



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:51 AM UTC

PDB ID : 8HLZ / pdb_00008hlz
EMDB ID : EMD-34886
Title : F8-A22-E4 complex of MPXV in hexameric form
Authors : Li, Y.N.; Shen, Y.P.; Hu, Z.W.; Yan, R.H.
Deposited on : 2022-12-02
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

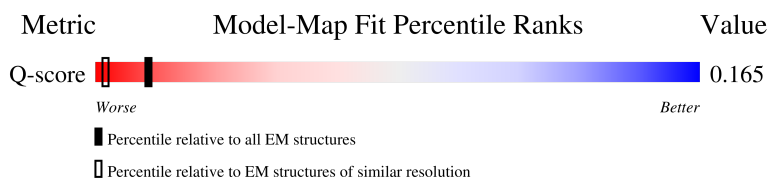
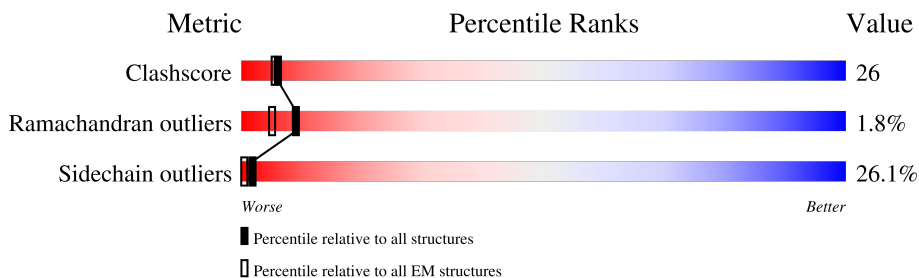
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	C	426	
1	F	426	
2	B	218	
2	E	218	

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Mol	Chain	Length	Quality of chain
3	A	1006	45% 43% 36% 13% 8%
3	D	1006	44% 35% 13% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24718 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 DNA polymerase processivity factor component A20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	370	Total	C	N	O	S	0	0
			3020	1937	495	578	10		
1	C	370	Total	C	N	O	S	0	0
			3020	1937	495	578	10		

- Molecule 2 is a protein called E4R.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	218	Total	C	N	O	S	0	0
			1772	1149	292	325	6		
2	B	218	Total	C	N	O	S	0	0
			1772	1149	292	325	6		

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	929	Total	C	N	O	S	0	0
			7567	4835	1262	1420	50		
3	A	929	Total	C	N	O	S	0	0
			7567	4835	1262	1420	50		

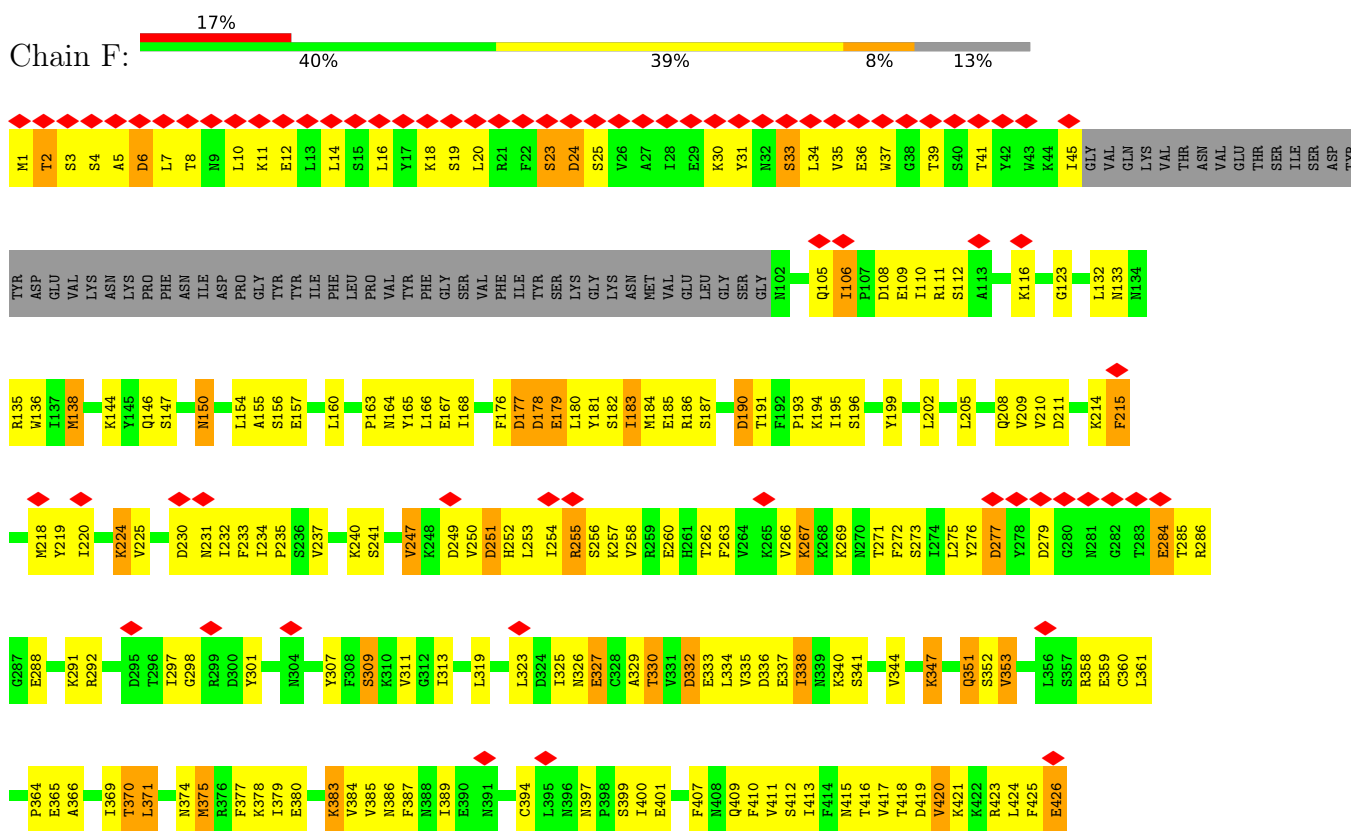
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	PHE	LEU	conflict	UNP A0A2L0AR76
A	108	PHE	LEU	conflict	UNP A0A2L0AR76

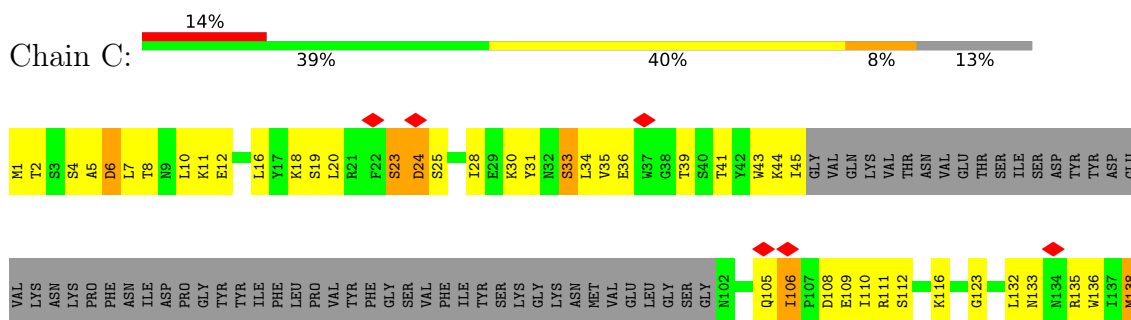
3 Residue-property plots

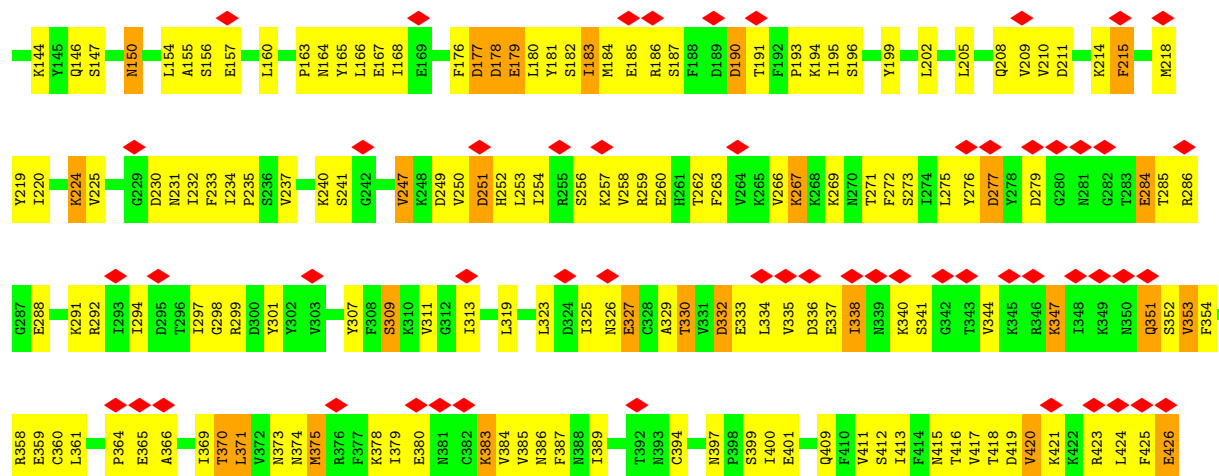
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA polymerase processivity factor component A20



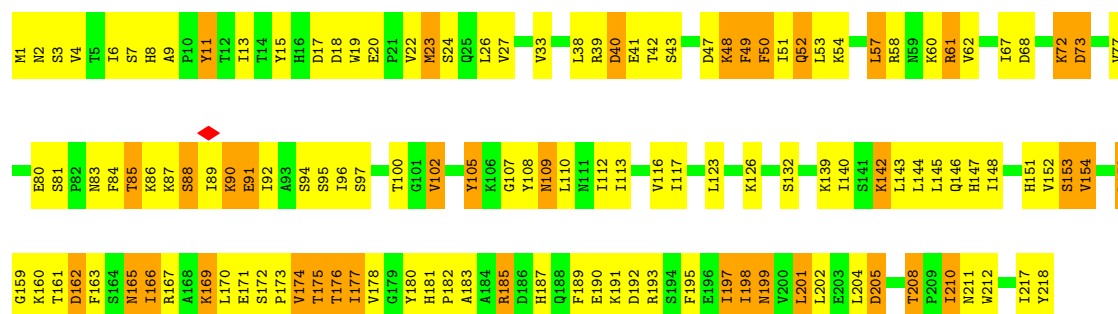
- Molecule 1: DNA polymerase processivity factor component A20





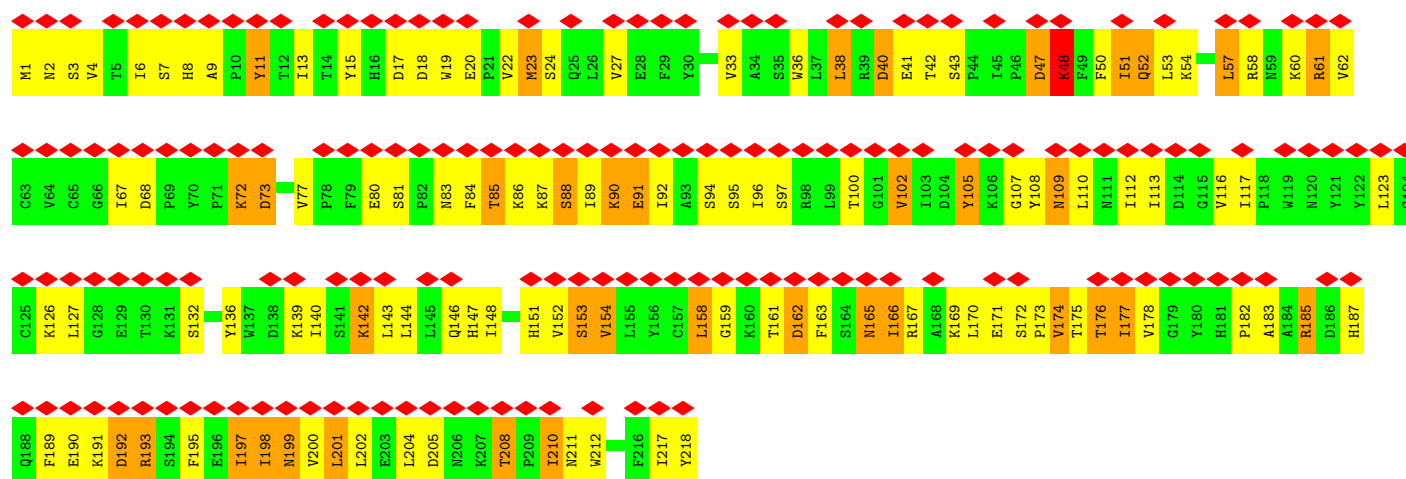
• Molecule 2: E4R

Chain E: 39% 43% 17%



• Molecule 2: E4R

Chain B: 41% 42% 17%



• Molecule 3: DNA polymerase

Chain D: 44% 35% 13% 8%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	391085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	315.36002, 315.36002, 315.36002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	C	0.35	0/3073	0.63	0/4142
1	F	0.35	0/3073	0.63	0/4142
2	B	0.36	0/1822	0.71	3/2479 (0.1%)
2	E	0.36	0/1822	0.70	2/2479 (0.1%)
3	A	0.47	0/7720	0.71	1/10418 (0.0%)
3	D	0.47	0/7720	0.71	1/10418 (0.0%)
All	All	0.43	0/25230	0.69	7/34078 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	788	LYS	N-CA-C	7.79	118.25	108.19
3	D	788	LYS	N-CA-C	7.79	118.23	108.19
2	B	192	ASP	N-CA-C	6.29	118.69	107.80
2	B	67	ILE	CA-C-N	-6.13	110.02	122.45
2	B	67	ILE	C-N-CA	-6.13	110.02	122.45
2	E	67	ILE	CA-C-N	-6.12	110.02	122.45
2	E	67	ILE	C-N-CA	-6.12	110.02	122.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3020	0	3035	142	0
1	F	3020	0	3035	151	0
2	B	1772	0	1764	96	0
2	E	1772	0	1764	99	0
3	A	7567	0	7528	425	0
3	D	7567	0	7528	405	0
All	All	24718	0	24654	1298	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 26.

