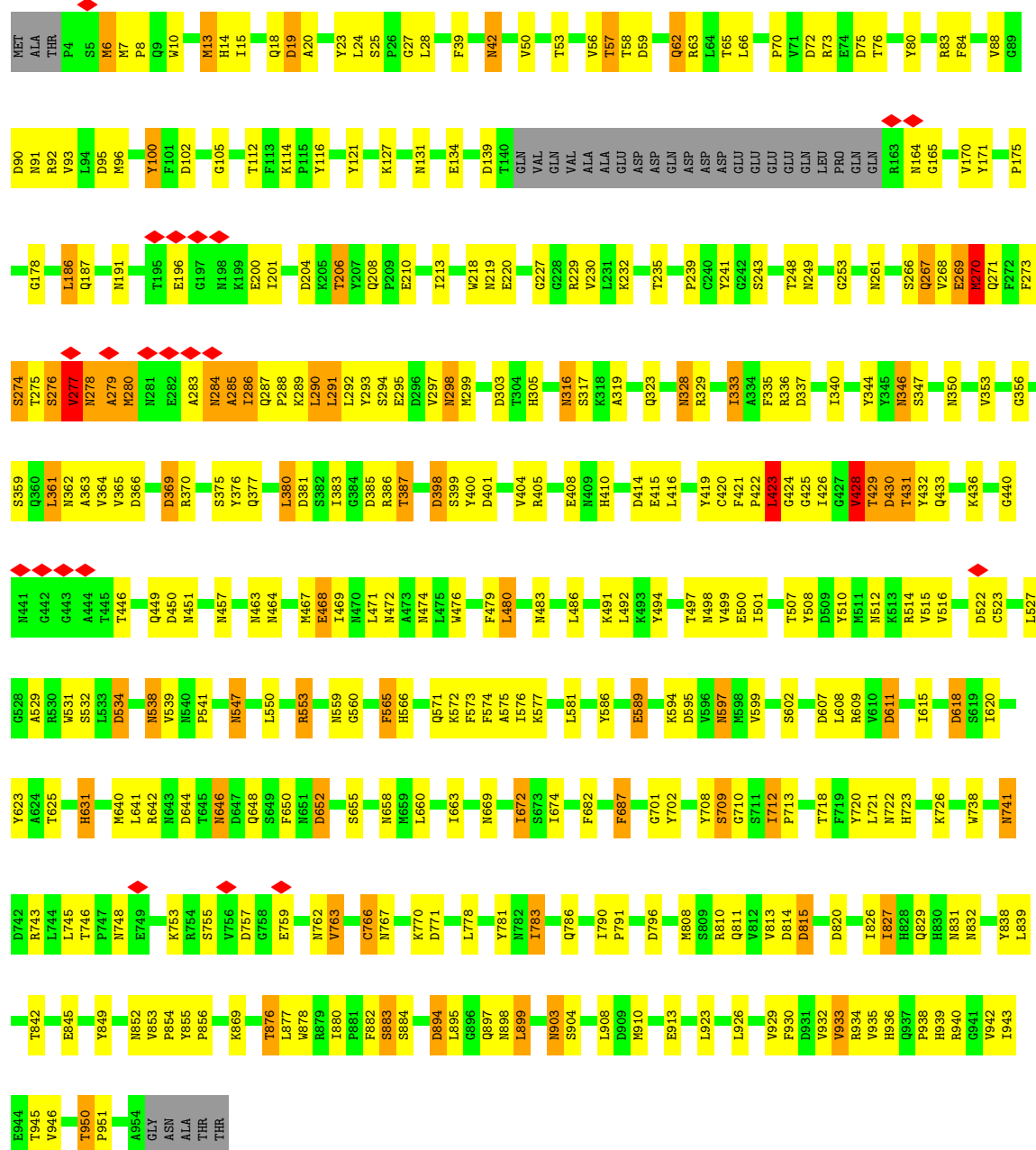
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



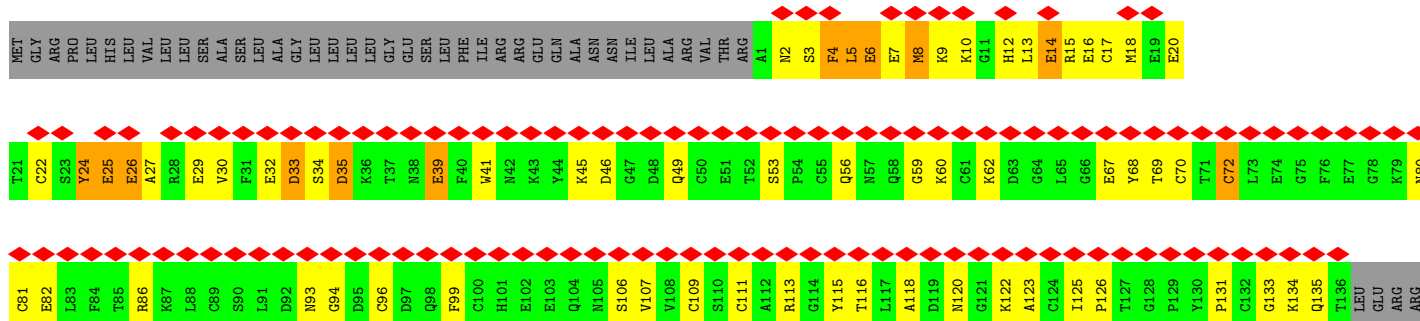
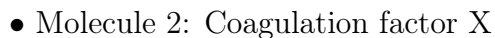


• Molecule 1: Hexon protein



• Molecule 1: Hexon protein







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3845	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	0.054	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	115.456, 205.568, 132.352	wwPDB
Map dimensions	146, 94, 82	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.408, 1.408, 1.4080001	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: CA, CGU

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	0.51	2/7595 (0.0%)	0.59	12/10330 (0.1%)
1	K	0.44	0/7587	0.53	4/10318 (0.0%)
1	L	0.58	4/7568 (0.1%)	0.65	12/10294 (0.1%)
2	Z	0.17	0/2918	0.41	1/3912 (0.0%)
All	All	0.49	6/25668 (0.0%)	0.57	29/34854 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	2
1	K	0	3
1	L	0	1
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	433	GLN	CA-C	-9.87	1.48	1.53
1	L	899	LEU	CA-C	-6.81	1.43	1.52
1	L	901	TYR	CA-C	-6.65	1.43	1.52
1	L	900	LEU	N-CA	-5.90	1.37	1.46
1	L	426	ILE	CA-C	-5.82	1.45	1.52
1	J	426	ILE	CA-C	-5.40	1.45	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	900	LEU	N-CA-C	-9.21	98.54	111.24
1	L	898	ASN	N-CA-C	-9.20	100.39	112.34
1	J	380	LEU	N-CA-C	-8.43	100.99	111.11
1	L	897	GLN	N-CA-C	-7.34	103.58	112.54
1	J	663	ILE	CB-CA-C	-7.13	102.96	110.16
1	L	739	PRO	N-CA-C	-6.93	98.20	112.47
1	L	736	VAL	N-CA-C	6.28	122.39	109.34
1	J	426	ILE	N-CA-C	-6.23	96.37	109.34
1	K	287	GLN	CA-C-N	-6.12	113.99	120.66
1	K	287	GLN	C-N-CA	-6.12	113.99	120.66
1	K	276	SER	N-CA-C	-6.07	106.20	113.97
1	L	738	TRP	CA-C-N	-6.06	112.27	119.84
1	L	738	TRP	C-N-CA	-6.06	112.27	119.84
1	J	374	LEU	N-CA-C	-5.79	104.97	111.28
2	Z	30	VAL	N-CA-C	-5.61	95.28	111.00
1	L	906	HIS	N-CA-C	5.59	117.34	108.79
1	J	663	ILE	CA-C-N	5.59	125.49	119.85
1	J	663	ILE	C-N-CA	5.59	125.49	119.85
1	J	433	GLN	CB-CA-C	-5.56	109.06	117.07
1	J	278	ASN	N-CA-C	-5.55	106.55	113.15
1	L	471	LEU	N-CA-C	5.53	117.77	111.02
1	J	658	ASN	N-CA-C	5.51	118.55	109.85
1	J	378	LEU	N-CA-C	-5.44	105.26	112.34
1	J	231	LEU	N-CA-C	5.35	117.45	108.73
1	L	853	VAL	CA-C-N	-5.33	113.17	119.84
1	L	853	VAL	C-N-CA	-5.33	113.17	119.84
1	J	277	VAL	N-CA-C	-5.33	104.58	112.04
1	K	277	VAL	N-CA-C	-5.33	104.22	111.89
1	L	738	TRP	N-CA-C	5.20	120.75	113.57

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	738	TRP	Peptide
1	J	853	VAL	Peptide
1	K	738	TRP	Peptide
1	K	853	VAL	Peptide
1	K	950	THR	Peptide
1	L	425	GLY	Mainchain

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	7402	0	7067	308	0
1	K	7393	0	7062	282	0
1	L	7374	0	7042	367	0
2	Z	3002	0	2796	124	0
3	Z	7	0	0	0	0
All	All	25178	0	23967	989	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 20.

