



Full wwPDB EM Validation Report ⓘ

Jul 8, 2024 – 10:28 AM EDT

PDB ID : 8GHN
EMDB ID : EMD-40037
Title : Composite model of the yeast Hir Complex with Asf1/H3/H4
Authors : Kim, H.J.; Murakami, K.
Deposited on : 2023-03-10
Resolution : 2.96 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

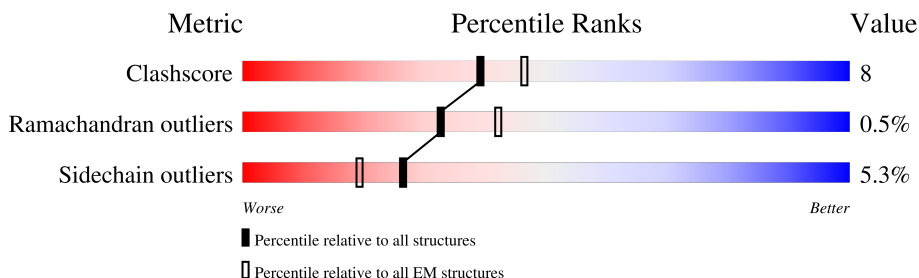
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

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




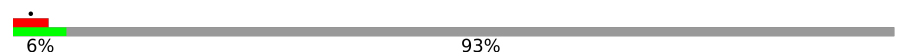

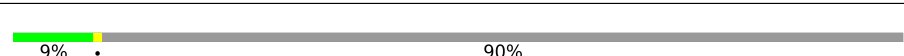

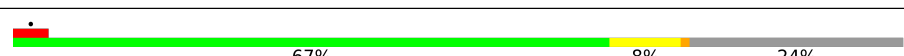
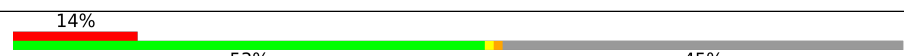
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	840	
1	G	840	
2	B	875	
2	C	875	
2	H	875	
2	I	875	
3	D	1648	
3	J	1648	

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Mol	Chain	Length	Quality of chain
4	E	625	 17% 80%
4	F	625	 6% 93%
4	K	625	 17% 80%
4	L	625	 9% 90%
5	M	136	 49% 47%
6	N	103	 67% 8% 24%
7	O	279	 14% 53% 45%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 59784 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 Protein HIR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	667	Total	C	N	O	S	0	0
			5272	3363	902	985	22		
1	G	651	Total	C	N	O	S	0	0
			5155	3289	880	964	22		

- Molecule 2 is a protein called Protein HIR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	800	Total	C	N	O	S	0	0
			6359	4053	1061	1214	31		
2	C	377	Total	C	N	O	S	0	0
			3022	1936	498	571	17		
2	H	800	Total	C	N	O	S	0	0
			6359	4053	1061	1214	31		
2	I	377	Total	C	N	O	S	0	0
			3022	1936	498	571	17		

- Molecule 3 is a protein called Histone transcription regulator 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1533	Total	C	N	O	S	0	0
			12616	8119	2086	2364	47		
3	J	1533	Total	C	N	O	S	0	0
			12617	8119	2086	2365	47		

- Molecule 4 is a protein called Histone promoter control protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	126	Total	C	N	O	S	0	0
			1012	651	162	198	1		
4	F	43	Total	C	N	O		0	0
			362	240	53	69			

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	126	Total	C	N	O	S	0	0
			1012	651	162	198	1		
4	L	64	Total	C	N	O		0	0
			540	356	76	108			

- Molecule 5 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	72	Total	C	N	O	0	0
			584	369	110	105		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	78	Total	C	N	O	0	0
			618	391	119	108		

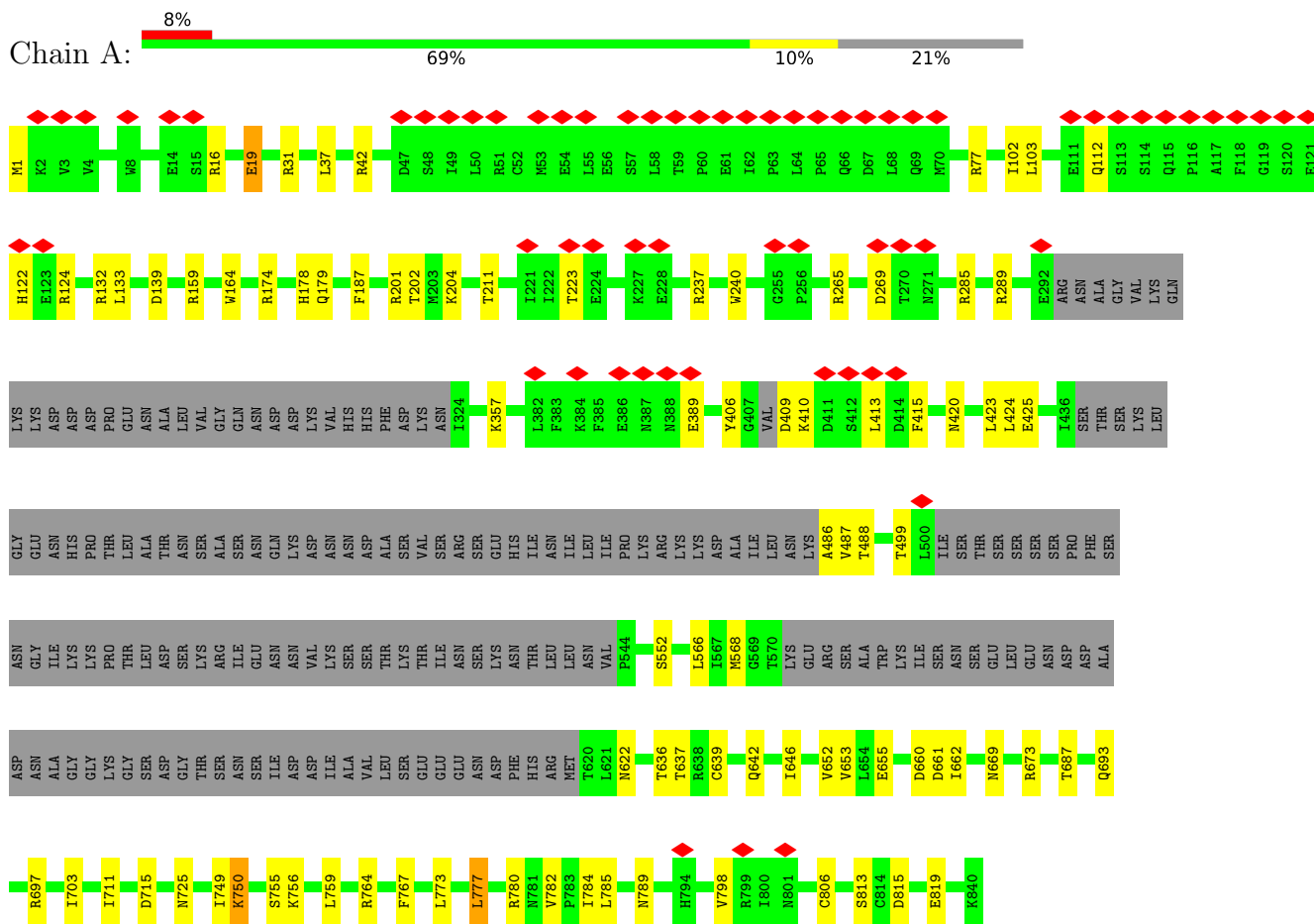
- Molecule 7 is a protein called Histone chaperone.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	154	Total	C	N	O	S	0	0
			1234	793	200	238	3		