All (1298) 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)
3:D:701:VAL:HA	3:D:715:ALA:CB	1.45	1.45
3:A:701:VAL:HA	3:A:715:ALA:CB	1.45	1.45
3:D:701:VAL:CA	3:D:715:ALA:HB2	1.55	1.35
3:A:701:VAL:CA	3:A:715:ALA:HB2	1.55	1.35
3:D:547:ILE:HD12	3:D:756:PHE:CE1	1.72	1.24
3:A:763:ASP:HB2	3:A:767:SER:HB3	1.22	1.20
3:D:604:ARG:HG3	3:D:611:GLU:OE1	1.40	1.19
3:A:701:VAL:CG1	3:A:715:ALA:HB3	1.74	1.16
3:D:701:VAL:CG1	3:D:715:ALA:HB3	1.74	1.16
3:A:45:GLU:OE1	3:A:46:ILE:HG12	1.44	1.15
3:D:45:GLU:OE1	3:D:46:ILE:HG12	1.46	1.14
3:D:547:ILE:CD1	3:D:756:PHE:CD1	2.33	1.12
3:D:799:ILE:HG23	3:D:982:LEU:HD13	1.12	1.11
3:D:540:MET:HA	3:D:797:ASN:HB2	1.22	1.10
3:A:540:MET:HA	3:A:797:ASN:HB3	1.20	1.07
3:A:799:ILE:HG23	3:A:982:LEU:HD13	1.12	1.06
3:A:608:LEU:O	3:A:609:ILE:HG23	1.55	1.06
3:D:608:LEU:O	3:D:609:ILE:HG23	1.55	1.05
3:A:701:VAL:HG12	3:A:715:ALA:HB3	1.06	1.04
3:A:547:ILE:HG12	3:A:794:VAL:H	1.21	1.04
3:A:799:ILE:HG23	3:A:982:LEU:CD1	1.88	1.03
3:D:546:LEU:HD23	3:D:548:PHE:CE2	1.94	1.02
3:D:701:VAL:HG12	3:D:715:ALA:HB3	1.06	1.02
3:D:799:ILE:HG23	3:D:982:LEU:CD1	1.88	1.02
3:A:763:ASP:CB	3:A:767:SER:HB3	1.90	1.01
1:C:256:SER:HB2	1:C:258:VAL:HG23	1.39	1.01
3:A:539:LYS:O	3:A:982:LEU:HG	1.63	0.99
3:D:547:ILE:CD1	3:D:756:PHE:HD1	1.75	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:533:VAL:HG13	3:D:803:LYS:HD2	1.46	0.98
3:A:533:VAL:HG13	3:A:803:LYS:HD2	1.45	0.97
3:D:539:LYS:O	3:D:982:LEU:HG	1.63	0.97
3:D:547:ILE:CD1	3:D:756:PHE:CE1	2.46	0.96
3:D:773:GLU:O	3:D:776:ARG:HB2	1.65	0.96
3:A:773:GLU:O	3:A:776:ARG:HB2	1.65	0.96
3:D:547:ILE:HD12	3:D:756:PHE:CD1	1.95	0.96
3:A:796:LYS:HG3	3:A:823:ARG:HH12	1.31	0.94
3:A:547:ILE:CG1	3:A:794:VAL:H	1.81	0.94
3:A:540:MET:CA	3:A:797:ASN:HB3	1.98	0.93
3:D:796:LYS:HG3	3:D:823:ARG:HH12	1.31	0.93
3:D:605:LEU:HD12	3:D:605:LEU:H	1.33	0.92
1:F:109:GLU:N	1:F:109:GLU:OE2	2.03	0.91
3:D:701:VAL:CA	3:D:715:ALA:CB	2.29	0.90
3:D:547:ILE:HD12	3:D:756:PHE:HE1	1.32	0.90
1:C:109:GLU:N	1:C:109:GLU:OE2	2.02	0.90
3:A:605:LEU:HD12	3:A:605:LEU:H	1.34	0.90
3:A:608:LEU:O	3:A:609:ILE:CG2	2.21	0.88
3:D:608:LEU:O	3:D:609:ILE:CG2	2.21	0.88
3:A:701:VAL:HG12	3:A:715:ALA:CB	2.00	0.88
3:D:840:LYS:O	3:D:841:ASN:HB2	1.73	0.87
3:A:840:LYS:O	3:A:841:ASN:HB2	1.72	0.87
3:D:540:MET:HA	3:D:797:ASN:CB	2.04	0.87
3:A:540:MET:HA	3:A:797:ASN:CB	2.03	0.87
3:A:701:VAL:CA	3:A:715:ALA:CB	2.29	0.85
2:E:50:PHE:HB3	2:E:53:LEU:HD13	1.56	0.85
3:D:542:SER:CB	3:D:758:GLU:HG3	2.06	0.85
3:A:542:SER:CB	3:A:758:GLU:HG3	2.06	0.84
3:A:542:SER:HB2	3:A:758:GLU:HG3	1.59	0.84
3:A:547:ILE:CG1	3:A:794:VAL:N	2.40	0.84
3:D:701:VAL:HG12	3:D:715:ALA:CB	2.00	0.84
3:D:542:SER:HB2	3:D:758:GLU:HG3	1.59	0.84
3:A:836:SER:HA	3:A:837:LYS:HE3	1.60	0.84
3:A:544:ASN:O	3:A:544:ASN:ND2	2.12	0.83
3:A:716:ASN:O	3:A:717:THR:OG1	1.96	0.83
2:E:48:LYS:HD2	2:E:48:LYS:N	1.93	0.82
3:D:544:ASN:O	3:D:544:ASN:ND2	2.12	0.82
3:D:838:PHE:HB2	3:D:960:LEU:HD22	1.62	0.82
3:D:836:SER:HA	3:D:837:LYS:HE3	1.59	0.81
3:A:45:GLU:HG3	3:A:46:ILE:H	1.44	0.81
3:D:45:GLU:HG3	3:D:46:ILE:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:SER:HB2	1:C:258:VAL:CG2	2.09	0.81
3:A:838:PHE:HB2	3:A:960:LEU:HD22	1.62	0.81
3:D:539:LYS:O	3:D:540:MET:CB	2.28	0.81
3:A:545:VAL:HG11	3:A:756:PHE:HB3	1.63	0.81
3:A:547:ILE:HD12	3:A:756:PHE:HE1	1.47	0.80
1:C:6:ASP:N	1:C:6:ASP:OD1	2.15	0.80
3:A:796:LYS:HG3	3:A:823:ARG:NH1	1.96	0.80
3:D:545:VAL:HG11	3:D:756:PHE:HB3	1.63	0.80
1:C:218:MET:HG2	1:C:266:VAL:HG11	1.63	0.80
3:A:688:THR:O	3:A:692:ARG:HB2	1.82	0.80
1:F:332:ASP:OD1	1:F:332:ASP:N	2.13	0.80
3:A:539:LYS:O	3:A:540:MET:CB	2.28	0.80
3:D:547:ILE:HG13	3:D:794:VAL:HB	1.63	0.79
3:D:688:THR:O	3:D:692:ARG:HB2	1.82	0.79
1:C:335:VAL:HG12	1:C:420:VAL:HG12	1.63	0.79
3:A:832:ARG:HD3	3:A:893:SER:HB2	1.64	0.79
3:D:832:ARG:HD3	3:D:893:SER:HB2	1.64	0.79
1:C:332:ASP:OD1	1:C:332:ASP:N	2.13	0.79
3:A:547:ILE:HG13	3:A:794:VAL:N	1.97	0.79
1:F:218:MET:HG2	1:F:266:VAL:HG11	1.63	0.79
1:F:135:ARG:HE	1:F:136:TRP:H	1.29	0.79
1:F:335:VAL:HG12	1:F:420:VAL:HG12	1.63	0.79
3:D:796:LYS:HG3	3:D:823:ARG:NH1	1.96	0.78
1:F:6:ASP:OD1	1:F:6:ASP:N	2.15	0.78
3:D:546:LEU:HD23	3:D:548:PHE:CZ	2.19	0.78
2:B:72:LYS:HZ2	2:B:72:LYS:HB2	1.46	0.78
3:D:540:MET:CA	3:D:797:ASN:HB2	2.09	0.78
1:F:179:GLU:HA	1:F:182:SER:HG	1.48	0.77
3:D:167:ILE:HD11	3:D:268:ASP:HA	1.66	0.77
3:D:796:LYS:CG	3:D:823:ARG:HH22	1.97	0.77
1:C:135:ARG:HE	1:C:136:TRP:H	1.29	0.77
1:F:190:ASP:N	1:F:190:ASP:OD1	2.16	0.77
3:A:406:ILE:O	3:A:407:ARG:NH1	2.16	0.77
3:A:167:ILE:HD11	3:A:268:ASP:HA	1.66	0.77
1:F:182:SER:HB2	1:F:186:ARG:HH12	1.50	0.77
1:F:179:GLU:HA	1:F:182:SER:OG	1.85	0.76
1:C:190:ASP:N	1:C:190:ASP:OD1	2.16	0.76
2:E:47:ASP:C	2:E:48:LYS:HD2	2.10	0.76
2:E:84:PHE:HE1	2:E:90:LYS:HA	1.50	0.76
3:D:799:ILE:CG2	3:D:982:LEU:HD13	2.06	0.76
2:E:84:PHE:HD2	2:E:107:GLY:HA2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:701:VAL:CG1	3:D:715:ALA:CB	2.61	0.76
3:A:701:VAL:HA	3:A:715:ALA:HB2	0.78	0.76
3:D:406:ILE:O	3:D:407:ARG:NH1	2.16	0.76
2:B:84:PHE:HE1	2:B:90:LYS:HA	1.50	0.76
3:A:796:LYS:CG	3:A:823:ARG:HH22	1.97	0.76
3:D:972:PHE:HA	3:D:975:LEU:HD12	1.68	0.76
3:A:972:PHE:HA	3:A:975:LEU:HD12	1.68	0.76
3:D:876:LEU:HD11	3:D:968:TYR:HB3	1.68	0.76
2:B:84:PHE:HD2	2:B:107:GLY:HA2	1.50	0.76
3:D:989:CYS:SG	3:D:990:ILE:N	2.58	0.75
3:A:876:LEU:HD11	3:A:968:TYR:HB3	1.68	0.75
3:A:989:CYS:SG	3:A:990:ILE:N	2.58	0.75
1:F:2:THR:HG1	2:B:192:ASP:CG	1.95	0.75
3:A:539:LYS:O	3:A:982:LEU:CG	2.34	0.75
3:D:779:ASN:HB2	3:D:789:ILE:HG22	1.68	0.75
3:D:701:VAL:HA	3:D:715:ALA:HB2	0.78	0.75
1:C:33:SER:O	1:C:36:GLU:HB3	1.86	0.75
3:A:43:THR:HG22	3:A:88:MET:HE1	1.68	0.75
3:A:808:THR:HG21	3:A:810:LYS:HE3	1.69	0.74
3:D:486:TYR:CE2	3:D:501:ILE:HD12	2.22	0.74
3:D:605:LEU:HD12	3:D:605:LEU:N	2.03	0.74
2:B:72:LYS:HB2	2:B:72:LYS:NZ	2.02	0.74
1:F:33:SER:O	1:F:36:GLU:HB3	1.86	0.74
3:A:840:LYS:HE2	3:A:843:ILE:HB	1.68	0.74
1:F:182:SER:HB2	1:F:186:ARG:NH1	2.03	0.74
3:D:361:LEU:HD11	3:D:371:ILE:HB	1.69	0.74
2:E:72:LYS:HB2	2:E:72:LYS:NZ	2.03	0.74
3:D:627:LEU:HD21	3:D:667:VAL:HG11	1.69	0.74
2:E:72:LYS:HB2	2:E:72:LYS:HZ2	1.52	0.74
3:D:539:LYS:O	3:D:982:LEU:CG	2.34	0.74
3:D:43:THR:HG22	3:D:88:MET:HE1	1.68	0.73
3:A:547:ILE:HD12	3:A:756:PHE:CE1	2.23	0.73
3:A:701:VAL:CG1	3:A:715:ALA:CB	2.61	0.73
3:A:779:ASN:HB2	3:A:789:ILE:HG22	1.68	0.73
3:D:45:GLU:HG3	3:D:46:ILE:N	2.04	0.73
3:D:796:LYS:HG3	3:D:823:ARG:HH22	1.52	0.73
1:C:351:GLN:O	1:C:421:LYS:NZ	2.21	0.73
3:A:486:TYR:CE2	3:A:501:ILE:HD12	2.22	0.73
2:E:6:ILE:HG22	2:E:27:VAL:HG13	1.69	0.73
3:D:546:LEU:CD2	3:D:548:PHE:CE2	2.72	0.73
3:D:840:LYS:O	3:D:841:ASN:CB	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:605:LEU:HD12	3:A:605:LEU:N	2.03	0.73
3:A:627:LEU:HD21	3:A:667:VAL:HG11	1.69	0.73
3:A:796:LYS:HG3	3:A:823:ARG:HH22	1.51	0.73
3:A:361:LEU:HD11	3:A:371:ILE:HB	1.69	0.73
3:A:840:LYS:O	3:A:841:ASN:CB	2.36	0.73
1:F:351:GLN:O	1:F:421:LYS:NZ	2.21	0.73
2:E:50:PHE:HB3	2:E:53:LEU:CD1	2.18	0.73
1:C:182:SER:HB2	1:C:186:ARG:HH12	1.53	0.73
3:D:701:VAL:N	3:D:715:ALA:HB2	2.04	0.73
3:D:808:THR:HG21	3:D:810:LYS:HE3	1.69	0.73
2:B:6:ILE:HG22	2:B:27:VAL:HG13	1.69	0.73
3:A:964:GLN:HB3	3:A:968:TYR:HE2	1.53	0.73
3:D:519:ARG:NH2	3:D:679:TYR:O	2.21	0.73
3:A:45:GLU:HG3	3:A:46:ILE:N	2.03	0.72
3:A:742:ARG:NH1	3:A:742:ARG:HG3	2.04	0.72
3:A:846:TYR:HE1	3:A:868:ILE:HB	1.54	0.72
1:C:177:ASP:H	1:C:180:LEU:HB2	1.52	0.72
3:D:604:ARG:HB2	3:D:605:LEU:HD12	1.71	0.72
3:D:700:SER:C	3:D:715:ALA:HB2	2.15	0.72
3:D:840:LYS:HE2	3:D:843:ILE:HB	1.68	0.72
1:F:177:ASP:H	1:F:180:LEU:HB2	1.52	0.72
3:D:964:GLN:HB3	3:D:968:TYR:HE2	1.53	0.72
3:A:701:VAL:N	3:A:715:ALA:HB2	2.04	0.72
3:D:609:ILE:N	3:D:609:ILE:HD13	2.05	0.71
3:D:249:LYS:NZ	3:D:283:LYS:O	2.21	0.71
1:C:179:GLU:HA	1:C:182:SER:OG	1.90	0.71
3:A:249:LYS:NZ	3:A:283:LYS:O	2.21	0.71
3:A:700:SER:C	3:A:715:ALA:HB2	2.15	0.71
3:D:523:LYS:O	3:D:674:ARG:NH2	2.23	0.71
3:D:846:TYR:HE1	3:D:868:ILE:HB	1.54	0.71
3:A:519:ARG:NH2	3:A:679:TYR:O	2.21	0.71
3:A:523:LYS:O	3:A:674:ARG:NH2	2.23	0.71
3:D:700:SER:O	3:D:715:ALA:HB2	1.91	0.71
1:C:182:SER:HB2	1:C:186:ARG:NH1	2.06	0.71
1:F:330:THR:N	1:F:333:GLU:OE2	2.20	0.71
1:C:330:THR:N	1:C:333:GLU:OE2	2.20	0.71
3:A:609:ILE:N	3:A:609:ILE:HD13	2.05	0.71
3:A:701:VAL:HA	3:A:715:ALA:CA	2.21	0.71
3:D:23:ARG:NH1	3:D:29:THR:OG1	2.24	0.70
3:D:742:ARG:HG3	3:D:742:ARG:NH1	2.05	0.70
3:A:23:ARG:NH1	3:A:29:THR:OG1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:700:SER:O	3:A:715:ALA:HB2	1.91	0.70
3:D:608:LEU:C	3:D:609:ILE:HG23	2.17	0.70
3:A:742:ARG:HG3	3:A:742:ARG:HH11	1.55	0.70
3:A:605:LEU:H	3:A:605:LEU:CD1	2.04	0.70
3:A:608:LEU:C	3:A:609:ILE:HG23	2.16	0.70
3:D:742:ARG:HG3	3:D:742:ARG:HH11	1.55	0.70
3:D:988:LEU:HA	3:D:991:SER:HB2	1.74	0.69
3:A:187:SER:O	3:A:188:TYR:CD1	2.45	0.69
3:A:821:PRO:HG2	3:A:823:ARG:HE	1.57	0.69
3:A:580:GLU:O	3:A:584:ASN:HB2	1.93	0.69
3:A:763:ASP:CG	3:A:767:SER:CA	2.65	0.69
3:A:799:ILE:CG2	3:A:982:LEU:HD13	2.06	0.69
3:D:187:SER:O	3:D:188:TYR:CD1	2.46	0.69
1:C:334:LEU:O	1:C:338:ILE:HG12	1.93	0.69
3:A:547:ILE:HG12	3:A:794:VAL:N	2.00	0.69
1:F:334:LEU:O	1:F:338:ILE:HG12	1.93	0.69
3:D:605:LEU:H	3:D:605:LEU:CD1	2.03	0.69
3:D:821:PRO:HG2	3:D:823:ARG:HE	1.57	0.69
2:B:18:ASP:OD1	2:B:58:ARG:NH2	2.20	0.69
2:B:47:ASP:O	2:B:48:LYS:HD2	1.93	0.69
3:D:580:GLU:O	3:D:584:ASN:HB2	1.93	0.69
3:D:574:SER:N	3:D:610:SER:OG	2.25	0.68
3:D:701:VAL:HA	3:D:715:ALA:CA	2.21	0.68
3:A:574:SER:N	3:A:610:SER:OG	2.25	0.68
3:A:988:LEU:HA	3:A:991:SER:HB2	1.74	0.68
3:A:763:ASP:CG	3:A:767:SER:HB3	2.19	0.68
3:D:840:LYS:HB3	3:D:889:LEU:O	1.94	0.68
3:A:81:ARG:HG2	3:A:81:ARG:HH11	1.59	0.68
3:D:872:LEU:HD21	3:D:972:PHE:HB3	1.75	0.67
3:A:411:LEU:HB2	3:A:414:GLY:H	1.60	0.67
3:A:872:LEU:HD21	3:A:972:PHE:HB3	1.75	0.67
3:A:18:LEU:HD21	3:A:110:ILE:HD11	1.75	0.67
2:B:62:VAL:HG23	2:B:154:VAL:HB	1.77	0.67
2:E:18:ASP:OD1	2:E:58:ARG:NH2	2.20	0.67
2:E:62:VAL:HG23	2:E:154:VAL:HB	1.77	0.67
3:A:546:LEU:HD23	3:A:771:ALA:HB2	1.76	0.67
3:D:547:ILE:HD13	3:D:756:PHE:HD1	1.57	0.67
3:A:796:LYS:HG3	3:A:823:ARG:NH2	2.10	0.67
3:D:18:LEU:HD21	3:D:110:ILE:HD11	1.75	0.67
1:C:183:ILE:HG13	1:C:184:MET:N	2.10	0.67
3:A:170:HIS:HB2	3:A:207:MET:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:411:LEU:HB2	3:D:414:GLY:H	1.60	0.67
2:B:36:TRP:NE1	3:A:179:PHE:HB3	2.09	0.67
2:E:40:ASP:N	2:E:40:ASP:OD1	2.28	0.66
3:D:546:LEU:CD2	3:D:548:PHE:HE2	2.09	0.66
3:D:634:ARG:HE	3:D:661:LYS:HB2	1.60	0.66
3:D:539:LYS:H	3:D:982:LEU:HA	1.59	0.66
3:A:840:LYS:HB3	3:A:889:LEU:O	1.94	0.66
1:F:194:LYS:NZ	1:F:196:SER:O	2.21	0.66
3:D:724:MET:N	3:D:724:MET:HE2	2.11	0.66
3:A:573:VAL:HA	3:A:610:SER:OG	1.95	0.66
1:C:194:LYS:NZ	1:C:196:SER:OG	2.29	0.66
3:A:81:ARG:HG2	3:A:81:ARG:NH1	2.10	0.66
3:A:724:MET:HE2	3:A:724:MET:N	2.11	0.66
3:A:777:LEU:HD23	3:A:781:ARG:HB3	1.77	0.66
3:D:81:ARG:HG2	3:D:81:ARG:HH11	1.59	0.66
3:D:796:LYS:HG3	3:D:823:ARG:NH2	2.10	0.66
1:F:183:ILE:HG13	1:F:184:MET:N	2.10	0.66
1:F:194:LYS:NZ	1:F:196:SER:OG	2.29	0.66
3:A:659:THR:O	3:A:663:VAL:HG13	1.96	0.66
3:D:81:ARG:HG2	3:D:81:ARG:NH1	2.10	0.65
3:D:573:VAL:HA	3:D:610:SER:OG	1.95	0.65
3:D:777:LEU:HD23	3:D:781:ARG:HB3	1.77	0.65
3:A:539:LYS:H	3:A:982:LEU:HA	1.59	0.65
3:A:701:VAL:HB	3:A:714:PHE:HB3	1.78	0.65
3:D:170:HIS:HB2	3:D:207:MET:HE1	1.77	0.65
3:D:687:CYS:O	3:D:688:THR:OG1	2.13	0.65
3:D:797:ASN:ND2	3:D:854:LEU:O	2.30	0.65
3:D:659:THR:O	3:D:663:VAL:HG13	1.96	0.65
3:D:765:ASP:O	3:D:768:ILE:HG13	1.97	0.65
3:A:547:ILE:HD11	3:A:794:VAL:HB	1.77	0.65
3:A:763:ASP:CG	3:A:767:SER:CB	2.70	0.65
2:E:26:LEU:HD21	2:E:50:PHE:HE2	1.62	0.65
3:A:833:ARG:O	3:A:835:VAL:HG13	1.97	0.65
3:D:486:TYR:CZ	3:D:663:VAL:HG12	2.31	0.64
2:B:40:ASP:OD1	2:B:40:ASP:N	2.28	0.64
1:C:288:GLU:OE2	1:C:288:GLU:N	2.24	0.64
3:A:486:TYR:CZ	3:A:663:VAL:HG12	2.31	0.64
3:A:634:ARG:HE	3:A:661:LYS:HB2	1.60	0.64
2:E:7:SER:OG	2:E:8:HIS:ND1	2.31	0.64
3:D:836:SER:CA	3:D:837:LYS:HE3	2.27	0.64
1:C:109:GLU:HG2	1:C:110:ILE:HG12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:761:SER:O	3:A:762:GLN:HB3	1.98	0.64
3:D:701:VAL:HB	3:D:714:PHE:HB3	1.78	0.64
3:D:779:ASN:HD22	3:D:789:ILE:HA	1.63	0.64
3:D:833:ARG:O	3:D:835:VAL:HG13	1.97	0.64
1:C:386:ASN:OD1	1:C:387:PHE:N	2.31	0.64
2:B:7:SER:OG	2:B:8:HIS:ND1	2.31	0.64
3:A:211:GLN:OE1	3:A:212:GLU:N	2.31	0.64
3:A:547:ILE:CD1	3:A:794:VAL:HB	2.27	0.64
1:F:109:GLU:HG2	1:F:110:ILE:HG12	1.80	0.64
3:A:521:GLU:OE1	3:A:522:THR:N	2.31	0.64
3:A:546:LEU:HD12	3:A:546:LEU:N	2.13	0.64
3:D:211:GLN:OE1	3:D:212:GLU:N	2.31	0.64
3:D:374:ASP:O	3:D:376:THR:N	2.31	0.64
3:D:521:GLU:OE1	3:D:522:THR:N	2.31	0.64
3:A:175:PHE:HD1	3:A:176:PRO:HD2	1.63	0.64
1:F:288:GLU:OE2	1:F:288:GLU:N	2.24	0.63
3:D:175:PHE:HD1	3:D:176:PRO:HD2	1.63	0.63
1:F:255:ARG:O	1:F:255:ARG:HG2	1.98	0.63
3:A:509:LEU:HD11	3:A:625:ARG:HE	1.63	0.63
1:C:155:ALA:HB1	1:C:160:LEU:HB2	1.80	0.63
3:A:551:ASN:HD21	3:A:788:LYS:HB2	1.63	0.63
1:F:155:ALA:HB1	1:F:160:LEU:HB2	1.80	0.63
3:D:551:ASN:HD21	3:D:788:LYS:HB2	1.63	0.63
1:F:386:ASN:OD1	1:F:387:PHE:N	2.31	0.63
3:D:184:SER:OG	3:D:185:HIS:ND1	2.23	0.63
3:A:538:GLN:NE2	3:A:984:ASP:OD2	2.31	0.63
1:F:353:VAL:HG12	1:F:417:VAL:HG13	1.80	0.63
2:E:199:ASN:HA	2:E:202:LEU:HB2	1.80	0.63
1:C:354:PHE:HE2	3:A:578:LEU:HD23	1.64	0.63
2:B:199:ASN:HA	2:B:202:LEU:HB2	1.80	0.63
3:A:836:SER:CA	3:A:837:LYS:HE3	2.28	0.63
3:D:538:GLN:NE2	3:D:984:ASP:OD2	2.31	0.62
3:A:779:ASN:HD22	3:A:789:ILE:HA	1.63	0.62
1:F:182:SER:O	1:F:185:GLU:HB3	1.99	0.62
3:A:762:GLN:O	3:A:762:GLN:HG3	1.99	0.62
1:F:251:ASP:OD1	1:F:251:ASP:N	2.20	0.62
3:A:801:GLN:O	3:A:801:GLN:HG2	1.99	0.62
1:C:182:SER:O	1:C:185:GLU:HB3	2.00	0.62
3:A:763:ASP:CG	3:A:767:SER:N	2.58	0.62
3:D:371:ILE:HD11	3:D:411:LEU:HD11	1.81	0.62
3:D:547:ILE:HG22	3:D:547:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:509:LEU:HD11	3:D:625:ARG:HE	1.63	0.62
3:A:209:THR:OG1	3:A:211:GLN:NE2	2.32	0.62
3:A:374:ASP:O	3:A:376:THR:N	2.31	0.62
3:A:609:ILE:HG12	3:A:609:ILE:O	2.00	0.62
3:A:78:ILE:HG21	3:A:569:VAL:HG12	1.81	0.62
3:D:209:THR:OG1	3:D:211:GLN:NE2	2.32	0.62
3:D:605:LEU:O	3:D:607:ASN:N	2.33	0.62
3:D:801:GLN:HG2	3:D:801:GLN:O	1.99	0.62
3:D:78:ILE:HG21	3:D:569:VAL:HG12	1.81	0.61
3:D:773:GLU:HA	3:D:776:ARG:HG3	1.82	0.61
1:F:14:LEU:HD11	2:B:200:VAL:HG13	1.82	0.61
3:A:371:ILE:HD11	3:A:411:LEU:HD11	1.81	0.61
3:D:540:MET:CB	3:D:982:LEU:HG	2.30	0.61
3:A:773:GLU:HA	3:A:776:ARG:HG3	1.82	0.61
3:A:605:LEU:O	3:A:607:ASN:N	2.33	0.61
2:E:48:LYS:O	2:E:49:PHE:HB2	2.01	0.61
3:D:609:ILE:HG12	3:D:609:ILE:O	2.00	0.61
3:A:540:MET:CB	3:A:982:LEU:HG	2.31	0.61
3:D:345:LYS:HD3	3:D:346:LEU:N	2.16	0.61
1:C:353:VAL:HG12	1:C:417:VAL:HG13	1.81	0.61
3:A:856:GLU:HB3	3:A:859:MET:HE1	1.83	0.60
3:D:454:ASP:OD1	3:D:457:ARG:NH2	2.34	0.60
3:A:720:ASN:ND2	3:A:721:PRO:O	2.35	0.60
3:A:742:ARG:HH11	3:A:742:ARG:CG	2.14	0.60
2:E:102:VAL:HG21	2:E:218:TYR:OH	2.02	0.60
3:D:363:ARG:NH2	3:D:426:ASN:O	2.35	0.60
3:D:620:GLU:OE2	3:D:628:ARG:NH1	2.34	0.60
2:B:84:PHE:CD2	2:B:107:GLY:HA2	2.35	0.60
3:A:45:GLU:CG	3:A:46:ILE:N	2.64	0.60
3:A:620:GLU:OE2	3:A:628:ARG:NH1	2.35	0.60
3:A:797:ASN:OD1	3:A:797:ASN:N	2.32	0.60
2:B:62:VAL:HG21	2:B:198:ILE:HD11	1.84	0.60
3:A:345:LYS:HD3	3:A:346:LEU:N	2.16	0.60
3:A:363:ARG:NH2	3:A:426:ASN:O	2.35	0.60
1:C:341:SER:OG	1:C:344:VAL:HG23	2.01	0.60
2:B:165:ASN:OD1	2:B:165:ASN:N	2.35	0.60
3:A:454:ASP:OD1	3:A:457:ARG:NH2	2.35	0.60
2:E:62:VAL:HG21	2:E:198:ILE:HD11	1.84	0.60
2:E:165:ASN:OD1	2:E:165:ASN:N	2.35	0.60
2:B:102:VAL:HG21	2:B:218:TYR:OH	2.02	0.60
3:D:546:LEU:O	3:D:547:ILE:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:372:GLY:O	3:A:414:GLY:HA3	2.02	0.60
3:D:45:GLU:CG	3:D:46:ILE:N	2.65	0.60
3:D:856:GLU:HB3	3:D:859:MET:HE1	1.83	0.60
3:D:720:ASN:ND2	3:D:721:PRO:O	2.35	0.59
3:A:526:PHE:HD1	3:A:526:PHE:N	2.00	0.59
3:A:763:ASP:O	3:A:764:VAL:HB	2.02	0.59
3:D:742:ARG:HH11	3:D:742:ARG:CG	2.14	0.59
3:A:526:PHE:N	3:A:526:PHE:CD1	2.70	0.59
3:D:331:LEU:O	3:D:335:ILE:HG13	2.03	0.59
1:C:291:LYS:HE2	1:C:389:ILE:HG23	1.84	0.59
3:A:547:ILE:HG13	3:A:794:VAL:HG23	1.84	0.59
3:D:372:GLY:HA3	3:D:415:PHE:CE1	2.38	0.59
3:A:135:ILE:HD11	3:A:141:HIS:HB2	1.85	0.59
3:D:372:GLY:O	3:D:414:GLY:HA3	2.02	0.59
3:D:23:ARG:NH2	3:D:257:ASP:OD2	2.36	0.59
3:D:135:ILE:HD11	3:D:141:HIS:HB2	1.85	0.59
3:D:526:PHE:N	3:D:526:PHE:CD1	2.70	0.59
3:D:533:VAL:CG1	3:D:803:LYS:HD2	2.25	0.59
3:D:60:MET:HE3	3:D:88:MET:HB3	1.85	0.59
3:D:997:PHE:CZ	1:C:183:ILE:HD13	2.37	0.59
3:D:175:PHE:CD1	3:D:176:PRO:HD2	2.37	0.59
2:E:84:PHE:CD2	2:E:107:GLY:HA2	2.35	0.58
3:D:526:PHE:N	3:D:526:PHE:HD1	2.00	0.58
3:D:547:ILE:HD11	3:D:756:PHE:CD1	2.32	0.58
3:A:533:VAL:CG1	3:A:803:LYS:HD2	2.25	0.58
1:F:24:ASP:OD1	1:F:24:ASP:N	2.36	0.58
3:D:846:TYR:CE1	3:D:868:ILE:HB	2.36	0.58
1:C:194:LYS:NZ	1:C:196:SER:O	2.22	0.58
3:A:14:GLU:N	3:A:14:GLU:OE2	2.35	0.58
3:A:331:LEU:O	3:A:335:ILE:HG13	2.03	0.58
3:A:372:GLY:HA3	3:A:415:PHE:CE1	2.38	0.58
1:F:123:GLY:O	1:F:144:LYS:NZ	2.29	0.58
1:F:291:LYS:HE2	1:F:389:ILE:HG23	1.84	0.58
3:D:713:ARG:O	3:D:714:PHE:HB2	2.03	0.58
3:A:60:MET:HE3	3:A:88:MET:HB3	1.85	0.58
3:A:544:ASN:OD1	3:A:762:GLN:OE1	2.21	0.58
3:A:687:CYS:O	3:A:688:THR:OG1	2.13	0.58
2:E:166:ILE:O	2:E:170:LEU:HD12	2.02	0.58
3:D:113:PHE:O	3:D:117:ASN:HB2	2.03	0.58
3:D:542:SER:HB3	3:D:758:GLU:HG3	1.85	0.58
3:D:547:ILE:HG12	3:D:794:VAL:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:796:LYS:HG3	3:D:823:ARG:CZ	2.33	0.58
3:A:184:SER:OG	3:A:185:HIS:ND1	2.23	0.58
3:A:713:ARG:O	3:A:714:PHE:HB2	2.03	0.58
1:F:179:GLU:CA	1:F:182:SER:HG	2.15	0.58
3:A:796:LYS:HG3	3:A:823:ARG:CZ	2.33	0.58
1:F:2:THR:OG1	2:B:192:ASP:CG	2.46	0.58
3:D:14:GLU:N	3:D:14:GLU:OE2	2.36	0.58
3:D:547:ILE:HD13	3:D:756:PHE:CD1	2.35	0.58
1:C:179:GLU:O	1:C:183:ILE:HG23	2.04	0.58
2:B:166:ILE:O	2:B:170:LEU:HD12	2.02	0.58
3:A:175:PHE:CD1	3:A:176:PRO:HD2	2.37	0.58
3:D:409:ASP:HB3	3:D:416:LYS:HB3	1.86	0.58
3:D:961:GLY:O	3:D:964:GLN:NE2	2.37	0.58
3:A:573:VAL:CA	3:A:610:SER:OG	2.52	0.58
1:F:254:ILE:C	1:F:256:SER:H	2.12	0.58
1:C:219:TYR:HB3	1:C:240:LYS:HG2	1.86	0.58
1:F:179:GLU:O	1:F:183:ILE:HG23	2.04	0.58
3:D:287:ARG:HD3	3:D:287:ARG:N	2.19	0.58
3:D:604:ARG:HG3	3:D:611:GLU:CD	2.25	0.58
3:A:113:PHE:O	3:A:117:ASN:HB2	2.03	0.58
3:A:187:SER:HB2	3:A:201:THR:HG23	1.86	0.57
3:D:533:VAL:HG13	3:D:803:LYS:CD	2.28	0.57
1:C:24:ASP:OD1	1:C:24:ASP:N	2.36	0.57
2:E:183:ALA:O	2:E:185:ARG:NH1	2.38	0.57
3:D:779:ASN:ND2	3:D:788:LYS:O	2.38	0.57
3:A:768:ILE:HD12	3:A:816:ASN:HB2	1.87	0.57
1:F:7:LEU:O	1:F:11:LYS:HG2	2.04	0.57
1:F:284:GLU:OE1	1:F:292:ARG:NH2	2.35	0.57
3:D:76:LEU:HD22	3:D:586:LEU:HB3	1.86	0.57
1:C:7:LEU:O	1:C:11:LYS:HG2	2.04	0.57
3:A:23:ARG:NH2	3:A:257:ASP:OD2	2.36	0.57
3:A:717:THR:HG22	3:A:719:SER:H	1.69	0.57
3:A:779:ASN:ND2	3:A:788:LYS:O	2.37	0.57
1:F:351:GLN:OE1	1:F:351:GLN:HA	2.05	0.57
3:D:14:GLU:CD	3:D:14:GLU:H	2.13	0.57
3:D:547:ILE:HG13	3:D:794:VAL:CB	2.34	0.57