All (989) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:899:LEU:HB3	1:L:902:ALA:H	1.32	0.95
1:K:274:SER:HB2	1:L:435:ILE:HG21	1.52	0.90
1:L:346:ASN:HD21	1:L:372:THR:H	1.08	0.90
1:L:421:PHE:HB3	1:L:422:PRO:HD2	1.54	0.88
1:L:431:THR:HG21	1:L:456:ARG:NH2	1.88	0.87
1:L:766:CYS:SG	1:L:767:ASN:N	2.48	0.87
1:K:277:VAL:HA	1:K:280:MET:HE2	1.55	0.86
1:J:459:ILE:HD11	1:L:292:LEU:HD11	1.59	0.85
1:L:849:TYR:HD1	1:L:850:PRO:HD2	1.41	0.85
1:J:766:CYS:SG	1:J:767:ASN:N	2.49	0.84
1:K:766:CYS:SG	1:K:767:ASN:N	2.50	0.84
1:J:433:GLN:HG3	1:L:278:ASN:HB3	1.61	0.83
2:Z:9:LYS:HG3	2:Z:10:LYS:H	1.44	0.82
1:K:274:SER:HB2	1:L:435:ILE:CG2	2.08	0.82
1:J:369:ASP:N	1:J:369:ASP:OD1	2.12	0.82
1:J:231:LEU:HD21	1:L:849:TYR:CE1	2.15	0.82
2:Z:5:LEU:O	2:Z:6:CGU:C	2.26	0.82
1:L:899:LEU:HB3	1:L:902:ALA:N	1.95	0.81
1:L:899:LEU:HD22	1:L:902:ALA:HB2	1.63	0.81
1:L:433:GLN:HE21	1:L:449:GLN:HG3	1.44	0.80
1:J:378:LEU:O	1:J:381:ASP:HB3	1.83	0.79
1:L:348:THR:H	1:L:368:GLN:HE22	1.28	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:4:PHE:O	2:Z:5:LEU:C	2.26	0.77
1:L:848:ALA:O	1:L:849:TYR:HB2	1.83	0.77
1:J:433:GLN:CD	1:L:276:SER:HA	2.10	0.76
1:J:350:ASN:HB3	1:J:591:ASN:HD22	1.49	0.76
2:Z:9:LYS:HG3	2:Z:10:LYS:N	2.01	0.75
2:Z:133:GLY:HA2	2:Z:391:TYR:HB2	1.68	0.75
1:L:346:ASN:ND2	1:L:372:THR:H	1.84	0.75
1:L:477:ARG:HD2	1:L:523:CYS:SG	2.27	0.75
1:K:369:ASP:O	1:K:658:ASN:ND2	2.20	0.74
1:J:464:ASN:OD1	1:J:464:ASN:N	2.15	0.74
1:J:178:GLY:HA3	1:J:186:LEU:HD11	1.69	0.74
1:J:254:GLN:O	1:J:297:VAL:HG12	1.88	0.74
1:K:277:VAL:O	1:K:280:MET:HG2	1.86	0.74
1:J:527:LEU:O	1:K:559:ASN:ND2	2.21	0.74
1:K:100:TYR:HE1	1:K:623:TYR:HB2	1.50	0.74
1:L:341:GLY:O	1:L:593:ARG:NH1	2.21	0.73
1:J:653:TYR:O	1:J:654:LEU:C	2.27	0.73
1:J:371:ASN:HB2	1:J:658:ASN:HD21	1.53	0.73
1:K:876:THR:OG1	1:K:877:LEU:N	2.20	0.73
1:K:277:VAL:O	1:K:278:ASN:C	2.32	0.73
1:L:346:ASN:HD21	1:L:372:THR:N	1.84	0.73
1:K:431:THR:HA	1:K:457:ASN:O	1.89	0.72
1:K:811:GLN:HE22	1:L:558:GLY:HA3	1.54	0.72
1:L:898:ASN:C	1:L:900:LEU:N	2.42	0.72
1:K:362:ASN:OD1	1:K:363:ALA:N	2.22	0.72
1:L:595:ASP:OD2	1:L:609:ARG:NH2	2.23	0.72
1:L:732:PHE:O	1:L:736:VAL:HG23	1.88	0.72
1:J:540:ASN:HD22	1:J:720:TYR:HE2	1.36	0.72
1:L:741:ASN:O	1:L:743:ARG:N	2.23	0.72
1:J:109:ARG:NH2	1:J:558:GLY:O	2.23	0.71
1:L:898:ASN:C	1:L:900:LEU:H	1.96	0.71
2:Z:118:ALA:HB2	2:Z:125:ILE:HD11	1.72	0.71
1:L:19:ASP:OD1	1:L:19:ASP:N	2.22	0.71
1:J:331:ASN:O	1:J:331:ASN:ND2	2.23	0.71
1:L:897:GLN:C	1:L:899:LEU:N	2.42	0.71
1:K:24:LEU:HD22	1:K:28:LEU:HD23	1.70	0.71
1:K:398:ASP:OD1	1:K:398:ASP:N	2.22	0.71
1:L:891:ALA:O	1:L:930:PHE:HZ	1.71	0.71
1:L:328:ASN:OD1	1:L:512:ASN:ND2	2.24	0.71
1:L:398:ASP:OD1	1:L:398:ASP:N	2.18	0.71
1:J:90:ASP:OD1	1:J:90:ASP:N	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:814:ASP:OD1	1:K:815:ASP:N	2.24	0.70
1:L:495:ASN:OD1	1:L:495:ASN:N	2.23	0.70
1:J:754:ARG:HE	1:J:758:GLY:HA3	1.57	0.70
1:L:62:GLN:OE1	1:L:92:ARG:NH1	2.24	0.70
1:K:436:LYS:HB3	1:K:450:ASP:HB2	1.74	0.70
1:K:420:CYS:SG	1:L:469:ILE:HB	2.31	0.69
1:L:98:SER:O	1:L:98:SER:OG	2.10	0.69
1:K:820:ASP:OD2	1:L:246:ARG:NH1	2.24	0.69
1:L:405:ARG:NH2	1:L:874:ASP:OD2	2.24	0.69
1:J:422:PRO:HG2	1:J:425:GLY:HA2	1.74	0.69
1:K:527:LEU:O	1:L:559:ASN:ND2	2.24	0.69
1:L:899:LEU:CB	1:L:902:ALA:H	2.05	0.69
1:J:379:LEU:O	1:J:383:ILE:HG23	1.93	0.69
1:J:759:GLU:OE1	1:J:762:ASN:ND2	2.25	0.69
1:L:898:ASN:O	1:L:901:TYR:N	2.26	0.69
2:Z:263:HIS:ND1	2:Z:290:THR:O	2.25	0.68
1:J:426:ILE:HG13	1:L:171:TYR:OH	1.93	0.68
1:K:682:PHE:HB3	1:K:882:PHE:HD2	1.58	0.68
1:K:759:GLU:O	1:L:104:ARG:NH1	2.27	0.68
1:K:289:LYS:O	1:K:290:LEU:HB2	1.93	0.68
1:J:467:MET:HG3	1:K:467:MET:HE2	1.76	0.68
1:J:303:ASP:OD1	1:J:303:ASP:N	2.27	0.67
1:J:642:ARG:NH1	1:J:939:HIS:O	2.27	0.67
1:L:275:THR:HB	1:L:277:VAL:HG13	1.76	0.67
1:K:42:ASN:OD1	1:K:42:ASN:N	2.19	0.67
2:Z:259:GLY:O	2:Z:297:ASN:ND2	2.27	0.67
1:J:58:THR:OG1	1:J:59:ASP:N	2.27	0.67
1:J:794:TYR:O	1:J:797:ARG:NH1	2.28	0.67
1:K:597:ASN:OD1	1:K:597:ASN:N	2.28	0.67
2:Z:304:PRO:HG2	2:Z:419:LEU:HD11	1.75	0.67
1:J:544:HIS:CD2	1:J:546:ARG:HB2	2.29	0.66
1:K:815:ASP:N	1:K:815:ASP:OD1	2.28	0.66
1:L:345:TYR:HE1	1:L:590:TRP:HZ2	1.41	0.66
1:K:19:ASP:OD1	1:K:19:ASP:N	2.21	0.66
2:Z:93:ASN:ND2	2:Z:96:CYS:O	2.28	0.66
1:L:435:ILE:HG13	1:L:436:LYS:N	2.10	0.66
1:J:314:ASP:N	1:J:314:ASP:OD1	2.24	0.66
2:Z:379:SER:HA	2:Z:397:VAL:HB	1.78	0.66
1:J:656:ALA:HB1	1:J:927:PHE:O	1.96	0.66
1:J:847:GLN:NE2	1:J:848:ALA:O	2.29	0.66
1:K:346:ASN:ND2	1:K:370:ARG:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:892:LEU:HD23	1:L:897:GLN:HE22	1.61	0.65
1:L:899:LEU:HD13	1:L:902:ALA:HB2	1.76	0.65
1:L:901:TYR:O	1:L:903:ASN:N	2.28	0.65
1:J:435:ILE:HD12	1:L:274:SER:OG	1.96	0.65
1:J:843:MET:HA	1:L:419:TYR:OH	1.96	0.65
1:L:844:ARG:O	1:L:844:ARG:NH1	2.27	0.65
1:J:282:GLU:HB3	1:J:285:ALA:CB	2.25	0.65
1:J:860:LYS:HG3	1:J:861:THR:HG23	1.78	0.65
1:J:275:THR:HG22	1:K:432:TYR:CE1	2.32	0.65
1:L:900:LEU:O	1:L:901:TYR:C	2.40	0.65
2:Z:380:GLY:HA2	2:Z:396:ILE:HG23	1.78	0.65
1:J:137:GLU:OE1	1:J:169:HIS:NE2	2.29	0.65
1:K:178:GLY:HA3	1:K:186:LEU:HD11	1.78	0.65
1:L:421:PHE:HB3	1:L:422:PRO:CD	2.27	0.65
1:J:346:ASN:ND2	1:J:370:ARG:O	2.30	0.65
1:J:114:LYS:NZ	1:J:116:TYR:O	2.29	0.65
1:K:366:ASP:HA	1:K:370:ARG:HH12	1.61	0.65
1:J:842:THR:OG1	1:J:843:MET:N	2.25	0.65
1:K:534:ASP:OD1	1:K:534:ASP:N	2.25	0.65
1:K:419:TYR:CE1	1:K:468:GLU:HG3	2.32	0.64
1:K:277:VAL:HA	1:K:280:MET:CE	2.25	0.64
1:L:547:ASN:OD1	1:L:550:LEU:N	2.26	0.64
1:L:736:VAL:HG12	1:L:737:SER:N	2.12	0.64
1:J:274:SER:O	1:K:433:GLN:N	2.30	0.64
1:L:736:VAL:HG12	1:L:737:SER:H	1.60	0.64
1:L:284:ASN:O	1:L:286:ILE:HD13	1.97	0.64
1:L:814:ASP:OD1	1:L:816:THR:N	2.20	0.64
1:J:709:SER:O	1:J:709:SER:OG	2.15	0.64
1:J:894:ASP:OD1	1:J:895:LEU:N	2.31	0.64
1:L:296:ASP:N	1:L:296:ASP:OD1	2.31	0.64
1:J:227:GLY:HA2	1:J:291:LEU:O	1.98	0.64
1:K:609:ARG:NH1	1:K:702:TYR:OH	2.31	0.64
1:K:762:ASN:O	1:L:566:HIS:NE2	2.30	0.64
1:L:373:GLU:O	1:L:376:TYR:N	2.31	0.64
1:K:139:ASP:HB3	1:K:164:ASN:HB3	1.79	0.63
2:Z:5:LEU:O	2:Z:8:MET:N	2.31	0.63
1:J:375:SER:O	1:J:376:TYR:C	2.37	0.63
1:J:574:PHE:HD2	1:J:651:ASN:O	1.82	0.63
1:J:112:THR:O	1:J:112:THR:OG1	2.15	0.63
1:J:611:ASP:OD1	1:J:611:ASP:N	2.31	0.63
1:K:642:ARG:NH1	1:K:939:HIS:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:899:LEU:HB3	1:L:902:ALA:CA	2.28	0.63
1:J:334:ALA:HB2	1:J:554:SER:HA	1.80	0.63
1:L:849:TYR:CD1	1:L:850:PRO:HD2	2.29	0.63
1:L:899:LEU:HD22	1:L:902:ALA:CB	2.28	0.63
2:Z:236:HIS:ND1	2:Z:282:ASP:OD2	2.30	0.63
1:J:658:ASN:N	1:J:658:ASN:OD1	2.30	0.63
1:L:198:ASN:O	1:L:199:LYS:C	2.40	0.63
1:K:838:TYR:HE1	1:L:212:GLN:HE21	1.47	0.62
1:J:432:TYR:C	1:J:433:GLN:HE21	2.07	0.62
1:J:571:GLN:OE1	1:J:572:LYS:N	2.32	0.62
1:K:883:SER:OG	1:K:884:SER:N	2.33	0.62
1:J:652:ASP:O	1:J:653:TYR:C	2.42	0.62
1:J:282:GLU:HB3	1:J:285:ALA:HB2	1.81	0.62
1:K:316:ASN:N	1:K:316:ASN:OD1	2.32	0.62
1:J:379:LEU:O	1:J:380:LEU:C	2.41	0.62
1:L:369:ASP:O	1:L:658:ASN:ND2	2.33	0.62
1:L:469:ILE:HG12	1:L:470:ASN:N	2.14	0.62
1:K:6:MET:SD	1:K:6:MET:N	2.65	0.62
2:Z:4:PHE:O	2:Z:6:CGU:N	2.33	0.62
2:Z:24:TYR:O	2:Z:26:CGU:N	2.33	0.62
2:Z:269:ILE:O	2:Z:285:VAL:N	2.33	0.62
1:K:280:MET:SD	2:Z:24:TYR:OH	2.53	0.62
1:K:611:ASP:N	1:K:611:ASP:OD1	2.33	0.61
1:L:50:VAL:HG12	1:L:51:ALA:H	1.64	0.61
1:K:90:ASP:OD1	1:K:940:ARG:NH1	2.31	0.61
1:K:114:LYS:NZ	1:K:116:TYR:O	2.32	0.61
1:K:709:SER:O	1:K:709:SER:OG	2.12	0.61
1:L:883:SER:OG	1:L:884:SER:N	2.32	0.61
1:K:652:ASP:OD1	1:K:655:SER:N	2.29	0.61
1:K:283:ALA:O	1:K:285:ALA:N	2.32	0.61
1:L:114:LYS:NZ	1:L:116:TYR:O	2.24	0.61
1:J:727:LYS:NZ	1:J:749:GLU:OE2	2.32	0.61
1:L:67:ARG:NH2	1:L:621:CYS:SG	2.73	0.61
1:J:119:THR:OG1	1:J:120:ALA:N	2.32	0.61
1:J:196:GLU:N	1:J:196:GLU:OE1	2.33	0.61
1:K:328:ASN:OD1	1:K:328:ASN:N	2.31	0.61
1:K:894:ASP:OD1	1:K:894:ASP:N	2.27	0.61
1:J:574:PHE:CD2	1:J:652:ASP:HB2	2.35	0.60
1:K:283:ALA:C	1:K:285:ALA:N	2.59	0.60
1:L:245:ALA:O	1:L:254:GLN:NE2	2.34	0.60
1:L:345:TYR:CE1	1:L:590:TRP:HZ2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:354:LEU:HD23	1:L:576:ILE:HG21	1.83	0.60
1:L:899:LEU:O	1:L:902:ALA:HA	2.01	0.60
1:K:672:ILE:HG13	1:K:910:MET:HB2	1.83	0.60
1:J:336:ARG:NE	1:J:598:MET:O	2.21	0.60
2:Z:115:TYR:HA	2:Z:125:ILE:O	2.01	0.60
1:K:7:MET:HG3	1:K:8:PRO:HD2	1.83	0.60
1:J:385:ASP:OD1	1:J:386:ARG:N	2.35	0.60
1:J:419:TYR:CE1	1:J:468:GLU:HG3	2.36	0.60
1:J:459:ILE:HG21	1:L:290:LEU:CD2	2.31	0.60
1:L:723:HIS:O	1:L:753:LYS:NZ	2.35	0.60
1:L:897:GLN:O	1:L:898:ASN:C	2.38	0.60
1:L:651:ASN:OD1	1:L:651:ASN:N	2.35	0.60
1:J:422:PRO:O	1:J:424:GLY:N	2.33	0.59
1:K:204:ASP:OD1	1:K:206:THR:OG1	2.20	0.59
1:K:763:VAL:HB	1:K:770:LYS:HG2	1.83	0.59
1:J:329:ARG:O	1:J:508:TYR:OH	2.20	0.59
1:J:355:ALA:HB2	1:J:362:ASN:HA	1.84	0.59
1:J:655:SER:O	1:J:656:ALA:HB2	2.01	0.59
1:L:345:TYR:O	1:L:346:ASN:HB2	2.03	0.59
1:L:433:GLN:NE2	1:L:449:GLN:HG3	2.16	0.59
1:L:834:GLY:HA3	1:L:847:GLN:O	2.02	0.59
1:J:42:ASN:OD1	1:J:42:ASN:N	2.35	0.59
2:Z:59:GLY:HA2	2:Z:72:CYS:HA	1.83	0.59
2:Z:309:ALA:HB3	2:Z:416:THR:HB	1.84	0.59
2:Z:10:LYS:O	2:Z:15:ARG:NH2	2.36	0.59
2:Z:229:PHE:O	2:Z:288:LEU:N	2.20	0.59
1:L:431:THR:HG21	1:L:456:ARG:HH21	1.66	0.59
1:L:768:MET:HE2	1:L:772:TRP:HD1	1.68	0.59
2:Z:15:ARG:NH2	2:Z:16:CGU:OE21	2.35	0.59
1:K:219:ASN:OD1	1:K:220:GLU:N	2.30	0.59
1:K:344:TYR:OH	1:K:701:GLY:O	2.21	0.59
1:K:646:ASN:OD1	1:K:646:ASN:N	2.32	0.59
1:L:830:HIS:O	1:L:830:HIS:ND1	2.30	0.59
1:K:284:ASN:C	1:K:286:ILE:H	2.10	0.59
1:K:757:ASP:OD1	1:K:757:ASP:N	2.35	0.59
1:L:739:PRO:HG2	1:L:740:GLY:H	1.67	0.59
1:L:755:SER:OG	1:L:756:VAL:N	2.34	0.59
2:Z:261:ALA:HB2	2:Z:295:ARG:HH22	1.68	0.59
1:K:270:MET:O	1:K:271:GLN:HG2	2.03	0.59
1:K:279:ALA:C	1:K:280:MET:SD	2.86	0.59
1:K:547:ASN:OD1	1:K:550:LEU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:219:ASN:OD1	1:L:220:GLU:N	2.35	0.59
1:L:861:THR:O	1:L:861:THR:OG1	2.16	0.58
1:L:905:ALA:O	1:L:906:HIS:CG	2.56	0.58
1:K:607:ASP:OD1	1:K:608:LEU:N	2.35	0.58
1:J:757:ASP:OD1	1:J:757:ASP:N	2.35	0.58
1:L:285:ALA:O	1:L:287:GLN:HG2	2.04	0.58
1:J:419:TYR:HE1	1:J:468:GLU:HG3	1.67	0.58
2:Z:263:HIS:ND1	2:Z:290:THR:OG1	2.36	0.58
1:J:237:MET:O	1:J:323:GLN:NE2	2.37	0.58
1:J:648:GLN:HB2	1:J:935:VAL:HB	1.85	0.58
1:J:121:TYR:HB2	1:J:242:GLY:HA2	1.86	0.58
1:K:333:ILE:HG12	1:K:602:SER:HA	1.85	0.58
1:K:839:LEU:H	1:K:839:LEU:HD23	1.68	0.58
1:L:415:GLU:OE1	1:L:415:GLU:N	2.37	0.58
1:J:609:ARG:HH12	1:J:704:PRO:HA	1.69	0.57
2:Z:329:GLU:HG2	2:Z:330:LYS:HG3	1.86	0.57
1:J:261:ASN:ND2	1:J:265:GLU:OE2	2.37	0.57
1:J:558:GLY:HA3	1:L:811:GLN:HE22	1.69	0.57
1:K:618:ASP:OD1	1:K:618:ASP:N	2.35	0.57
1:L:334:ALA:HB2	1:L:554:SER:HA	1.85	0.57
1:L:609:ARG:NH1	1:L:702:TYR:OH	2.38	0.57
2:Z:106:SER:OG	2:Z:107:VAL:N	2.37	0.57
1:J:507:THR:OG1	1:J:508:TYR:N	2.35	0.57
1:K:838:TYR:O	1:K:839:LEU:C	2.47	0.57
1:L:479:PHE:O	1:L:480:LEU:C	2.43	0.57
1:L:804:ASN:ND2	1:L:875:ARG:HB3	2.19	0.57
1:L:240:CYS:O	1:L:243:SER:OG	2.22	0.57
1:L:607:ASP:OD1	1:L:608:LEU:N	2.38	0.57
1:L:864:ASP:OD1	1:L:864:ASP:N	2.38	0.57
1:J:371:ASN:HB2	1:J:658:ASN:ND2	2.19	0.57
1:J:390:PHE:HD1	1:L:802:PHE:HZ	1.52	0.57
1:K:743:ARG:HB3	1:L:64:LEU:HD12	1.85	0.57
1:L:408:GLU:HG2	1:L:410:HIS:NE2	2.20	0.57
1:J:494:TYR:OH	1:J:839:LEU:O	2.21	0.57
1:K:366:ASP:OD1	1:K:370:ARG:NH1	2.38	0.57
1:L:694:GLU:OE1	1:L:720:TYR:OH	2.22	0.57
1:L:697:SER:HB3	1:L:703:ASP:OD2	2.04	0.57
1:L:901:TYR:O	1:L:902:ALA:C	2.46	0.57
1:K:329:ARG:NH2	1:K:486:LEU:O	2.37	0.57
1:K:399:SER:OG	1:K:400:TYR:N	2.36	0.57
1:L:853:VAL:O	1:L:855:TYR:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:421:PHE:CD1	1:J:421:PHE:N	2.73	0.56
1:J:742:ASP:OD1	1:J:742:ASP:N	2.35	0.56
1:K:277:VAL:CA	1:K:280:MET:HE2	2.33	0.56
1:L:112:THR:O	1:L:112:THR:OG1	2.23	0.56
1:K:298:ASN:OD1	1:K:298:ASN:N	2.37	0.56
1:L:441:ASN:C	1:L:443:GLY:H	2.13	0.56
1:J:74:GLU:HG2	1:J:81:LYS:HB3	1.86	0.56
1:J:949:ARG:NH2	1:J:952:PHE:O	2.38	0.56
1:L:753:LYS:NZ	1:L:915:ASP:OD2	2.31	0.56
1:L:373:GLU:O	1:L:374:LEU:C	2.48	0.56
1:L:751:GLU:OE1	1:L:754:ARG:NH1	2.38	0.56
1:J:270:MET:HG2	1:J:293:TYR:HE1	1.71	0.56
1:J:398:ASP:HB2	1:J:547:ASN:HD21	1.71	0.56
1:K:829:GLN:HA	1:K:852:ASN:HD21	1.70	0.56
1:L:892:LEU:HD13	1:L:930:PHE:CE2	2.40	0.56
1:J:80:TYR:HE1	1:J:592:PHE:HB2	1.71	0.56
1:L:741:ASN:O	1:L:742:ASP:C	2.49	0.56
1:L:738:TRP:N	1:L:739:PRO:HD2	2.21	0.56
1:L:899:LEU:O	1:L:900:LEU:HB2	2.05	0.56
1:J:251:ASN:O	1:L:828:HIS:ND1	2.40	0.56
1:J:574:PHE:CD2	1:J:651:ASN:O	2.59	0.56
1:K:100:TYR:CE1	1:K:623:TYR:HB2	2.36	0.56
1:K:276:SER:C	1:K:278:ASN:N	2.57	0.56
1:K:510:TYR:OH	1:K:514:ARG:NH1	2.39	0.56
1:L:345:TYR:HE1	1:L:590:TRP:CZ2	2.23	0.56
1:L:894:ASP:OD1	1:L:894:ASP:N	2.28	0.56
1:J:341:GLY:O	1:J:593:ARG:NH1	2.38	0.55
1:J:186:LEU:HB2	1:J:291:LEU:HD23	1.88	0.55
1:K:284:ASN:C	1:K:286:ILE:N	2.65	0.55
1:J:899:LEU:O	1:J:903:ASN:ND2	2.34	0.55
1:K:574:PHE:HA	1:K:577:LYS:HE3	1.89	0.55
1:L:336:ARG:NH2	1:L:598:MET:O	2.30	0.55
1:J:422:PRO:HG2	1:J:425:GLY:CA	2.35	0.55
1:K:811:GLN:NE2	1:L:558:GLY:HA3	2.21	0.55
1:L:78:TYR:HA	1:L:594:LYS:HB2	1.89	0.55
1:J:210:GLU:HB2	1:J:213:ILE:HG13	1.89	0.55
1:L:893:THR:O	1:L:894:ASP:C	2.49	0.55
1:J:751:GLU:O	1:J:769:THR:OG1	2.20	0.55
1:L:362:ASN:OD1	1:L:363:ALA:N	2.40	0.55
2:Z:24:TYR:O	2:Z:27:ALA:N	2.33	0.55
1:J:231:LEU:HD21	1:L:849:TYR:HE1	1.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:450:ASP:OD1	1:J:451:ASN:N	2.39	0.55
1:J:471:LEU:CD2	1:L:471:LEU:HD11	2.37	0.55
1:K:336:ARG:HH12	1:K:712:ILE:HG13	1.71	0.55
1:L:597:ASN:OD1	1:L:597:ASN:N	2.40	0.55
2:Z:208:TRP:O	2:Z:225:ILE:N	2.40	0.55
1:K:369:ASP:OD1	1:K:369:ASP:N	2.37	0.55
1:L:751:GLU:O	1:L:769:THR:OG1	2.20	0.55
1:L:853:VAL:O	1:L:854:PRO:C	2.45	0.55
2:Z:135:GLN:OE1	2:Z:135:GLN:N	2.40	0.55
1:J:205:LYS:HB2	1:J:268:VAL:HG11	1.89	0.54
2:Z:263:HIS:CE1	2:Z:290:THR:HG1	2.25	0.54
1:K:277:VAL:C	1:K:279:ALA:N	2.63	0.54
1:K:421:PHE:CZ	1:L:835:PHE:HD2	2.24	0.54
1:L:58:THR:OG1	1:L:59:ASP:N	2.40	0.54
1:J:551:ARG:O	1:J:555:MET:HG3	2.08	0.54
1:J:674:ILE:HB	1:J:908:LEU:HB3	1.90	0.54
1:K:607:ASP:OD1	1:K:609:ARG:N	2.40	0.54
1:L:132:SER:HB3	1:L:172:ALA:HA	1.89	0.54
1:J:73:ARG:NH2	1:J:75:ASP:OD2	2.41	0.54
1:J:849:TYR:CD1	1:J:850:PRO:HD2	2.42	0.54
1:L:894:ASP:O	1:L:896:GLY:N	2.41	0.54
1:L:905:ALA:C	1:L:906:HIS:CG	2.85	0.54
1:J:380:LEU:O	1:J:381:ASP:C	2.49	0.54
1:J:421:PHE:HB3	1:J:422:PRO:HD2	1.89	0.54