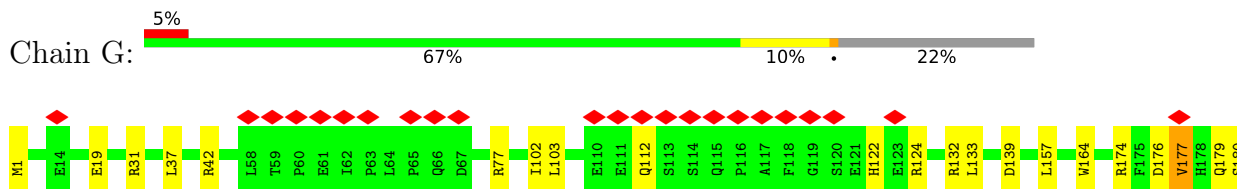
3 Residue-property plots

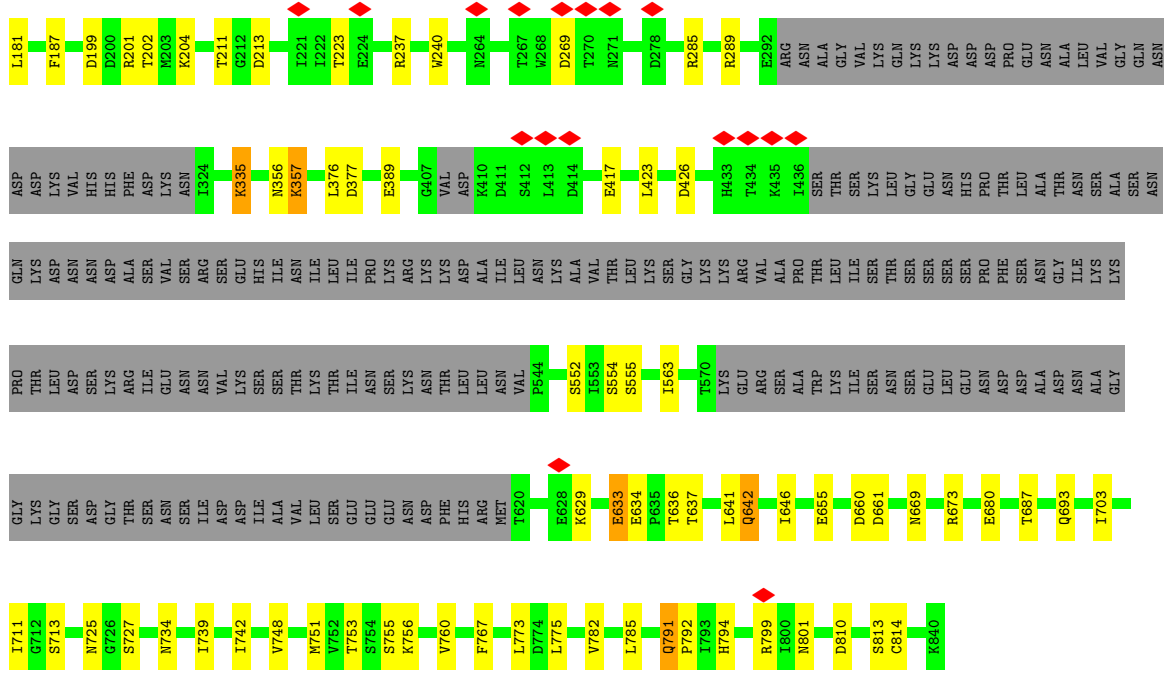
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Protein HIR1