3:D:573:VAL:CA	3:D:610:SER:OG	2.52	0.57
3:D:763:ASP:O	3:D:764:VAL:HB	2.03	0.57
1:C:123:GLY:O	1:C:144:LYS:NZ	2.29	0.57
1:C:330:THR:OG1	1:C:333:GLU:HG3	2.05	0.57
3:D:964:GLN:HB3	3:D:968:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLU:OE1	1:C:292:ARG:NH2	2.35	0.57
3:A:409:ASP:HB3	3:A:416:LYS:HB3	1.86	0.57
2:E:57:LEU:HB3	2:E:151:HIS:CD2	2.39	0.57
3:D:532:LYS:HG3	3:D:533:VAL:N	2.19	0.57
2:B:57:LEU:HB3	2:B:151:HIS:CD2	2.39	0.57
2:B:183:ALA:O	2:B:185:ARG:NH1	2.37	0.57
3:A:961:GLY:O	3:A:964:GLN:NE2	2.37	0.57
1:F:215:PHE:CD1	1:F:215:PHE:C	2.83	0.57
3:A:983:LEU:HD22	3:A:983:LEU:H	1.70	0.57
2:E:89:ILE:HD11	2:E:108:TYR:HD2	1.69	0.56
3:D:187:SER:HB2	3:D:201:THR:HG23	1.86	0.56
3:D:983:LEU:H	3:D:983:LEU:HD22	1.70	0.56
3:A:45:GLU:OE1	3:A:46:ILE:CG1	2.35	0.56
1:F:219:TYR:HB3	1:F:240:LYS:HG2	1.86	0.56
2:E:50:PHE:CD1	2:E:50:PHE:N	2.73	0.56
2:E:205:ASP:OD1	1:C:44:LYS:HD3	2.05	0.56
3:D:117:ASN:OD1	3:D:145:PRO:HB2	2.05	0.56
1:C:215:PHE:CD1	1:C:215:PHE:C	2.83	0.56
1:C:351:GLN:OE1	1:C:351:GLN:HA	2.05	0.56
2:B:84:PHE:CE1	2:B:90:LYS:HA	2.37	0.56
2:B:89:ILE:HD11	2:B:108:TYR:HD2	1.69	0.56
3:A:763:ASP:OD1	3:A:770:ILE:HD12	2.05	0.56
3:A:846:TYR:CE1	3:A:868:ILE:HB	2.36	0.56
1:F:167:GLU:HB3	1:F:199:TYR:CE1	2.40	0.56
3:D:363:ARG:NH2	3:D:425:PRO:O	2.38	0.56
3:D:837:LYS:O	3:D:888:GLU:N	2.39	0.56
2:B:167:ARG:HH22	2:B:173:PRO:HA	1.70	0.56
3:A:76:LEU:HD22	3:A:586:LEU:HB3	1.86	0.56
3:A:363:ARG:NH2	3:A:425:PRO:O	2.38	0.56
3:A:532:LYS:HG3	3:A:533:VAL:N	2.19	0.56
3:A:837:LYS:O	3:A:888:GLU:N	2.39	0.56
1:F:167:GLU:HB3	1:F:199:TYR:HE1	1.71	0.56
3:D:45:GLU:OE1	3:D:46:ILE:CG1	2.37	0.56
3:D:551:ASN:OD1	3:D:551:ASN:N	2.35	0.56
2:B:88:SER:O	2:B:92:ILE:HG12	2.06	0.56
3:A:390:THR:HG22	3:A:391:THR:HG23	1.88	0.56
1:F:330:THR:OG1	1:F:333:GLU:HG3	2.04	0.56
2:E:167:ARG:HH22	2:E:173:PRO:HA	1.70	0.56
3:D:637:TYR:HA	3:D:640:MET:HG3	1.87	0.56
3:A:117:ASN:OD1	3:A:145:PRO:HB2	2.05	0.56
3:A:540:MET:C	3:A:797:ASN:HB3	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:745:PHE:HE2	3:A:774:LEU:HD22	1.70	0.56
1:F:3:SER:C	2:B:193:ARG:HH12	2.14	0.56
1:C:167:GLU:HB3	1:C:199:TYR:CE1	2.40	0.56
1:C:219:TYR:HD1	1:C:240:LYS:HB3	1.71	0.56
3:A:444:TYR:CE2	3:A:455:MET:HE1	2.41	0.56
3:A:825:ASN:OD1	3:A:828:THR:N	2.39	0.56
2:E:88:SER:O	2:E:92:ILE:HG12	2.06	0.56
3:D:319:HIS:CE1	3:D:495:GLU:HG2	2.41	0.56
1:C:108:ASP:OD1	1:C:111:ARG:NH2	2.39	0.56
2:B:72:LYS:O	2:B:73:ASP:HB2	2.04	0.56
3:A:287:ARG:N	3:A:287:ARG:HD3	2.19	0.56
3:A:369:THR:OG1	3:A:418:VAL:HG22	2.05	0.56
2:E:26:LEU:HD21	2:E:50:PHE:CE2	2.40	0.56
2:E:72:LYS:O	2:E:73:ASP:HB2	2.04	0.56
3:A:170:HIS:O	3:A:181:ASN:ND2	2.30	0.56
3:A:746:ARG:HD2	3:A:760:ASP:OD2	2.06	0.56
2:E:3:SER:HA	2:E:13:ILE:O	2.06	0.55
3:D:369:THR:OG1	3:D:418:VAL:HG22	2.05	0.55
3:D:444:TYR:CE2	3:D:455:MET:HE1	2.41	0.55
3:D:745:PHE:HE2	3:D:774:LEU:HD22	1.70	0.55
1:C:135:ARG:HE	1:C:136:TRP:N	2.02	0.55
1:C:167:GLU:HB3	1:C:199:TYR:HE1	1.71	0.55
1:C:257:LYS:O	1:C:259:ARG:HG3	2.06	0.55
3:A:865:CYS:O	3:A:869:LEU:HD12	2.06	0.55
3:D:707:LEU:HD13	3:D:742:ARG:HE	1.71	0.55
1:C:220:ILE:HD12	1:C:237:VAL:HG13	1.88	0.55
3:A:14:GLU:CD	3:A:14:GLU:H	2.13	0.55
3:A:699:GLU:OE2	3:A:755:VAL:HG22	2.06	0.55
1:F:108:ASP:OD1	1:F:111:ARG:NH2	2.39	0.55
3:D:183:ILE:HD12	3:D:245:LEU:HD21	1.89	0.55
3:D:514:LYS:N	3:D:514:LYS:HD2	2.21	0.55
2:B:18:ASP:OD2	2:B:57:LEU:N	2.27	0.55
3:A:286:PHE:HB2	3:A:295:VAL:HG23	1.88	0.55
3:D:699:GLU:OE2	3:D:755:VAL:HG22	2.06	0.55
3:A:707:LEU:HD13	3:A:742:ARG:HE	1.71	0.55
1:F:219:TYR:HD1	1:F:240:LYS:HB3	1.71	0.55
3:D:286:PHE:HB2	3:D:295:VAL:HG23	1.88	0.55
1:C:336:ASP:O	1:C:340:LYS:HG2	2.06	0.55
2:B:3:SER:HA	2:B:13:ILE:O	2.07	0.55
3:A:637:TYR:HA	3:A:640:MET:HG3	1.87	0.55
3:D:746:ARG:HD2	3:D:760:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:821:PRO:HG3	3:D:823:ARG:HH21	1.72	0.55
1:C:416:THR:O	1:C:420:VAL:HG22	2.07	0.55
3:A:319:HIS:CE1	3:A:495:GLU:HG2	2.41	0.55
2:B:187:HIS:HB3	2:B:190:GLU:HG3	1.89	0.55
1:F:16:LEU:HD21	1:F:30:LYS:HD2	1.89	0.55
3:D:390:THR:HG22	3:D:391:THR:HG23	1.88	0.55
1:C:16:LEU:HD21	1:C:30:LYS:HD2	1.89	0.55
3:A:778:ILE:HG23	3:A:779:ASN:H	1.72	0.55
1:F:336:ASP:O	1:F:340:LYS:HG2	2.06	0.54
3:A:774:LEU:O	3:A:778:ILE:HG22	2.07	0.54
3:D:825:ASN:OD1	3:D:828:THR:N	2.39	0.54
3:A:183:ILE:HD12	3:A:245:LEU:HD21	1.89	0.54
1:F:334:LEU:HD23	1:F:420:VAL:HG11	1.89	0.54
3:D:778:ILE:HG23	3:D:779:ASN:H	1.72	0.54
3:D:865:CYS:O	3:D:869:LEU:HD12	2.06	0.54
3:A:514:LYS:HD2	3:A:514:LYS:N	2.21	0.54
3:A:821:PRO:HG3	3:A:823:ARG:HH21	1.72	0.54
1:F:220:ILE:HD12	1:F:237:VAL:HG13	1.88	0.54
3:A:547:ILE:HG13	3:A:794:VAL:CB	2.38	0.54
1:F:135:ARG:HE	1:F:136:TRP:N	2.02	0.54
3:D:774:LEU:O	3:D:778:ILE:HG22	2.07	0.54
1:C:247:VAL:HG12	1:C:252:HIS:CE1	2.43	0.54
1:F:178:ASP:HA	1:F:181:TYR:CZ	2.43	0.54
2:B:153:SER:O	2:B:153:SER:OG	2.26	0.54
3:A:836:SER:C	3:A:837:LYS:HG3	2.33	0.54
3:D:700:SER:OG	3:D:701:VAL:N	2.41	0.54
1:F:247:VAL:HG12	1:F:252:HIS:CE1	2.42	0.54
2:E:153:SER:O	2:E:153:SER:OG	2.26	0.54
1:C:329:ALA:N	1:C:333:GLU:OE2	2.41	0.54
3:A:964:GLN:HB3	3:A:968:TYR:CE2	2.39	0.54
3:A:974:ARG:O	3:A:977:SER:N	2.41	0.54
1:F:416:THR:O	1:F:420:VAL:HG22	2.07	0.54
1:C:267:LYS:HG3	1:C:276:TYR:CD1	2.43	0.54
1:C:334:LEU:HD23	1:C:420:VAL:HG11	1.89	0.54
1:C:178:ASP:HA	1:C:181:TYR:CZ	2.43	0.54
1:C:193:PRO:HA	1:C:272:PHE:CZ	2.43	0.53
1:F:2:THR:OG1	2:B:192:ASP:OD2	2.26	0.53
1:F:193:PRO:HA	1:F:272:PHE:CZ	2.43	0.53
2:E:84:PHE:CE1	2:E:90:LYS:HA	2.37	0.53
2:E:187:HIS:HB3	2:E:190:GLU:HG3	1.89	0.53
3:D:742:ARG:HG3	3:D:742:ARG:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:SER:HB3	3:A:758:GLU:HG3	1.85	0.53
3:D:542:SER:O	3:D:758:GLU:CD	2.52	0.53
3:A:542:SER:O	3:A:758:GLU:CD	2.52	0.53
3:D:767:SER:O	3:D:770:ILE:HB	2.09	0.53
1:C:16:LEU:HD11	1:C:31:TYR:HB2	1.91	0.53
1:F:16:LEU:HD11	1:F:31:TYR:HB2	1.91	0.53
3:A:577:ARG:C	3:A:579:GLU:H	2.17	0.53
1:F:329:ALA:N	1:F:333:GLU:OE2	2.41	0.53
3:A:187:SER:HB3	3:A:459:CYS:SG	2.49	0.53
3:D:187:SER:HB3	3:D:459:CYS:SG	2.49	0.53
3:D:208:LEU:HB2	3:D:213:ILE:HD11	1.91	0.53
3:D:577:ARG:C	3:D:579:GLU:H	2.17	0.53
3:D:836:SER:C	3:D:837:LYS:HG3	2.33	0.53
3:D:974:ARG:O	3:D:977:SER:N	2.41	0.53
3:A:700:SER:OG	3:A:701:VAL:N	2.41	0.53
1:F:267:LYS:HG3	1:F:276:TYR:CD1	2.43	0.53
2:E:18:ASP:OD2	2:E:57:LEU:N	2.28	0.53
3:D:840:LYS:HG2	3:D:841:ASN:H	1.74	0.52
1:C:193:PRO:HA	1:C:272:PHE:CE2	2.43	0.52
2:B:172:SER:O	2:B:174:VAL:N	2.41	0.52
3:A:551:ASN:OD1	3:A:551:ASN:N	2.35	0.52
3:A:849:ARG:O	3:A:853:MET:HE2	2.10	0.52
3:D:547:ILE:CG1	3:D:794:VAL:H	2.21	0.52
3:D:716:ASN:N	3:D:716:ASN:OD1	2.42	0.52
3:D:842:MET:O	3:D:845:THR:N	2.43	0.52
3:A:604:ARG:HB3	3:A:605:LEU:HD12	1.90	0.52
3:A:715:ALA:O	3:A:716:ASN:HB3	2.08	0.52
1:F:193:PRO:HA	1:F:272:PHE:CE2	2.43	0.52
1:C:373:ASN:OD1	3:A:577:ARG:HG3	2.10	0.52
3:A:240:SER:OG	3:A:241:GLU:N	2.42	0.52
3:A:717:THR:HG22	3:A:718:LEU:N	2.23	0.52
3:A:742:ARG:HG3	3:A:742:ARG:O	2.09	0.52
3:A:842:MET:O	3:A:845:THR:N	2.42	0.52
2:B:57:LEU:HG	2:B:151:HIS:CG	2.45	0.52
3:A:442:GLN:HA	3:A:445:LYS:HG3	1.91	0.52
1:F:30:LYS:HE2	1:F:34:LEU:HG	1.91	0.52
2:E:57:LEU:HG	2:E:151:HIS:CG	2.45	0.52
3:D:849:ARG:O	3:D:853:MET:HE2	2.10	0.52
3:A:703:ASN:N	3:A:714:PHE:O	2.43	0.52
2:E:23:MET:HG3	2:E:24:SER:N	2.25	0.52
3:A:208:LEU:HB2	3:A:213:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:GLU:OE1	2:B:127:LEU:HB3	2.10	0.52
3:A:724:MET:N	3:A:724:MET:CE	2.73	0.52
1:F:375:MET:HB3	1:F:389:ILE:HA	1.92	0.52
3:D:703:ASN:N	3:D:714:PHE:O	2.43	0.52
1:F:132:LEU:HD22	1:F:193:PRO:HD2	1.92	0.51
1:C:375:MET:HB3	1:C:389:ILE:HA	1.92	0.51
3:A:666:SER:O	3:A:666:SER:OG	2.27	0.51
3:D:836:SER:C	3:D:837:LYS:HE3	2.35	0.51
3:D:876:LEU:CD1	3:D:968:TYR:HB3	2.40	0.51
1:C:251:ASP:OD1	1:C:251:ASP:N	2.20	0.51
3:A:609:ILE:N	3:A:609:ILE:CD1	2.73	0.51
1:F:37:TRP:HZ3	3:A:674:ARG:HH22	1.58	0.51
1:C:370:THR:O	1:C:374:ASN:ND2	2.43	0.51
1:F:253:LEU:HD12	1:F:258:VAL:HG21	1.92	0.51
3:D:442:GLN:HA	3:D:445:LYS:HG3	1.91	0.51
2:E:18:ASP:HB3	2:E:57:LEU:HB2	1.93	0.51
3:D:525:LYS:HE3	3:D:527:PRO:HA	1.93	0.51
1:C:30:LYS:HE2	1:C:34:LEU:HG	1.92	0.51
3:A:546:LEU:N	3:A:546:LEU:CD1	2.73	0.51
3:A:840:LYS:HG2	3:A:841:ASN:H	1.74	0.51
2:E:172:SER:O	2:E:174:VAL:N	2.41	0.51
3:D:1:MET:N	3:D:129:GLU:OE2	2.35	0.51
1:F:5:ALA:O	1:F:8:THR:OG1	2.25	0.51
1:F:230:ASP:O	1:F:232:ILE:HG13	2.11	0.51
3:D:399:GLU:O	3:D:401:ILE:N	2.44	0.51
3:D:724:MET:N	3:D:724:MET:CE	2.73	0.51
1:C:132:LEU:HD22	1:C:193:PRO:HD2	1.92	0.51
3:D:568:LEU:HB2	3:D:615:PHE:CE1	2.46	0.50
1:C:230:ASP:O	1:C:232:ILE:HG13	2.11	0.50
3:D:717:THR:HG22	3:D:729:ILE:CG2	2.41	0.50
1:F:12:GLU:HB3	1:F:30:LYS:HE3	1.94	0.50
1:F:377:PHE:CE2	3:D:578:LEU:HD22	2.46	0.50
3:D:240:SER:OG	3:D:241:GLU:N	2.42	0.50
3:D:810:LYS:N	3:D:822:GLU:O	2.44	0.50
1:C:253:LEU:HD12	1:C:258:VAL:HG21	1.92	0.50
3:A:525:LYS:HE3	3:A:527:PRO:HA	1.93	0.50
2:B:18:ASP:HB3	2:B:57:LEU:HB2	1.93	0.50
3:A:810:LYS:N	3:A:822:GLU:O	2.44	0.50
3:D:609:ILE:N	3:D:609:ILE:CD1	2.73	0.50
3:D:687:CYS:C	3:D:689:SER:H	2.20	0.50
2:B:23:MET:HG3	2:B:24:SER:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:568:LEU:HB2	3:A:615:PHE:CE1	2.46	0.50
3:A:836:SER:C	3:A:837:LYS:HE3	2.36	0.50
2:E:40:ASP:OD2	2:E:126:LYS:HE3	2.12	0.50
3:A:533:VAL:HG13	3:A:803:LYS:CD	2.28	0.50
1:F:370:THR:O	1:F:374:ASN:ND2	2.43	0.50
1:C:12:GLU:HB3	1:C:30:LYS:HE3	1.93	0.50
3:A:701:VAL:HG11	3:A:717:THR:O	2.12	0.50
2:E:110:LEU:HD12	2:E:113:ILE:HD12	1.94	0.50
3:A:43:THR:OG1	3:A:46:ILE:HG13	2.12	0.50
3:A:526:PHE:CE2	3:A:604:ARG:HD2	2.46	0.50
3:A:538:GLN:OE1	3:A:746:ARG:NH2	2.41	0.50
3:A:777:LEU:O	3:A:781:ARG:N	2.23	0.50
2:B:40:ASP:OD2	2:B:126:LYS:HE3	2.12	0.50
2:B:110:LEU:HD12	2:B:113:ILE:HD12	1.94	0.50
3:A:763:ASP:OD2	3:A:767:SER:N	2.45	0.50
1:F:319:LEU:O	1:F:323:LEU:HD12	2.12	0.49
3:D:876:LEU:HD13	3:D:972:PHE:CD2	2.47	0.49
2:B:15:TYR:CZ	2:B:53:LEU:HD22	2.47	0.49
3:A:687:CYS:C	3:A:689:SER:H	2.20	0.49
3:D:170:HIS:O	3:D:181:ASN:ND2	2.30	0.49
3:D:714:PHE:CZ	3:D:782:VAL:HG21	2.47	0.49
3:D:842:MET:O	3:D:843:ILE:C	2.54	0.49
1:C:319:LEU:O	1:C:323:LEU:HD12	2.12	0.49
3:A:399:GLU:O	3:A:401:ILE:N	2.44	0.49
3:A:773:GLU:C	3:A:776:ARG:HB2	2.35	0.49
3:D:547:ILE:CD1	3:D:756:PHE:HE1	2.04	0.49
3:A:714:PHE:CZ	3:A:782:VAL:HG21	2.47	0.49
1:F:256:SER:HB3	1:F:258:VAL:CG2	2.43	0.49
3:D:666:SER:O	3:D:666:SER:OG	2.27	0.49
3:D:766:LYS:CD	3:D:766:LYS:C	2.86	0.49
3:A:763:ASP:OD1	3:A:767:SER:CB	2.59	0.49
3:A:590:LYS:HG3	3:A:591:TYR:N	2.28	0.49
1:F:225:VAL:HB	1:F:233:PHE:HB3	1.95	0.49
1:F:424:LEU:HD22	1:F:425:PHE:CE1	2.48	0.49
2:E:15:TYR:CZ	2:E:53:LEU:HD22	2.47	0.49
3:D:526:PHE:HD2	3:D:604:ARG:HB3	1.77	0.49
3:D:604:ARG:N	3:D:611:GLU:OE1	2.46	0.49
1:C:225:VAL:HB	1:C:233:PHE:HB3	1.95	0.49
2:B:36:TRP:HE1	3:A:179:PHE:HB3	1.77	0.49
3:A:682:ALA:O	3:A:686:SER:OG	2.29	0.49
3:A:876:LEU:HD13	3:A:972:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:PRO:HB3	2:E:189:PHE:HB3	1.94	0.49
3:D:223:ARG:CG	3:D:223:ARG:HH11	2.26	0.49
2:B:107:GLY:H	2:B:217:ILE:HB	1.77	0.49
3:A:412:GLU:OE1	3:A:413:ASN:HB2	2.12	0.49
2:E:15:TYR:HD2	2:E:23:MET:HB3	1.77	0.49
1:C:5:ALA:O	1:C:8:THR:OG1	2.25	0.49
3:A:842:MET:O	3:A:843:ILE:C	2.54	0.49
3:D:209:THR:HG23	3:D:212:GLU:OE2	2.13	0.49
1:C:219:TYR:HB2	1:C:263:PHE:CE2	2.48	0.49
1:C:424:LEU:HD22	1:C:425:PHE:CE1	2.48	0.49
1:F:183:ILE:HD13	3:A:997:PHE:CZ	2.48	0.48
1:F:219:TYR:CD1	1:F:240:LYS:HB3	2.47	0.48
3:D:412:GLU:OE1	3:D:413:ASN:HB2	2.12	0.48
1:C:378:LYS:HB3	1:C:386:ASN:HB3	1.95	0.48
2:B:15:TYR:HD2	2:B:23:MET:HB3	1.77	0.48
3:A:604:ARG:N	3:A:611:GLU:OE1	2.46	0.48
3:D:682:ALA:O	3:D:686:SER:OG	2.29	0.48
2:B:87:LYS:HZ1	2:B:185:ARG:HH12	1.60	0.48
2:E:62:VAL:O	2:E:116:VAL:HA	2.14	0.48
2:E:169:LYS:HB2	2:E:169:LYS:HE3	1.56	0.48
2:E:187:HIS:O	2:E:190:GLU:HB2	2.13	0.48
3:D:2:ASP:OD1	3:D:2:ASP:N	2.46	0.48
3:D:625:ARG:O	3:D:629:THR:HG23	2.13	0.48
3:D:773:GLU:C	3:D:776:ARG:HB2	2.35	0.48
3:D:777:LEU:O	3:D:781:ARG:N	2.23	0.48
3:A:763:ASP:CG	3:A:767:SER:HA	2.38	0.48
1:F:219:TYR:HB2	1:F:263:PHE:CE2	2.48	0.48
3:D:43:THR:OG1	3:D:46:ILE:HG13	2.12	0.48
3:D:590:LYS:HG3	3:D:591:TYR:N	2.28	0.48
1:C:219:TYR:CD1	1:C:240:LYS:HB3	2.47	0.48
2:B:182:PRO:HB3	2:B:189:PHE:HB3	1.94	0.48
3:A:41:VAL:HG13	3:A:60:MET:HE1	1.94	0.48
1:F:417:VAL:HA	1:F:420:VAL:CG2	2.43	0.48
2:E:87:LYS:HZ1	2:E:185:ARG:HH12	1.62	0.48
3:D:72:ILE:HA	3:D:571:VAL:HG22	1.96	0.48
3:A:209:THR:HG23	3:A:212:GLU:OE2	2.13	0.48
3:A:625:ARG:O	3:A:629:THR:HG23	2.13	0.48
3:A:681:TYR:HE1	3:A:685:LYS:HZ2	1.59	0.48
2:E:107:GLY:H	2:E:217:ILE:HB	1.77	0.48
2:E:158:LEU:HD23	2:E:182:PRO:HD3	1.96	0.48
3:D:41:VAL:HG13	3:D:60:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:538:GLN:OE1	3:D:746:ARG:NH2	2.41	0.48
3:A:750:GLY:HA2	3:A:755:VAL:HA	1.96	0.48
3:A:762:GLN:O	3:A:763:ASP:C	2.55	0.48
2:E:109:ASN:OD1	2:E:109:ASN:C	2.57	0.48
3:D:706:GLU:HA	3:D:711:MET:HB3	1.96	0.48
1:C:383:LYS:HE2	1:C:415:ASN:HB3	1.96	0.48
3:A:124:CYS:SG	3:A:155:ARG:HA	2.54	0.48
3:A:223:ARG:CG	3:A:223:ARG:HH11	2.26	0.48
3:A:766:LYS:O	3:A:769:GLU:HG3	2.14	0.48
1:F:178:ASP:HA	1:F:181:TYR:CE1	2.49	0.48
3:A:170:HIS:HB2	3:A:207:MET:CE	2.42	0.48
3:A:364:GLY:O	3:A:423:THR:OG1	2.31	0.48
1:F:271:THR:HG23	1:F:272:PHE:CD2	2.49	0.48
1:F:366:ALA:O	1:F:369:ILE:N	2.33	0.48
1:F:383:LYS:HE2	1:F:415:ASN:HB3	1.96	0.48
3:D:700:SER:O	3:D:715:ALA:CB	2.61	0.48
3:D:750:GLY:HA2	3:D:755:VAL:HA	1.96	0.48
1:C:178:ASP:HA	1:C:181:TYR:CE1	2.49	0.48
2:B:62:VAL:O	2:B:116:VAL:HA	2.14	0.48
2:B:174:VAL:HG12	2:B:176:THR:HG22	1.96	0.48
3:A:142:CYS:SG	3:A:143:ASP:N	2.87	0.48
3:A:706:GLU:HA	3:A:711:MET:HB3	1.95	0.48
2:E:142:LYS:O	2:E:146:GLN:HG2	2.13	0.47
3:D:54:PRO:HB3	3:D:91:ILE:HD11	1.96	0.47
3:D:652:ILE:HG22	3:D:653:TYR:CD1	2.49	0.47
3:D:748:VAL:HG12	3:D:757:THR:HA	1.96	0.47
1:C:417:VAL:HA	1:C:420:VAL:CG2	2.44	0.47
2:B:83:ASN:OD1	2:B:85:THR:HB	2.14	0.47
2:B:158:LEU:HD23	2:B:182:PRO:HD3	1.96	0.47
3:A:630:PHE:CD2	3:A:663:VAL:HG23	2.49	0.47
3:A:779:ASN:ND2	3:A:789:ILE:HA	2.29	0.47
1:F:177:ASP:N	1:F:180:LEU:HB2	2.24	0.47
1:F:378:LYS:HB3	1:F:386:ASN:HB3	1.95	0.47
3:D:124:CYS:SG	3:D:155:ARG:HA	2.54	0.47
3:D:630:PHE:CD2	3:D:663:VAL:HG23	2.49	0.47
2:B:202:LEU:HD23	2:B:202:LEU:HA	1.66	0.47
3:A:229:GLU:HA	3:A:229:GLU:OE1	2.14	0.47
3:A:230:MET:HE3	3:A:237:VAL:HG21	1.96	0.47
3:D:345:LYS:HD3	3:D:346:LEU:H	1.78	0.47
1:C:176:PHE:HD1	1:C:210:VAL:HG11	1.79	0.47
1:C:177:ASP:N	1:C:180:LEU:HB2	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:HIS:O	2:B:190:GLU:HB2	2.14	0.47
3:A:546:LEU:HD13	3:A:757:THR:O	2.15	0.47
1:F:110:ILE:HD11	1:F:135:ARG:NH2	2.30	0.47
1:F:176:PHE:HD1	1:F:210:VAL:HG11	1.79	0.47
3:D:351:LYS:HG3	3:D:432:SER:OG	2.14	0.47
1:C:285:THR:HG22	1:C:286:ARG:H	1.80	0.47
1:C:366:ALA:O	1:C:369:ILE:N	2.33	0.47
3:A:547:ILE:HG13	3:A:794:VAL:CG2	2.44	0.47
3:A:652:ILE:HG22	3:A:653:TYR:CD1	2.49	0.47
3:D:364:GLY:O	3:D:423:THR:OG1	2.31	0.47
3:D:873:GLU:HB2	3:D:992:PHE:HE2	1.79	0.47
2:B:142:LYS:O	2:B:146:GLN:HG2	2.14	0.47
3:A:748:VAL:HG12	3:A:757:THR:HA	1.96	0.47
3:D:763:ASP:HB2	3:D:767:SER:HB3	1.95	0.47
3:D:768:ILE:HG12	3:D:795:TYR:OH	2.15	0.47
1:C:332:ASP:O	1:C:335:VAL:HG22	2.14	0.47
2:B:61:ARG:NE	2:B:208:THR:HG23	2.29	0.47
3:A:54:PRO:HB3	3:A:91:ILE:HD11	1.96	0.47
3:A:525:LYS:HG3	3:A:527:PRO:HD3	1.97	0.47
3:A:808:THR:HB	3:A:810:LYS:HG3	1.95	0.47
2:E:61:ARG:NE	2:E:208:THR:HG23	2.29	0.47
2:E:83:ASN:OD1	2:E:85:THR:HB	2.14	0.47
3:D:7:ASN:C	3:D:7:ASN:OD1	2.57	0.47
3:D:81:ARG:HH11	3:D:81:ARG:CG	2.23	0.47
3:D:230:MET:HE3	3:D:237:VAL:HG21	1.96	0.47
3:D:316:THR:OG1	3:D:317:THR:N	2.48	0.47
3:D:702:LEU:HD23	3:D:702:LEU:HA	1.54	0.47
3:D:779:ASN:ND2	3:D:789:ILE:HA	2.29	0.47
3:D:808:THR:HB	3:D:810:LYS:HG3	1.95	0.47
3:D:835:VAL:HG23	3:D:836:SER:N	2.29	0.47
1:C:110:ILE:HD11	1:C:135:ARG:NH2	2.30	0.47
1:C:271:THR:HG23	1:C:272:PHE:CD2	2.49	0.47
2:B:60:LYS:HA	2:B:60:LYS:HD3	1.68	0.47
3:A:7:ASN:OD1	3:A:7:ASN:C	2.57	0.47
3:A:72:ILE:HA	3:A:571:VAL:HG22	1.96	0.47
3:A:81:ARG:HH11	3:A:81:ARG:CG	2.23	0.47
3:A:835:VAL:HG23	3:A:836:SER:N	2.29	0.47
3:A:873:GLU:HB2	3:A:992:PHE:HE2	1.80	0.47
3:A:876:LEU:CD1	3:A:968:TYR:HB3	2.40	0.47
1:F:409:GLN:O	1:F:413:ILE:HG22	2.15	0.47
3:D:226:SER:OG	3:D:227:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:542:SER:O	3:D:758:GLU:OE2	2.33	0.47
3:A:711:MET:SD	3:A:732:ILE:HD11	2.55	0.47
3:A:837:LYS:HA	3:A:890:PHE:CD1	2.50	0.47
3:A:839:HIS:CE1	3:A:967:PHE:HB2	2.50	0.47
3:D:525:LYS:HG3	3:D:527:PRO:HD3	1.97	0.47
3:D:711:MET:SD	3:D:732:ILE:HD11	2.55	0.47
2:E:9:ALA:HA	2:E:11:TYR:CD1	2.49	0.47
2:E:174:VAL:HG12	2:E:176:THR:HG22	1.96	0.47
3:A:46:ILE:O	3:A:50:LEU:HB2	2.15	0.47
3:D:540:MET:C	3:D:542:SER:N	2.73	0.46
3:D:839:HIS:CE1	3:D:967:PHE:HB2	2.50	0.46
3:A:542:SER:O	3:A:758:GLU:OE2	2.33	0.46
1:F:335:VAL:CG1	1:F:420:VAL:HG12	2.39	0.46
2:B:109:ASN:OD1	2:B:109:ASN:C	2.56	0.46
3:A:351:LYS:HG3	3:A:432:SER:OG	2.14	0.46
1:F:35:VAL:HA	1:F:45:ILE:HG12	1.98	0.46
2:E:175:THR:HA	1:C:43:TRP:CD1	2.51	0.46
3:D:170:HIS:HB2	3:D:207:MET:CE	2.42	0.46
3:D:701:VAL:CB	3:D:715:ALA:CB	2.92	0.46
3:D:837:LYS:HA	3:D:890:PHE:CD1	2.50	0.46
1:C:35:VAL:HA	1:C:45:ILE:HG12	1.98	0.46
2:B:9:ALA:HA	2:B:11:TYR:CD1	2.49	0.46
3:A:2:ASP:OD1	3:A:2:ASP:N	2.46	0.46
3:A:134:LYS:HD3	3:A:134:LYS:HA	1.54	0.46
3:A:540:MET:C	3:A:542:SER:N	2.73	0.46
1:F:176:PHE:H	1:F:210:VAL:HG11	1.80	0.46
1:F:379:ILE:HG23	1:F:383:LYS:H	1.81	0.46
3:A:219:ARG:HH21	3:A:453:LEU:HD12	1.81	0.46
3:A:345:LYS:HD3	3:A:346:LEU:H	1.78	0.46
3:A:446:ASP:OD1	3:A:446:ASP:N	2.40	0.46
3:A:700:SER:O	3:A:715:ALA:CB	2.61	0.46
1:F:218:MET:O	1:F:263:PHE:HA	2.15	0.46
3:D:46:ILE:O	3:D:50:LEU:HB2	2.15	0.46
3:D:142:CYS:SG	3:D:143:ASP:N	2.87	0.46
3:D:407:ARG:HB2	3:D:418:VAL:HB	1.98	0.46
1:C:176:PHE:H	1:C:210:VAL:HG11	1.80	0.46
2:B:9:ALA:HA	2:B:11:TYR:HD1	1.81	0.46
2:B:105:TYR:N	2:B:105:TYR:CD1	2.84	0.46
3:A:407:ARG:HB2	3:A:418:VAL:HB	1.98	0.46
3:D:270:ARG:O	3:D:274:ASN:HB2	2.15	0.46
3:D:437:ASP:C	3:D:438:ILE:HG12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:GLN:O	1:C:413:ILE:HG22	2.15	0.46
1:C:397:ASN:OD1	1:C:399:SER:N	2.49	0.46
2:B:177:ILE:HD12	2:B:177:ILE:HA	1.73	0.46
3:A:270:ARG:O	3:A:274:ASN:HB2	2.15	0.46
3:A:543:ASN:O	3:A:544:ASN:CG	2.59	0.46
2:E:9:ALA:HA	2:E:11:TYR:HD1	1.81	0.46
2:E:19:TRP:CE3	2:E:147:HIS:HD2	2.33	0.46
3:D:539:LYS:O	3:D:982:LEU:HA	2.16	0.46
3:A:297:LEU:HD11	3:A:320:VAL:HG22	1.98	0.46
3:A:437:ASP:C	3:A:438:ILE:HG12	2.40	0.46
3:A:680:SER:OG	3:A:683:SER:OG	2.27	0.46
3:A:701:VAL:CB	3:A:715:ALA:CB	2.92	0.46
3:A:759:ILE:HG22	3:A:762:GLN:H	1.81	0.46
1:F:325:ILE:HB	1:F:337:GLU:CD	2.41	0.46
1:F:332:ASP:O	1:F:335:VAL:HG22	2.14	0.46
3:D:229:GLU:OE1	3:D:229:GLU:HA	2.14	0.46
3:D:397:VAL:HG23	3:D:401:ILE:O	2.16	0.46
3:D:411:LEU:HB2	3:D:414:GLY:C	2.41	0.46
3:D:744:ARG:NH1	3:D:744:ARG:HG3	2.31	0.46
3:D:852:GLU:O	3:D:855:SER:OG	2.34	0.46
3:A:411:LEU:HB2	3:A:414:GLY:C	2.41	0.46
3:A:536:PRO:HA	3:A:749:TYR:CD1	2.51	0.46