1:K:655:SER:OG	1:K:929:VAL:O	2.21	0.54
1:L:464:ASN:N	1:L:464:ASN:OD1	2.40	0.54
1:L:904:SER:O	1:L:905:ALA:HB2	2.08	0.54
1:K:898:ASN:OD1	1:K:899:LEU:N	2.41	0.54
1:L:315:ASP:N	1:L:315:ASP:OD1	2.40	0.54
1:L:419:TYR:HE1	1:L:468:GLU:OE2	1.91	0.54
1:L:897:GLN:C	1:L:899:LEU:H	2.16	0.54
1:K:713:PRO:HB3	1:K:718:THR:O	2.08	0.54
1:J:249:ASN:ND2	1:J:253:GLY:H	2.04	0.54
1:K:75:ASP:OD1	1:K:594:LYS:NZ	2.41	0.54
1:J:383:ILE:HG13	1:J:384:GLY:N	2.22	0.53
1:J:751:GLU:OE2	1:J:754:ARG:NH1	2.40	0.53
1:K:62:GLN:OE1	1:K:92:ARG:NH1	2.41	0.53
1:L:346:ASN:ND2	1:L:370:ARG:O	2.40	0.53
2:Z:5:LEU:HA	2:Z:8:MET:HE3	1.88	0.53
2:Z:49:GLN:HB3	2:Z:68:TYR:HB3	1.90	0.53
2:Z:226:LEU:HD11	2:Z:232:LEU:HB2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:814:ASP:OD1	1:J:816:THR:N	2.33	0.53
1:K:831:ASN:ND2	1:K:854:PRO:HG3	2.23	0.53
1:K:903:ASN:O	1:K:903:ASN:ND2	2.39	0.53
1:L:652:ASP:OD1	1:L:655:SER:N	2.40	0.53
1:L:654:LEU:HD21	1:L:926:LEU:HD21	1.90	0.53
2:Z:265:VAL:HG13	2:Z:286:LEU:HB3	1.90	0.53
1:K:855:TYR:HD1	1:K:856:PRO:HD2	1.73	0.53
1:L:707:THR:O	1:L:707:THR:OG1	2.23	0.53
1:L:899:LEU:CD2	1:L:902:ALA:HB2	2.35	0.53
1:J:811:GLN:NE2	1:K:560:GLY:H	2.07	0.53
1:J:931:ASP:HB2	1:J:949:ARG:HG3	1.90	0.53
1:K:297:VAL:HG23	1:K:299:MET:H	1.73	0.53
1:L:647:ASP:HB2	1:L:934:ARG:HE	1.74	0.53
1:L:894:ASP:C	1:L:896:GLY:H	2.16	0.53
1:J:233:LYS:O	1:J:234:THR:C	2.50	0.53
1:K:786:GLN:HG2	1:L:95:ASP:OD2	2.09	0.53
1:K:936:HIS:CD2	1:K:938:PRO:HD3	2.44	0.53
1:L:477:ARG:O	1:L:478:ASN:C	2.48	0.53
1:L:758:GLY:O	1:L:762:ASN:ND2	2.41	0.53
2:Z:17:CYS:HA	2:Z:22:CYS:HB2	1.89	0.53
1:J:297:VAL:HG23	1:J:297:VAL:O	2.08	0.53
1:K:229:ARG:NE	1:K:295:GLU:OE2	2.40	0.53
1:J:561:ARG:HD3	1:J:562:TYR:CE1	2.43	0.53
1:L:571:GLN:OE1	1:L:572:LYS:N	2.42	0.53
2:Z:326:ARG:HB2	2:Z:375:CYS:HB3	1.91	0.53
1:K:408:GLU:OE1	1:L:551:ARG:NH2	2.42	0.53
1:K:650:PHE:HB2	1:K:933:VAL:HG13	1.91	0.53
1:L:189:GLY:O	1:L:201:ILE:HG13	2.09	0.53
1:L:782:ASN:HD21	1:L:888:SER:HB3	1.73	0.53
1:J:371:ASN:CB	1:J:658:ASN:HD21	2.20	0.53
2:Z:235:ALA:HA	2:Z:284:ALA:HB2	1.90	0.53
1:J:741:ASN:OD1	1:J:741:ASN:N	2.43	0.52
1:J:831:ASN:OD1	1:J:832:ASN:N	2.42	0.52
1:K:83:ARG:HA	1:K:589:GLU:HB2	1.90	0.52
1:J:63:ARG:NE	1:L:742:ASP:OD1	2.42	0.52
1:K:73:ARG:NH2	1:K:618:ASP:O	2.38	0.52
1:K:422:PRO:O	1:K:423:LEU:C	2.51	0.52
1:L:281:ASN:CG	1:L:282:GLU:H	2.16	0.52
1:J:544:HIS:CD2	1:J:546:ARG:H	2.28	0.52
1:L:815:ASP:N	1:L:815:ASP:OD1	2.42	0.52
2:Z:228:GLU:HB3	2:Z:292:ILE:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:105:GLY:HA2	1:J:618:ASP:OD1	2.10	0.52
1:J:270:MET:HG2	1:J:293:TYR:CE1	2.43	0.52
1:K:83:ARG:HB2	1:K:589:GLU:OE1	2.10	0.52
1:L:134:GLU:HB3	1:L:170:VAL:HG22	1.91	0.52
1:L:768:MET:HE2	1:L:772:TRP:CD1	2.43	0.52
2:Z:111:CYS:HB3	2:Z:115:TYR:CB	2.39	0.52
2:Z:116:THR:O	2:Z:125:ILE:N	2.43	0.52
1:K:479:PHE:HE1	1:K:483:ASN:HD22	1.56	0.52
1:L:534:ASP:OD1	1:L:534:ASP:N	2.41	0.52
1:J:830:HIS:ND1	1:J:830:HIS:O	2.43	0.52
1:K:936:HIS:HD2	1:K:938:PRO:HD3	1.75	0.52
1:L:676:SER:HA	1:L:906:HIS:O	2.09	0.52
2:Z:12:HIS:HB3	2:Z:15:ARG:HB3	1.91	0.52
1:J:463:ASN:HD21	1:L:215:GLU:HB2	1.75	0.52
1:J:627:PHE:O	1:J:629:MET:N	2.41	0.52
1:K:450:ASP:OD1	1:K:451:ASN:N	2.43	0.52
1:L:285:ALA:O	1:L:286:ILE:C	2.46	0.52
1:L:347:SER:HA	1:L:368:GLN:NE2	2.24	0.52
1:J:811:GLN:CD	1:K:560:GLY:H	2.18	0.51
1:K:420:CYS:O	1:K:421:PHE:CG	2.63	0.51
1:K:440:GLY:HA2	1:K:446:THR:HG22	1.91	0.51
1:K:950:THR:HG23	1:K:951:PRO:HD2	1.92	0.51
1:L:897:GLN:O	1:L:899:LEU:N	2.43	0.51
1:L:899:LEU:O	1:L:900:LEU:C	2.50	0.51
2:Z:56:GLN:H	2:Z:81:CYS:HB2	1.76	0.51
1:J:116:TYR:CD2	1:L:527:LEU:HG	2.45	0.51
1:J:230:VAL:O	1:J:294:SER:HA	2.09	0.51
1:J:653:TYR:O	1:J:655:SER:HB2	2.10	0.51
1:J:935:VAL:HG22	1:J:945:THR:HG22	1.92	0.51
1:K:491:LYS:O	1:K:492:LEU:HD23	2.10	0.51
1:J:35:THR:O	1:J:35:THR:OG1	2.27	0.51
1:J:467:MET:HB3	1:L:421:PHE:O	2.09	0.51
2:Z:46:ASP:OD1	2:Z:46:ASP:N	2.43	0.51
1:J:425:GLY:C	1:J:426:ILE:HG12	2.35	0.51
1:K:663:ILE:HD11	1:K:923:LEU:HB2	1.92	0.51
1:K:422:PRO:O	1:K:425:GLY:N	2.26	0.51
1:L:200:GLU:N	1:L:200:GLU:OE1	2.43	0.51
1:L:778:LEU:HD23	1:L:783:ILE:O	2.10	0.51
2:Z:415:VAL:O	2:Z:419:LEU:N	2.44	0.51
1:K:230:VAL:O	1:K:294:SER:HA	2.10	0.51
2:Z:94:GLY:HA3	2:Z:107:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:416:THR:HA	2:Z:419:LEU:HD12	1.93	0.51
1:J:656:ALA:HA	1:J:929:VAL:HG22	1.93	0.51
1:J:559:ASN:CG	1:L:529:ALA:HB2	2.35	0.51
1:L:343:MET:O	1:L:344:TYR:C	2.54	0.51
1:L:422:PRO:HG2	1:L:425:GLY:H	1.76	0.51
1:J:282:GLU:HB3	1:J:285:ALA:HB3	1.93	0.51
1:J:375:SER:OG	1:J:376:TYR:N	2.44	0.51
1:K:429:THR:O	1:K:430:ASP:HB2	2.11	0.51
1:L:381:ASP:OD2	1:L:798:MET:HB3	2.11	0.51
1:K:333:ILE:HD11	1:K:608:LEU:HD21	1.92	0.50
1:K:230:VAL:HG12	1:K:293:TYR:O	2.10	0.50
1:K:267:GLN:O	1:K:269:GLU:HG3	2.11	0.50
2:Z:2:ASN:ND2	2:Z:26:CGU:OE11	2.44	0.50
1:J:755:SER:OG	1:J:757:ASP:OD1	2.25	0.50
2:Z:9:LYS:CG	2:Z:10:LYS:H	2.10	0.50
1:J:435:ILE:HG12	1:J:435:ILE:O	2.09	0.50
1:K:280:MET:SD	2:Z:24:TYR:CE2	3.05	0.50
1:K:433:GLN:HE21	1:K:449:GLN:HG3	1.77	0.50
1:L:878:TRP:HA	1:L:878:TRP:CE3	2.47	0.50
1:J:116:TYR:HD2	1:L:527:LEU:HG	1.76	0.50
1:L:36:GLU:OE2	1:L:42:ASN:ND2	2.45	0.50
1:L:237:MET:HG3	1:L:316:ASN:ND2	2.26	0.50
1:J:459:ILE:CG2	1:J:460:GLY:N	2.73	0.50
1:K:356:GLY:O	1:K:359:SER:OG	2.23	0.50
1:K:687:PHE:CE1	1:K:878:TRP:HB2	2.46	0.50
1:L:55:ASP:N	1:L:55:ASP:OD1	2.43	0.50
1:L:892:LEU:C	1:L:893:THR:OG1	2.54	0.50
1:L:894:ASP:C	1:L:896:GLY:N	2.70	0.50
2:Z:272:ASN:HD21	2:Z:273:ARG:HE	1.60	0.50
1:K:491:LYS:C	1:K:492:LEU:HD23	2.36	0.50
1:J:413:GLU:O	1:J:472:ASN:ND2	2.44	0.50
1:J:618:ASP:OD1	1:J:618:ASP:N	2.45	0.50
1:J:854:PRO:HG2	1:K:121:TYR:CE2	2.46	0.50
1:K:335:PHE:CZ	1:K:565:PHE:HE2	2.30	0.50
1:J:62:GLN:NE2	1:J:92:ARG:HD3	2.27	0.49
1:J:218:TRP:CZ3	1:J:219:ASN:HB3	2.47	0.49
1:K:232:LYS:HG3	1:K:295:GLU:O	2.12	0.49
1:K:283:ALA:C	1:K:285:ALA:H	2.18	0.49
1:L:373:GLU:O	1:L:375:SER:N	2.45	0.49
1:J:435:ILE:HD13	1:J:435:ILE:H	1.76	0.49
1:K:401:ASP:HB3	1:K:404:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:595:ASP:OD1	1:L:598:MET:N	2.38	0.49
1:L:727:LYS:NZ	1:L:751:GLU:OE2	2.45	0.49
1:J:366:ASP:OD1	1:J:367:LEU:N	2.45	0.49
1:J:433:GLN:O	1:J:434:ALA:HB2	2.12	0.49
2:Z:399:TRP:NE1	2:Z:411:ILE:HG21	2.27	0.49
1:J:738:TRP:O	1:J:740:GLY:N	2.45	0.49
1:K:191:ASN:HB2	1:K:201:ILE:HD11	1.94	0.49
1:L:738:TRP:O	1:L:738:TRP:CG	2.64	0.49
1:J:59:ASP:N	1:J:59:ASP:OD1	2.42	0.49
1:J:235:THR:HG22	1:J:236:PRO:HD3	1.94	0.49
1:K:266:SER:OG	1:K:267:GLN:N	2.46	0.49
1:K:276:SER:C	1:K:278:ASN:H	2.20	0.49
1:K:422:PRO:O	1:K:424:GLY:N	2.45	0.49
2:Z:4:PHE:CG	2:Z:5:LEU:N	2.80	0.49
2:Z:35:ASP:N	2:Z:35:ASP:OD1	2.45	0.49
1:K:56:VAL:HG12	1:K:57:THR:HG22	1.94	0.49
1:K:134:GLU:HB3	1:K:170:VAL:HG22	1.94	0.49
1:K:280:MET:HE3	2:Z:24:TYR:HE2	1.77	0.49
1:J:121:TYR:CD2	1:J:244:TYR:HB2	2.48	0.49
1:L:602:SER:OG	1:L:709:SER:OG	2.20	0.49
1:L:678:ASN:OD1	1:L:679:TRP:N	2.45	0.49
1:L:739:PRO:CG	1:L:740:GLY:H	2.25	0.49
1:J:390:PHE:CD1	1:L:802:PHE:HZ	2.31	0.49
1:J:680:ALA:O	1:J:951:PRO:HG3	2.13	0.49
1:L:899:LEU:HB3	1:L:902:ALA:HB2	1.94	0.49
2:Z:318:THR:HA	2:Z:343:PRO:HA	1.95	0.49
1:K:827:ILE:HG23	1:K:839:LEU:HD11	1.95	0.49
1:L:446:THR:O	1:L:447:TRP:CG	2.66	0.49
1:L:713:PRO:HB3	1:L:718:THR:O	2.13	0.49
1:L:771:ASP:OD1	1:L:772:TRP:N	2.46	0.49
2:Z:245:LYS:HD3	2:Z:264:GLU:HG2	1.94	0.49
1:J:339:PHE:HD2	1:J:342:LEU:HD12	1.78	0.49
1:K:336:ARG:NH1	1:K:712:ILE:HG13	2.28	0.49
1:L:606:ASN:OD1	1:L:606:ASN:N	2.38	0.49
2:Z:41:TRP:CH2	2:Z:45:LYS:HE2	2.48	0.49
2:Z:238:LEU:HA	2:Z:244:PHE:CZ	2.48	0.49
2:Z:393:VAL:HG12	2:Z:415:VAL:HG21	1.94	0.49
1:J:668:THR:O	1:J:913:GLU:HA	2.13	0.48
1:J:781:TYR:HB2	1:J:783:ILE:HG13	1.94	0.48
1:L:286:ILE:HD13	1:L:286:ILE:H	1.77	0.48
1:J:80:TYR:CE1	1:J:592:PHE:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:MET:HE1	1:K:576:ILE:HD12	1.96	0.48
1:K:105:GLY:HA2	1:K:618:ASP:OD1	2.13	0.48
1:K:271:GLN:O	1:K:273:PHE:HD1	1.95	0.48
1:L:90:ASP:OD1	1:L:90:ASP:N	2.46	0.48
1:L:352:GLY:HA3	1:L:590:TRP:CE3	2.48	0.48
2:Z:252:ASN:ND2	2:Z:255:GLN:HB3	2.28	0.48
1:K:414:ASP:HA	1:L:478:ASN:HD21	1.78	0.48
1:L:431:THR:HG21	1:L:456:ARG:CZ	2.40	0.48
1:L:489:PRO:HG2	1:L:535:TYR:HB3	1.96	0.48
1:J:276:SER:O	1:J:279:ALA:HB3	2.12	0.48
1:K:755:SER:OG	1:K:757:ASP:OD1	2.26	0.48
1:L:93:VAL:HB	1:L:580:LEU:HD11	1.95	0.48
1:L:199:LYS:HD2	1:L:199:LYS:HA	1.50	0.48
1:L:737:SER:C	1:L:739:PRO:HD2	2.38	0.48
1:K:58:THR:OG1	1:K:59:ASP:N	2.47	0.48
1:K:249:ASN:HD21	1:K:253:GLY:HA3	1.78	0.48
1:L:830:HIS:HB2	1:L:833:SER:HB3	1.96	0.48
2:Z:120:ASN:HD21	2:Z:123:ALA:HB3	1.78	0.48
1:J:245:ALA:HB3	1:J:254:GLN:HG2	1.96	0.48
1:J:493:LYS:HG2	1:J:516:VAL:HB	1.94	0.48
1:K:317:SER:OG	1:K:319:ALA:N	2.47	0.48
1:K:428:VAL:HA	2:Z:4:PHE:HE1	1.79	0.48
1:L:736:VAL:O	1:L:737:SER:HB2	2.14	0.48
2:Z:207:PRO:HB2	2:Z:299:ALA:H	1.79	0.48
1:J:215:GLU:HB2	1:K:463:ASN:ND2	2.29	0.48
1:K:227:GLY:HA2	1:K:291:LEU:O	2.14	0.48
1:K:428:VAL:O	1:K:429:THR:HB	2.13	0.48
1:L:652:ASP:O	1:L:655:SER:OG	2.30	0.48
1:J:688:THR:OG1	1:J:689:ARG:N	2.46	0.48
1:K:239:PRO:HG3	1:K:323:GLN:HG3	1.96	0.48
1:K:385:ASP:OD1	1:K:386:ARG:N	2.46	0.48
1:K:571:GLN:OE1	1:K:573:PHE:N	2.31	0.48
1:L:652:ASP:OD1	1:L:654:LEU:N	2.47	0.48
1:J:254:GLN:N	1:J:254:GLN:OE1	2.46	0.48
1:J:377:GLN:O	1:J:378:LEU:C	2.54	0.48
1:J:578:ASN:HB2	1:J:650:PHE:CZ	2.49	0.48
1:L:376:TYR:HD2	1:L:572:LYS:HB3	1.79	0.48
2:Z:94:GLY:O	2:Z:122:LYS:NZ	2.33	0.48
2:Z:213:ILE:HA	2:Z:219:GLY:HA2	1.96	0.48
1:L:642:ARG:NH1	1:L:938:PRO:O	2.45	0.47
1:L:885:ASN:OD1	1:L:885:ASN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:25:SER:O	1:K:27:GLY:N	2.47	0.47
1:L:304:THR:HG22	1:L:327:PRO:HA	1.96	0.47
1:L:694:GLU:HG2	1:L:708:TYR:CE2	2.49	0.47
2:Z:41:TRP:HH2	2:Z:45:LYS:HE2	1.78	0.47
1:K:210:GLU:HB2	1:K:213:ILE:HG13	1.95	0.47
2:Z:109:CYS:SG	2:Z:122:LYS:HA	2.55	0.47
1:J:56:VAL:O	1:J:630:ALA:N	2.44	0.47
1:J:127:LYS:N	1:L:468:GLU:OE1	2.44	0.47
1:J:459:ILE:HD13	1:L:290:LEU:HD23	1.96	0.47
1:J:653:TYR:O	1:J:655:SER:N	2.47	0.47
1:K:781:TYR:CE2	1:K:791:PRO:HG3	2.50	0.47
1:L:10:TRP:HB3	1:L:15:ILE:HG22	1.96	0.47
1:L:348:THR:N	1:L:368:GLN:HE22	2.05	0.47
2:Z:270:LYS:HA	2:Z:284:ALA:HA	1.95	0.47
1:J:46:ARG:HG2	1:L:651:ASN:HD21	1.79	0.47
1:J:458:GLU:O	1:J:459:ILE:HG13	2.13	0.47
1:L:333:ILE:HD11	1:L:608:LEU:HD11	1.96	0.47
1:J:457:ASN:N	1:J:457:ASN:OD1	2.46	0.47
1:L:642:ARG:NH1	1:L:939:HIS:O	2.36	0.47
1:J:423:LEU:N	1:J:423:LEU:HD23	2.30	0.47
1:J:786:GLN:NE2	1:K:95:ASP:OD2	2.48	0.47
1:K:267:GLN:HE21	1:K:267:GLN:HA	1.79	0.47
1:K:811:GLN:OE1	1:L:560:GLY:N	2.48	0.47
1:L:345:TYR:O	1:L:346:ASN:CB	2.61	0.47
1:L:352:GLY:HA3	1:L:590:TRP:CZ3	2.50	0.47
1:L:507:THR:OG1	1:L:508:TYR:N	2.46	0.47
1:L:878:TRP:HA	1:L:878:TRP:HE3	1.79	0.47
1:L:898:ASN:O	1:L:900:LEU:N	2.47	0.47
1:L:900:LEU:C	1:L:902:ALA:N	2.68	0.47
2:Z:211:LEU:HD13	2:Z:324:PHE:HD2	1.80	0.47
1:J:415:GLU:N	1:J:415:GLU:OE2	2.48	0.47
1:J:422:PRO:HG2	1:J:425:GLY:H	1.80	0.47
1:J:433:GLN:HE21	1:J:433:GLN:N	2.12	0.47
1:J:828:HIS:N	1:J:828:HIS:CD2	2.82	0.47
1:K:415:GLU:N	1:K:415:GLU:OE1	2.48	0.47
1:L:379:LEU:O	1:L:383:ILE:HG23	2.15	0.47
2:Z:210:ALA:O	2:Z:223:GLY:N	2.47	0.47
1:J:274:SER:O	1:K:433:GLN:HB3	2.15	0.47
1:J:345:TYR:O	1:J:347:SER:N	2.48	0.47
1:K:73:ARG:NE	1:K:80:TYR:OH	2.48	0.47
1:J:377:GLN:C	1:J:379:LEU:N	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:386:ARG:HD2	1:J:386:ARG:HA	1.59	0.47
1:K:687:PHE:CD1	1:K:878:TRP:HB2	2.49	0.47
1:K:845:GLU:HB2	1:L:214:GLY:HA3	1.97	0.47
1:K:854:PRO:HG2	1:L:121:TYR:CD1	2.50	0.47
1:L:741:ASN:O	1:L:743:ARG:HG2	2.15	0.47
2:Z:397:VAL:HG22	2:Z:412:TYR:CD2	2.50	0.47
1:J:544:HIS:HD2	1:J:546:ARG:HB2	1.76	0.46
1:K:274:SER:OG	1:K:288:PRO:HA	2.15	0.46
1:K:845:GLU:OE1	1:L:214:GLY:N	2.42	0.46
1:L:237:MET:HG3	1:L:316:ASN:HD21	1.79	0.46
1:L:716:ASP:OD1	1:L:717:GLY:N	2.49	0.46
2:Z:233:THR:O	2:Z:284:ALA:N	2.46	0.46
1:L:418:ASN:HD22	1:L:471:LEU:HD12	1.80	0.46
1:L:953:SER:OG	1:L:954:ALA:N	2.49	0.46
1:K:105:GLY:HA2	1:K:618:ASP:CG	2.40	0.46
1:K:299:MET:HE3	1:K:299:MET:HB2	1.74	0.46
2:Z:134:LYS:NZ	2:Z:389:ASP:O	2.45	0.46
1:J:309:LYS:NZ	1:J:312:LYS:O	2.39	0.46
1:K:279:ALA:HB3	1:K:280:MET:CE	2.45	0.46
2:Z:231:ILE:N	2:Z:286:LEU:O	2.30	0.46
1:J:404:VAL:HG11	1:J:544:HIS:CE1	2.50	0.46
1:J:682:PHE:HB3	1:J:882:PHE:CD2	2.51	0.46
1:L:726:LYS:O	1:L:752:ILE:HG13	2.16	0.46
1:J:282:GLU:O	1:J:285:ALA:HB3	2.15	0.46
1:K:464:ASN:OD1	1:K:464:ASN:N	2.48	0.46
1:K:708:TYR:CZ	1:K:710:GLY:HA3	2.50	0.46
1:L:332:TYR:HE1	1:L:545:HIS:HB2	1.81	0.46
1:J:459:ILE:HG23	1:J:460:GLY:N	2.31	0.46
2:Z:12:HIS:CE1	2:Z:14:CGU:HB2	2.50	0.46
2:Z:126:PRO:HB3	2:Z:131:PRO:HG3	1.96	0.46
1:J:343:MET:HG2	1:J:592:PHE:HE1	1.81	0.46
1:L:217:GLN:HG3	1:L:220:GLU:HB2	1.97	0.46
1:L:704:PRO:HG2	1:L:705:TYR:CD1	2.50	0.46
1:L:852:ASN:CG	1:L:852:ASN:O	2.55	0.46
1:J:23:TYR:HD1	1:J:24:LEU:N	2.14	0.46
1:J:123:ALA:H	1:L:832:ASN:HD21	1.63	0.46
1:J:728:VAL:HG13	1:J:750:PHE:HB2	1.97	0.46
1:J:872:LEU:HD23	1:J:872:LEU:HA	1.56	0.46
1:K:303:ASP:N	1:K:303:ASP:OD1	2.48	0.46
1:K:682:PHE:HB3	1:K:882:PHE:CD2	2.46	0.46
1:L:458:GLU:O	1:L:459:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:561:ARG:NH1	1:L:562:TYR:OH	2.47	0.46
1:L:899:LEU:CG	1:L:902:ALA:HB2	2.46	0.46
2:Z:263:HIS:HD1	2:Z:290:THR:HG1	1.59	0.46
1:J:463:ASN:ND2	1:L:215:GLU:HB2	2.31	0.46
1:K:827:ILE:HG22	1:K:838:TYR:OH	2.15	0.46
1:L:250:SER:O	1:L:250:SER:OG	2.31	0.46
1:L:691:LYS:HA	1:L:921:THR:HG22	1.98	0.46
2:Z:111:CYS:HB3	2:Z:115:TYR:HB3	1.96	0.46
1:J:235:THR:HG22	1:J:236:PRO:CD	2.46	0.45
1:K:25:SER:O	1:K:28:LEU:N	2.43	0.45
1:K:277:VAL:HG22	1:K:280:MET:HG3	1.98	0.45
1:K:753:LYS:HB2	1:K:767:ASN:OD1	2.16	0.45
1:K:778:LEU:HD23	1:K:783:ILE:O	2.15	0.45
1:L:818:TYR:HE1	1:L:820:ASP:HB2	1.82	0.45
1:J:270:MET:HE3	1:J:270:MET:HB2	1.90	0.45
1:J:509:ASP:OD1	1:J:510:TYR:N	2.49	0.45
1:K:65:THR:O	1:K:66:LEU:HD23	2.16	0.45
1:K:538:ASN:N	1:K:538:ASN:OD1	2.47	0.45
1:L:339:PHE:CE1	1:L:394:ASN:HB3	2.51	0.45
1:J:275:THR:HA	1:K:432:TYR:HA	1.98	0.45
1:J:820:ASP:OD1	1:J:820:ASP:N	2.48	0.45
1:K:283:ALA:O	1:K:284:ASN:C	2.59	0.45
1:L:335:PHE:HE2	1:L:565:PHE:HD2	1.65	0.45
1:J:76:THR:OG1	1:J:79:SER:O	2.34	0.45
1:L:196:GLU:HB2	1:L:199:LYS:HD3	1.98	0.45
2:Z:223:GLY:HA2	2:Z:380:GLY:O	2.16	0.45
2:Z:344:TYR:HH	2:Z:383:HIS:CD2	2.29	0.45
1:K:387:THR:O	1:K:387:THR:OG1	2.26	0.45
1:K:430:ASP:O	1:K:431:THR:C	2.57	0.45