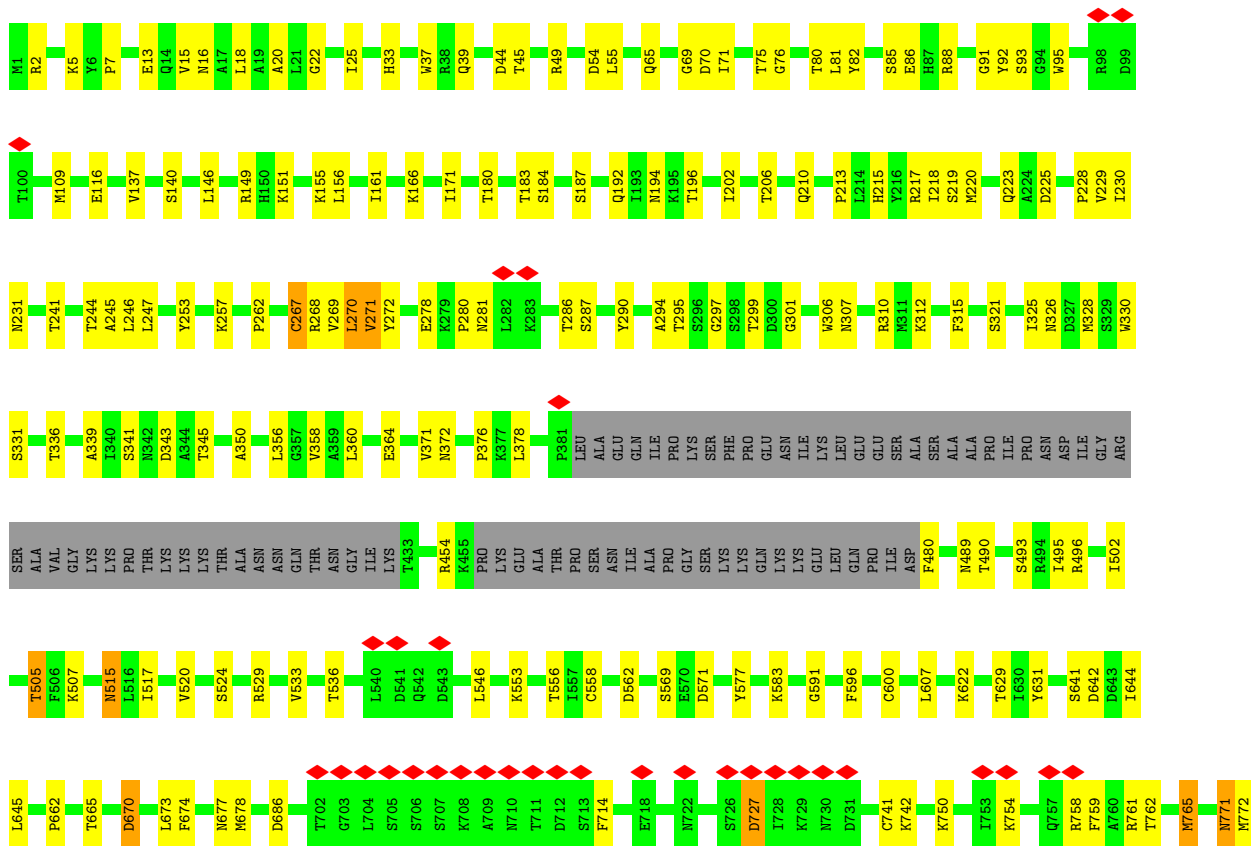


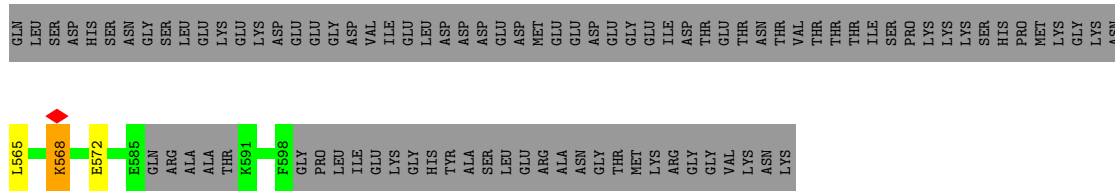
- Molecule 1: Protein HIR1



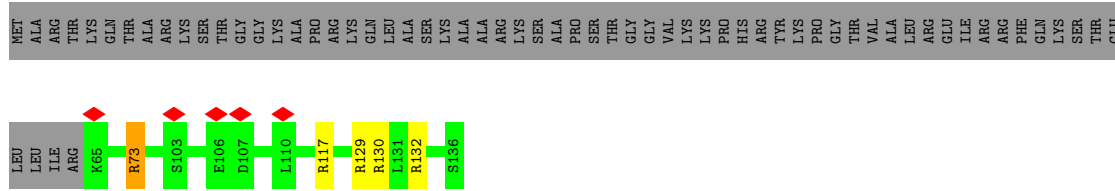


• Molecule 2: Protein HIR2

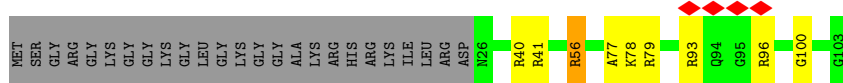




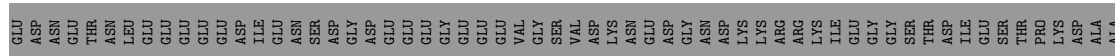
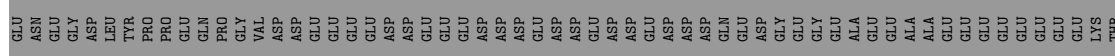
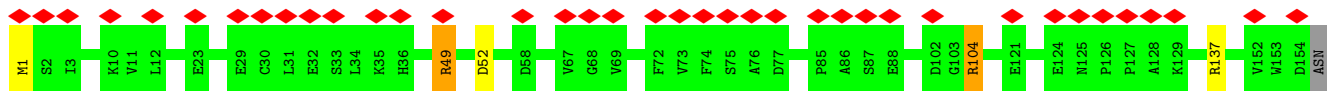
• Molecule 5: Histone H3



• Molecule 6: Histone H4



• Molecule 7: Histone chaperone



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	639629	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.190	Depositor
Minimum map value	0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	723.52, 754.8, 618.8	wwPDB
Map dimensions	532, 555, 455	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	A	0.55	0/5386	0.89	10/7300 (0.1%)
1	G	0.56	0/5269	0.89	11/7144 (0.2%)
2	B	0.30	0/6482	0.55	1/8786 (0.0%)
2	C	0.32	0/3080	0.67	7/4171 (0.2%)
2	H	0.30	0/6482	0.55	1/8786 (0.0%)
2	I	0.35	0/3080	0.72	9/4171 (0.2%)
3	D	0.32	0/12889	0.57	8/17409 (0.0%)
3	J	0.32	0/12890	0.56	8/17410 (0.0%)
4	E	0.27	0/1032	0.43	0/1397
4	F	0.76	0/370	0.92	2/500 (0.4%)
4	K	0.28	0/1032	0.43	0/1397
4	L	0.76	0/552	0.92	2/747 (0.3%)
5	M	0.71	0/590	1.12	6/789 (0.8%)
6	N	0.76	0/625	1.21	9/837 (1.1%)
7	O	0.67	0/1263	1.01	4/1722 (0.2%)
All	All	0.40	0/61022	0.67	78/82566 (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
2	C	0	2
2	I	0	1
3	D	0	4
3	J	0	4
4	F	0	1
4	L	0	1
5	M	0	1
6	N	0	2
7	O	0	2
All	All	0	18

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	174	ARG	NE-CZ-NH2	10.89	125.74	120.30
1	A	174	ARG	NE-CZ-NH2	10.85	125.73	120.30
3	D	814	LEU	CA-CB-CG	9.55	137.27	115.30
2	I	562	ASP	CB-CG-OD1	9.43	126.79	118.30
2	C	481	LEU	CA-CB-CG	9.20	136.47	115.30
6	N	41	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	G	642	GLN	CA-CB-CG	8.50	132.09	113.40
3	D	197	LEU	CA-CB-CG	8.29	134.37	115.30
3	D	255	ASP	CB-CG-OD1	8.18	125.66	118.30
2	C	540	LEU	CA-CB-CG	8.13	134.01	115.30
1	A	237	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	G	237	ARG	NE-CZ-NH2	8.06	124.33	120.30
2	I	764	LEU	CA-CB-CG	8.06	133.84	115.30
5	M	130	ARG	NE-CZ-NH2	7.71	124.16	120.30
2	C	541	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	413	LEU	CA-CB-CG	7.65	132.89	115.30
6	N	40	ARG	NE-CZ-NH1	-7.63	116.48	120.30
1	G	791	GLN	CA-CB-CG	7.53	129.97	113.40
3	J	755	LEU	CA-CB-CG	7.45	132.44	115.30
2	I	871	MET	CG-SD-CE	7.42	112.06	100.20
2	I	871	MET	CA-CB-CG	7.32	125.75	113.30
7	O	137	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	289	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	G	289	ARG	NE-CZ-NH2	7.22	123.91	120.30
5	M	73	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	77	ARG	NE-CZ-NH2	7.02	123.81	120.30
6	N	79	ARG	NE-CZ-NH2	7.00	123.80	120.30
5	M	132	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	G	77	ARG	NE-CZ-NH2	6.97	123.78	120.30
2	I	485	LEU	CA-CB-CG	6.85	131.05	115.30
7	O	49	ARG	NE-CZ-NH1	-6.80	116.90	120.30
6	N	40	ARG	NE-CZ-NH2	6.79	123.70	120.30
3	J	755	LEU	CB-CG-CD1	-6.76	99.50	111.00
2	I	860	VAL	CG1-CB-CG2	-6.76	100.09	110.90
1	A	124	ARG	NE-CZ-NH2	6.71	123.66	120.30
6	N	56	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	G	124	ARG	NE-CZ-NH2	6.70	123.65	120.30
7	O	104	ARG	NE-CZ-NH2	6.68	123.64	120.30
2	I	540	LEU	CA-CB-CG	6.66	130.61	115.30
3	J	814	LEU	CA-CB-CG	6.50	130.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	129	ARG	NE-CZ-NH2	6.48	123.54	120.30
3	D	814	LEU	CB-CG-CD2	6.32	121.75	111.00
6	N	96	ARG	NE-CZ-NH2	6.22	123.41	120.30
5	M	117	ARG	NE-CZ-NH2	6.17	123.39	120.30
3	J	783	MET	CA-CB-CG	6.14	123.74	113.30
2	I	653	LEU	CA-CB-CG	6.11	129.34	115.30
1	G	42	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	42	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	285	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	285	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	201	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	G	201	ARG	NE-CZ-NH2	5.81	123.21	120.30
3	D	775	ILE	CG1-CB-CG2	-5.69	98.88	111.40
2	B	772	MET	CA-CB-CG	5.67	122.94	113.30
2	C	814	MET	CB-CG-SD	5.67	129.40	112.40
1	G	31	ARG	NE-CZ-NH2	5.67	123.13	120.30
3	J	803	MET	CA-CB-CG	5.66	122.92	113.30
4	L	466	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	31	ARG	NE-CZ-NH2	5.62	123.11	120.30
7	O	49	ARG	NE-CZ-NH2	5.60	123.10	120.30
2	H	767	GLU	CA-CB-CG	5.58	125.69	113.40
3	J	934	PHE	N-CA-CB	5.56	120.61	110.60
3	J	446	ASP	C-N-CA	5.56	135.59	121.70
2	I	476	GLN	CA-CB-CG	5.54	125.59	113.40
2	C	764	LEU	CA-CB-CG	5.54	128.04	115.30
4	F	466	TYR	CB-CG-CD2	-5.54	117.68	121.00
6	N	56	ARG	NH1-CZ-NH2	-5.53	113.31	119.40
2	C	756	LEU	CA-CB-CG	5.47	127.89	115.30
2	C	487	LEU	CA-CB-CG	5.41	127.73	115.30
3	D	239	MET	CB-CG-SD	5.34	128.43	112.40
4	L	466	TYR	CB-CG-CD1	5.33	124.20	121.00
4	F	466	TYR	CB-CG-CD1	5.26	124.16	121.00
3	D	759	LEU	CA-CB-CG	5.25	127.37	115.30
5	M	73	ARG	NE-CZ-NH1	-5.25	117.68	120.30
6	N	93	ARG	NE-CZ-NH2	5.24	122.92	120.30
3	D	446	ASP	C-N-CA	5.20	134.70	121.70
3	J	69	MET	CA-CB-CG	5.15	122.06	113.30
6	N	56	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	476	GLN	Peptide
2	C	636	PRO	Peptide
3	D	10	ASN	Peptide
3	D	444	GLN	Peptide
3	D	445	ASN	Peptide
3	D	901	ARG	Sidechain
4	F	466	TYR	Sidechain
2	I	477	PRO	Peptide
3	J	444	GLN	Peptide
3	J	587	ARG	Peptide
3	J	826	ARG	Sidechain
3	J	901	ARG	Sidechain
4	L	466	TYR	Sidechain
5	M	73	ARG	Sidechain
6	N	100	GLY	Peptide
6	N	56	ARG	Sidechain
7	O	104	ARG	Sidechain
7	O	49	ARG	Sidechain