1:F:285:THR:HG22	1:F:286:ARG:H	1.80	0.46
3:D:543:ASN:O	3:D:544:ASN:CG	2.59	0.46
2:B:163:PHE:HD1	2:B:166:ILE:HG21	1.81	0.46
3:A:316:THR:OG1	3:A:317:THR:N	2.48	0.46
3:A:699:GLU:OE1	3:A:748:VAL:HG23	2.16	0.46
3:D:219:ARG:HH21	3:D:453:LEU:HD12	1.81	0.45
3:D:292:LYS:HB2	3:D:292:LYS:HE2	1.44	0.45
3:D:717:THR:HG22	3:D:729:ILE:HG21	1.96	0.45
1:C:325:ILE:HB	1:C:337:GLU:CD	2.41	0.45
3:A:539:LYS:O	3:A:982:LEU:HA	2.16	0.45
3:A:685:LYS:O	3:A:689:SER:OG	2.29	0.45
1:F:110:ILE:HG13	1:F:136:TRP:CD1	2.51	0.45
3:D:823:ARG:HA	3:D:823:ARG:HD3	1.58	0.45
1:C:214:LYS:HA	1:C:214:LYS:HD3	1.68	0.45
1:C:218:MET:O	1:C:263:PHE:HA	2.15	0.45
3:A:702:LEU:HD23	3:A:702:LEU:HA	1.54	0.45
1:F:20:LEU:HA	1:F:23:SER:OG	2.17	0.45
2:E:163:PHE:HD1	2:E:166:ILE:HG21	1.81	0.45
3:D:95:LYS:HD3	3:D:95:LYS:HA	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:785:ASN:O	3:D:787:PHE:N	2.49	0.45
2:B:210:ILE:HD12	2:B:210:ILE:HA	1.72	0.45
3:A:226:SER:OG	3:A:227:LEU:N	2.47	0.45
3:A:552:SER:O	3:A:552:SER:OG	2.34	0.45
3:A:743:PHE:CD1	3:A:743:PHE:N	2.84	0.45
1:F:397:ASN:OD1	1:F:399:SER:N	2.49	0.45
2:E:105:TYR:CD1	2:E:105:TYR:N	2.84	0.45
2:E:201:LEU:N	2:E:201:LEU:HD13	2.32	0.45
3:D:576:ASN:HD21	3:D:579:GLU:HG3	1.82	0.45
3:D:743:PHE:N	3:D:743:PHE:CD1	2.84	0.45
2:B:19:TRP:CE3	2:B:147:HIS:HD2	2.33	0.45
2:B:210:ILE:HG21	2:B:212:TRP:CE2	2.51	0.45
3:A:576:ASN:HD21	3:A:579:GLU:HG3	1.82	0.45
3:D:374:ASP:O	3:D:376:THR:HG23	2.17	0.45
3:D:759:ILE:HG22	3:D:762:GLN:H	1.81	0.45
1:C:215:PHE:C	1:C:215:PHE:HD1	2.25	0.45
1:C:276:TYR:C	1:C:277:ASP:O	2.56	0.45
3:A:717:THR:HG22	3:A:719:SER:N	2.32	0.45
3:A:876:LEU:HD13	3:A:972:PHE:CE2	2.52	0.45
1:F:215:PHE:C	1:F:215:PHE:HD1	2.24	0.45
1:F:256:SER:CB	1:F:258:VAL:HG23	2.46	0.45
3:D:685:LYS:O	3:D:689:SER:OG	2.29	0.45
3:D:699:GLU:OE1	3:D:748:VAL:HG23	2.16	0.45
3:D:739:ILE:HG13	3:D:741:TYR:CE1	2.52	0.45
3:D:997:PHE:CE1	1:C:183:ILE:HD13	2.52	0.45
1:C:224:LYS:O	1:C:235:PRO:HA	2.17	0.45
1:C:225:VAL:HA	1:C:234:ILE:O	2.17	0.45
3:A:213:ILE:HG21	3:A:223:ARG:HH12	1.82	0.45
3:A:244:LEU:HD23	3:A:245:LEU:HD23	1.99	0.45
3:A:397:VAL:HG23	3:A:401:ILE:O	2.16	0.45
1:F:195:ILE:HD12	1:F:211:ASP:OD2	2.17	0.45
2:E:105:TYR:N	2:E:105:TYR:HD1	2.15	0.45
3:D:223:ARG:HH11	3:D:223:ARG:HG3	1.82	0.45
3:D:397:VAL:C	3:D:399:GLU:H	2.25	0.45
1:C:335:VAL:CG1	1:C:420:VAL:HG12	2.39	0.45
3:A:223:ARG:HH11	3:A:223:ARG:HG3	1.82	0.45
3:A:696:LEU:O	3:A:700:SER:HB3	2.17	0.45
2:E:22:VAL:HB	2:E:143:LEU:HD21	1.98	0.45
2:E:210:ILE:HG21	2:E:212:TRP:CE2	2.51	0.45
3:D:398:ASP:OD1	3:D:430:LYS:HB2	2.17	0.45
3:D:526:PHE:CD2	3:D:604:ARG:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:692:ARG:O	3:D:696:LEU:HG	2.17	0.45
1:C:110:ILE:HG13	1:C:136:TRP:CD1	2.51	0.45
3:A:95:LYS:HA	3:A:95:LYS:HD3	1.63	0.45
3:A:763:ASP:CB	3:A:767:SER:H	2.28	0.45
1:F:276:TYR:C	1:F:277:ASP:O	2.56	0.45
2:E:18:ASP:CB	2:E:57:LEU:HB2	2.47	0.45
1:C:20:LEU:HA	1:C:23:SER:OG	2.17	0.45
1:C:195:ILE:HD12	1:C:211:ASP:OD2	2.17	0.45
1:C:358:ARG:NH1	1:C:359:GLU:OE1	2.50	0.45
3:A:785:ASN:O	3:A:787:PHE:N	2.49	0.45
3:D:785:ASN:HB3	3:D:786:ASN:H	1.62	0.45
1:C:379:ILE:HG23	1:C:383:LYS:H	1.81	0.45
2:B:7:SER:HG	2:B:8:HIS:CE1	2.33	0.45
2:B:22:VAL:HB	2:B:143:LEU:HD21	1.98	0.45
2:B:105:TYR:N	2:B:105:TYR:HD1	2.15	0.45
3:A:1:MET:N	3:A:129:GLU:OE2	2.35	0.45
1:F:224:LYS:O	1:F:235:PRO:HA	2.17	0.44
3:D:709:ASN:HB3	3:D:737:LEU:HD13	1.99	0.44
3:D:876:LEU:HD13	3:D:972:PHE:CE2	2.52	0.44
3:A:269:LEU:O	3:A:273:THR:HG22	2.16	0.44
3:A:374:ASP:HB3	3:A:375:THR:H	1.56	0.44
3:A:533:VAL:CG1	3:A:803:LYS:CD	2.93	0.44
3:D:222:LEU:HD22	3:D:234:ARG:HG2	2.00	0.44
3:D:223:ARG:HG3	3:D:223:ARG:NH1	2.33	0.44
3:D:269:LEU:O	3:D:273:THR:HG22	2.17	0.44
3:D:403:CYS:SG	3:D:419:LEU:HB3	2.58	0.44
3:D:696:LEU:O	3:D:700:SER:HB3	2.17	0.44
3:D:767:SER:O	3:D:770:ILE:HG13	2.17	0.44
3:A:398:ASP:OD1	3:A:430:LYS:HB2	2.17	0.44
3:A:717:THR:CG2	3:A:718:LEU:N	2.80	0.44
3:A:744:ARG:NH1	3:A:744:ARG:HG3	2.31	0.44
1:F:232:ILE:HG23	1:F:307:TYR:HB3	1.99	0.44
3:D:103:THR:OG1	3:D:104:MET:N	2.50	0.44
3:D:213:ILE:HG21	3:D:223:ARG:HH12	1.82	0.44
3:D:275:ARG:O	3:D:279:LEU:HG	2.17	0.44
3:D:297:LEU:HD11	3:D:320:VAL:HG22	1.98	0.44
3:D:701:VAL:HA	3:D:715:ALA:N	2.32	0.44
2:B:113:ILE:O	2:B:116:VAL:HG22	2.17	0.44
2:B:201:LEU:HD13	2:B:201:LEU:N	2.32	0.44
3:A:397:VAL:C	3:A:399:GLU:H	2.25	0.44
3:A:438:ILE:HD12	3:A:458:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542:SER:O	3:A:758:GLU:CG	2.65	0.44
3:A:692:ARG:O	3:A:696:LEU:HG	2.17	0.44
1:F:379:ILE:HG21	3:D:582:ILE:HD13	2.00	0.44
1:F:383:LYS:CE	1:F:415:ASN:HB3	2.48	0.44
3:D:407:ARG:HA	3:D:407:ARG:HD3	1.81	0.44
2:B:195:PHE:C	2:B:197:ILE:H	2.25	0.44
3:A:213:ILE:O	3:A:217:VAL:HG23	2.18	0.44
3:A:763:ASP:HB3	3:A:767:SER:H	1.82	0.44
3:D:542:SER:O	3:D:758:GLU:CG	2.65	0.44
3:A:514:LYS:HD2	3:A:514:LYS:H	1.82	0.44
3:A:934:CYS:O	3:A:966:ILE:HD13	2.18	0.44
1:F:358:ARG:NH1	1:F:359:GLU:OE1	2.50	0.44
2:E:72:LYS:O	2:E:86:LYS:NZ	2.50	0.44
3:D:485:THR:OG1	3:D:659:THR:HG21	2.17	0.44
3:D:766:LYS:C	3:D:768:ILE:N	2.73	0.44
1:C:232:ILE:HG23	1:C:307:TYR:HB3	1.99	0.44
2:B:50:PHE:HB3	2:B:53:LEU:HD13	2.00	0.44
3:A:716:ASN:C	3:A:717:THR:HG1	2.10	0.44
3:A:823:ARG:HA	3:A:823:ARG:HD3	1.58	0.44
3:A:852:GLU:O	3:A:855:SER:OG	2.34	0.44
2:E:15:TYR:CE1	2:E:53:LEU:HD13	2.53	0.44
3:D:536:PRO:HA	3:D:749:TYR:CD1	2.51	0.44
3:A:76:LEU:HD12	3:A:76:LEU:HA	1.79	0.44
3:A:701:VAL:HA	3:A:715:ALA:N	2.32	0.44
2:E:113:ILE:O	2:E:116:VAL:HG22	2.17	0.44
3:D:681:TYR:HE1	3:D:685:LYS:HZ2	1.62	0.44
3:D:934:CYS:O	3:D:966:ILE:HD13	2.17	0.44
1:C:383:LYS:CE	1:C:415:ASN:HB3	2.48	0.44
2:B:72:LYS:O	2:B:86:LYS:NZ	2.51	0.44
3:A:103:THR:OG1	3:A:104:MET:N	2.50	0.44
3:A:544:ASN:HD22	3:A:544:ASN:C	2.24	0.44
3:A:698:LEU:HD12	3:A:698:LEU:HA	1.64	0.44
3:A:811:TYR:CE1	3:A:813:ALA:HB2	2.53	0.44
3:A:866:ILE:HG22	3:A:867:ASP:N	2.32	0.44
2:E:72:LYS:NZ	2:E:72:LYS:CB	2.74	0.44
2:E:195:PHE:C	2:E:197:ILE:H	2.25	0.44
3:A:275:ARG:O	3:A:279:LEU:HG	2.17	0.44
3:A:292:LYS:HB2	3:A:292:LYS:HE2	1.44	0.44
3:A:485:THR:OG1	3:A:659:THR:HG21	2.17	0.44
1:F:179:GLU:HA	1:F:179:GLU:OE1	2.18	0.43
3:A:374:ASP:O	3:A:376:THR:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:639:LYS:O	3:A:642:LYS:N	2.51	0.43
3:A:724:MET:HE3	3:A:724:MET:HB2	1.80	0.43
1:F:144:LYS:O	1:F:205:LEU:HD11	2.18	0.43
1:F:154:LEU:O	1:F:157:GLU:N	2.51	0.43
1:F:225:VAL:HA	1:F:234:ILE:O	2.17	0.43
2:E:210:ILE:HD12	2:E:210:ILE:HA	1.72	0.43
3:D:533:VAL:CG1	3:D:803:LYS:CD	2.93	0.43
3:D:880:PHE:CE1	3:D:965:ARG:HB3	2.53	0.43
3:A:268:ASP:O	3:A:272:ILE:HG13	2.18	0.43
3:D:187:SER:O	3:D:188:TYR:CG	2.71	0.43
1:C:378:LYS:HD2	1:C:378:LYS:HA	1.87	0.43
2:B:15:TYR:CE1	2:B:53:LEU:HD13	2.53	0.43
3:A:403:CYS:SG	3:A:419:LEU:HB3	2.58	0.43
3:A:486:TYR:CZ	3:A:501:ILE:HD12	2.53	0.43
3:A:709:ASN:HB3	3:A:737:LEU:HD13	1.99	0.43
1:F:387:PHE:CE1	1:F:411:VAL:HG21	2.53	0.43
3:D:438:ILE:HD12	3:D:458:TYR:CE2	2.53	0.43
3:D:639:LYS:O	3:D:642:LYS:N	2.51	0.43
3:D:768:ILE:C	3:D:770:ILE:N	2.73	0.43
3:D:811:TYR:CE1	3:D:813:ALA:HB2	2.53	0.43
3:D:876:LEU:HD12	3:D:876:LEU:HA	1.63	0.43
1:C:266:VAL:HA	1:C:276:TYR:H	1.83	0.43
1:C:387:PHE:CE1	1:C:411:VAL:HG21	2.53	0.43
3:A:739:ILE:HG13	3:A:741:TYR:CE1	2.52	0.43
1:F:214:LYS:HA	1:F:214:LYS:HD3	1.68	0.43
1:F:297:ILE:HG13	1:F:298:GLY:N	2.32	0.43
1:F:360:CYS:C	1:F:361:LEU:HD12	2.44	0.43
3:D:14:GLU:N	3:D:14:GLU:CD	2.76	0.43
2:B:18:ASP:CB	2:B:57:LEU:HB2	2.47	0.43
3:A:222:LEU:HD22	3:A:234:ARG:HG2	2.00	0.43
3:A:223:ARG:HG3	3:A:223:ARG:NH1	2.33	0.43
3:A:407:ARG:HA	3:A:407:ARG:HD3	1.81	0.43
3:A:768:ILE:CD1	3:A:816:ASN:HB2	2.49	0.43
2:E:145:LEU:HD12	2:E:145:LEU:HA	1.78	0.43
3:D:265:HIS:CE1	3:D:330:ASP:HB2	2.53	0.43
3:D:407:ARG:HB2	3:D:418:VAL:CG2	2.48	0.43
3:D:811:TYR:HE1	3:D:813:ALA:HB2	1.84	0.43
3:D:866:ILE:HG22	3:D:867:ASP:N	2.32	0.43
1:C:250:VAL:O	1:C:254:ILE:HG13	2.19	0.43
1:C:360:CYS:C	1:C:361:LEU:HD12	2.44	0.43
2:B:48:LYS:HG3	2:B:51:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:227:LEU:HD12	3:A:227:LEU:HA	1.78	0.43
3:A:265:HIS:CE1	3:A:330:ASP:HB2	2.53	0.43
3:A:636:ARG:HG2	3:A:637:TYR:N	2.31	0.43
3:A:779:ASN:HB3	3:A:788:LYS:C	2.44	0.43
1:F:266:VAL:HA	1:F:276:TYR:H	1.83	0.43
2:E:7:SER:HG	2:E:8:HIS:CE1	2.34	0.43
3:D:268:ASP:O	3:D:272:ILE:HG13	2.18	0.43
3:D:481:ALA:O	3:D:485:THR:OG1	2.37	0.43
3:D:700:SER:C	3:D:715:ALA:CB	2.88	0.43
3:D:766:LYS:O	3:D:766:LYS:HD3	2.19	0.43
1:C:154:LEU:O	1:C:157:GLU:N	2.51	0.43
1:F:30:LYS:C	1:F:30:LYS:HD3	2.44	0.43
3:D:244:LEU:HD23	3:D:245:LEU:HD23	1.99	0.43
3:D:341:LEU:HB2	3:D:344:TYR:CE1	2.54	0.43
3:D:779:ASN:HA	3:D:783:LEU:HD12	2.00	0.43
1:C:30:LYS:HD3	1:C:30:LYS:C	2.44	0.43
1:C:144:LYS:O	1:C:205:LEU:HD11	2.18	0.43
2:B:167:ARG:NH2	2:B:173:PRO:HA	2.34	0.43
3:D:213:ILE:O	3:D:217:VAL:HG23	2.18	0.43
3:D:514:LYS:HD2	3:D:514:LYS:H	1.82	0.43
3:D:697:TYR:O	3:D:701:VAL:HG22	2.19	0.43
3:A:526:PHE:CE2	3:A:604:ARG:CD	3.01	0.43
3:A:705:ALA:CB	3:A:744:ARG:HB2	2.49	0.43
3:A:779:ASN:HA	3:A:783:LEU:HD12	2.00	0.43
3:A:991:SER:O	3:A:995:ARG:HG3	2.19	0.43
3:D:215:GLU:O	3:D:219:ARG:HB2	2.19	0.43
3:D:991:SER:O	3:D:995:ARG:HG3	2.19	0.43
1:C:231:ASN:O	1:C:309:SER:HA	2.19	0.43
1:C:297:ILE:HG13	1:C:298:GLY:N	2.33	0.43
3:A:187:SER:O	3:A:188:TYR:CG	2.71	0.43
3:A:574:SER:H	3:A:610:SER:HG	1.65	0.43
3:A:744:ARG:HG3	3:A:744:ARG:HH11	1.84	0.43
1:F:337:GLU:HA	1:F:340:LYS:HE3	2.01	0.42
3:D:779:ASN:HB3	3:D:788:LYS:C	2.44	0.42
3:A:407:ARG:HB2	3:A:418:VAL:CG2	2.48	0.42
3:A:547:ILE:HG13	3:A:794:VAL:HB	2.01	0.42
3:A:724:MET:CE	3:A:724:MET:H	2.32	0.42
1:C:164:ASN:O	1:C:166:LEU:HG	2.20	0.42
3:A:341:LEU:HB2	3:A:344:TYR:CE1	2.54	0.42
3:A:880:PHE:CE1	3:A:965:ARG:HB3	2.53	0.42
1:F:106:ILE:HG23	1:F:136:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:ASN:O	1:F:309:SER:HA	2.19	0.42
1:F:286:ARG:NH2	1:F:401:GLU:OE2	2.52	0.42
1:F:371:LEU:CD1	1:F:400:ILE:HG23	2.49	0.42
3:D:227:LEU:HD12	3:D:227:LEU:HA	1.78	0.42
3:D:705:ALA:CB	3:D:744:ARG:HB2	2.49	0.42
3:D:738:PRO:HG2	3:D:769:GLU:OE2	2.20	0.42
1:C:337:GLU:HA	1:C:340:LYS:HE3	2.01	0.42
2:E:39:ARG:HE	2:E:39:ARG:HB2	1.63	0.42
2:E:202:LEU:HD23	2:E:202:LEU:HA	1.66	0.42
3:D:486:TYR:CZ	3:D:501:ILE:HD12	2.53	0.42
3:D:734:LYS:HA	3:D:734:LYS:HD3	1.81	0.42
3:D:840:LYS:HB2	3:D:890:PHE:CZ	2.54	0.42
1:C:106:ILE:HG23	1:C:136:TRP:CE2	2.55	0.42
2:B:41:GLU:OE1	2:B:127:LEU:CB	2.68	0.42
3:A:215:GLU:O	3:A:219:ARG:HB2	2.19	0.42
3:A:577:ARG:C	3:A:579:GLU:N	2.78	0.42
3:A:697:TYR:O	3:A:701:VAL:HG22	2.19	0.42
3:A:729:ILE:H	3:A:729:ILE:HG13	1.59	0.42
1:F:413:ILE:O	1:F:417:VAL:HG12	2.20	0.42
3:D:828:THR:C	3:D:830:GLU:H	2.27	0.42
1:C:413:ILE:O	1:C:417:VAL:HG12	2.20	0.42
1:C:423:ARG:C	1:C:426:GLU:HB3	2.45	0.42
3:A:481:ALA:O	3:A:485:THR:OG1	2.37	0.42
3:A:832:ARG:HH21	3:A:834:ASP:HB2	1.84	0.42
3:A:837:LYS:HA	3:A:890:PHE:HD1	1.85	0.42
2:E:47:ASP:O	2:E:48:LYS:HE2	2.20	0.42
3:D:741:TYR:HE2	3:D:766:LYS:NZ	2.17	0.42
3:D:837:LYS:HA	3:D:890:PHE:HD1	1.85	0.42
3:D:865:CYS:SG	3:D:985:ASN:ND2	2.93	0.42
1:C:138:MET:HB3	1:C:138:MET:HE2	1.70	0.42
3:A:87:ASP:OD1	3:A:87:ASP:N	2.52	0.42
3:A:828:THR:C	3:A:830:GLU:H	2.27	0.42
1:F:3:SER:O	2:B:193:ARG:NH1	2.52	0.42
1:F:250:VAL:O	1:F:254:ILE:HG13	2.19	0.42
2:B:2:ASN:OD1	2:B:2:ASN:N	2.51	0.42
3:A:865:CYS:SG	3:A:985:ASN:ND2	2.93	0.42
1:F:326:ASN:OD1	1:F:327:GLU:N	2.53	0.42
1:F:423:ARG:C	1:F:426:GLU:HB3	2.45	0.42
2:E:48:LYS:O	2:E:49:PHE:CB	2.67	0.42
2:E:159:GLY:HA3	2:E:162:ASP:OD1	2.20	0.42
2:E:177:ILE:HD12	2:E:177:ILE:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:195:PHE:CD2	2:E:212:TRP:CZ2	3.08	0.42
3:D:87:ASP:N	3:D:87:ASP:OD1	2.52	0.42
3:D:552:SER:OG	3:D:552:SER:O	2.34	0.42
3:A:553:LEU:HD12	3:A:553:LEU:HA	1.89	0.42
3:A:759:ILE:CG2	3:A:762:GLN:H	2.33	0.42
3:A:811:TYR:HE1	3:A:813:ALA:HB2	1.84	0.42
1:F:12:GLU:HB3	1:F:30:LYS:NZ	2.35	0.42
1:F:347:LYS:HE3	1:F:347:LYS:HB3	1.71	0.42
1:F:378:LYS:CB	1:F:386:ASN:HB3	2.50	0.42
2:E:60:LYS:HA	2:E:60:LYS:HD3	1.68	0.42
3:D:876:LEU:HD22	3:D:972:PHE:CB	2.50	0.42
1:C:286:ARG:NH2	1:C:401:GLU:OE2	2.52	0.42
1:C:326:ASN:OD1	1:C:327:GLU:N	2.53	0.42
2:B:11:TYR:HD1	2:B:11:TYR:N	2.17	0.42
2:B:87:LYS:O	2:B:91:GLU:HG2	2.20	0.42
3:A:546:LEU:HD23	3:A:771:ALA:CB	2.49	0.42
3:A:840:LYS:HB2	3:A:890:PHE:CZ	2.54	0.42
2:E:11:TYR:HD1	2:E:11:TYR:N	2.17	0.42
2:E:167:ARG:NH2	2:E:173:PRO:HA	2.34	0.42
3:D:818:LYS:N	3:D:818:LYS:HD3	2.34	0.42
1:C:184:MET:HA	1:C:187:SER:OG	2.20	0.42
1:C:371:LEU:CD1	1:C:400:ILE:HG23	2.49	0.42
1:C:378:LYS:CB	1:C:386:ASN:HB3	2.50	0.42
3:A:602:GLU:HA	3:A:603:PRO:HD3	1.93	0.42
1:F:164:ASN:O	1:F:166:LEU:HG	2.20	0.41
1:F:256:SER:HB3	1:F:258:VAL:HG23	2.01	0.41
2:E:2:ASN:N	2:E:2:ASN:OD1	2.51	0.41
2:E:52:GLN:NE2	2:E:77:VAL:HG13	2.35	0.41
3:D:288:SER:OG	3:D:293:GLU:HB3	2.20	0.41
3:D:528:TYR:CD1	3:D:528:TYR:N	2.88	0.41
1:C:146:GLN:HG2	1:C:150:ASN:OD1	2.20	0.41
1:C:179:GLU:HA	1:C:179:GLU:OE1	2.18	0.41
2:B:92:ILE:HD11	2:B:182:PRO:HG2	2.02	0.41
2:B:195:PHE:CD2	2:B:212:TRP:CZ2	3.08	0.41
3:D:317:THR:HG22	3:D:319:HIS:NE2	2.35	0.41
3:D:744:ARG:HG3	3:D:744:ARG:HH11	1.84	0.41
3:D:809:MET:HG3	3:D:825:ASN:C	2.45	0.41
3:D:832:ARG:HH21	3:D:834:ASP:HB2	1.84	0.41
2:B:48:LYS:HG3	2:B:51:ILE:CG1	2.50	0.41
1:F:146:GLN:HG2	1:F:150:ASN:OD1	2.20	0.41
1:F:163:PRO:HD2	1:F:165:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:547:ILE:HD11	3:D:756:PHE:CE1	2.48	0.41
2:B:52:GLN:HE22	2:B:77:VAL:HA	1.85	0.41
3:A:528:TYR:CD1	3:A:528:TYR:N	2.88	0.41
2:E:19:TRP:CD1	2:E:53:LEU:O	2.73	0.41
2:E:87:LYS:O	2:E:91:GLU:HG2	2.20	0.41
3:D:453:LEU:HD23	3:D:453:LEU:HA	1.85	0.41
3:D:839:HIS:CE1	3:D:890:PHE:HZ	2.39	0.41
1:C:28:ILE:H	1:C:28:ILE:HG13	1.75	0.41
2:B:19:TRP:CD1	2:B:53:LEU:O	2.73	0.41
3:A:140:TYR:N	3:A:140:TYR:CD1	2.88	0.41
3:A:288:SER:OG	3:A:293:GLU:HB3	2.20	0.41
3:A:876:LEU:HD22	3:A:972:PHE:CB	2.50	0.41
2:E:52:GLN:HE22	2:E:77:VAL:HA	1.85	0.41
3:D:140:TYR:CD1	3:D:140:TYR:N	2.88	0.41
3:D:767:SER:O	3:D:770:ILE:CB	2.68	0.41
1:C:12:GLU:HB3	1:C:30:LYS:NZ	2.35	0.41
1:C:163:PRO:HD2	1:C:165:TYR:CE2	2.55	0.41
1:C:294:ILE:HD13	1:C:294:ILE:HA	1.82	0.41
1:C:344:VAL:HA	1:C:347:LYS:NZ	2.36	0.41
2:B:195:PHE:HD2	2:B:212:TRP:CZ2	2.38	0.41
3:A:809:MET:HG3	3:A:825:ASN:C	2.45	0.41
3:A:839:HIS:CE1	3:A:890:PHE:HZ	2.39	0.41
1:F:36:GLU:CD	3:A:524:GLN:HG3	2.45	0.41
1:F:184:MET:HA	1:F:187:SER:OG	2.20	0.41
3:D:465:LEU:HD23	3:D:465:LEU:HA	1.83	0.41
3:D:553:LEU:HD12	3:D:553:LEU:HA	1.90	0.41
2:B:11:TYR:CD1	2:B:11:TYR:N	2.88	0.41
3:A:317:THR:HG22	3:A:319:HIS:NE2	2.35	0.41
3:A:803:LYS:C	3:A:805:LYS:H	2.29	0.41
3:D:275:ARG:HH21	3:D:279:LEU:HD11	1.85	0.41
3:D:812:SER:O	3:D:812:SER:OG	2.37	0.41
1:C:299:ARG:HA	1:C:299:ARG:HD3	1.85	0.41
2:B:159:GLY:HA3	2:B:162:ASP:OD1	2.20	0.41
3:A:690:ILE:HG23	3:A:722:PHE:CZ	2.56	0.41
2:E:11:TYR:CD1	2:E:11:TYR:N	2.88	0.41
2:E:17:ASP:HA	2:E:20:GLU:HG2	2.03	0.41
2:E:96:ILE:O	2:E:100:THR:HG23	2.20	0.41
3:D:69:ASP:CG	3:D:521:GLU:HB2	2.46	0.41
3:D:581:GLU:O	3:D:585:GLN:HG3	2.20	0.41
1:C:154:LEU:HA	1:C:157:GLU:OE1	2.21	0.41
3:A:547:ILE:CG1	3:A:794:VAL:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:581:GLU:O	3:A:585:GLN:HG3	2.20	0.41
3:A:818:LYS:N	3:A:818:LYS:HD3	2.35	0.41
1:F:254:ILE:C	1:F:256:SER:N	2.77	0.41
2:E:13:ILE:HG23	2:E:15:TYR:CE1	2.56	0.41
2:E:181:HIS:HA	2:E:182:PRO:HD3	1.97	0.41
3:D:75:ASN:HB2	3:D:76:LEU:H	1.69	0.41
3:D:398:ASP:O	3:D:399:GLU:HB2	2.21	0.41
3:D:544:ASN:ND2	3:D:544:ASN:C	2.78	0.41
3:D:724:MET:CE	3:D:724:MET:H	2.33	0.41
3:D:839:HIS:ND1	3:D:890:PHE:HZ	2.19	0.41
1:C:276:TYR:O	1:C:277:ASP:O	2.38	0.41
1:C:285:THR:HG22	1:C:286:ARG:N	2.35	0.41
2:B:38:LEU:H	2:B:38:LEU:HG	1.71	0.41
2:B:52:GLN:NE2	2:B:77:VAL:HG13	2.35	0.41
3:A:435:LYS:HZ3	3:A:435:LYS:HG3	1.70	0.41
3:A:608:LEU:C	3:A:609:ILE:CG2	2.84	0.41
3:A:763:ASP:CB	3:A:767:SER:CB	2.79	0.41
3:A:763:ASP:O	3:A:764:VAL:CB	2.65	0.41
1:F:177:ASP:HB3	1:F:178:ASP:H	1.74	0.41
2:E:147:HIS:CE1	2:E:151:HIS:HE1	2.39	0.41
2:E:195:PHE:HD2	2:E:212:TRP:CZ2	2.38	0.41
3:D:759:ILE:CG2	3:D:762:GLN:H	2.33	0.41
3:D:803:LYS:C	3:D:805:LYS:H	2.29	0.41
1:C:251:ASP:HA	1:C:254:ILE:HD12	2.03	0.41
2:B:17:ASP:HA	2:B:20:GLU:HG2	2.03	0.41
3:A:214:GLN:OE1	3:A:214:GLN:HA	2.20	0.41
3:A:803:LYS:C	3:A:805:LYS:N	2.78	0.41
1:F:138:MET:HE2	1:F:138:MET:HB3	1.70	0.40
1:F:251:ASP:HA	1:F:254:ILE:HD12	2.03	0.40
1:F:269:LYS:HB3	1:F:272:PHE:O	2.22	0.40
1:F:276:TYR:O	1:F:277:ASP:O	2.38	0.40
1:F:407:PHE:O	1:F:410:PHE:N	2.55	0.40
2:E:107:GLY:N	2:E:217:ILE:HB	2.37	0.40
3:D:126:SER:HB3	3:D:151:LYS:HD3	2.02	0.40
3:D:214:GLN:OE1	3:D:214:GLN:HA	2.21	0.40
3:D:745:PHE:N	3:D:745:PHE:CD1	2.89	0.40
3:D:872:LEU:HG	3:D:972:PHE:CD2	2.56	0.40
3:A:734:LYS:HD3	3:A:734:LYS:HA	1.80	0.40
3:A:783:LEU:HD23	3:A:783:LEU:HA	1.96	0.40
1:F:154:LEU:HA	1:F:157:GLU:OE1	2.21	0.40
1:F:297:ILE:HD12	1:F:301:TYR:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:VAL:HA	1:F:347:LYS:NZ	2.36	0.40
3:D:542:SER:CB	3:D:758:GLU:CG	2.90	0.40
3:D:803:LYS:C	3:D:805:LYS:N	2.78	0.40
1:C:108:ASP:N	1:C:109:GLU:OE2	2.54	0.40
2:B:107:GLY:N	2:B:217:ILE:HB	2.36	0.40
3:A:40:TYR:HB2	3:A:91:ILE:HG23	2.02	0.40
3:A:69:ASP:CG	3:A:521:GLU:HB2	2.45	0.40
3:A:110:ILE:HD12	3:A:110:ILE:HA	1.84	0.40
3:A:275:ARG:HH21	3:A:279:LEU:HD11	1.85	0.40
3:A:367:GLU:HA	3:A:419:LEU:O	2.22	0.40
1:F:7:LEU:O	1:F:10:LEU:HG	2.22	0.40
1:F:123:GLY:O	1:F:144:LYS:HG3	2.22	0.40
3:D:346:LEU:HA	3:D:349:ILE:HD11	2.03	0.40
3:D:540:MET:O	3:D:542:SER:N	2.54	0.40
1:C:7:LEU:O	1:C:10:LEU:HG	2.22	0.40
1:C:297:ILE:HD12	1:C:301:TYR:HB2	2.04	0.40
2:B:136:TYR:CE1	3:A:179:PHE:CE1	3.09	0.40
3:A:960:LEU:H	3:A:960:LEU:HG	1.69	0.40
2:E:92:ILE:HD11	2:E:182:PRO:HG2	2.02	0.40
3:D:40:TYR:HB2	3:D:91:ILE:HG23	2.02	0.40
3:D:120:SER:HA	3:D:121:PRO:HD3	1.94	0.40
3:A:126:SER:HB3	3:A:151:LYS:HD3	2.02	0.40
3:A:346:LEU:HA	3:A:349:ILE:HD11	2.03	0.40
3:A:470:TRP:CD1	3:A:470:TRP:C	3.00	0.40
3:A:762:GLN:HG2	3:A:858:ARG:HH21	1.86	0.40
3:A:796:LYS:HD3	3:A:796:LYS:HA	1.60	0.40
3:A:839:HIS:ND1	3:A:890:PHE:HZ	2.19	0.40
1:F:12:GLU:HB3	1:F:30:LYS:CE	2.52	0.40
1:F:285:THR:HG22	1:F:286:ARG:N	2.36	0.40
2:E:160:LYS:HB2	2:E:180:TYR:CE1	2.57	0.40
3:D:40:TYR:HB2	3:D:91:ILE:CG2	2.52	0.40
3:D:264:GLY:HA2	3:D:268:ASP:HB2	2.04	0.40
3:D:321:ASN:O	3:D:321:ASN:CG	2.65	0.40
3:D:481:ALA:HB2	3:D:655:SER:OG	2.22	0.40
3:D:690:ILE:HG23	3:D:722:PHE:CZ	2.56	0.40
1:C:269:LYS:HB3	1:C:272:PHE:O	2.22	0.40
2:B:15:TYR:HD2	2:B:23:MET:CB	2.34	0.40
2:B:96:ILE:O	2:B:100:THR:HG23	2.20	0.40
3:A:215:GLU:OE1	3:A:449:LEU:HD23	2.21	0.40
3:A:493:VAL:HG12	3:A:494:PHE:CD2	2.57	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	C	366/426 (86%)	333 (91%)	31 (8%)	2 (0%)	24	57
1	F	366/426 (86%)	332 (91%)	31 (8%)	3 (1%)	16	49
2	B	216/218 (99%)	199 (92%)	15 (7%)	2 (1%)	14	47
2	E	216/218 (99%)	198 (92%)	16 (7%)	2 (1%)	14	47
3	A	919/1006 (91%)	769 (84%)	128 (14%)	22 (2%)	4	29
3	D	919/1006 (91%)	768 (84%)	129 (14%)	22 (2%)	4	29
All	All	3002/3300 (91%)	2599 (87%)	350 (12%)	53 (2%)	9	34