1:K:581:LEU:HD21	1:K:586:TYR:CE1	2.51	0.45
1:K:771:ASP:OD1	1:K:771:ASP:N	2.48	0.45
1:L:843:MET:HE3	1:L:844:ARG:HH12	1.81	0.45
1:J:422:PRO:HG2	1:J:425:GLY:N	2.31	0.45
1:K:386:ARG:HD2	1:K:386:ARG:HA	1.67	0.45
1:K:531:TRP:CZ3	1:K:810:ARG:HG2	2.52	0.45
1:L:441:ASN:C	1:L:443:GLY:N	2.75	0.45
1:L:688:THR:OG1	1:L:689:ARG:N	2.49	0.45
1:J:398:ASP:OD1	1:J:398:ASP:N	2.40	0.45
1:K:14:HIS:CD2	1:K:23:TYR:CZ	3.04	0.45
1:K:648:GLN:HB2	1:K:935:VAL:HB	1.98	0.45
1:J:275:THR:OG1	1:J:277:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:375:SER:C	1:J:377:GLN:N	2.71	0.45
2:Z:99:PHE:HZ	2:Z:304:PRO:HA	1.82	0.45
2:Z:115:TYR:CD1	2:Z:126:PRO:HA	2.52	0.45
1:J:409:ASN:HD21	1:J:527:LEU:HD12	1.82	0.45
1:J:811:GLN:HE22	1:K:560:GLY:H	1.64	0.45
1:K:571:GLN:OE1	1:K:572:LYS:N	2.50	0.45
1:K:574:PHE:CD1	1:K:652:ASP:HB2	2.52	0.45
1:K:808:MET:HE3	1:K:808:MET:HB2	1.87	0.45
1:L:538:ASN:OD1	1:L:538:ASN:N	2.49	0.45
1:J:814:ASP:OD1	1:J:817:LYS:N	2.49	0.45
1:K:722:ASN:ND2	1:K:876:THR:HG23	2.32	0.45
1:L:829:GLN:HE21	1:L:853:VAL:CG1	2.30	0.45
1:J:121:TYR:CE2	1:J:244:TYR:HB2	2.52	0.44
1:J:374:LEU:O	1:J:374:LEU:HD12	2.18	0.44
1:J:681:ALA:HB2	1:K:10:TRP:CZ2	2.51	0.44
1:J:825:GLY:O	1:J:829:GLN:HG3	2.15	0.44
1:K:13:MET:HE3	1:K:13:MET:HB3	1.71	0.44
1:L:421:PHE:CB	1:L:422:PRO:HD2	2.38	0.44
1:L:895:LEU:HD13	1:L:895:LEU:HA	1.68	0.44
1:K:337:ASP:O	1:K:340:ILE:HG13	2.18	0.44
2:Z:321:VAL:HG22	2:Z:383:HIS:HD1	1.82	0.44
1:J:230:VAL:HG12	1:J:293:TYR:O	2.18	0.44
1:J:232:LYS:HB3	1:J:232:LYS:HE2	1.45	0.44
1:J:390:PHE:CE2	1:J:392:MET:HB3	2.52	0.44
1:K:57:THR:OG1	1:K:58:THR:N	2.50	0.44
1:K:280:MET:HG3	2:Z:24:TYR:CE2	2.53	0.44
1:L:254:GLN:HB2	1:L:297:VAL:HG12	1.98	0.44
1:L:276:SER:C	1:L:278:ASN:N	2.70	0.44
1:L:277:VAL:C	1:L:279:ALA:N	2.73	0.44
1:L:422:PRO:HG2	1:L:425:GLY:CA	2.47	0.44
1:L:602:SER:HG	1:L:709:SER:HG	1.56	0.44
2:Z:245:LYS:HA	2:Z:265:VAL:HG23	2.00	0.44
1:K:574:PHE:CG	1:K:575:ALA:N	2.85	0.44
1:K:854:PRO:HG2	1:L:121:TYR:CE1	2.53	0.44
2:Z:228:GLU:HB3	2:Z:292:ILE:N	2.32	0.44
1:J:797:ARG:N	1:J:800:SER:OG	2.51	0.44
1:K:196:GLU:OE1	1:K:196:GLU:N	2.51	0.44
1:K:335:PHE:O	1:K:553:ARG:HD2	2.18	0.44
1:K:380:LEU:HD23	1:K:380:LEU:HA	1.71	0.44
1:L:899:LEU:CD1	1:L:902:ALA:HB2	2.43	0.44
2:Z:99:PHE:CZ	2:Z:304:PRO:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:321:VAL:HG22	2:Z:383:HIS:ND1	2.33	0.44
1:J:276:SER:C	1:J:279:ALA:H	2.24	0.44
1:J:480:LEU:HD23	1:J:480:LEU:HA	1.68	0.44
1:J:734:SER:O	1:J:734:SER:OG	2.32	0.44
1:K:70:PRO:HG3	1:K:84:PHE:CE2	2.53	0.44
1:K:187:GLN:HG3	1:K:200:GLU:HB3	1.99	0.44
1:K:277:VAL:O	1:K:279:ALA:N	2.51	0.44
1:K:278:ASN:O	1:K:280:MET:N	2.50	0.44
1:L:542:PHE:CE2	1:L:718:THR:HB	2.52	0.44
1:L:678:ASN:OD1	1:L:680:ALA:N	2.47	0.44
1:L:820:ASP:OD1	1:L:820:ASP:N	2.49	0.44
1:J:422:PRO:C	1:J:424:GLY:H	2.24	0.44
1:J:627:PHE:HD1	1:J:628:PRO:HD2	1.82	0.44
1:K:268:VAL:C	1:K:269:GLU:HG3	2.42	0.44
1:K:522:ASP:OD1	1:K:523:CYS:N	2.46	0.44
2:Z:419:LEU:HA	2:Z:422:ILE:HD12	1.98	0.44
1:J:373:GLU:O	1:J:374:LEU:C	2.59	0.44
1:J:876:THR:OG1	1:J:877:LEU:N	2.50	0.44
1:K:376:TYR:CD2	1:K:572:LYS:HG2	2.53	0.44
1:K:398:ASP:HA	1:K:547:ASN:HD21	1.82	0.44
2:Z:214:ASN:HB3	2:Z:220:PHE:HE2	1.82	0.44
1:J:328:ASN:H	1:J:328:ASN:ND2	2.15	0.44
1:J:526:ASN:OD1	1:J:810:ARG:NH1	2.50	0.44
1:J:687:PHE:CE1	1:J:878:TRP:HB2	2.53	0.44
1:K:290:LEU:HD23	1:K:290:LEU:O	2.18	0.44
2:Z:6:CGU:C	2:Z:8:MET:H	2.31	0.44
2:Z:111:CYS:HB3	2:Z:115:TYR:HB2	1.99	0.44
2:Z:414:LYS:HB3	2:Z:417:ALA:HB3	2.00	0.44
1:J:66:LEU:HD23	1:J:66:LEU:HA	1.67	0.43
1:K:839:LEU:HD23	1:K:839:LEU:N	2.28	0.43
2:Z:56:GLN:N	2:Z:80:ASN:O	2.51	0.43
2:Z:235:ALA:HB2	2:Z:283:ILE:O	2.18	0.43
2:Z:271:HIS:CE1	2:Z:281:PHE:HB3	2.52	0.43
1:J:811:GLN:OE1	1:K:560:GLY:N	2.50	0.43
1:K:127:LYS:HE3	1:K:241:TYR:CZ	2.53	0.43
1:K:722:ASN:HD22	1:K:876:THR:HG23	1.83	0.43
1:L:96:MET:HE3	1:L:96:MET:HB3	1.79	0.43
1:L:901:TYR:C	1:L:903:ASN:N	2.76	0.43
1:J:804:ASN:ND2	1:J:875:ARG:HB3	2.33	0.43
1:K:430:ASP:O	1:K:432:TYR:CD2	2.71	0.43
1:K:595:ASP:OD1	1:K:597:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:449:GLN:NE2	1:L:450:ASP:O	2.52	0.43
1:J:485:ALA:HA	1:J:488:LEU:HD12	2.00	0.43
1:J:574:PHE:CG	1:J:652:ASP:HB2	2.53	0.43
1:L:111:PRO:N	1:L:561:ARG:HH21	2.17	0.43
1:J:239:PRO:HG3	1:J:323:GLN:HG3	2.00	0.43
1:J:428:VAL:HG23	1:J:428:VAL:O	2.18	0.43
1:J:527:LEU:HD23	1:K:116:TYR:CD1	2.52	0.43
1:J:551:ARG:HD2	1:L:410:HIS:CE1	2.53	0.43
1:J:847:GLN:HG2	1:K:175:PRO:HG3	2.01	0.43
2:Z:232:LEU:HD21	2:Z:396:ILE:HD11	1.99	0.43
1:J:111:PRO:N	1:J:561:ARG:HH21	2.16	0.43
1:J:284:ASN:O	1:J:284:ASN:ND2	2.45	0.43
1:J:752:ILE:O	1:J:769:THR:OG1	2.36	0.43
1:K:416:LEU:HB2	1:L:478:ASN:OD1	2.19	0.43
1:K:852:ASN:OD1	1:K:852:ASN:N	2.47	0.43
1:J:189:GLY:HA3	1:J:201:ILE:HD12	2.01	0.43
1:J:405:ARG:CZ	1:J:541:PRO:HG3	2.48	0.43
1:K:741:ASN:HB3	1:L:61:SER:HA	1.99	0.43
1:L:299:MET:HE2	1:L:299:MET:HB2	1.94	0.43
1:L:422:PRO:O	1:L:423:LEU:C	2.61	0.43
2:Z:62:LYS:HB3	2:Z:69:THR:HB	2.00	0.43
1:J:835:PHE:HD1	1:L:421:PHE:CE1	2.37	0.43
1:K:139:ASP:OD2	1:K:165:GLY:N	2.51	0.43
1:K:429:THR:OG1	1:K:430:ASP:N	2.50	0.43
1:K:476:TRP:NE1	1:K:480:LEU:HD12	2.33	0.43
1:K:507:THR:OG1	1:K:508:TYR:N	2.51	0.43
1:K:581:LEU:HD11	1:K:586:TYR:CE2	2.54	0.43
1:L:597:ASN:CG	1:L:609:ARG:HE	2.26	0.43
1:L:719:PHE:O	1:L:875:ARG:N	2.48	0.43
1:L:728:VAL:HB	1:L:912:PHE:CD1	2.53	0.43
2:Z:336:ARG:O	2:Z:338:LYS:HG2	2.18	0.43
1:J:557:LEU:HD23	1:J:557:LEU:HA	1.76	0.43
1:L:229:ARG:HH21	1:L:295:GLU:CD	2.25	0.43
1:L:286:ILE:HG12	1:L:286:ILE:O	2.19	0.43
1:L:843:MET:HE2	1:L:843:MET:HB3	1.87	0.43
1:J:351:MET:HE2	1:J:366:ASP:HB3	2.01	0.43
1:J:431:THR:O	1:J:432:TYR:CG	2.72	0.43
1:J:895:LEU:HA	1:J:895:LEU:HD23	1.70	0.43
1:J:936:HIS:CD2	1:J:938:PRO:HD3	2.54	0.43
1:K:20:ALA:HA	1:K:23:TYR:CE2	2.54	0.43
1:K:289:LYS:O	1:K:290:LEU:CB	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:494:TYR:CE1	1:K:515:VAL:HG12	2.54	0.43
1:L:848:ALA:O	1:L:849:TYR:CB	2.59	0.43
2:Z:325:GLY:N	2:Z:378:ASP:OD1	2.46	0.43
1:J:316:ASN:OD1	1:J:316:ASN:N	2.52	0.42
1:J:433:GLN:CG	1:L:275:THR:O	2.67	0.42
1:K:72:ASP:OD1	1:K:73:ARG:N	2.50	0.42
1:K:218:TRP:CZ3	1:K:424:GLY:HA3	2.54	0.42
1:K:531:TRP:CD2	1:K:810:ARG:HD3	2.54	0.42
1:L:441:ASN:O	1:L:443:GLY:N	2.52	0.42
1:L:503:ASP:OD1	1:L:503:ASP:N	2.51	0.42
1:L:899:LEU:HB3	1:L:902:ALA:CB	2.48	0.42
2:Z:251:ARG:NH1	2:Z:337:LEU:HB3	2.34	0.42
1:J:94:LEU:HB2	1:J:626:PHE:CE1	2.54	0.42
1:J:249:ASN:CG	1:J:251:ASN:H	2.26	0.42
1:J:459:ILE:HG21	1:L:290:LEU:HD23	2.00	0.42
1:J:497:THR:HG22	1:J:498:ASN:CG	2.44	0.42
1:J:887:MET:HB3	1:J:887:MET:HE2	1.70	0.42
1:K:280:MET:SD	2:Z:24:TYR:CZ	3.11	0.42
1:L:196:GLU:HB2	1:L:199:LYS:HG2	2.00	0.42
1:L:371:ASN:HD21	1:L:715:LEU:HD23	1.84	0.42
1:L:525:ILE:HD12	1:L:525:ILE:HA	1.91	0.42
1:L:814:ASP:OD1	1:L:815:ASP:N	2.52	0.42
2:Z:233:THR:HG23	2:Z:284:ALA:HB3	2.00	0.42
2:Z:309:ALA:HA	2:Z:313:LEU:HB2	2.00	0.42
2:Z:344:TYR:HE1	2:Z:363:PHE:HE2	1.67	0.42
1:J:808:MET:HB2	1:J:808:MET:HE3	1.62	0.42
1:L:440:GLY:HA3	1:L:445:THR:HA	2.00	0.42
1:L:596:VAL:HG11	1:L:613:ALA:O	2.19	0.42
2:Z:24:TYR:O	2:Z:25:CGU:C	2.67	0.42
2:Z:306:ARG:O	2:Z:416:THR:OG1	2.37	0.42
1:J:237:MET:HE2	1:J:316:ASN:HA	2.01	0.42
1:J:431:THR:CG2	1:J:456:ARG:HB3	2.49	0.42
1:J:807:PRO:C	1:J:808:MET:HG3	2.44	0.42
1:K:935:VAL:HG22	1:K:945:THR:HG22	2.02	0.42
1:L:345:TYR:HE2	1:L:572:LYS:HB2	1.85	0.42
1:L:370:ARG:O	1:L:370:ARG:HG2	2.18	0.42
1:J:130:PRO:HG3	1:J:321:LEU:HD23	2.01	0.42
1:J:381:ASP:CG	1:J:382:SER:N	2.72	0.42
1:J:531:TRP:NE1	1:J:532:SER:O	2.52	0.42
1:J:678:ASN:OD1	1:J:679:TRP:N	2.52	0.42
1:J:722:ASN:ND2	1:J:876:THR:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:249:ASN:ND2	1:K:253:GLY:HA3	2.34	0.42
1:K:430:ASP:OD1	1:K:430:ASP:C	2.62	0.42
1:L:196:GLU:HB2	1:L:199:LYS:CD	2.49	0.42
1:L:450:ASP:OD1	1:L:451:ASN:N	2.52	0.42
1:L:705:TYR:CD1	1:L:705:TYR:N	2.87	0.42
1:J:655:SER:O	1:J:656:ALA:CB	2.66	0.42
1:K:270:MET:HE3	1:K:270:MET:H	1.85	0.42
1:K:899:LEU:HD23	1:K:899:LEU:HA	1.80	0.42
1:K:930:PHE:HB2	1:K:950:THR:HG22	2.02	0.42
1:L:455:GLU:H	1:L:455:GLU:HG3	1.56	0.42
1:L:550:LEU:HD12	1:L:550:LEU:HA	1.80	0.42
2:Z:304:PRO:O	2:Z:419:LEU:HD13	2.19	0.42
1:J:83:ARG:HA	1:J:589:GLU:HB2	2.02	0.42
1:J:382:SER:OG	1:J:653:TYR:HE2	2.01	0.42
1:J:426:ILE:HD12	1:L:171:TYR:CE1	2.54	0.42
1:K:112:THR:O	1:K:112:THR:OG1	2.31	0.42
1:L:647:ASP:OD2	1:L:934:ARG:NE	2.53	0.42
2:Z:364:CYS:HB3	2:Z:409:TYR:CG	2.54	0.42
1:J:7:MET:N	1:J:8:PRO:HD2	2.35	0.42
1:J:120:ALA:HB2	1:L:527:LEU:HD23	2.02	0.42
1:J:304:THR:N	1:J:328:ASN:HD21	2.17	0.42
1:J:426:ILE:HG22	1:L:173:GLN:NE2	2.35	0.42
1:J:582:LEU:HD23	1:J:582:LEU:HA	1.91	0.42
1:L:510:TYR:CD1	1:L:510:TYR:C	2.97	0.42
1:L:872:LEU:HD23	1:L:872:LEU:HA	1.75	0.42
2:Z:8:MET:HE2	2:Z:8:MET:HB2	1.72	0.42
2:Z:33:ASP:CG	2:Z:34:SER:H	2.27	0.42
1:J:212:GLN:OE1	1:L:830:HIS:HB3	2.19	0.42
1:J:653:TYR:HB3	1:J:654:LEU:H	1.71	0.42
1:J:883:SER:OG	1:J:886:PHE:N	2.53	0.42
1:K:91:ASN:HD22	1:K:631:HIS:CD2	2.37	0.42
1:K:674:ILE:HB	1:K:908:LEU:HB3	2.01	0.42
1:K:849:TYR:OH	1:L:295:GLU:OE2	2.26	0.42
1:L:345:TYR:CE2	1:L:572:LYS:HB2	2.55	0.42
1:L:369:ASP:OD1	1:L:949:ARG:NH1	2.49	0.42
1:L:376:TYR:CD2	1:L:572:LYS:HB3	2.55	0.42
1:L:481:TYR:HE2	1:L:518:PRO:HG3	1.84	0.42
1:L:736:VAL:CG1	1:L:737:SER:H	2.24	0.42
1:L:899:LEU:O	1:L:902:ALA:N	2.53	0.42
1:J:229:ARG:H	1:L:847:GLN:HE22	1.67	0.42
1:J:422:PRO:CG	1:J:425:GLY:HA2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:506:ASN:OD1	1:J:506:ASN:N	2.53	0.42
1:K:497:THR:HG22	1:K:498:ASN:OD1	2.20	0.42
1:K:529:ALA:HB2	1:L:559:ASN:CG	2.44	0.42
1:L:422:PRO:HG2	1:L:425:GLY:N	2.35	0.42
1:L:653:TYR:CD1	1:L:653:TYR:C	2.98	0.42
1:L:858:ILE:HG13	1:L:859:GLY:N	2.35	0.42
1:J:622:LEU:HD12	1:J:623:TYR:H	1.84	0.41
1:K:291:LEU:HD12	1:K:292:LEU:N	2.34	0.41
1:K:329:ARG:H	1:K:329:ARG:HG3	1.56	0.41
1:K:531:TRP:NE1	1:K:532:SER:O	2.53	0.41
1:K:934:ARG:HB2	1:L:13:MET:HE1	2.02	0.41
1:L:256:VAL:HG23	1:L:296:ASP:O	2.20	0.41
1:L:607:ASP:OD1	1:L:609:ARG:N	2.26	0.41
1:L:733:ASP:O	1:L:734:SER:OG	2.32	0.41
1:K:726:LYS:HB2	1:K:913:GLU:O	2.20	0.41
1:J:338:ASN:HD21	1:J:395:GLN:HB2	1.85	0.41
1:K:340:ILE:HD11	1:K:377:GLN:HE21	1.86	0.41
1:K:472:ASN:OD1	1:L:475:LEU:HD21	2.20	0.41
1:K:720:TYR:CD1	1:K:721:LEU:HG	2.55	0.41
1:L:632:ASN:O	1:L:636:THR:HG23	2.20	0.41
2:Z:39:CGU:N	2:Z:39:CGU:CD2	2.84	0.41
2:Z:199:GLN:O	2:Z:339:MET:N	2.52	0.41
2:Z:328:HIS:ND1	2:Z:329:GLU:O	2.53	0.41
1:J:112:THR:HG21	1:J:611:ASP:OD2	2.21	0.41
1:J:233:LYS:HE3	1:J:233:LYS:HB2	1.72	0.41
1:L:663:ILE:HG23	1:L:670:VAL:HG21	2.03	0.41
1:L:705:TYR:N	1:L:705:TYR:HD1	2.18	0.41
1:L:727:LYS:HB3	1:L:727:LYS:HE2	1.68	0.41
2:Z:213:ILE:HD11	2:Z:217:ASN:HA	2.02	0.41
2:Z:384:VAL:HG12	2:Z:393:VAL:HA	2.02	0.41
1:J:41:LEU:HD23	1:J:41:LEU:HA	1.81	0.41
1:J:297:VAL:O	1:J:298:ASN:C	2.62	0.41
1:J:451:ASN:N	1:J:451:ASN:OD1	2.53	0.41
1:J:782:ASN:HD21	1:J:888:SER:HB3	1.86	0.41
1:L:367:LEU:O	1:L:369:ASP:N	2.51	0.41
1:L:410:HIS:CD2	1:L:410:HIS:N	2.86	0.41
1:L:819:LYS:H	1:L:819:LYS:HD2	1.85	0.41
1:K:328:ASN:HB3	1:K:512:ASN:HD21	1.85	0.41
1:L:367:LEU:HD23	1:L:367:LEU:HA	1.77	0.41
1:L:373:GLU:C	1:L:375:SER:N	2.78	0.41
1:L:826:ILE:HA	1:L:829:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:289:LYS:HB2	1:J:289:LYS:HE3	1.82	0.41
1:K:171:TYR:CE2	1:L:426:ILE:HG13	2.56	0.41
1:L:376:TYR:HD1	1:L:376:TYR:O	2.03	0.41
2:Z:247:ARG:HG3	2:Z:262:VAL:HG22	2.02	0.41
1:J:107:LEU:HD11	1:J:600:LEU:HD21	2.02	0.41
1:J:124:LEU:N	1:L:832:ASN:OD1	2.36	0.41
1:J:328:ASN:HB3	1:J:512:ASN:HD21	1.86	0.41
1:K:781:TYR:CD2	1:K:791:PRO:HG3	2.56	0.41
1:L:333:ILE:CD1	1:L:608:LEU:HD11	2.51	0.41
1:L:480:LEU:O	1:L:481:TYR:C	2.61	0.41
1:J:20:ALA:HA	1:J:23:TYR:CE1	2.56	0.41
1:J:110:GLY:C	1:J:561:ARG:HH21	2.29	0.41
1:J:292:LEU:HA	1:J:292:LEU:HD23	1.85	0.41
1:J:597:ASN:ND2	1:J:706:TYR:O	2.54	0.41
1:K:640:MET:HE3	1:K:640:MET:HB2	1.98	0.41
1:K:660:LEU:HD23	1:K:660:LEU:HA	1.90	0.41
1:K:720:TYR:O	1:K:723:HIS:NE2	2.54	0.41
1:K:781:TYR:OH	1:K:796:ASP:OD1	2.34	0.41
1:K:934:ARG:HH12	1:L:14:HIS:HE1	1.68	0.41
1:L:757:ASP:OD1	1:L:757:ASP:N	2.54	0.41
1:L:757:ASP:C	1:L:759:GLU:H	2.28	0.41
1:L:828:HIS:CD2	1:L:828:HIS:N	2.86	0.41
2:Z:60:LYS:O	2:Z:70:CYS:HA	2.21	0.41
2:Z:306:ARG:HH21	2:Z:307:ASP:CG	2.29	0.41
1:J:10:TRP:N	1:J:10:TRP:CD1	2.89	0.41
1:J:46:ARG:HG2	1:L:651:ASN:ND2	2.36	0.41
1:J:467:MET:SD	1:L:467:MET:HG3	2.60	0.41
1:J:627:PHE:HD2	1:K:39:PHE:HD2	1.68	0.41
1:K:364:VAL:HG13	1:K:573:PHE:HE2	1.85	0.41
1:L:447:TRP:HA	1:L:447:TRP:CE3	2.55	0.41
1:L:531:TRP:CE2	1:L:810:ARG:HD3	2.55	0.41
1:L:677:ARG:HG3	1:L:679:TRP:NE1	2.36	0.41
1:J:380:LEU:HD23	1:J:380:LEU:HA	1.66	0.40
1:J:659:MET:HB3	1:J:661:TYR:CE1	2.56	0.40
1:K:88:VAL:HG21	1:K:581:LEU:HD23	2.02	0.40
1:K:204:ASP:O	1:K:208:GLN:HB2	2.21	0.40
1:L:335:PHE:CE2	1:L:565:PHE:HD2	2.40	0.40
1:L:346:ASN:ND2	1:L:371:ASN:HA	2.36	0.40
1:L:803:ARG:HB3	1:L:804:ASN:OD1	2.20	0.40
1:K:13:MET:H	1:K:13:MET:HG2	1.55	0.40
1:K:414:ASP:N	1:K:414:ASP:OD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:832:ASN:HD21	1:L:123:ALA:H	1.69	0.40
1:L:366:ASP:OD1	1:L:367:LEU:N	2.50	0.40
1:L:577:LYS:HG2	1:L:578:ASN:OD1	2.21	0.40
1:J:332:TYR:N	1:J:603:SER:OG	2.50	0.40
1:J:426:ILE:O	1:J:427:GLY:C	2.64	0.40
1:K:361:LEU:HD22	1:K:362:ASN:H	1.87	0.40
1:K:405:ARG:CZ	1:K:541:PRO:HG3	2.50	0.40
1:L:450:ASP:CG	1:L:452:THR:H	2.24	0.40
1:L:531:TRP:CD1	1:L:532:SER:N	2.89	0.40
1:L:899:LEU:O	1:L:902:ALA:CA	2.67	0.40
2:Z:283:ILE:HD12	2:Z:418:PHE:CD2	2.55	0.40
1:J:233:LYS:H	1:J:233:LYS:HG3	1.30	0.40
1:J:433:GLN:HG2	1:L:275:THR:O	2.22	0.40
1:J:654:LEU:HD11	1:J:926:LEU:CD2	2.52	0.40
1:K:102:ASP:OD1	1:K:566:HIS:HE1	2.04	0.40
1:L:399:SER:OG	1:L:400:TYR:N	2.52	0.40
1:L:728:VAL:HB	1:L:912:PHE:CE1	2.56	0.40
2:Z:231:ILE:HG12	2:Z:288:LEU:HD11	2.04	0.40
1:J:656:ALA:HB2	1:J:928:GLU:HA	2.04	0.40
1:J:929:VAL:HG12	1:J:951:PRO:HD2	2.04	0.40
1:K:280:MET:HE3	2:Z:24:TYR:CE2	2.55	0.40
1:K:934:ARG:HH12	1:L:14:HIS:CE1	2.39	0.40
1:L:716:ASP:CG	1:L:718:THR:HG1	2.27	0.40
1:L:892:LEU:O	1:L:892:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	927/959 (97%)	820 (88%)	92 (10%)	15 (2%)	7 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	925/959 (96%)	799 (86%)	117 (13%)	9 (1%)	12	45
1	L	923/959 (96%)	767 (83%)	132 (14%)	24 (3%)	4	29
2	Z	362/488 (74%)	328 (91%)	29 (8%)	5 (1%)	9	39
All	All	3137/3365 (93%)	2714 (86%)	370 (12%)	53 (2%)	9	36