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	A	5272	0	5314	80	0
1	G	5155	0	5180	54	0
2	B	6359	0	6419	111	0
2	C	3022	0	3048	42	0
2	H	6359	0	6419	109	0
2	I	3022	0	3048	29	0
3	D	12616	0	12567	273	0
3	J	12617	0	12567	273	0
4	E	1012	0	1019	13	0
4	F	362	0	345	3	0
4	K	1012	0	1019	15	0
4	L	540	0	504	5	0
5	M	584	0	614	0	0
6	N	618	0	660	23	0
7	O	1234	0	1219	0	0
All	All	59784	0	59942	932	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 8.

All (932) 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:10:ASN:CA	3:D:11:ILE:HG22	1.26	1.61
3:D:1634:LYS:HD3	6:N:78:LYS:CB	1.29	1.61
3:D:10:ASN:CB	3:D:11:ILE:HG22	1.27	1.59
3:D:10:ASN:HB3	3:D:11:ILE:CG2	1.22	1.57
3:D:379:VAL:HG21	3:D:923:HIS:CD2	1.45	1.48
3:D:1634:LYS:CD	6:N:78:LYS:CB	1.87	1.48
3:D:10:ASN:CB	3:D:11:ILE:CG2	1.80	1.45
1:A:16:ARG:CG	1:A:488:THR:HG22	1.45	1.44
3:D:1634:LYS:CD	6:N:78:LYS:HB3	1.50	1.35
1:A:16:ARG:CD	1:A:488:THR:HG21	1.55	1.34
3:D:1634:LYS:CD	6:N:78:LYS:HB2	1.53	1.32
1:G:213:ASP:OD2	2:H:714:PHE:CZ	1.83	1.31
1:A:16:ARG:NE	1:A:488:THR:CG2	1.93	1.31
1:A:16:ARG:HG3	1:A:488:THR:CG2	1.63	1.29
1:A:16:ARG:CD	1:A:488:THR:CG2	2.10	1.28
3:D:884:ILE:CG2	3:D:930:SER:HB3	1.63	1.27
1:A:406:TYR:CD1	1:A:409:ASP:OD1	1.92	1.23
1:A:16:ARG:CG	1:A:488:THR:CG2	2.17	1.16
1:A:16:ARG:NE	1:A:488:THR:HG21	1.57	1.16
3:D:1634:LYS:HD2	6:N:78:LYS:HB2	1.16	1.13
3:D:902:THR:HB	3:D:905:GLU:HB2	1.28	1.12
3:D:10:ASN:HA	3:D:11:ILE:HG22	1.19	1.11
1:A:16:ARG:HE	1:A:488:THR:CG2	1.56	1.10
3:D:818:LEU:HB3	3:D:889:LEU:HD11	1.32	1.09
3:J:891:LEU:HD21	3:J:914:ILE:HD11	1.13	1.09
1:A:265:ARG:NH1	1:A:409:ASP:OD2	1.86	1.08
1:A:16:ARG:HD2	1:A:488:THR:HG21	1.35	1.08
1:A:179:GLN:O	2:B:765:MET:HB2	1.51	1.08
3:D:379:VAL:HG21	3:D:923:HIS:NE2	1.70	1.07
3:J:891:LEU:CD2	3:J:914:ILE:HD11	1.83	1.06
1:G:213:ASP:CG	2:H:714:PHE:CZ	2.27	1.05
1:A:16:ARG:HE	1:A:488:THR:HG23	0.94	1.05
3:D:1634:LYS:HB2	6:N:78:LYS:HD3	1.39	1.05
1:A:406:TYR:HD1	1:A:409:ASP:CG	1.59	1.04
3:D:379:VAL:CG2	3:D:923:HIS:CD2	2.42	1.03
3:D:884:ILE:HG22	3:D:930:SER:HB3	1.31	1.03
1:G:213:ASP:OD2	2:H:714:PHE:CE1	2.12	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TYR:CD1	1:A:409:ASP:CG	2.30	1.02
3:D:10:ASN:CA	3:D:11:ILE:CG2	2.23	1.00
1:A:265:ARG:NE	1:A:409:ASP:OD1	1.96	0.98
1:A:16:ARG:NE	1:A:488:THR:HG23	1.68	0.97
3:J:891:LEU:HD11	3:J:910:THR:HG23	1.48	0.94
3:D:884:ILE:HG22	3:D:930:SER:CB	1.98	0.93
3:D:1634:LYS:HD2	6:N:78:LYS:CB	1.76	0.93
3:J:826:ARG:HB3	3:J:828:GLU:HG2	1.50	0.93
3:J:380:HIS:HE1	3:J:920:LEU:HD11	1.34	0.92
1:A:265:ARG:HE	1:A:409:ASP:CG	1.71	0.92
3:J:827:TRP:HB3	3:J:940:LYS:HG2	1.53	0.91
3:D:1634:LYS:CB	6:N:78:LYS:HD3	2.01	0.90
3:J:891:LEU:HD21	3:J:914:ILE:CD1	2.00	0.90
3:D:880:LYS:HB3	3:D:929:ALA:HB2	1.51	0.90
1:A:406:TYR:CE1	1:A:409:ASP:OD1	2.26	0.89
3:D:10:ASN:CB	3:D:11:ILE:HG23	1.70	0.89
1:A:159:ARG:CZ	2:B:765:MET:HG3	2.02	0.88
3:D:10:ASN:CG	3:D:11:ILE:CG2	2.41	0.88
1:A:159:ARG:NE	2:B:765:MET:HG2	1.88	0.87
3:D:822:LEU:HB3	3:D:827:TRP:CE3	2.10	0.86
3:D:10:ASN:ND2	3:D:11:ILE:CG2	2.39	0.86
1:G:213:ASP:CG	2:H:714:PHE:HZ	1.78	0.85
3:D:10:ASN:ND2	3:D:11:ILE:HG21	1.92	0.85
3:D:386:GLU:OE1	3:D:916:SER:HB3	1.77	0.84
3:J:376:VAL:CG1	3:J:923:HIS:NE2	2.40	0.84
1:G:213:ASP:OD1	2:H:714:PHE:HZ	1.59	0.84
1:A:179:GLN:O	2:B:765:MET:CB	2.25	0.84
1:A:159:ARG:CZ	2:B:765:MET:CG	2.57	0.83
3:D:880:LYS:C	3:D:929:ALA:HB1	1.99	0.83
3:D:884:ILE:CG2	3:D:930:SER:CB	2.54	0.82
3:D:884:ILE:HG21	3:D:930:SER:HB3	1.61	0.82
3:J:380:HIS:CE1	3:J:920:LEU:HD11	2.14	0.82
3:D:881:ASP:OD1	3:D:929:ALA:HA	1.78	0.81
3:J:826:ARG:HB3	3:J:828:GLU:CG	2.11	0.81
3:D:10:ASN:HB3	3:D:11:ILE:HG23	0.82	0.81
3:D:10:ASN:HD22	3:D:11:ILE:CG2	1.94	0.81
3:J:849:PHE:CZ	3:J:882:ILE:HG21	2.16	0.81
1:A:159:ARG:NH2	2:B:765:MET:HG3	1.96	0.80
1:G:213:ASP:OD1	2:H:714:PHE:CZ	2.33	0.80
3:D:10:ASN:HA	3:D:11:ILE:CG2	2.01	0.80
3:J:888:THR:HG23	3:J:937:LEU:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1634:LYS:HB2	6:N:78:LYS:CD	2.11	0.79