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	374	ASP
3	D	375	THR
3	D	540	MET
3	D	544	ASN
3	D	547	ILE
3	D	604	ARG
3	D	609	ILE
3	D	764	VAL
3	D	765	ASP
2	B	48	LYS
3	A	374	ASP
3	A	375	THR
3	A	540	MET
3	A	544	ASN
3	A	609	ILE
3	A	716	ASN
3	A	763	ASP
3	A	764	VAL
3	A	765	ASP
3	D	75	ASN

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Mol	Chain	Res	Type
3	D	786	ASN
3	D	798	LEU
3	D	841	ASN
3	A	75	ASN
3	A	604	ARG
3	A	786	ASN
3	A	798	LEU
3	A	841	ASN
1	F	277	ASP
1	F	364	PRO
3	D	543	ASN
3	D	607	ASN
3	D	714	PHE
3	D	716	ASN
1	C	277	ASP
1	C	364	PRO
3	A	543	ASN
3	A	607	ASN
3	A	714	PHE
3	A	717	THR
1	F	255	ARG
2	E	49	PHE
2	E	73	ASP
3	D	803	LYS
2	B	73	ASP
3	A	803	LYS
3	D	546	LEU
3	D	606	PRO
3	D	610	SER
3	A	606	PRO
3	A	610	SER
3	D	400	ASP
3	A	400	ASP