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	280	MET
1	J	423	LEU
1	J	426	ILE
1	J	653	TYR
1	K	279	ALA
1	K	290	LEU
1	K	430	ASP
1	L	428	VAL
1	L	444	ALA
1	L	737	SER
1	L	742	ASP
1	L	849	TYR
1	L	853	VAL
1	L	902	ALA
2	Z	4	PHE
2	Z	5	LEU
2	Z	24	TYR
1	J	235	THR
1	J	428	VAL
1	J	431	THR
1	J	655	SER
1	K	284	ASN
1	K	429	THR
1	L	199	LYS
1	L	346	ASN
1	L	442	GLY
1	L	736	VAL
1	L	895	LEU
2	Z	18	MET
1	J	381	ASP
1	J	424	GLY
1	J	434	ALA
1	J	459	ILE

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Mol	Chain	Res	Type
1	K	285	ALA
1	K	428	VAL
1	L	374	LEU
1	L	427	GLY
1	K	270	MET
1	L	283	ALA
1	L	373	GLU
1	L	447	TRP
1	L	481	TYR
1	L	741	ASN
1	L	904	SER
2	Z	33	ASP
1	J	654	LEU
1	L	893	THR
1	J	236	PRO
1	K	423	LEU
1	L	369	ASP
1	J	662	PRO
1	L	850	PRO
1	L	854	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	799/824 (97%)	674 (84%)	125 (16%)	2	15
1	K	799/824 (97%)	683 (86%)	116 (14%)	3	16
1	L	797/824 (97%)	660 (83%)	137 (17%)	2	13
2	Z	313/408 (77%)	287 (92%)	26 (8%)	10	33
All	All	2708/2880 (94%)	2304 (85%)	404 (15%)	5	16