3:J:910:THR:HG21	3:J:945:PHE:HE2	1.45	0.79
3:J:880:LYS:HB3	3:J:926:PHE:HD1	1.46	0.79
3:J:376:VAL:HG12	3:J:923:HIS:NE2	1.96	0.79
1:A:406:TYR:HB3	1:A:409:ASP:OD2	1.82	0.79
3:J:898:ALA:HB1	3:J:906:GLN:HA	1.64	0.79
3:D:881:ASP:N	3:D:929:ALA:HB1	1.98	0.78
3:D:10:ASN:HD22	3:D:11:ILE:HG21	1.46	0.78
3:J:891:LEU:HG	3:J:941:LEU:HD12	1.67	0.77
3:D:881:ASP:CG	3:D:930:SER:H	1.87	0.77
3:J:812:GLY:HA3	3:J:882:ILE:HG23	1.65	0.76
3:J:891:LEU:CD2	3:J:914:ILE:CD1	2.62	0.76
3:D:379:VAL:HG21	3:D:923:HIS:HD2	1.41	0.75
3:D:880:LYS:HB3	3:D:929:ALA:CB	2.17	0.74
3:D:884:ILE:HG21	3:D:929:ALA:O	1.87	0.74
3:D:379:VAL:HG12	3:D:920:LEU:HD13	1.70	0.74
1:G:356:ASN:C	4:L:565:LEU:HD13	2.08	0.74
1:A:265:ARG:NE	1:A:409:ASP:CG	2.38	0.73
3:D:379:VAL:CG2	3:D:923:HIS:NE2	2.48	0.73
3:J:902:THR:HB	3:J:905:GLU:HB2	1.69	0.73
3:J:879:MET:HG3	3:J:880:LYS:N	2.03	0.73
3:J:380:HIS:HE1	3:J:920:LEU:CD1	2.02	0.73
3:J:850:TYR:OH	3:J:920:LEU:HD22	1.89	0.72
3:D:383:PHE:HE2	3:D:917:LEU:CD2	2.01	0.72
3:D:902:THR:O	3:D:906:GLN:N	2.23	0.72
3:D:1634:LYS:HZ3	6:N:78:LYS:C	1.92	0.71
3:J:880:LYS:HB2	3:J:929:ALA:HB3	1.70	0.71
2:B:215:HIS:H	2:B:268:ARG:HH21	1.37	0.71
1:A:357:LYS:HZ3	1:A:487:VAL:CG2	2.04	0.71
3:J:826:ARG:O	3:J:828:GLU:HG2	1.91	0.70
1:A:265:ARG:CZ	1:A:409:ASP:OD2	2.39	0.70
3:J:891:LEU:HD22	3:J:914:ILE:HG12	1.74	0.70
3:D:881:ASP:OD1	3:D:929:ALA:CA	2.39	0.70
3:D:884:ILE:CB	3:D:930:SER:HB3	2.21	0.70
3:D:10:ASN:C	3:D:11:ILE:HG22	2.11	0.69
3:J:10:ASN:C	3:J:12:GLU:H	1.94	0.69
2:H:215:HIS:H	2:H:268:ARG:HH21	1.37	0.69
1:A:357:LYS:NZ	1:A:487:VAL:CG2	2.55	0.69
3:J:390:LEU:HD22	3:J:909:GLU:HB3	1.73	0.69
3:D:23:ARG:HH22	3:D:72:ASN:HD21	1.41	0.69
3:J:880:LYS:HB2	3:J:929:ALA:CB	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:881:ASP:O	3:D:930:SER:HB2	1.93	0.68
3:D:1634:LYS:HD3	6:N:78:LYS:HB3	0.69	0.68
3:J:891:LEU:HD22	3:J:914:ILE:CG1	2.22	0.68
3:J:892:TYR:HB2	3:J:937:LEU:HD11	1.75	0.68
1:A:159:ARG:CD	2:B:765:MET:HG2	2.24	0.68
3:D:881:ASP:OD1	3:D:930:SER:N	2.25	0.68
3:J:898:ALA:O	3:J:906:GLN:HB2	1.94	0.68
3:J:744:ILE:HG12	3:J:755:LEU:HD11	1.76	0.67
3:D:914:ILE:O	3:D:918:HIS:HB2	1.94	0.67
3:J:849:PHE:HB3	3:J:883:MET:SD	2.35	0.67
3:J:888:THR:CG2	3:J:937:LEU:HB3	2.24	0.67
3:D:697:ILE:HG13	3:D:715:HIS:HE1	1.60	0.67
3:J:910:THR:HG21	3:J:945:PHE:CE2	2.28	0.67
1:G:176:ASP:HB2	2:H:761:ARG:NH1	2.10	0.66
3:D:914:ILE:HG12	3:D:938:ALA:HB1	1.76	0.66
3:J:868:PHE:HE2	3:J:879:MET:HG2	1.61	0.66
3:D:1634:LYS:NZ	6:N:77:ALA:O	2.27	0.66
3:J:898:ALA:C	3:J:906:GLN:HB2	2.16	0.66
1:A:357:LYS:NZ	1:A:487:VAL:HG21	2.11	0.65
3:J:383:PHE:CD2	3:J:916:SER:HB3	2.32	0.65
3:J:880:LYS:HB3	3:J:926:PHE:CD1	2.30	0.64
3:J:1452:LYS:O	3:J:1456:TYR:HB2	1.97	0.64
3:D:827:TRP:CG	3:D:937:LEU:HD13	2.32	0.64
3:J:825:ASN:O	3:J:826:ARG:HB2	1.98	0.64
3:J:879:MET:HG3	3:J:880:LYS:H	1.63	0.64
3:J:1189:ASP:OD1	3:J:1189:ASP:N	2.31	0.64
2:B:71:ILE:HA	2:B:85:SER:HA	1.80	0.64
1:A:669:ASN:HA	1:A:687:THR:HG22	1.79	0.63
3:D:1634:LYS:CE	6:N:78:LYS:O	2.45	0.63
2:H:71:ILE:HA	2:H:85:SER:HA	1.80	0.63
2:C:866:ARG:HA	2:C:869:LYS:HE2	1.80	0.63
1:G:179:GLN:HB2	2:H:765:MET:CB	2.28	0.63
3:D:1452:LYS:O	3:D:1456:TYR:HB2	1.97	0.63
1:G:552:SER:HB3	2:H:600:CYS:HB2	1.81	0.63
1:A:16:ARG:HG3	1:A:488:THR:HG22	0.68	0.63
3:D:1189:ASP:OD1	3:D:1189:ASP:N	2.31	0.63
3:J:850:TYR:OH	3:J:920:LEU:CD2	2.47	0.63
3:J:380:HIS:CE1	3:J:920:LEU:CD1	2.79	0.63
3:D:376:VAL:HB	3:D:924:PHE:CZ	2.34	0.62
3:D:960:CYS:HG	3:D:976:HIS:HE2	1.46	0.62
3:D:1634:LYS:NZ	6:N:78:LYS:C	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:956:GLN:NE2	3:J:960:CYS:SG	2.71	0.62
3:D:880:LYS:C	3:D:929:ALA:CB	2.67	0.62
3:D:1182:LYS:NZ	3:D:1189:ASP:OD2	2.31	0.62
3:J:888:THR:HA	3:J:937:LEU:HD22	1.81	0.62
3:D:1281:SER:O	3:D:1285:ASN:ND2	2.33	0.62
3:J:1281:SER:O	3:J:1285:ASN:ND2	2.33	0.61
3:J:202:ILE:HA	3:J:205:ARG:HB3	1.82	0.61
3:J:376:VAL:HG12	3:J:923:HIS:CE1	2.35	0.61
2:I:477:PRO:HD2	2:I:478:ILE:HD12	1.82	0.61