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	C	346/396 (87%)	277 (80%)	69 (20%)	1	7
1	F	346/396 (87%)	275 (80%)	71 (20%)	1	7
2	B	200/200 (100%)	134 (67%)	66 (33%)	0	2
2	E	200/200 (100%)	132 (66%)	68 (34%)	0	2
3	A	853/928 (92%)	627 (74%)	226 (26%)	0	3
3	D	853/928 (92%)	624 (73%)	229 (27%)	0	3
All	All	2798/3048 (92%)	2069 (74%)	729 (26%)	2	3

All (729) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1	MET
1	F	2	THR
1	F	4	SER
1	F	6	ASP
1	F	18	LYS
1	F	19	SER
1	F	23	SER
1	F	24	ASP
1	F	25	SER
1	F	33	SER
1	F	39	THR
1	F	41	THR
1	F	105	GLN
1	F	106	ILE
1	F	112	SER
1	F	116	LYS
1	F	133	ASN
1	F	138	MET
1	F	147	SER
1	F	150	ASN
1	F	156	SER
1	F	168	ILE
1	F	177	ASP
1	F	178	ASP
1	F	179	GLU
1	F	183	ILE
1	F	190	ASP
1	F	191	THR
1	F	202	LEU
1	F	208	GLN

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Mol	Chain	Res	Type
1	F	209	VAL
1	F	215	PHE
1	F	224	LYS
1	F	241	SER
1	F	247	VAL
1	F	249	ASP
1	F	251	ASP
1	F	257	LYS
1	F	260	GLU
1	F	262	THR
1	F	267	LYS
1	F	273	SER
1	F	275	LEU
1	F	279	ASP
1	F	284	GLU
1	F	309	SER
1	F	311	VAL
1	F	313	ILE
1	F	327	GLU
1	F	330	THR
1	F	332	ASP
1	F	338	ILE
1	F	341	SER
1	F	347	LYS
1	F	351	GLN
1	F	352	SER
1	F	353	VAL
1	F	365	GLU
1	F	370	THR
1	F	371	LEU
1	F	375	MET
1	F	380	GLU
1	F	383	LYS
1	F	384	VAL
1	F	385	VAL
1	F	394	CYS
1	F	412	SER
1	F	418	THR
1	F	419	ASP
1	F	420	VAL
1	F	426	GLU
2	E	1	MET

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Mol	Chain	Res	Type
2	E	4	VAL
2	E	11	TYR
2	E	23	MET
2	E	33	VAL
2	E	38	LEU
2	E	40	ASP
2	E	41	GLU
2	E	42	THR
2	E	43	SER
2	E	48	LYS
2	E	50	PHE
2	E	51	ILE
2	E	52	GLN
2	E	54	LYS
2	E	57	LEU
2	E	61	ARG
2	E	68	ASP
2	E	72	LYS
2	E	80	GLU
2	E	81	SER
2	E	85	THR
2	E	88	SER
2	E	90	LYS
2	E	91	GLU
2	E	94	SER
2	E	95	SER
2	E	97	SER
2	E	102	VAL
2	E	105	TYR
2	E	109	ASN
2	E	112	ILE
2	E	117	ILE
2	E	123	LEU
2	E	132	SER
2	E	139	LYS
2	E	140	ILE
2	E	142	LYS
2	E	144	LEU
2	E	148	ILE
2	E	152	VAL
2	E	153	SER
2	E	154	VAL

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Mol	Chain	Res	Type
2	E	158	LEU
2	E	161	THR
2	E	162	ASP
2	E	165	ASN
2	E	166	ILE
2	E	169	LYS
2	E	171	GLU
2	E	174	VAL
2	E	175	THR
2	E	176	THR
2	E	177	ILE
2	E	178	VAL
2	E	185	ARG
2	E	191	LYS
2	E	192	ASP
2	E	193	ARG
2	E	197	ILE
2	E	198	ILE
2	E	199	ASN
2	E	201	LEU
2	E	204	LEU
2	E	205	ASP
2	E	208	THR
2	E	210	ILE
2	E	211	ASN
3	D	2	ASP
3	D	7	ASN
3	D	11	SER
3	D	14	GLU
3	D	15	ASN
3	D	18	LEU
3	D	22	SER
3	D	25	ARG
3	D	28	GLU
3	D	29	THR
3	D	32	ILE
3	D	42	VAL
3	D	48	GLN
3	D	50	LEU
3	D	62	LYS
3	D	81	ARG
3	D	85	VAL

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Mol	Chain	Res	Type
3	D	87	ASP
3	D	88	MET
3	D	96	LYS
3	D	98	SER
3	D	105	ASP
3	D	117	ASN
3	D	122	ASP
3	D	127	LEU
3	D	134	LYS
3	D	135	ILE
3	D	137	ASN
3	D	139	CYS
3	D	140	TYR
3	D	142	CYS
3	D	144	ASP
3	D	158	ILE
3	D	167	ILE
3	D	172	ASP
3	D	175	PHE
3	D	177	SER
3	D	178	VAL
3	D	184	SER
3	D	187	SER
3	D	189	CYS
3	D	193	LEU
3	D	194	SER
3	D	196	LYS
3	D	201	THR
3	D	203	ILE
3	D	207	MET
3	D	208	LEU
3	D	209	THR
3	D	210	GLU
3	D	211	GLN
3	D	214	GLN
3	D	219	ARG
3	D	223	ARG
3	D	226	SER
3	D	229	GLU
3	D	234	ARG
3	D	237	VAL
3	D	238	LEU

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Mol	Chain	Res	Type
3	D	240	SER
3	D	245	LEU
3	D	251	LEU
3	D	253	GLU
3	D	271	TYR
3	D	274	ASN
3	D	277	GLU
3	D	278	LEU
3	D	280	THR
3	D	282	GLU
3	D	283	LYS
3	D	287	ARG
3	D	292	LYS
3	D	301	GLU
3	D	316	THR
3	D	320	VAL
3	D	333	SER
3	D	335	ILE
3	D	338	SER
3	D	339	GLU
3	D	340	LYS
3	D	345	LYS
3	D	348	SER
3	D	350	SER
3	D	356	CYS
3	D	357	MET
3	D	360	VAL
3	D	367	GLU
3	D	369	THR
3	D	371	ILE
3	D	374	ASP
3	D	376	THR
3	D	377	ASP
3	D	381	LYS
3	D	388	VAL
3	D	390	THR
3	D	399	GLU
3	D	401	ILE
3	D	406	ILE
3	D	411	LEU
3	D	412	GLU
3	D	416	LYS

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Mol	Chain	Res	Type
3	D	417	VAL
3	D	420	SER
3	D	421	CYS
3	D	428	ILE
3	D	430	LYS
3	D	431	LEU
3	D	435	LYS
3	D	438	ILE
3	D	451	ILE
3	D	455	MET
3	D	462	ASP
3	D	479	THR
3	D	485	THR
3	D	487	VAL
3	D	488	LEU
3	D	493	VAL
3	D	500	THR
3	D	511	LEU
3	D	512	GLU
3	D	514	LYS
3	D	518	VAL
3	D	521	GLU
3	D	522	THR
3	D	526	PHE
3	D	528	TYR
3	D	532	LYS
3	D	542	SER
3	D	544	ASN
3	D	545	VAL
3	D	549	ASP
3	D	551	ASN
3	D	558	CYS
3	D	568	LEU
3	D	571	VAL
3	D	572	VAL
3	D	585	GLN
3	D	588	LEU
3	D	590	LYS
3	D	598	THR
3	D	599	VAL
3	D	602	GLU
3	D	605	LEU

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Mol	Chain	Res	Type
3	D	608	LEU
3	D	609	ILE
3	D	622	THR
3	D	636	ARG
3	D	638	LYS
3	D	640	MET
3	D	645	THR
3	D	652	ILE
3	D	655	SER
3	D	657	GLN
3	D	663	VAL
3	D	666	SER
3	D	670	LEU
3	D	678	LEU
3	D	685	LYS
3	D	686	SER
3	D	694	MET
3	D	702	LEU
3	D	716	ASN
3	D	717	THR
3	D	719	SER
3	D	724	MET
3	D	729	ILE
3	D	732	ILE
3	D	733	VAL
3	D	735	THR
3	D	736	SER
3	D	742	ARG
3	D	744	ARG
3	D	758	GLU
3	D	759	ILE
3	D	762	GLN
3	D	763	ASP
3	D	765	ASP
3	D	766	LYS
3	D	772	LYS
3	D	776	ARG
3	D	777	LEU
3	D	778	ILE
3	D	799	ILE
3	D	803	LYS
3	D	808	THR

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Mol	Chain	Res	Type
3	D	812	SER
3	D	815	SER
3	D	818	LYS
3	D	819	SER
3	D	824	ILE
3	D	828	THR
3	D	829	SER
3	D	831	THR
3	D	832	ARG
3	D	834	ASP
3	D	835	VAL
3	D	836	SER
3	D	837	LYS
3	D	844	LYS
3	D	845	THR
3	D	847	LYS
3	D	850	LEU
3	D	853	MET
3	D	854	LEU
3	D	855	SER
3	D	856	GLU
3	D	858	ARG
3	D	859	MET
3	D	861	SER
3	D	865	CYS
3	D	866	ILE
3	D	867	ASP
3	D	872	LEU
3	D	873	GLU
3	D	893	SER
3	D	932	TYR
3	D	938	VAL
3	D	960	LEU
3	D	962	SER
3	D	966	ILE
3	D	969	GLU
3	D	970	VAL
3	D	978	GLU
3	D	980	VAL
3	D	983	LEU
3	D	987	VAL
3	D	988	LEU

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Mol	Chain	Res	Type
3	D	990	ILE
3	D	991	SER
1	C	1	MET
1	C	2	THR
1	C	4	SER
1	C	6	ASP
1	C	18	LYS
1	C	19	SER
1	C	23	SER
1	C	24	ASP
1	C	25	SER
1	C	33	SER
1	C	39	THR
1	C	41	THR
1	C	105	GLN
1	C	106	ILE
1	C	112	SER
1	C	116	LYS
1	C	133	ASN
1	C	138	MET
1	C	147	SER
1	C	150	ASN
1	C	156	SER
1	C	168	ILE
1	C	177	ASP
1	C	178	ASP
1	C	179	GLU
1	C	183	ILE
1	C	190	ASP
1	C	191	THR
1	C	202	LEU
1	C	208	GLN
1	C	209	VAL
1	C	215	PHE
1	C	224	LYS
1	C	241	SER
1	C	247	VAL
1	C	249	ASP
1	C	251	ASP
1	C	260	GLU
1	C	262	THR
1	C	267	LYS