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	16	SER

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Mol	Chain	Res	Type
1	J	23	TYR
1	J	25	SER
1	J	29	VAL
1	J	35	THR
1	J	37	THR
1	J	39	PHE
1	J	42	ASN
1	J	47	ASN
1	J	54	HIS
1	J	55	ASP
1	J	57	THR
1	J	58	THR
1	J	64	LEU
1	J	71	VAL
1	J	75	ASP
1	J	80	TYR
1	J	90	ASP
1	J	91	ASN
1	J	93	VAL
1	J	112	THR
1	J	116	TYR
1	J	119	THR
1	J	188	ILE
1	J	232	LYS
1	J	233	LYS
1	J	235	THR
1	J	249	ASN
1	J	258	VAL
1	J	261	ASN
1	J	268	VAL
1	J	275	THR
1	J	278	ASN
1	J	284	ASN
1	J	286	ILE
1	J	298	ASN
1	J	299	MET
1	J	303	ASP
1	J	305	HIS
1	J	307	SER
1	J	314	ASP
1	J	317	SER
1	J	324	GLN

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Mol	Chain	Res	Type
1	J	328	ASN
1	J	329	ARG
1	J	331	ASN
1	J	342	LEU
1	J	365	VAL
1	J	369	ASP
1	J	374	LEU
1	J	383	ILE
1	J	395	GLN
1	J	400	TYR
1	J	405	ARG
1	J	406	ILE
1	J	410	HIS
1	J	412	THR
1	J	423	LEU
1	J	426	ILE
1	J	431	THR
1	J	433	GLN
1	J	435	ILE
1	J	445	THR
1	J	452	THR
1	J	456	ARG
1	J	457	ASN
1	J	459	ILE
1	J	464	ASN
1	J	467	MET
1	J	468	GLU
1	J	474	ASN
1	J	488	LEU
1	J	500	GLU
1	J	501	ILE
1	J	504	ASN
1	J	507	THR
1	J	527	LEU
1	J	554	SER
1	J	556	LEU
1	J	567	ILE
1	J	580	LEU
1	J	581	LEU
1	J	599	VAL
1	J	608	LEU
1	J	611	ASP

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Mol	Chain	Res	Type
1	J	615	ILE
1	J	618	ASP
1	J	620	ILE
1	J	633	THR
1	J	638	GLU
1	J	650	PHE
1	J	658	ASN
1	J	659	MET
1	J	663	ILE
1	J	683	ARG
1	J	687	PHE
1	J	695	THR
1	J	698	LEU
1	J	712	ILE
1	J	728	VAL
1	J	730	ILE
1	J	734	SER
1	J	741	ASN
1	J	742	ASP
1	J	746	THR
1	J	769	THR
1	J	783	ILE
1	J	813	VAL
1	J	842	THR
1	J	845	GLU
1	J	847	GLN
1	J	849	TYR
1	J	858	ILE
1	J	863	VAL
1	J	865	SER
1	J	869	LYS
1	J	883	SER
1	J	893	THR
1	J	895	LEU
1	J	914	VAL
1	J	915	ASP
1	J	919	GLU
1	J	925	VAL
1	J	932	VAL
1	J	950	THR
1	K	6	MET
1	K	13	MET

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Mol	Chain	Res	Type
1	K	15	ILE
1	K	18	GLN
1	K	19	ASP
1	K	42	ASN
1	K	50	VAL
1	K	53	THR
1	K	57	THR
1	K	62	GLN
1	K	63	ARG
1	K	76	THR
1	K	93	VAL
1	K	100	TYR
1	K	131	ASN
1	K	186	LEU
1	K	206	THR
1	K	235	THR
1	K	243	SER
1	K	248	THR
1	K	261	ASN
1	K	267	GLN
1	K	269	GLU
1	K	270	MET
1	K	274	SER
1	K	275	THR
1	K	277	VAL
1	K	278	ASN
1	K	280	MET
1	K	286	ILE
1	K	291	LEU
1	K	298	ASN
1	K	305	HIS
1	K	316	ASN
1	K	328	ASN
1	K	333	ILE
1	K	346	ASN
1	K	347	SER
1	K	350	ASN
1	K	353	VAL
1	K	361	LEU
1	K	365	VAL
1	K	369	ASP
1	K	375	SER

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Mol	Chain	Res	Type
1	K	380	LEU
1	K	381	ASP
1	K	383	ILE
1	K	387	THR
1	K	398	ASP
1	K	410	HIS
1	K	423	LEU
1	K	426	ILE
1	K	428	VAL
1	K	431	THR
1	K	468	GLU
1	K	469	ILE
1	K	471	LEU
1	K	474	ASN
1	K	480	LEU
1	K	499	VAL
1	K	500	GLU
1	K	501	ILE
1	K	516	VAL
1	K	534	ASP
1	K	538	ASN
1	K	539	VAL
1	K	547	ASN
1	K	553	ARG
1	K	565	PHE
1	K	589	GLU
1	K	597	ASN
1	K	599	VAL
1	K	611	ASP
1	K	615	ILE
1	K	618	ASP
1	K	620	ILE
1	K	625	THR
1	K	631	HIS
1	K	641	LEU
1	K	644	ASP
1	K	646	ASN
1	K	652	ASP
1	K	669	ASN
1	K	672	ILE
1	K	687	PHE
1	K	709	SER

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Mol	Chain	Res	Type
1	K	712	ILE
1	K	741	ASN
1	K	745	LEU
1	K	746	THR
1	K	748	ASN
1	K	763	VAL
1	K	766	CYS
1	K	783	ILE
1	K	790	ILE
1	K	813	VAL
1	K	815	ASP
1	K	826	ILE
1	K	827	ILE
1	K	842	THR
1	K	869	LYS
1	K	876	THR
1	K	880	ILE
1	K	883	SER
1	K	894	ASP
1	K	895	LEU
1	K	897	GLN
1	K	899	LEU
1	K	903	ASN
1	K	904	SER
1	K	926	LEU
1	K	932	VAL
1	K	933	VAL
1	K	942	VAL
1	K	943	ILE
1	K	946	VAL
1	L	15	ILE
1	L	19	ASP
1	L	25	SER
1	L	50	VAL
1	L	54	HIS
1	L	55	ASP
1	L	58	THR
1	L	64	LEU
1	L	69	ILE
1	L	79	SER
1	L	85	THR
1	L	96	MET

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Mol	Chain	Res	Type
1	L	98	SER
1	L	104	ARG
1	L	112	THR
1	L	198	ASN
1	L	199	LYS
1	L	201	ILE
1	L	206	THR
1	L	243	SER
1	L	244	TYR
1	L	246	ARG
1	L	248	THR
1	L	254	GLN
1	L	264	LEU
1	L	275	THR
1	L	277	VAL
1	L	278	ASN
1	L	280	MET
1	L	284	ASN
1	L	286	ILE
1	L	298	ASN
1	L	301	THR
1	L	307	SER
1	L	315	ASP
1	L	333	ILE
1	L	340	ILE
1	L	342	LEU
1	L	343	MET
1	L	345	TYR
1	L	347	SER
1	L	348	THR
1	L	350	ASN
1	L	361	LEU
1	L	367	LEU
1	L	368	GLN
1	L	383	ILE
1	L	398	ASP
1	L	399	SER
1	L	420	CYS
1	L	426	ILE
1	L	428	VAL
1	L	429	THR
1	L	430	ASP

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Mol	Chain	Res	Type
1	L	436	LYS
1	L	438	THR
1	L	441	ASN
1	L	445	THR
1	L	446	THR
1	L	450	ASP
1	L	455	GLU
1	L	459	ILE
1	L	461	VAL
1	L	469	ILE
1	L	477	ARG
1	L	482	SER
1	L	488	LEU
1	L	495	ASN
1	L	497	THR
1	L	498	ASN
1	L	501	ILE
1	L	507	THR
1	L	511	MET
1	L	516	VAL
1	L	521	VAL
1	L	523	CYS
1	L	534	ASP
1	L	539	VAL
1	L	554	SER
1	L	556	LEU
1	L	557	LEU
1	L	565	PHE
1	L	569	VAL
1	L	573	PHE
1	L	574	PHE
1	L	579	LEU
1	L	581	LEU
1	L	595	ASP
1	L	597	ASN
1	L	599	VAL
1	L	601	GLN
1	L	603	SER
1	L	606	ASN
1	L	608	LEU
1	L	610	VAL
1	L	641	LEU

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Mol	Chain	Res	Type
1	L	648	GLN
1	L	651	ASN
1	L	655	SER
1	L	658	ASN
1	L	660	LEU
1	L	663	ILE
1	L	668	THR
1	L	683	ARG
1	L	705	TYR
1	L	707	THR
1	L	728	VAL
1	L	730	ILE
1	L	736	VAL
1	L	741	ASN
1	L	752	ILE
1	L	759	GLU
1	L	762	ASN
1	L	766	CYS
1	L	783	ILE
1	L	790	ILE
1	L	815	ASP
1	L	820	ASP
1	L	836	VAL
1	L	843	MET
1	L	850	PRO
1	L	853	VAL
1	L	861	THR
1	L	864	ASP
1	L	878	TRP
1	L	880	ILE
1	L	883	SER
1	L	892	LEU
1	L	893	THR
1	L	894	ASP
1	L	895	LEU
1	L	897	GLN
1	L	901	TYR
1	L	903	ASN
1	L	921	THR
1	L	936	HIS
1	L	950	THR
2	Z	3	SER

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Mol	Chain	Res	Type
2	Z	8	MET
2	Z	13	LEU
2	Z	35	ASP
2	Z	53	SER
2	Z	67	GLU
2	Z	72	CYS
2	Z	82	GLU
2	Z	86	ARG
2	Z	113	ARG
2	Z	213	ILE
2	Z	224	THR
2	Z	228	GLU
2	Z	230	TYR
2	Z	231	ILE
2	Z	257	GLU
2	Z	266	GLU
2	Z	298	VAL
2	Z	313	LEU
2	Z	322	SER
2	Z	324	PHE
2	Z	342	VAL
2	Z	345	VAL
2	Z	352	LEU
2	Z	368	ASP
2	Z	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	328	ASN
1	J	331	ASN
1	J	338	ASN
1	J	377	GLN
1	J	474	ASN
1	J	512	ASN
1	J	543	ASN
1	J	544	HIS
1	J	591	ASN
1	J	786	GLN
1	K	254	GLN
1	K	271	GLN
1	K	346	ASN

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Mol	Chain	Res	Type
1	K	433	GLN
1	K	547	ASN
1	K	631	HIS
1	K	666	ASN
1	K	762	ASN
1	K	830	HIS
1	L	173	GLN
1	L	187	GLN
1	L	254	GLN
1	L	267	GLN
1	L	346	ASN
1	L	368	GLN
1	L	433	GLN
1	L	470	ASN
1	L	741	ASN
2	Z	2	ASN
2	Z	42	ASN
2	Z	252	ASN

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	3,2	9,11,12	1.57	1 (11%)	10,14,16	0.86	0
2	CGU	Z	6	2	9,11,12	1.24	0	10,14,16	1.63	2 (20%)
2	CGU	Z	32	2	9,11,12	1.53	1 (11%)	10,14,16	0.81	0
2	CGU	Z	39	2	9,11,12	1.50	1 (11%)	10,14,16	1.06	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CGU	Z	20	3,2	9,11,12	1.37	1 (11%)	10,14,16	0.85	0
2	CGU	Z	26	2	9,11,12	1.70	1 (11%)	10,14,16	0.98	0
2	CGU	Z	29	3,2	9,11,12	2.43	4 (44%)	10,14,16	0.87	0
2	CGU	Z	19	3,2	9,11,12	1.40	0	10,14,16	0.88	0
2	CGU	Z	16	3,2	9,11,12	1.31	0	10,14,16	0.83	0
2	CGU	Z	7	3,2	9,11,12	1.17	0	10,14,16	1.02	1 (10%)
2	CGU	Z	14	3,2	9,11,12	1.42	1 (11%)	10,14,16	0.85	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	3,2	-	8/13/14/16	-
2	CGU	Z	6	2	-	3/13/14/16	-
2	CGU	Z	32	2	-	9/13/14/16	-
2	CGU	Z	39	2	-	7/13/14/16	-
2	CGU	Z	20	3,2	-	4/13/14/16	-
2	CGU	Z	26	2	-	4/13/14/16	-
2	CGU	Z	29	3,2	-	6/13/14/16	-
2	CGU	Z	19	3,2	-	10/13/14/16	-
2	CGU	Z	16	3,2	-	0/13/14/16	-
2	CGU	Z	7	3,2	-	7/13/14/16	-
2	CGU	Z	14	3,2	-	10/13/14/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	29	CGU	CA-N	-4.15	1.36	1.48
2	Z	29	CGU	CG-CD1	3.53	1.56	1.52
2	Z	29	CGU	CG-CD2	3.25	1.56	1.52
2	Z	26	CGU	CG-CD2	3.20	1.56	1.52
2	Z	39	CGU	CG-CD2	2.64	1.55	1.52
2	Z	25	CGU	CG-CD2	2.42	1.55	1.52
2	Z	29	CGU	O-C	2.20	1.28	1.20
2	Z	32	CGU	CG-CD1	2.19	1.54	1.52
2	Z	14	CGU	CG-CD2	2.07	1.54	1.52
2	Z	20	CGU	CG-CD2	2.01	1.54	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	6	CGU	CB-CA-C	-3.93	104.94	110.99
2	Z	6	CGU	CB-CA-N	-2.80	104.36	110.48
2	Z	7	CGU	CB-CA-C	-2.22	107.57	110.99
2	Z	39	CGU	CB-CG-CD1	-2.02	109.00	113.11

There are no chirality outliers.