3:J:850:TYR:CZ	3:J:920:LEU:HD21	2.36	0.61
3:J:1182:LYS:NZ	3:J:1189:ASP:OD2	2.31	0.61
3:J:1539:GLN:O	3:J:1543:VAL:HB	2.01	0.61
3:D:881:ASP:HA	3:D:930:SER:N	2.16	0.61
3:J:891:LEU:HD13	3:J:914:ILE:HG13	1.83	0.60
1:A:159:ARG:CZ	2:B:765:MET:HG2	2.27	0.60
3:D:1539:GLN:O	3:D:1543:VAL:HB	2.01	0.60
3:D:902:THR:CB	3:D:905:GLU:HB2	2.18	0.60
3:J:939:GLU:HB3	3:J:957:ILE:HG21	1.83	0.60
3:D:956:GLN:NE2	3:D:960:CYS:SG	2.71	0.60
2:H:95:TRP:HA	2:H:109:MET:HG2	1.83	0.60
4:F:598:PHE:CE1	3:J:16:TYR:HD2	2.20	0.60
3:J:670:TYR:HB3	3:J:673:TYR:HB2	1.84	0.60
2:B:95:TRP:HA	2:B:109:MET:HG2	1.83	0.60
2:B:267:CYS:HA	2:B:297:GLY:HA2	1.84	0.60
3:D:708:SER:HB2	3:D:712:SER:HB3	1.83	0.60
3:D:69:MET:SD	3:D:69:MET:N	2.75	0.60
3:D:383:PHE:HE2	3:D:917:LEU:HD23	1.65	0.59
3:J:902:THR:O	3:J:906:GLN:N	2.23	0.59
3:D:1634:LYS:HD3	6:N:78:LYS:CA	2.24	0.59
2:H:267:CYS:HA	2:H:297:GLY:HA2	1.84	0.59
2:H:65:GLN:NE2	2:H:69:GLY:O	2.35	0.59
2:H:520:VAL:HG22	2:H:533:VAL:HG22	1.83	0.59
3:J:1362:GLN:OE1	3:J:1387:ARG:NH2	2.35	0.59
3:D:133:THR:HG21	3:D:156:GLU:HB2	1.85	0.59
3:D:952:LEU:HA	3:D:955:LYS:HE2	1.85	0.59
3:J:133:THR:HG21	3:J:156:GLU:HB2	1.84	0.59
2:C:840:LYS:HE3	2:C:844:ARG:HD3	1.85	0.59
3:D:1430:ILE:HG12	3:D:1440:VAL:HG22	1.85	0.59
1:G:629:LYS:O	1:G:633:GLU:HB3	2.00	0.59
3:J:526:ILE:O	3:J:672:ASN:ND2	2.36	0.59
1:A:406:TYR:CD1	1:A:409:ASP:OD2	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:815:ASP:OD1	2:B:815:ASP:N	2.36	0.59
2:B:65:GLN:NE2	2:B:69:GLY:O	2.35	0.58
3:D:1362:GLN:OE1	3:D:1387:ARG:NH2	2.35	0.58
3:D:1634:LYS:CE	6:N:78:LYS:HB2	2.28	0.58
2:B:187:SER:HA	2:B:206:THR:HA	1.85	0.58
2:B:490:THR:O	2:B:496:ARG:NH1	2.35	0.58
3:D:376:VAL:HB	3:D:924:PHE:HZ	1.67	0.58
3:D:912:GLU:O	3:D:916:SER:OG	2.21	0.58
3:J:827:TRP:HA	3:J:827:TRP:CE3	2.37	0.58
3:D:383:PHE:HE2	3:D:917:LEU:HD21	1.67	0.58
3:D:811:ILE:HA	3:D:814:LEU:HD23	1.85	0.58
1:G:669:ASN:HA	1:G:687:THR:HG22	1.84	0.58
1:G:357:LYS:HB3	1:G:376:LEU:HB2	1.85	0.58
2:B:480:PHE:N	2:B:502:ILE:O	2.36	0.58
3:D:1304:LYS:HG2	3:D:1308:GLN:HE22	1.69	0.58
1:G:176:ASP:HB2	2:H:761:ARG:HH12	1.69	0.58
1:G:792:PRO:HB2	2:H:485:LEU:HD23	1.86	0.58
2:H:217:ARG:HB3	2:H:269:VAL:HG13	1.84	0.58
3:J:952:LEU:HA	3:J:955:LYS:HE2	1.85	0.58
4:K:499:LYS:NZ	4:K:573:ASP:O	2.37	0.58
3:J:1430:ILE:HG12	3:J:1440:VAL:HG22	1.85	0.58
3:J:5:ASN:OD1	3:J:11:ILE:N	2.23	0.58
2:H:187:SER:HA	2:H:206:THR:HA	1.85	0.58
3:J:1270:LYS:HD2	3:J:1278:LEU:HD21	1.85	0.58
2:B:271:VAL:HG23	2:B:294:ALA:HB3	1.86	0.57
1:G:179:GLN:HB2	2:H:765:MET:HB3	1.86	0.57
2:C:637:SER:OG	2:C:638:LEU:N	2.36	0.57
3:D:445:ASN:H	3:D:588:ILE:HG22	1.70	0.57
3:D:1270:LYS:HD2	3:D:1278:LEU:HD21	1.85	0.57
4:E:499:LYS:NZ	4:E:573:ASP:O	2.37	0.57
2:H:271:VAL:HG23	2:H:294:ALA:HB3	1.86	0.57
3:D:456:GLU:HG2	3:D:588:ILE:HD13	1.85	0.57
3:J:383:PHE:CE2	3:J:916:SER:HB2	2.40	0.57
2:H:280:PRO:HA	2:H:287:SER:HA	1.85	0.57
3:J:1304:LYS:HG2	3:J:1308:GLN:HE22	1.69	0.57
3:J:903:PRO:HA	3:J:906:GLN:OE1	2.05	0.57
3:J:1356:ASN:HA	3:J:1359:PHE:HB2	1.86	0.57
2:C:859:GLN:O	2:C:862:ARG:NH2	2.38	0.57
3:D:156:GLU:HG2	3:D:181:MET:HE1	1.87	0.57
3:D:822:LEU:HD13	3:D:827:TRP:HE3	1.69	0.57
3:D:1356:ASN:HA	3:D:1359:PHE:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:853:LEU:HD21	3:J:926:PHE:CE1	2.39	0.57
2:B:217:ARG:HB3	2:B:269:VAL:HG13	1.85	0.57
1:A:102:ILE:HG12	1:A:132:ARG:HH11	1.70	0.57
1:A:357:LYS:HZ3	1:A:487:VAL:HG23	1.69	0.57
3:D:230:GLU:OE1	3:D:234:GLN:NE2	2.38	0.57
2:B:280:PRO:HA	2:B:287:SER:HA	1.85	0.57
3:J:812:GLY:CA	3:J:882:ILE:HG23	2.33	0.57
1:G:725:ASN:O	2:I:639:ARG:NH2	2.38	0.56
1:A:646:ILE:O	1:A:673:ARG:NH2	2.38	0.56
2:B:520:VAL:HG22	2:B:533:VAL:HG22	1.86	0.56
3:D:74:SER:HB3	3:D:77:LEU:HG	1.87	0.56
3:D:379:VAL:HG12	3:D:920:LEU:CD1	2.34	0.56
2:I:764:LEU:HD12	2:I:765:MET:HB3	1.87	0.56
3:J:884:ILE:HD12	3:J:934:PHE:HB2	1.87	0.56
2:C:698:THR:HA	2:C:744:ASN:HD21	1.69	0.56
3:J:822:LEU:HB3	3:J:827:TRP:CZ3	2.40	0.56
1:G:767:PHE:HB2	1:G:782:VAL:HB	1.87	0.56