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Mol	Chain	Res	Type
1	C	273	SER
1	C	275	LEU
1	C	279	ASP
1	C	284	GLU
1	C	309	SER
1	C	311	VAL
1	C	313	ILE
1	C	327	GLU
1	C	330	THR
1	C	332	ASP
1	C	338	ILE
1	C	347	LYS
1	C	351	GLN
1	C	352	SER
1	C	353	VAL
1	C	365	GLU
1	C	370	THR
1	C	371	LEU
1	C	375	MET
1	C	380	GLU
1	C	383	LYS
1	C	384	VAL
1	C	385	VAL
1	C	394	CYS
1	C	412	SER
1	C	418	THR
1	C	419	ASP
1	C	420	VAL
1	C	426	GLU
2	B	1	MET
2	B	4	VAL
2	B	11	TYR
2	B	23	MET
2	B	33	VAL
2	B	38	LEU
2	B	40	ASP
2	B	42	THR
2	B	43	SER
2	B	47	ASP
2	B	48	LYS
2	B	51	ILE
2	B	52	GLN

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Mol	Chain	Res	Type
2	B	54	LYS
2	B	57	LEU
2	B	61	ARG
2	B	68	ASP
2	B	72	LYS
2	B	80	GLU
2	B	81	SER
2	B	85	THR
2	B	88	SER
2	B	90	LYS
2	B	91	GLU
2	B	94	SER
2	B	95	SER
2	B	97	SER
2	B	102	VAL
2	B	105	TYR
2	B	109	ASN
2	B	112	ILE
2	B	117	ILE
2	B	123	LEU
2	B	132	SER
2	B	139	LYS
2	B	140	ILE
2	B	142	LYS
2	B	144	LEU
2	B	148	ILE
2	B	152	VAL
2	B	153	SER
2	B	154	VAL
2	B	158	LEU
2	B	161	THR
2	B	162	ASP
2	B	165	ASN
2	B	166	ILE
2	B	169	LYS
2	B	171	GLU
2	B	174	VAL
2	B	175	THR
2	B	176	THR
2	B	177	ILE
2	B	178	VAL
2	B	185	ARG

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Mol	Chain	Res	Type
2	B	191	LYS
2	B	193	ARG
2	B	197	ILE
2	B	198	ILE
2	B	199	ASN
2	B	201	LEU
2	B	204	LEU
2	B	205	ASP
2	B	208	THR
2	B	210	ILE
2	B	211	ASN
3	A	2	ASP
3	A	7	ASN
3	A	11	SER
3	A	14	GLU
3	A	15	ASN
3	A	18	LEU
3	A	22	SER
3	A	25	ARG
3	A	28	GLU
3	A	29	THR
3	A	32	ILE
3	A	42	VAL
3	A	48	GLN
3	A	50	LEU
3	A	62	LYS
3	A	81	ARG
3	A	85	VAL
3	A	87	ASP
3	A	88	MET
3	A	96	LYS
3	A	98	SER
3	A	105	ASP
3	A	117	ASN
3	A	122	ASP
3	A	127	LEU
3	A	134	LYS
3	A	135	ILE
3	A	137	ASN
3	A	139	CYS
3	A	140	TYR
3	A	142	CYS

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Mol	Chain	Res	Type
3	A	144	ASP
3	A	158	ILE
3	A	167	ILE
3	A	172	ASP
3	A	175	PHE
3	A	177	SER
3	A	178	VAL
3	A	184	SER
3	A	187	SER
3	A	189	CYS
3	A	193	LEU
3	A	194	SER
3	A	196	LYS
3	A	201	THR
3	A	203	ILE
3	A	207	MET
3	A	208	LEU
3	A	209	THR
3	A	210	GLU
3	A	211	GLN
3	A	214	GLN
3	A	219	ARG
3	A	223	ARG
3	A	226	SER
3	A	229	GLU
3	A	234	ARG
3	A	237	VAL
3	A	238	LEU
3	A	240	SER
3	A	245	LEU
3	A	251	LEU
3	A	253	GLU
3	A	271	TYR
3	A	274	ASN
3	A	277	GLU
3	A	278	LEU
3	A	280	THR
3	A	282	GLU
3	A	283	LYS
3	A	287	ARG
3	A	292	LYS
3	A	301	GLU

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Mol	Chain	Res	Type
3	A	316	THR
3	A	320	VAL
3	A	333	SER
3	A	335	ILE
3	A	338	SER
3	A	339	GLU
3	A	340	LYS
3	A	345	LYS
3	A	348	SER
3	A	350	SER
3	A	356	CYS
3	A	357	MET
3	A	360	VAL
3	A	367	GLU
3	A	369	THR
3	A	371	ILE
3	A	374	ASP
3	A	376	THR
3	A	377	ASP
3	A	381	LYS
3	A	388	VAL
3	A	390	THR
3	A	399	GLU
3	A	401	ILE
3	A	406	ILE
3	A	411	LEU
3	A	412	GLU
3	A	416	LYS
3	A	417	VAL
3	A	420	SER
3	A	421	CYS
3	A	428	ILE
3	A	430	LYS
3	A	431	LEU
3	A	435	LYS
3	A	438	ILE
3	A	451	ILE
3	A	455	MET
3	A	462	ASP
3	A	479	THR
3	A	485	THR
3	A	487	VAL

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Mol	Chain	Res	Type
3	A	488	LEU
3	A	493	VAL
3	A	500	THR
3	A	511	LEU
3	A	512	GLU
3	A	514	LYS
3	A	518	VAL
3	A	521	GLU
3	A	522	THR
3	A	526	PHE
3	A	528	TYR
3	A	532	LYS
3	A	542	SER
3	A	544	ASN
3	A	545	VAL
3	A	546	LEU
3	A	549	ASP
3	A	551	ASN
3	A	558	CYS
3	A	568	LEU
3	A	571	VAL
3	A	572	VAL
3	A	585	GLN
3	A	588	LEU
3	A	590	LYS
3	A	598	THR
3	A	599	VAL
3	A	602	GLU
3	A	605	LEU
3	A	608	LEU
3	A	609	ILE
3	A	622	THR
3	A	636	ARG
3	A	638	LYS
3	A	640	MET
3	A	645	THR
3	A	652	ILE
3	A	655	SER
3	A	657	GLN
3	A	663	VAL
3	A	666	SER
3	A	670	LEU

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Mol	Chain	Res	Type
3	A	678	LEU
3	A	685	LYS
3	A	686	SER
3	A	694	MET
3	A	702	LEU
3	A	719	SER
3	A	724	MET
3	A	729	ILE
3	A	732	ILE
3	A	733	VAL
3	A	735	THR
3	A	736	SER
3	A	742	ARG
3	A	744	ARG
3	A	758	GLU
3	A	759	ILE
3	A	763	ASP
3	A	772	LYS
3	A	776	ARG
3	A	777	LEU
3	A	778	ILE
3	A	797	ASN
3	A	799	ILE
3	A	803	LYS
3	A	808	THR
3	A	812	SER
3	A	815	SER
3	A	818	LYS
3	A	819	SER
3	A	824	ILE
3	A	828	THR
3	A	829	SER
3	A	831	THR
3	A	832	ARG
3	A	834	ASP
3	A	835	VAL
3	A	836	SER
3	A	837	LYS
3	A	844	LYS
3	A	845	THR
3	A	847	LYS
3	A	850	LEU

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Mol	Chain	Res	Type
3	A	853	MET
3	A	854	LEU
3	A	855	SER
3	A	856	GLU
3	A	858	ARG
3	A	859	MET
3	A	861	SER
3	A	865	CYS
3	A	866	ILE
3	A	867	ASP
3	A	872	LEU
3	A	873	GLU
3	A	893	SER
3	A	932	TYR
3	A	938	VAL
3	A	960	LEU
3	A	962	SER
3	A	966	ILE
3	A	969	GLU
3	A	970	VAL
3	A	978	GLU
3	A	980	VAL
3	A	983	LEU
3	A	987	VAL
3	A	988	LEU
3	A	990	ILE
3	A	991	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	270	ASN
1	F	388	ASN
2	E	52	GLN
2	E	151	HIS
2	E	181	HIS
2	E	199	ASN
3	D	15	ASN
3	D	36	HIS
3	D	413	ASN
3	D	426	ASN
3	D	562	ASN

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Mol	Chain	Res	Type
3	D	585	GLN
3	D	657	GLN
3	D	720	ASN
3	D	762	GLN
3	D	786	ASN
3	D	937	ASN
3	D	985	ASN
1	C	270	ASN
2	B	52	GLN
2	B	151	HIS
2	B	181	HIS
3	A	15	ASN
3	A	36	HIS
3	A	274	ASN
3	A	413	ASN
3	A	426	ASN
3	A	562	ASN
3	A	576	ASN
3	A	585	GLN
3	A	657	GLN
3	A	786	ASN
3	A	937	ASN
3	A	985	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

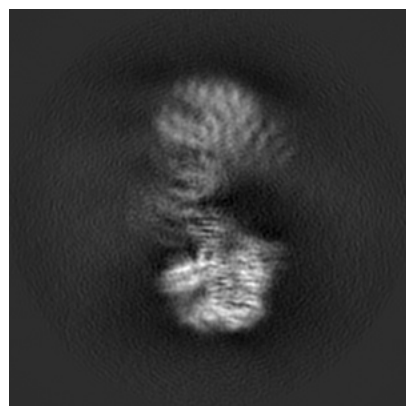
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34886. These allow visual inspection of the internal detail of the map and identification of artifacts.

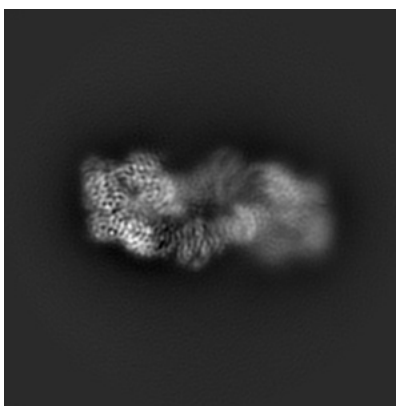
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

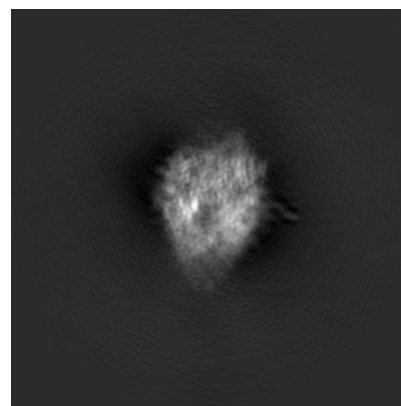
6.1.1 Primary map



X

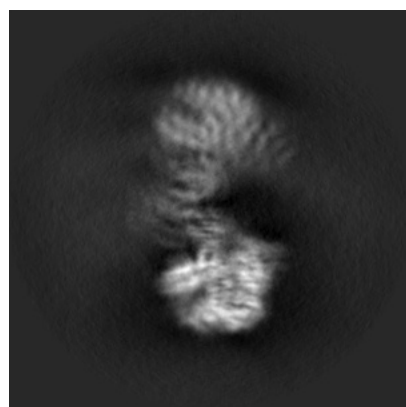


Y

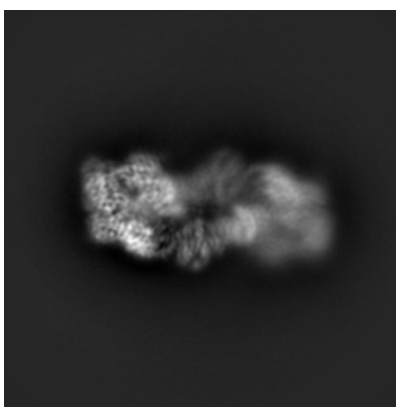


Z

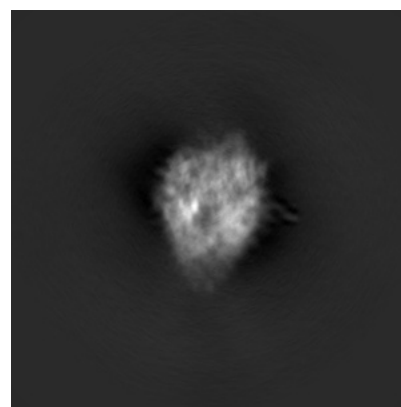
6.1.2 Raw map



X



Y

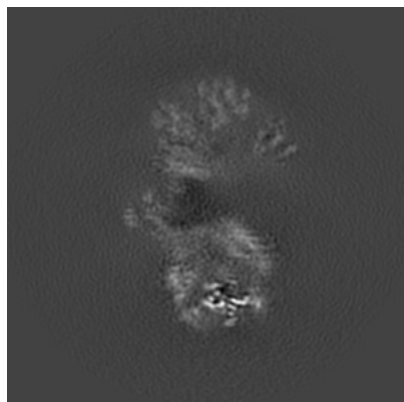


Z

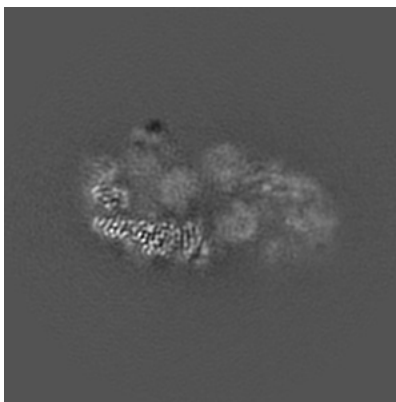
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

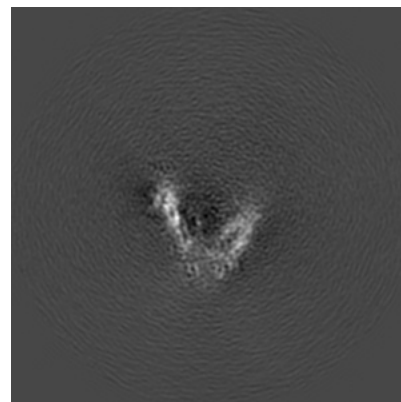
6.2.1 Primary map



X Index: 144

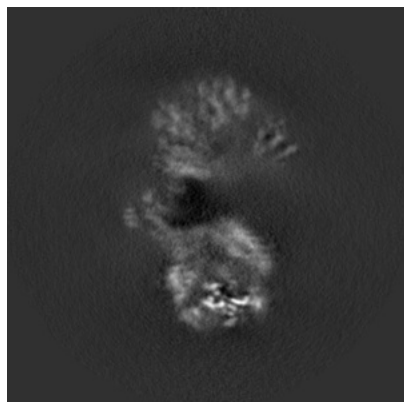


Y Index: 144

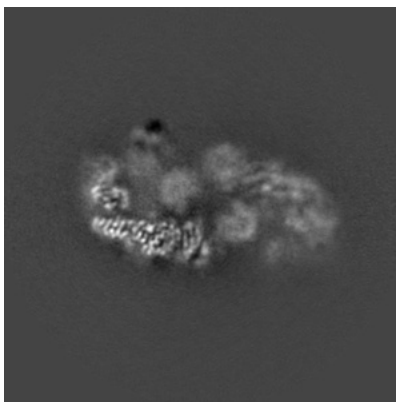


Z Index: 144

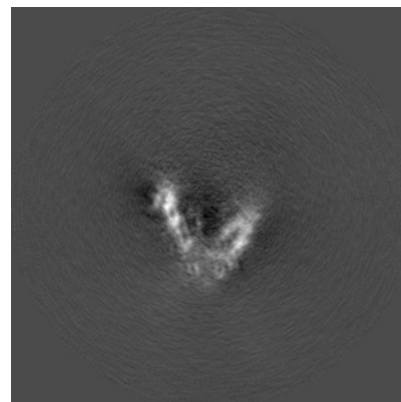
6.2.2 Raw map



X Index: 144



Y Index: 144

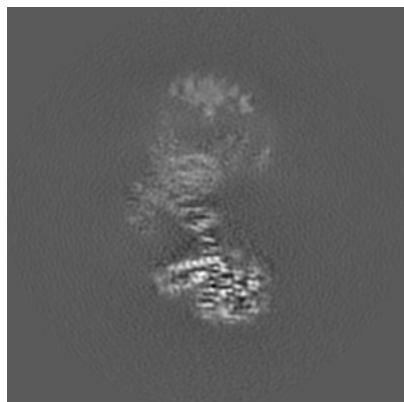


Z Index: 144

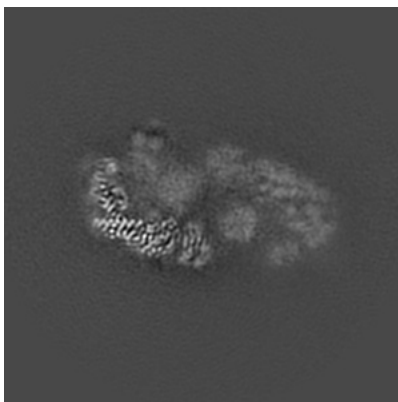
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

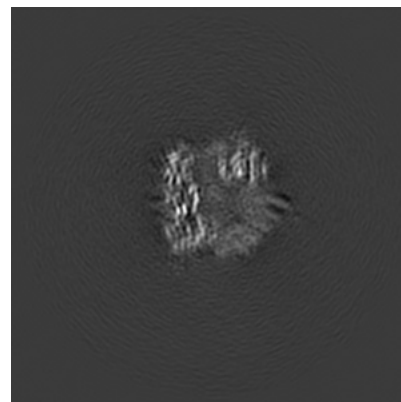
6.3.1 Primary map



X Index: 129

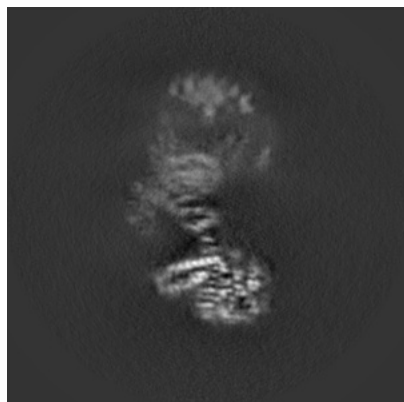


Y Index: 147

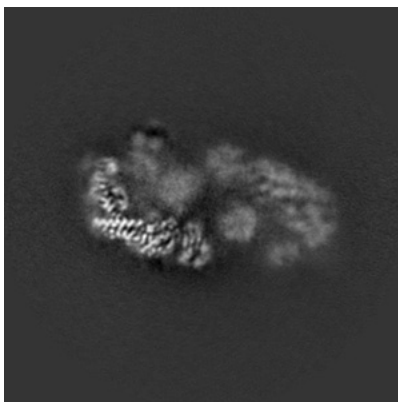


Z Index: 98

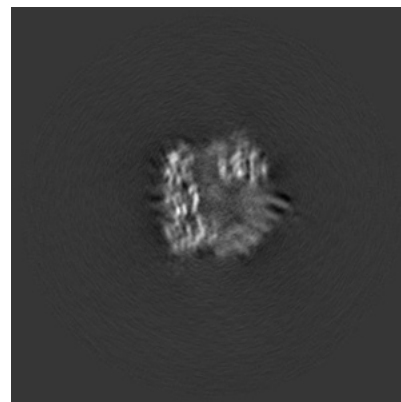
6.3.2 Raw map



X Index: 129



Y Index: 147

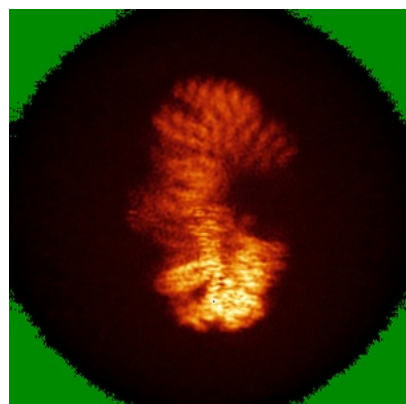


Z Index: 98

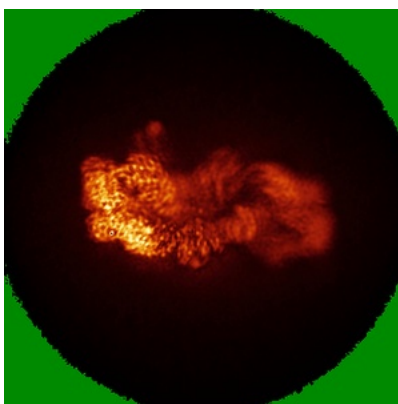
The images above show the largest variance slices of the map in three orthogonal directions.