All (68) torsion outliers are listed below:

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

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

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	25	CGU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	6	CGU	3	0
2	Z	39	CGU	1	0
2	Z	26	CGU	2	0
2	Z	16	CGU	1	0
2	Z	14	CGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.

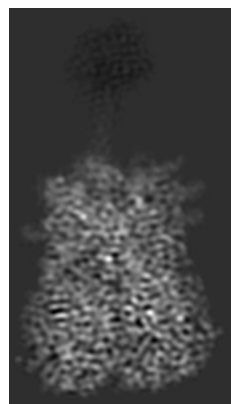
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45744. These allow visual inspection of the internal detail of the map and identification of artifacts.

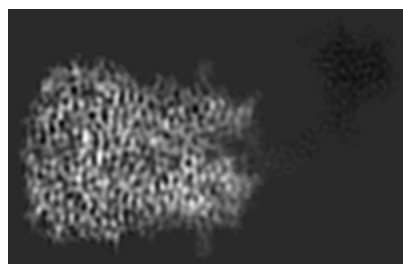
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

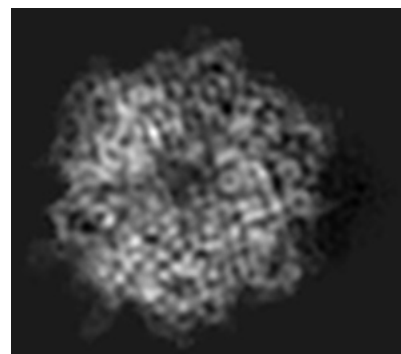
6.1.1 Primary map



X

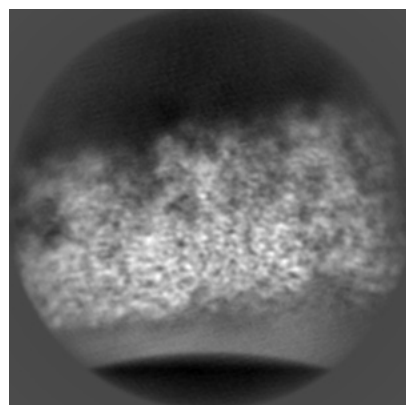


Y

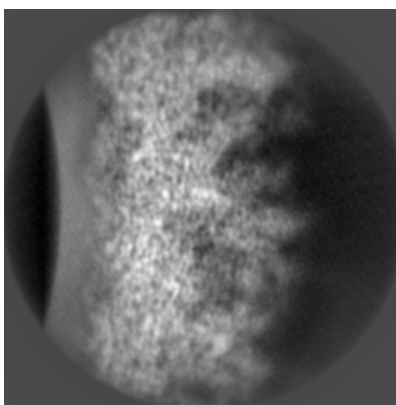


Z

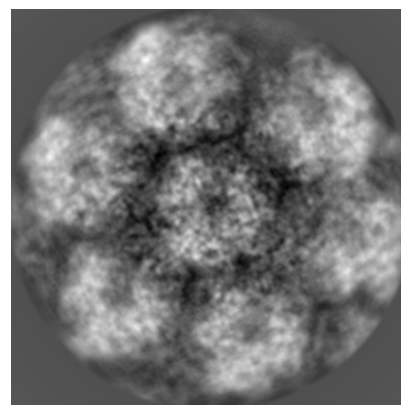
6.1.2 Raw map



X



Y

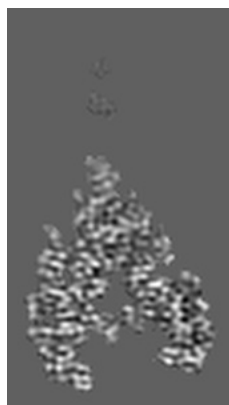


Z

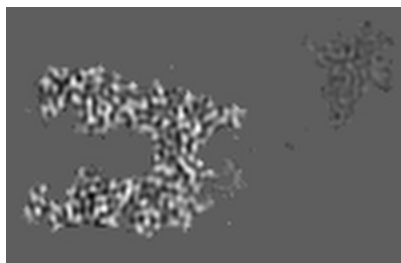
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

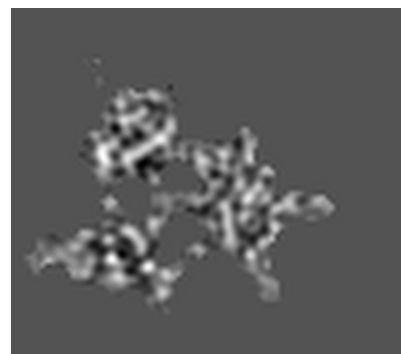
6.2.1 Primary map



X Index: 47

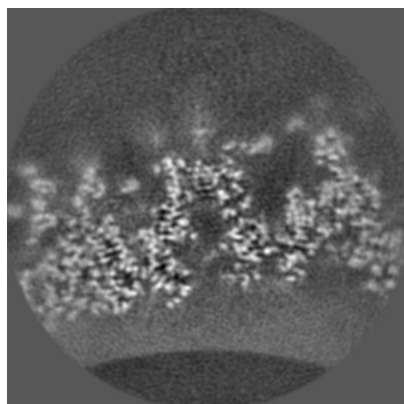


Y Index: 41

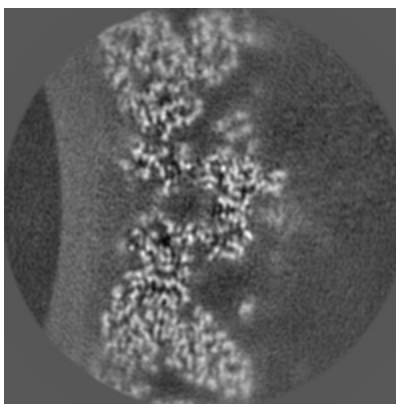


Z Index: 73

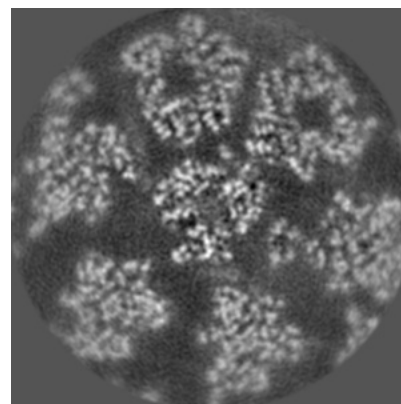
6.2.2 Raw map



X Index: 100



Y Index: 100

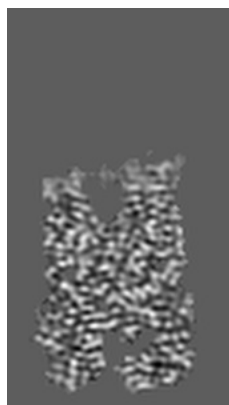


Z Index: 100

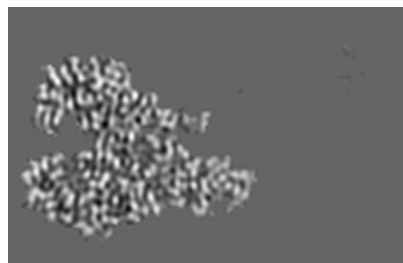
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

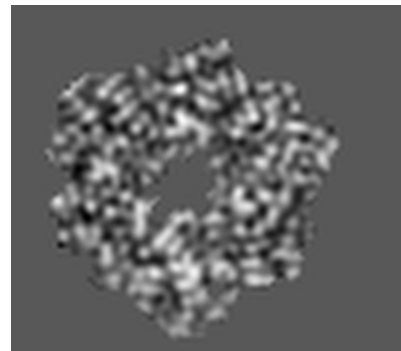
6.3.1 Primary map



X Index: 29

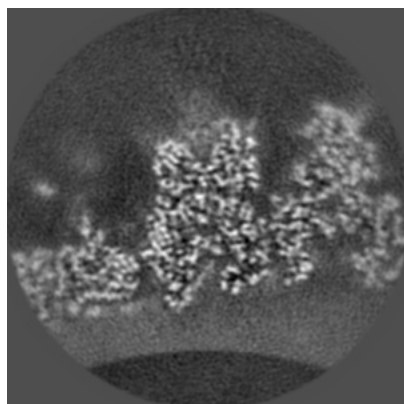


Y Index: 53

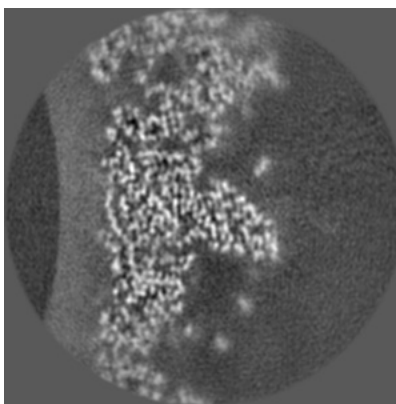


Z Index: 33

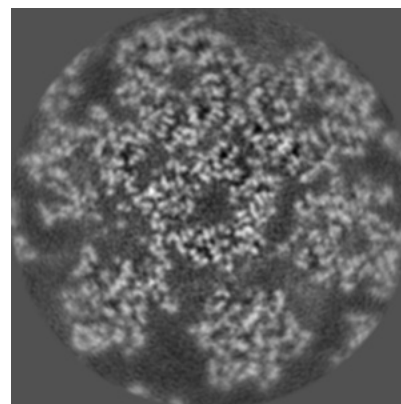
6.3.2 Raw map



X Index: 92



Y Index: 80



Z Index: 91

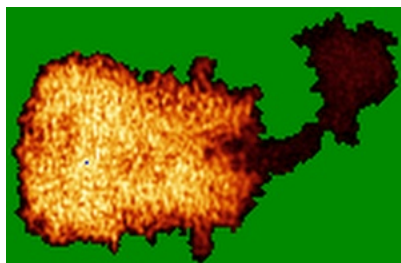
The images above show the largest variance slices of the map in three orthogonal directions.

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

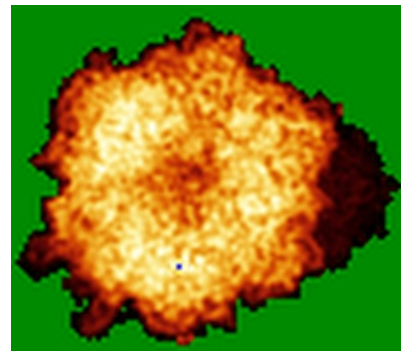
6.4.1 Primary map



X

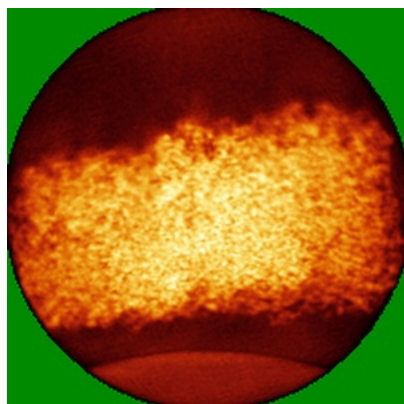


Y

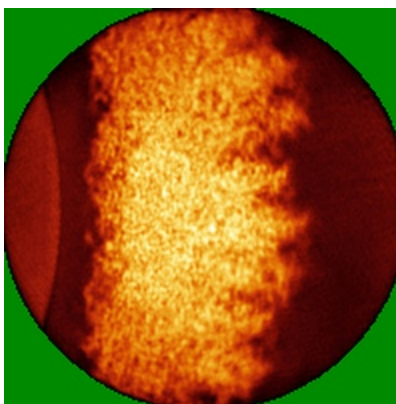


Z

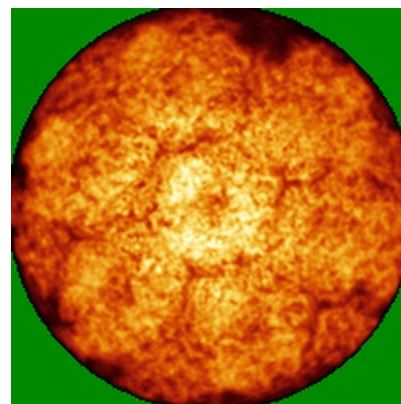
6.4.2 Raw map



X



Y

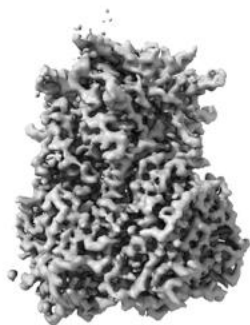


Z

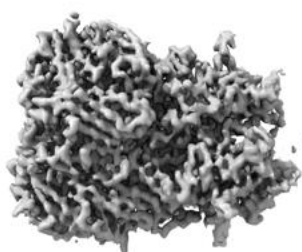
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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

6.5.2 Raw map



X



Y



Z

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.

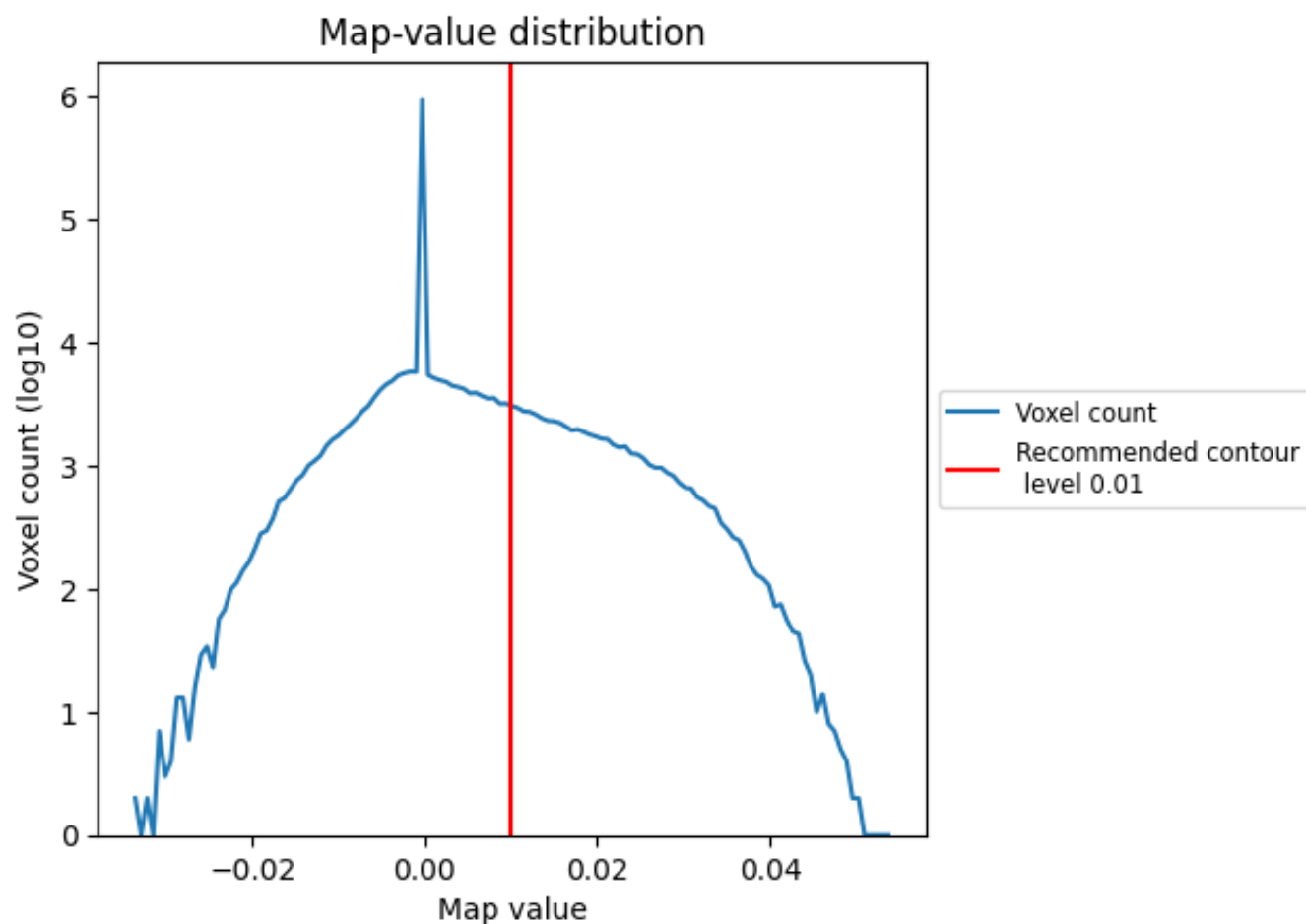
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