2:I:488:PRO:HD2	2:I:491:SER:HB3	1.87	0.56
3:J:876:SER:HB2	3:J:880:LYS:HE3	1.86	0.56
3:J:934:PHE:O	3:J:935:LEU:C	2.44	0.56
2:B:44:ASP:HB3	2:B:49:ARG:HB2	1.87	0.56
2:H:2:ARG:HB2	2:H:350:ALA:HB3	1.87	0.56
2:I:755:ASN:OD1	2:I:758:ARG:NH1	2.38	0.56
2:H:315:PHE:HB2	4:K:473:VAL:HB	1.88	0.56
3:J:442:PHE:HA	3:J:805:LEU:HD13	1.86	0.56
1:A:357:LYS:HZ3	1:A:487:VAL:HG21	1.67	0.56
2:B:315:PHE:HB2	4:E:473:VAL:HB	1.88	0.56
1:G:357:LYS:HB2	1:G:377:ASP:HB3	1.87	0.56
3:J:1180:TYR:O	3:J:1185:ARG:NH2	2.39	0.56
1:A:725:ASN:O	2:C:639:ARG:NH2	2.39	0.56
3:D:896:LEU:O	3:D:900:LEU:HG	2.06	0.56
4:F:598:PHE:CZ	3:J:16:TYR:HD2	2.24	0.56
2:H:44:ASP:HB3	2:H:49:ARG:HB2	1.86	0.56
3:D:826:ARG:HG2	3:D:940:LYS:HD3	1.87	0.55
3:D:949:ASP:OD1	3:D:949:ASP:N	2.39	0.55
3:D:1634:LYS:HZ2	6:N:78:LYS:HB2	1.71	0.55
3:J:853:LEU:CD2	3:J:926:PHE:CZ	2.89	0.55
3:J:1114:ARG:HA	3:J:1117:LYS:HD2	1.88	0.55
3:D:645:ASP:O	3:D:695:GLN:NE2	2.38	0.55
1:G:755:SER:OG	1:G:756:LYS:N	2.37	0.55
2:B:870:GLU:HG3	3:J:175:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1114:ARG:HA	3:D:1117:LYS:HD2	1.88	0.55
3:J:10:ASN:C	3:J:12:GLU:N	2.60	0.55
1:G:102:ILE:HG12	1:G:132:ARG:HH11	1.70	0.55
2:H:247:LEU:HD13	2:H:253:TYR:HB3	1.88	0.55
2:B:2:ARG:HB2	2:B:350:ALA:HB3	1.87	0.55
3:D:928:ASP:OD1	3:D:928:ASP:N	2.40	0.55
3:D:1180:TYR:O	3:D:1185:ARG:NH2	2.39	0.55
2:I:654:CYS:HB2	2:I:664:VAL:HG22	1.89	0.55
3:J:898:ALA:CB	3:J:906:GLN:HA	2.36	0.55
2:B:225:ASP:N	2:B:225:ASP:OD1	2.39	0.55
3:J:949:ASP:N	3:J:949:ASP:OD1	2.39	0.55
2:B:192:GLN:NE2	2:B:376:PRO:O	2.33	0.55
3:D:272:SER:HB3	3:D:276:ARG:HH21	1.72	0.55
3:J:9:SER:HB2	3:J:12:GLU:HB3	1.89	0.55
3:J:935:LEU:HD11	3:J:978:THR:HG21	1.89	0.55
4:K:578:ASP:OD1	4:K:578:ASP:N	2.40	0.55
3:J:1110:ASP:OD1	3:J:1110:ASP:N	2.39	0.55
3:J:928:ASP:OD1	3:J:928:ASP:N	2.40	0.55
2:B:515:ASN:OD1	2:B:515:ASN:N	2.40	0.54
2:H:515:ASN:OD1	2:H:515:ASN:N	2.39	0.54
3:J:383:PHE:HD2	3:J:916:SER:HB3	1.71	0.54
3:D:524:ARG:HD3	3:D:563:TYR:HB3	1.88	0.54
3:D:822:LEU:HB3	3:D:827:TRP:CZ3	2.41	0.54
1:G:157:LEU:HD22	1:G:181:LEU:HB3	1.89	0.54
2:H:225:ASP:OD1	2:H:225:ASP:N	2.39	0.54
2:B:247:LEU:HD13	2:B:253:TYR:HB3	1.88	0.54
3:D:960:CYS:HG	3:D:976:HIS:CD2	2.24	0.54
3:D:1059:THR:HA	3:D:1177:SER:HB2	1.89	0.54
1:G:157:LEU:CD2	1:G:181:LEU:HB3	2.37	0.54
2:H:192:GLN:NE2	2:H:376:PRO:O	2.33	0.54
1:A:655:GLU:HB2	1:A:662:ILE:HD11	1.90	0.54
1:A:755:SER:OG	1:A:756:LYS:N	2.38	0.54
3:D:1110:ASP:OD1	3:D:1110:ASP:N	2.39	0.54
4:E:578:ASP:N	4:E:578:ASP:OD1	2.40	0.54
3:J:853:LEU:HD21	3:J:926:PHE:CZ	2.43	0.54
3:J:891:LEU:CD1	3:J:910:THR:HG23	2.28	0.54
2:H:815:ASP:OD1	2:H:815:ASP:N	2.39	0.54
3:J:869:PHE:HE2	3:J:924:PHE:HB3	1.72	0.54
1:A:159:ARG:NE	2:B:765:MET:CG	2.63	0.54
2:C:694:GLN:NE2	2:C:773:GLU:OE1	2.41	0.54
3:D:383:PHE:CE2	3:D:917:LEU:CD2	2.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1059:THR:HA	3:J:1177:SER:HB2	1.89	0.54
3:J:891:LEU:CD2	3:J:914:ILE:CG1	2.86	0.54
2:H:758:ARG:HA	2:H:761:ARG:HD2	1.90	0.53
3:J:386:GLU:OE1	3:J:915:TRP:HZ3	1.91	0.53
3:J:673:TYR:HB3	3:J:676:ILE:HD12	1.90	0.53
2:B:183:THR:HG1	2:B:187:SER:HG	1.55	0.53
3:D:1188:ASP:OD1	3:D:1188:ASP:N	2.39	0.53
3:J:1188:ASP:N	3:J:1188:ASP:OD1	2.39	0.53
3:D:881:ASP:CA	3:D:929:ALA:HB1	2.38	0.53
3:D:83:LEU:O	3:D:87:ASN:ND2	2.42	0.53
3:D:383:PHE:CE2	3:D:917:LEU:HD23	2.44	0.53
3:D:905:GLU:HA	3:D:908:ILE:HD12	1.91	0.53
3:D:955:LYS:HA	3:D:966:ILE:HD12	1.90	0.53
4:F:598:PHE:CE1	3:J:16:TYR:CD2	2.97	0.53
2:H:642:ASP:OD1	2:H:642:ASP:N	2.40	0.53
3:J:849:PHE:CD2	3:J:886:LEU:HD11	2.44	0.53
2:B:642:ASP:OD1	2:B:642:ASP:N	2.41	0.53
3:D:817:GLN:O	3:D:820:ALA:HB3	2.08	0.53
3:D:443:ASN:HB3	3:D:589:GLN:HA	1.91	0.53
3:J:902:THR:CB	3:J:905:GLU:HB2	2.39	0.53
2:B:45:THR:HG21	2:B:55:LEU:HD22	1.91	0.53
3:D:910:THR:O	3:D:914:ILE:HD12	2.08	0.53
3:D:1520:TYR:HA	3:D:1524:ILE:HD12	1.90	0.53
3:D:169:ARG:NH2	2:I:561:GLY:O	2.42	0.53
3:D:478:ARG:NH1	3:D:482:ASP:OD1	2.42	0.53
3:J:1252:GLU:OE1	4:K:500:ARG:NH1	2.42	0.53