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

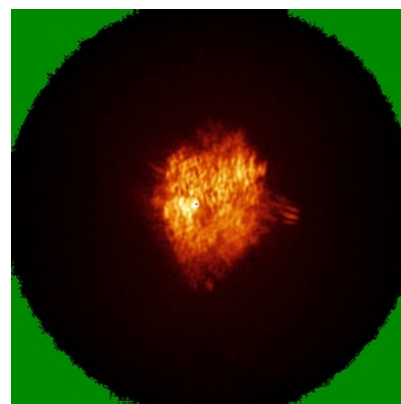
6.4.1 Primary map



X



Y

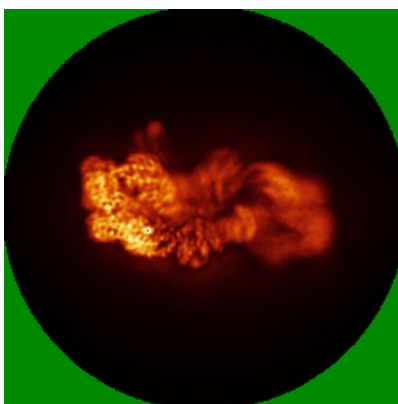


Z

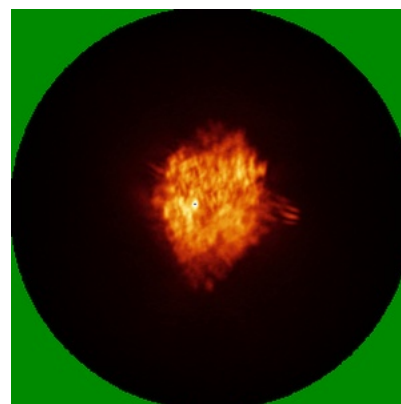
6.4.2 Raw map



X



Y

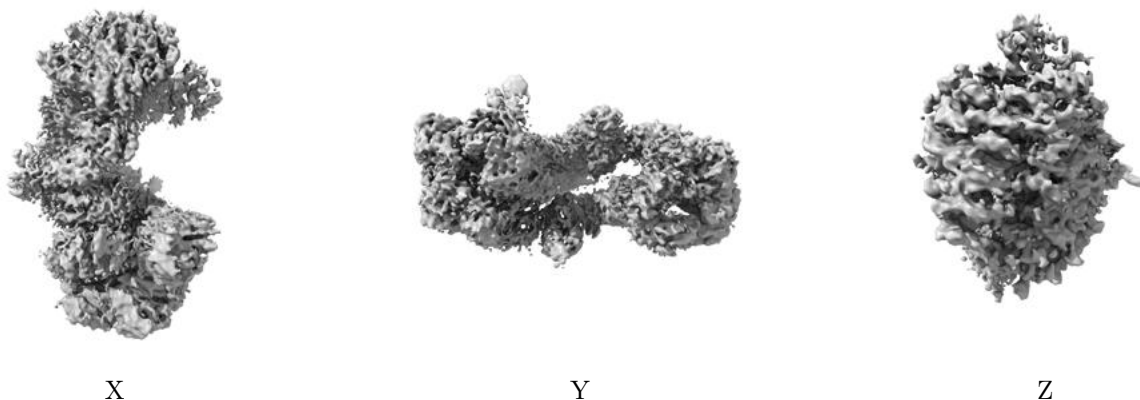


Z

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 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

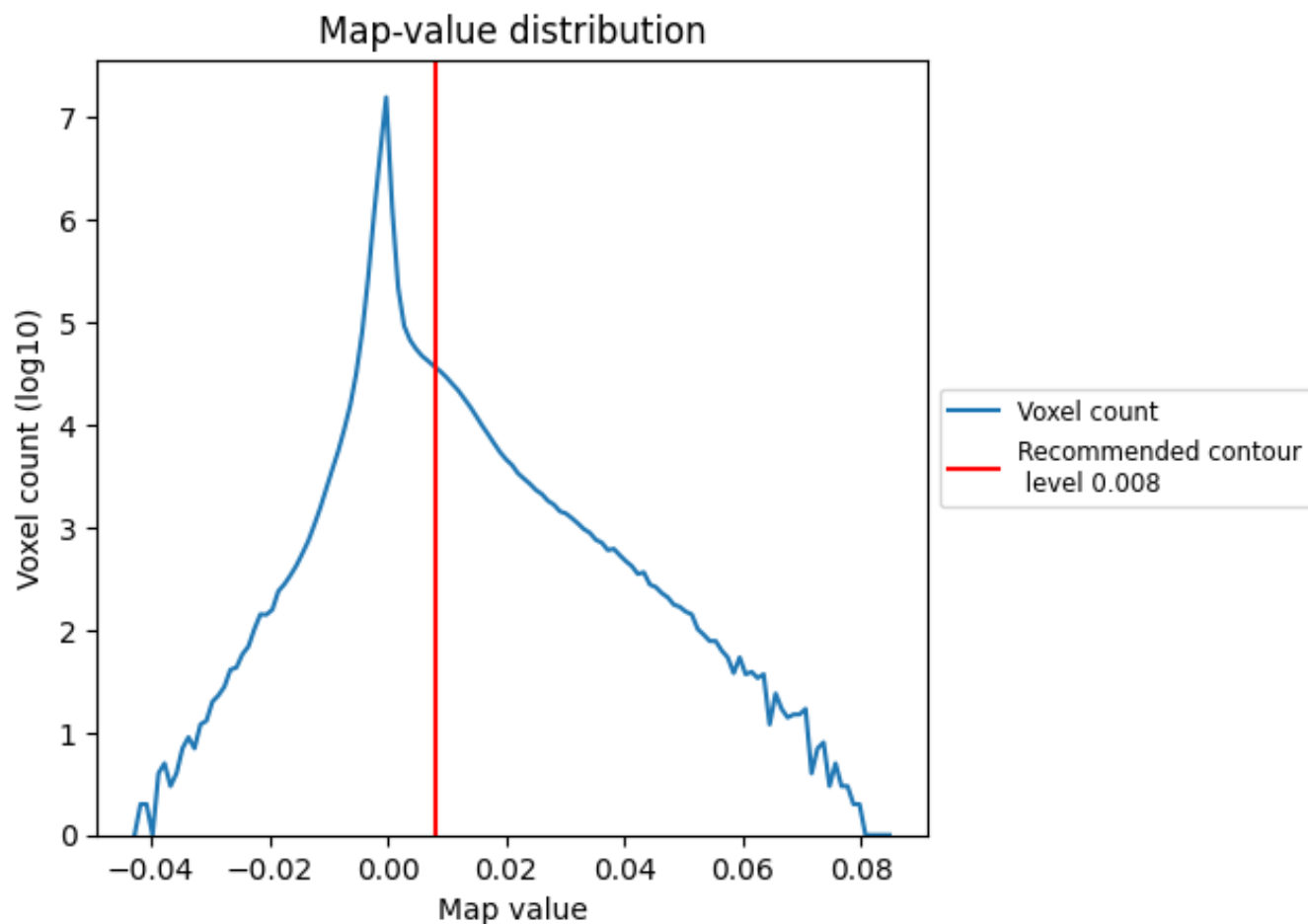
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

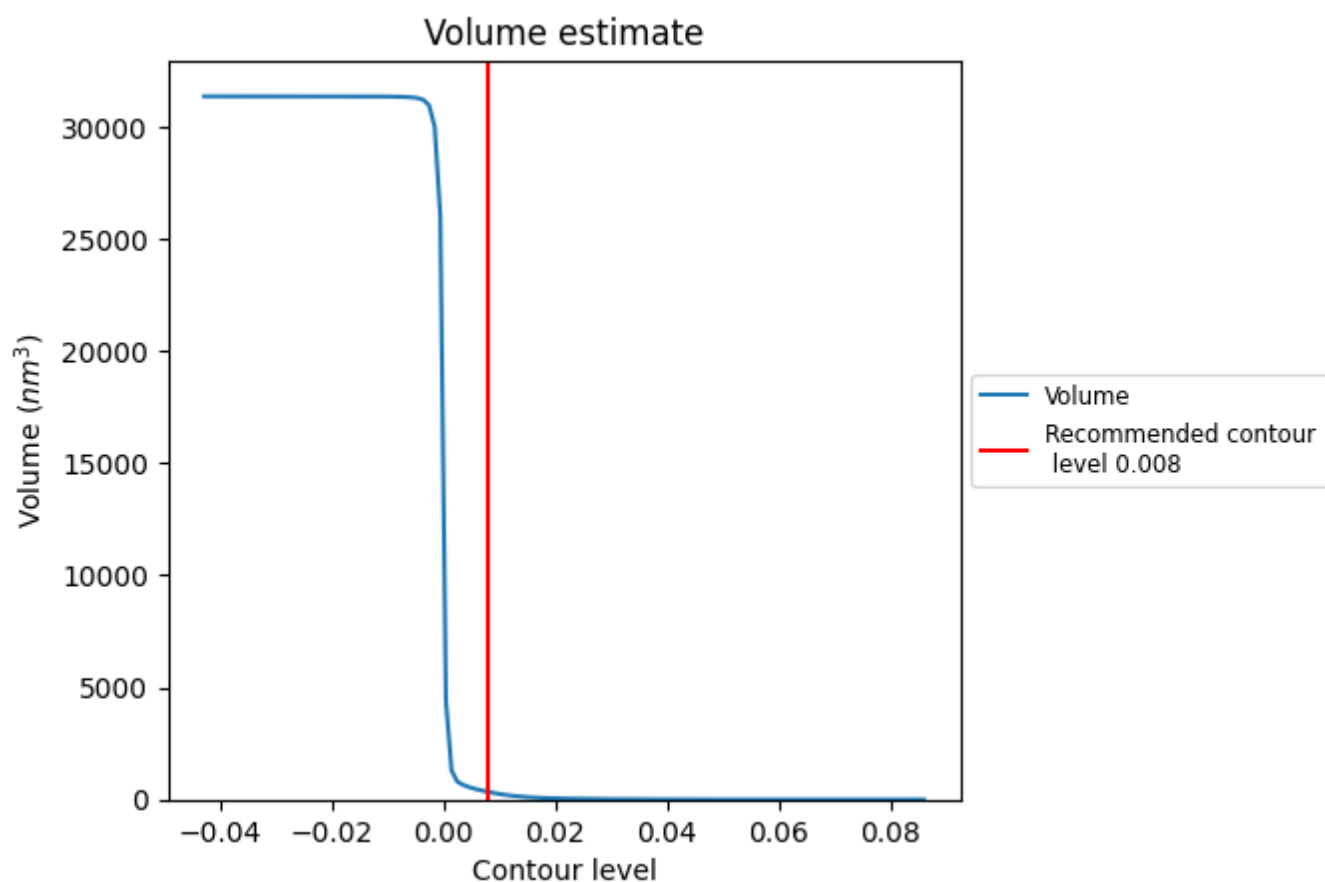
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

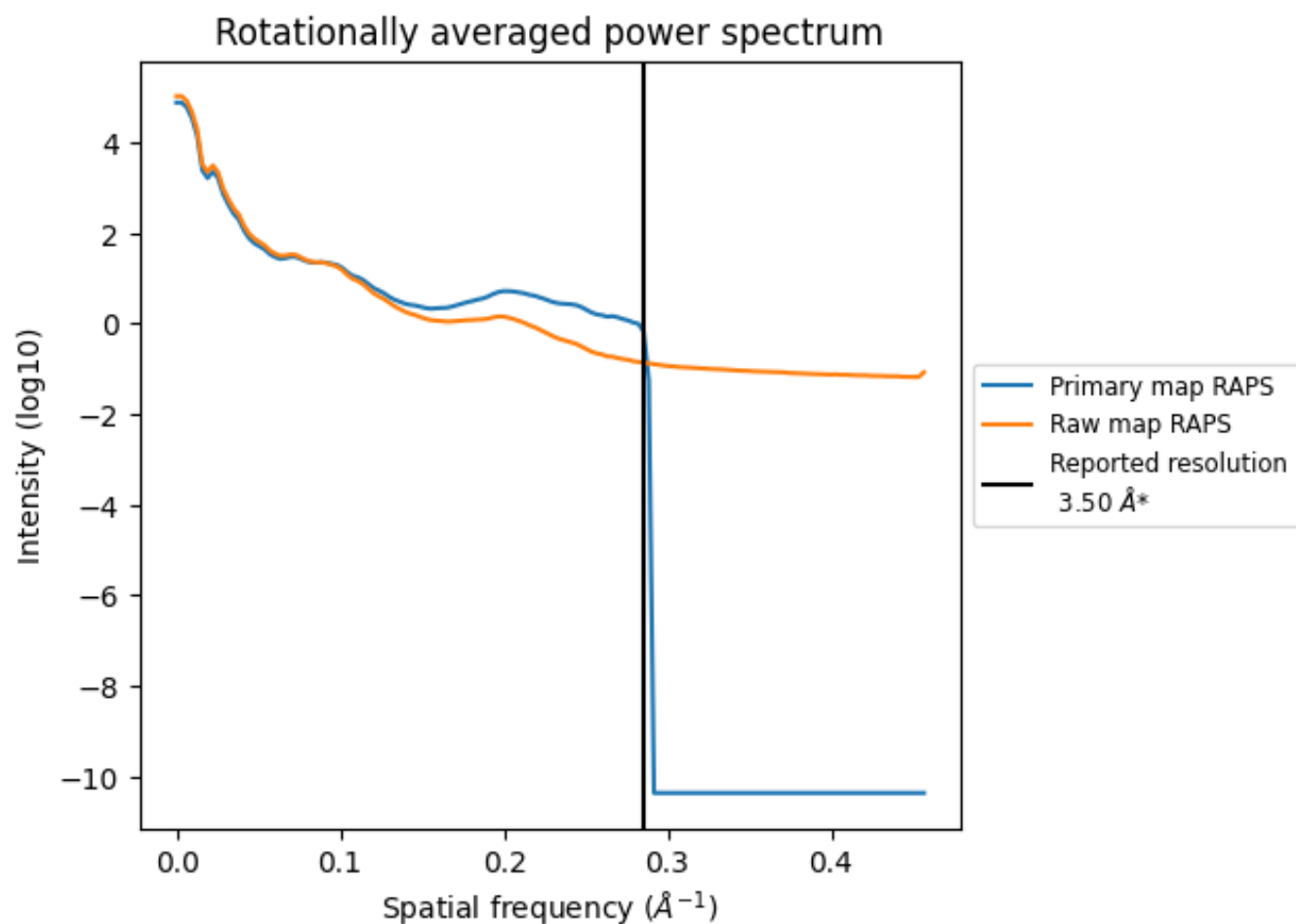
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 306 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

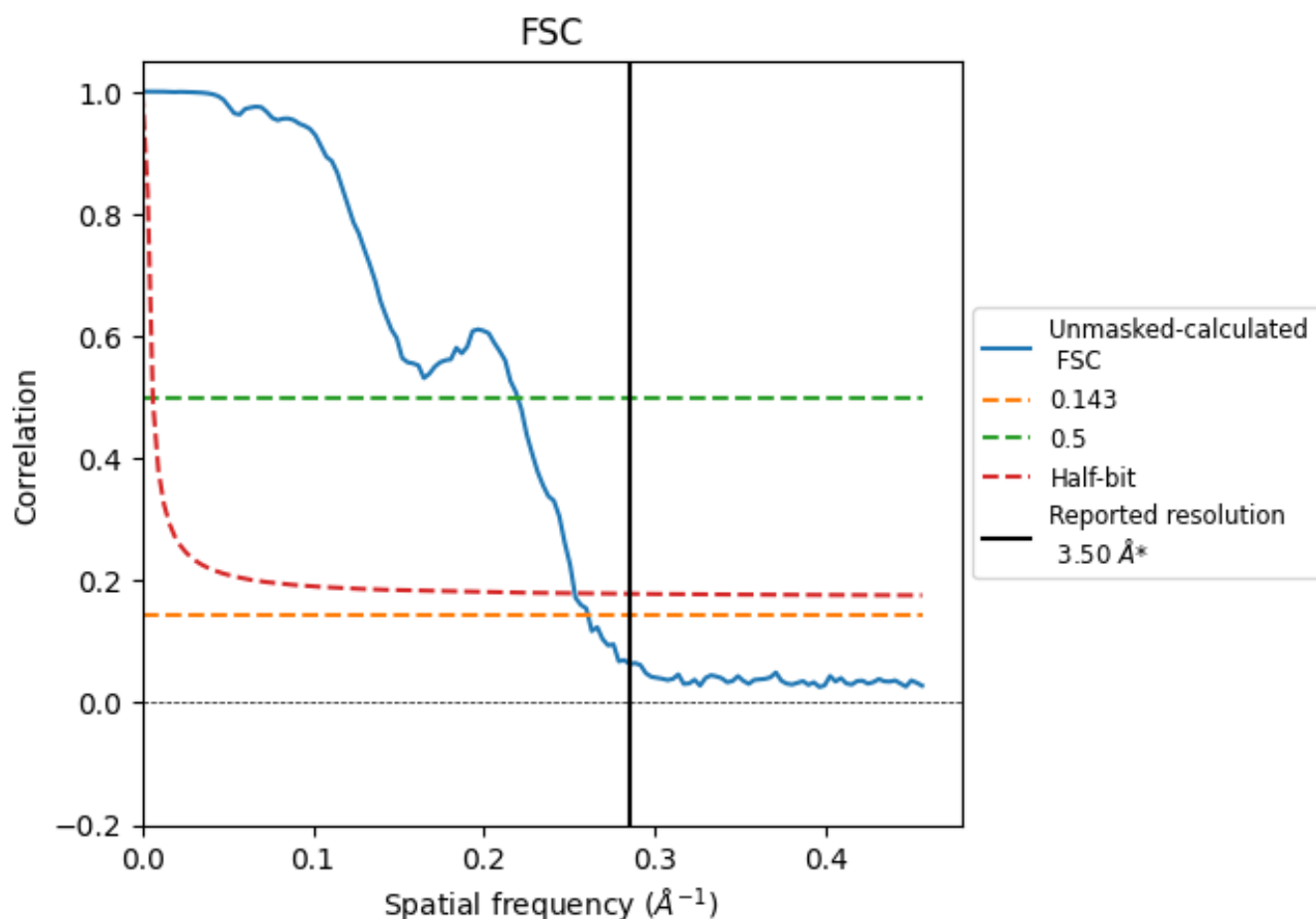


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	4.55	3.95

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

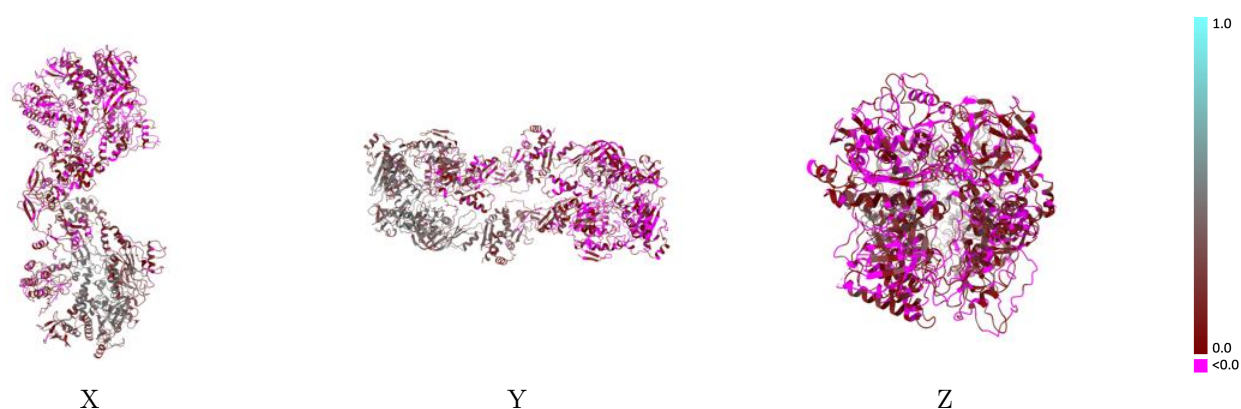
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-34886 and PDB model 8HLZ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

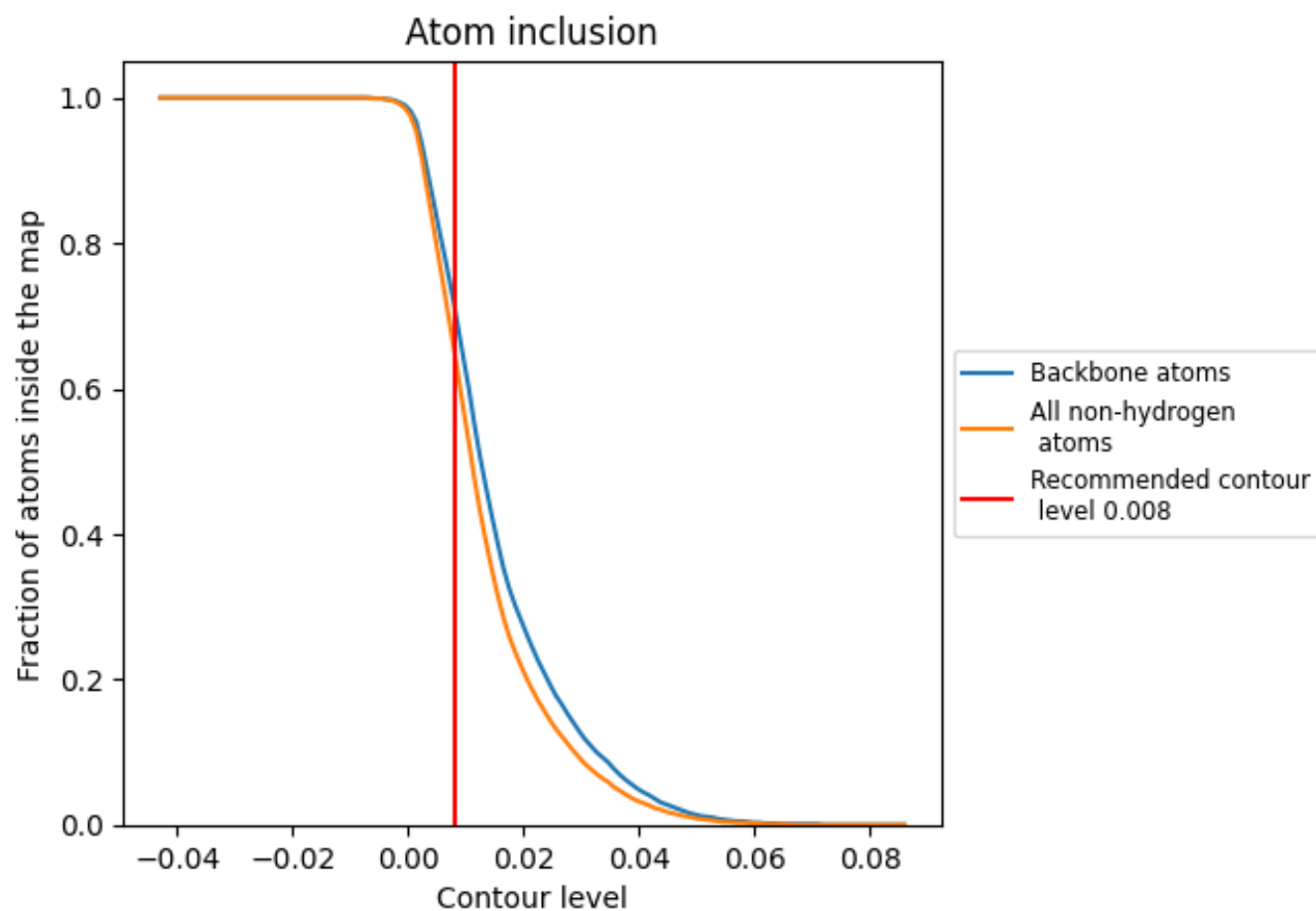


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 65% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6530	0.1650
A	0.4480	0.0340
B	0.2230	0.0160
C	0.7080	0.1090
D	0.8710	0.3220
E	0.9050	0.2750
F	0.6750	0.1810

1.0

0.0

<0.0