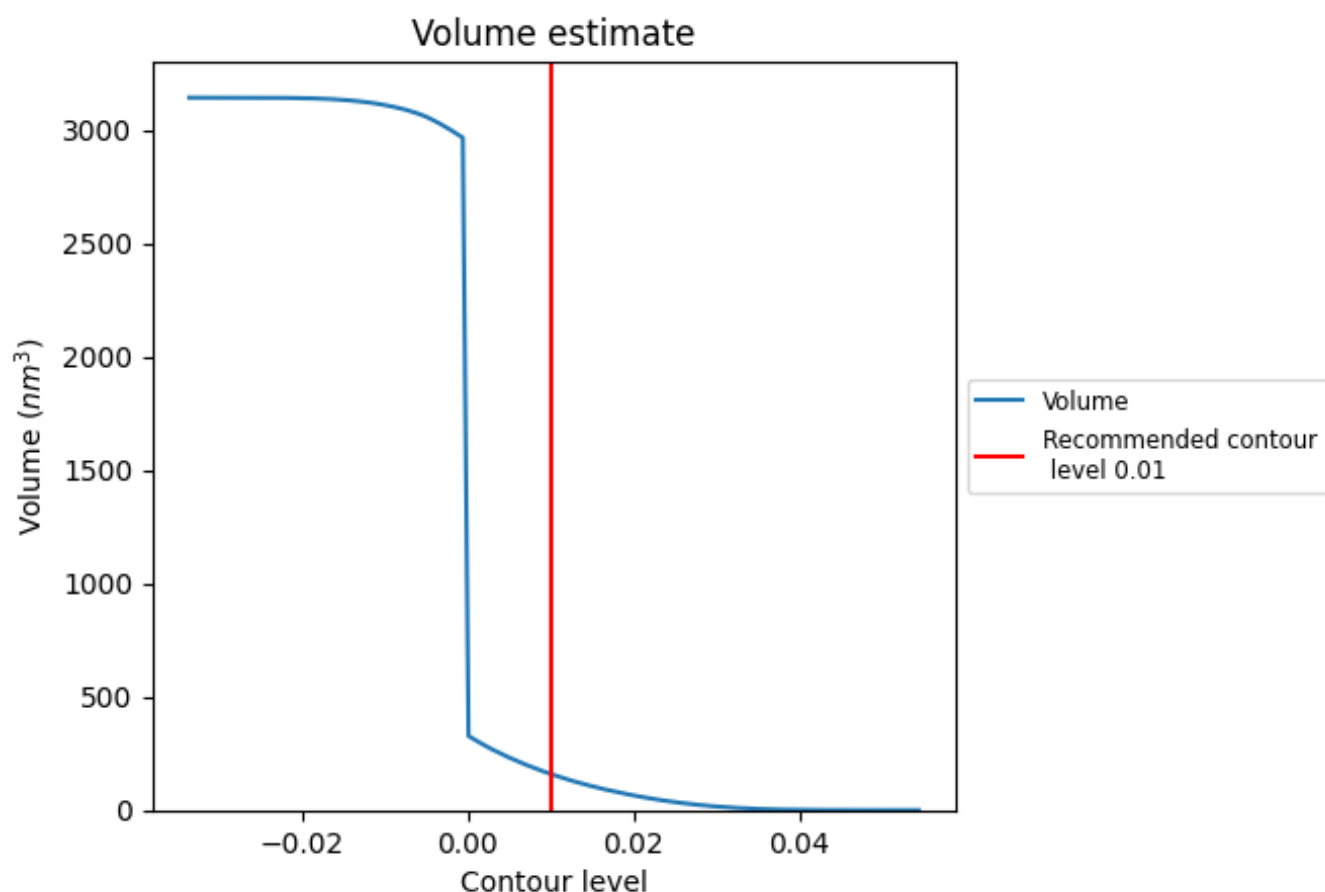
This section contains the results of statistical analysis of the map.

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 160 nm³; this corresponds to an approximate mass of 144 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.

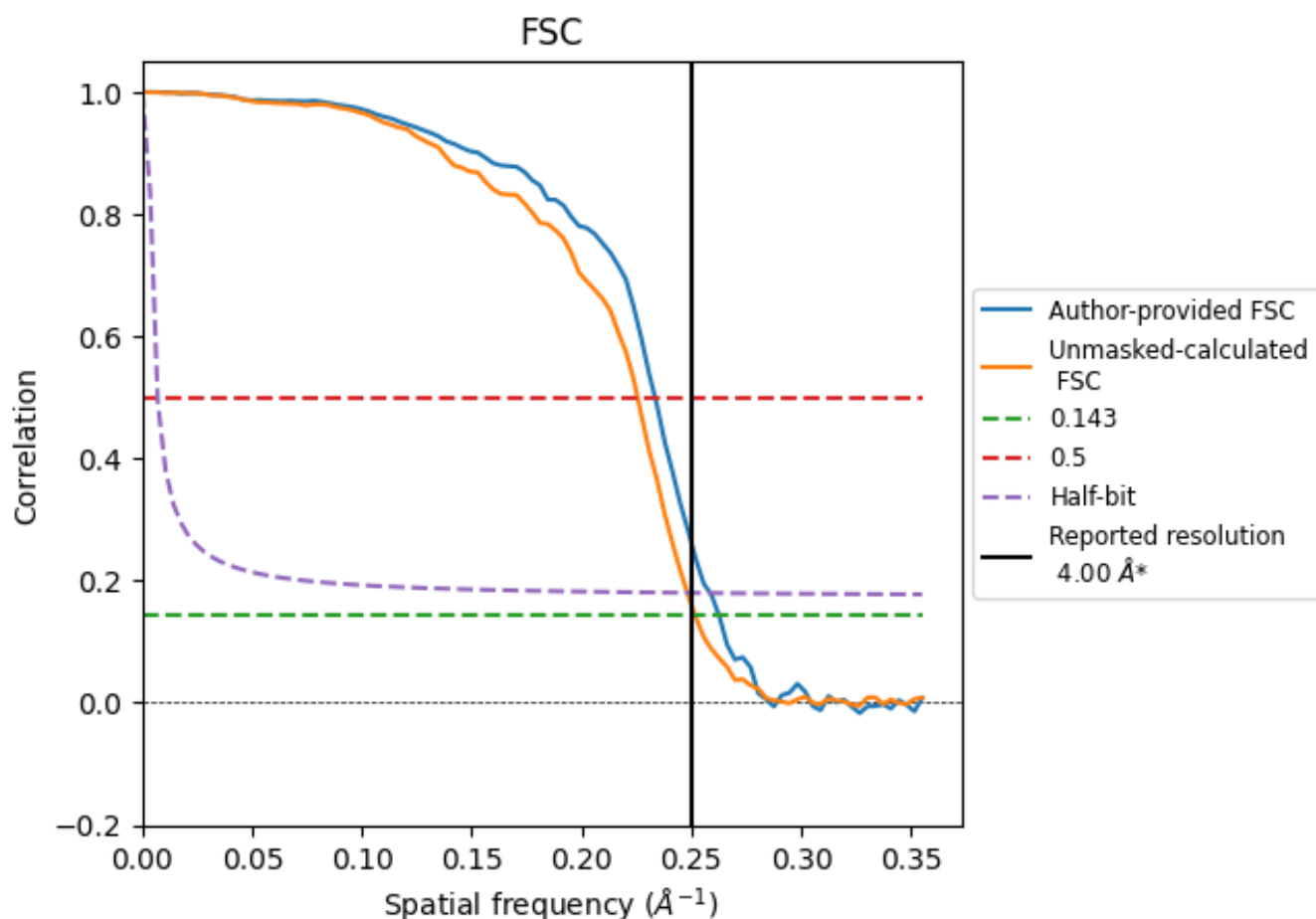
7.3 Rotationally averaged power spectrum [i](#)

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

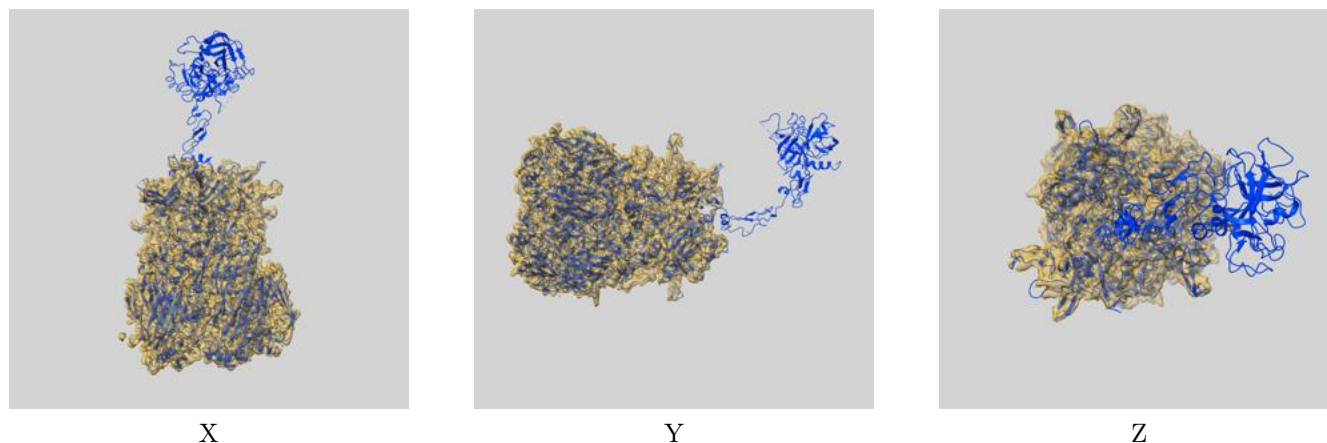
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.81	4.28	3.87
Unmasked-calculated*	3.97	4.43	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

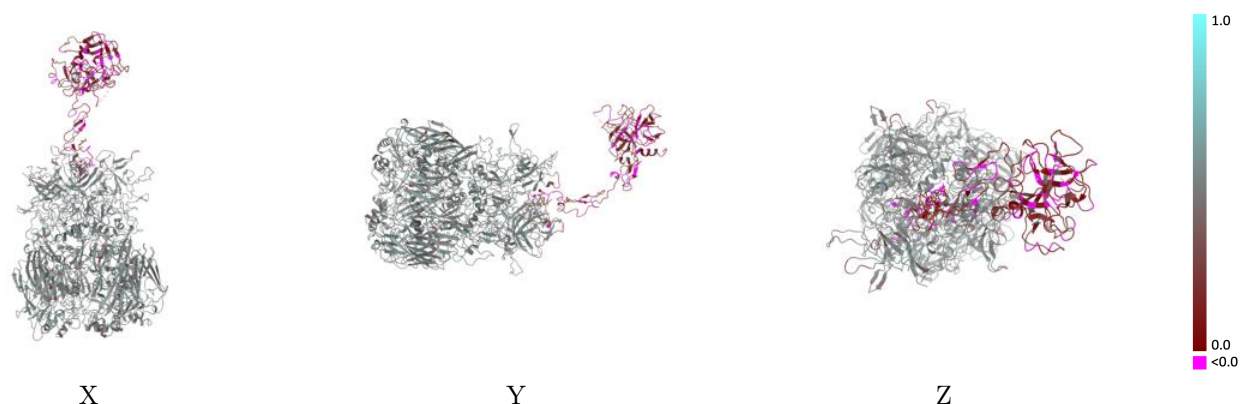
This section contains information regarding the fit between EMDB map EMD-45744 and PDB model 9CM9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



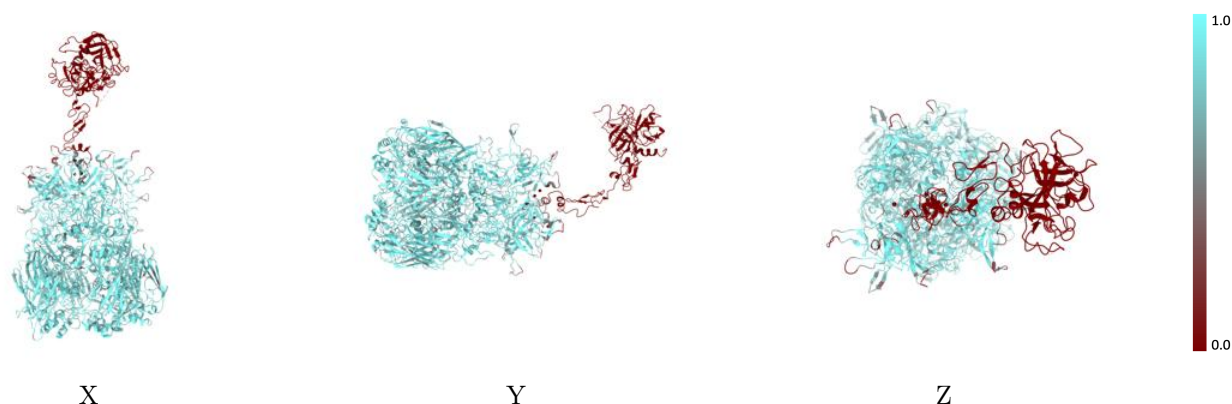
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



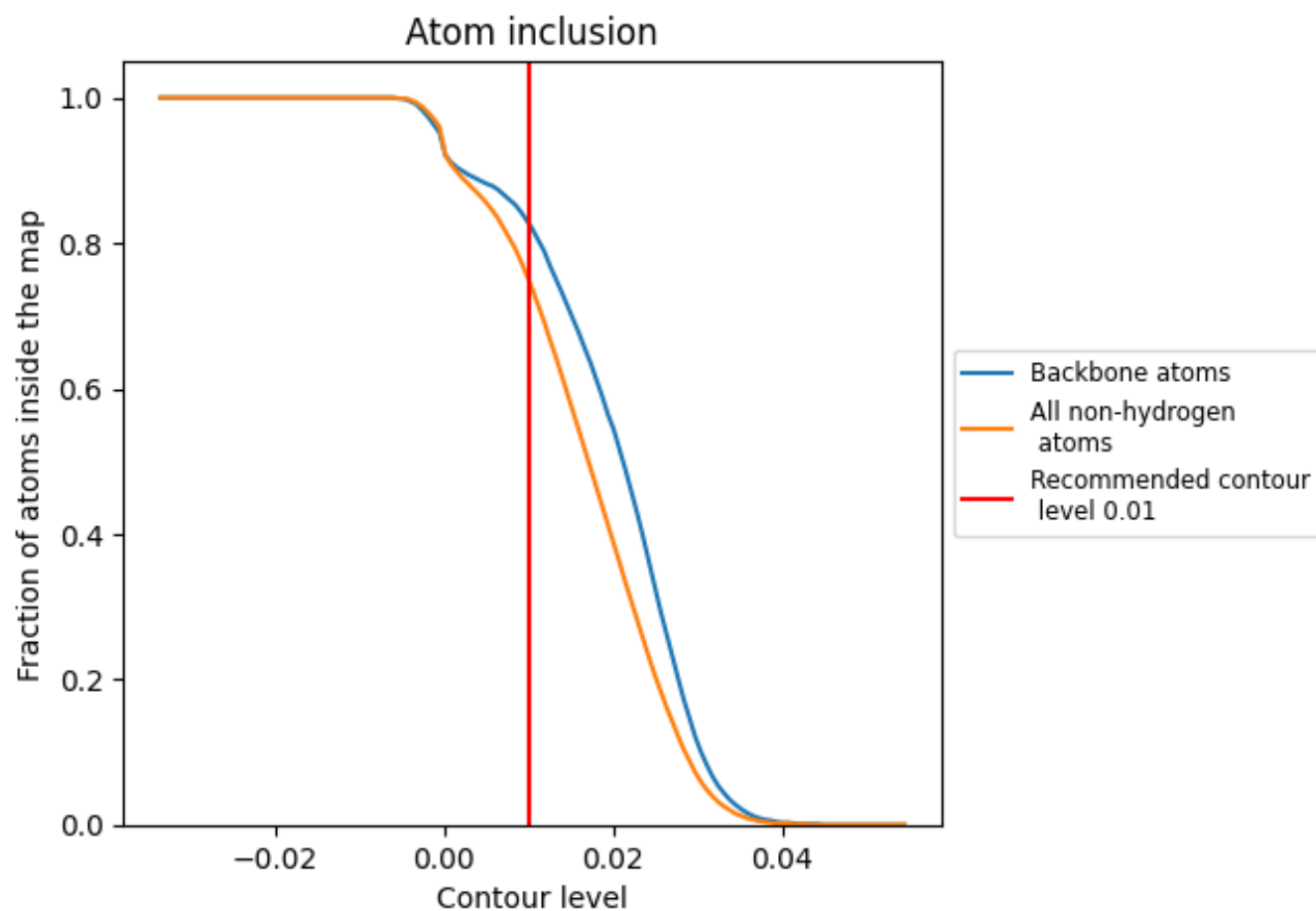
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 75% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7490	0.4590
J	0.8470	0.4990
K	0.8410	0.5000
L	0.8510	0.5030
Z	0.0320	0.1530