3:J:1520:TYR:HA	3:J:1524:ILE:HD12	1.90	0.52
1:A:566:LEU:HG	2:B:645:LEU:HD12	1.91	0.52
2:C:856:ASP:OD1	2:C:856:ASP:N	2.41	0.52
2:H:183:THR:HG1	2:H:187:SER:HG	1.56	0.52
3:J:390:LEU:HD22	3:J:909:GLU:CB	2.39	0.52
3:J:955:LYS:HA	3:J:966:ILE:HD12	1.90	0.52
3:D:884:ILE:HB	3:D:930:SER:HB3	1.91	0.52
3:D:1252:GLU:OE1	4:E:500:ARG:NH1	2.42	0.52
1:A:19:GLU:OE1	1:A:486:ALA:HA	2.09	0.52
2:C:634:LEU:O	2:C:639:ARG:NH1	2.42	0.52
3:D:1269:ILE:O	3:D:1273:ASP:N	2.43	0.52
2:H:45:THR:HG21	2:H:55:LEU:HD22	1.91	0.52
3:J:737:ASP:HB3	3:J:740:MET:HG3	1.91	0.52
1:A:159:ARG:NH2	2:B:765:MET:CG	2.67	0.52
2:B:328:MET:HA	2:B:339:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:431:LEU:HD11	3:D:852:VAL:HG22	1.92	0.52
1:A:552:SER:HB3	2:B:600:CYS:HB2	1.92	0.52
2:I:634:LEU:O	2:I:639:ARG:NH1	2.43	0.52
3:J:1269:ILE:O	3:J:1273:ASP:N	2.43	0.52
3:J:850:TYR:CZ	3:J:920:LEU:CD2	2.93	0.52
3:D:208:LEU:HD11	3:D:214:ILE:HG21	1.91	0.52
3:D:773:GLN:OE1	3:D:830:SER:HB2	2.10	0.52
2:B:677:ASN:HD22	2:B:790:ARG:HH22	1.58	0.51
4:K:439:ILE:HA	4:K:454:ILE:HG12	1.92	0.51
3:J:5:ASN:HA	3:J:14:GLU:HG3	1.91	0.51
2:C:841:ASP:OD1	2:C:841:ASP:N	2.42	0.51
3:D:1357:GLN:O	3:D:1360:GLN:NE2	2.44	0.51
1:G:180:SER:HB3	1:G:199:ASP:HB2	1.92	0.51
2:H:228:PRO:HG3	2:H:272:TYR:HE1	1.76	0.51
2:H:328:MET:HA	2:H:339:ALA:HA	1.91	0.51
2:H:569:SER:OG	2:H:571:ASP:OD1	2.28	0.51
3:D:909:GLU:HA	3:D:912:GLU:HB2	1.93	0.51
3:D:1389:LEU:HD13	3:D:1408:ILE:HG13	1.92	0.51
2:B:228:PRO:HG3	2:B:272:TYR:HE1	1.76	0.51
3:D:1058:HIS:O	3:D:1063:ALA:N	2.44	0.51
4:E:439:ILE:HA	4:E:454:ILE:HG12	1.92	0.51
3:J:75:PRO:HA	3:J:78:ASP:HB2	1.93	0.51
3:J:376:VAL:HG11	3:J:923:HIS:NE2	2.23	0.51
3:J:969:ASP:OD1	3:J:969:ASP:N	2.43	0.51
2:B:5:LYS:HE3	2:B:345:THR:HG21	1.93	0.51
3:D:710:THR:HA	3:D:713:GLU:HB2	1.91	0.51
1:G:179:GLN:N	2:H:765:MET:HG3	2.25	0.51
2:H:5:LYS:HE3	2:H:345:THR:HG21	1.93	0.51
3:J:878:LYS:O	3:J:881:ASP:HB2	2.11	0.51
3:J:1389:LEU:HD13	3:J:1408:ILE:HG13	1.92	0.51
3:D:442:PHE:HA	3:D:805:LEU:HD13	1.93	0.51
3:D:1634:LYS:HB3	6:N:78:LYS:HD3	1.90	0.51
2:H:684:VAL:HG11	2:H:739:LEU:HD13	1.93	0.51
3:J:1058:HIS:O	3:J:1063:ALA:N	2.44	0.51
3:J:1357:GLN:O	3:J:1360:GLN:NE2	2.44	0.51
1:A:777:LEU:HD22	2:C:679:GLU:HG3	1.93	0.50
3:D:937:LEU:HD12	3:D:941:LEU:HG	1.92	0.50
3:D:1188:ASP:HA	3:D:1191:LYS:HD2	1.93	0.50
3:J:876:SER:O	3:J:880:LYS:HG3	2.11	0.50
2:B:219:SER:H	2:B:270:LEU:HD23	1.76	0.50
1:G:655:GLU:OE2	3:J:503:HIS:NE2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:563:ILE:HG23	2:H:498:ALA:HB3	1.93	0.50
2:I:655:SER:OG	2:I:656:ILE:N	2.44	0.50
3:J:826:ARG:O	3:J:827:TRP:C	2.49	0.50
3:D:880:LYS:CB	3:D:929:ALA:HB2	2.35	0.50
2:H:219:SER:H	2:H:270:LEU:HD23	1.76	0.50
3:J:587:ARG:HG3	3:J:593:SER:HB3	1.91	0.50
1:A:660:ASP:OD2	1:A:660:ASP:N	2.36	0.50
2:B:192:GLN:HB2	2:B:202:ILE:HD13	1.93	0.50
2:H:16:ASN:HA	2:H:326:ASN:HD22	1.77	0.50
3:J:3:MET:O	3:J:14:GLU:OE2	2.28	0.50
3:J:1087:SER:O	3:J:1091:SER:OG	2.27	0.50
3:D:969:ASP:N	3:D:969:ASP:OD1	2.43	0.50
3:D:1128:GLU:HA	3:D:1131:ILE:HD12	1.92	0.50
3:J:1243:ILE:HG21	4:K:587:ARG:HD3	1.92	0.50
1:A:646:ILE:HG23	1:A:652:VAL:HG21	1.93	0.50
2:B:15:VAL:O	2:B:326:ASN:ND2	2.45	0.50
2:B:229:VAL:N	2:B:245:ALA:O	2.39	0.50
3:D:1243:ILE:HG21	4:E:587:ARG:HD3	1.92	0.50
3:D:1634:LYS:HE2	6:N:78:LYS:O	2.11	0.50
2:H:15:VAL:O	2:H:326:ASN:ND2	2.45	0.50
3:J:464:LEU:HD13	3:J:751:LEU:HD13	1.92	0.50
3:J:1188:ASP:HA	3:J:1191:LYS:HD2	1.93	0.50
3:D:804:LEU:HD11	3:D:848:PHE:HZ	1.77	0.50
2:H:229:VAL:HB	2:H:245:ALA:HB3	1.94	0.50
3:J:645:ASP:O	3:J:695:GLN:NE2	2.45	0.50
3:J:1298:ASN:O	3:J:1302:VAL:N	2.42	0.50
3:D:1515:LEU:HD22	3:D:1578:GLY:HA3	1.93	0.50
2:H:192:GLN:HB2	2:H:202:ILE:HD13	1.93	0.50
1:A:103:LEU:HD23	1:A:133:LEU:HD12	1.94	0.49
2:B:16:ASN:HA	2:B:326:ASN:HD22	1.77	0.49
2:I:815:ASP:N	2:I:815:ASP:OD2	2.45	0.49
3:J:1304:LYS:O	3:J:1308:GLN:NE2	2.45	0.49
1:A:425:GLU:OE2	2:B:858:ARG:NH1	2.45	0.49
2:B:229:VAL:HB	2:B:245:ALA:HB3	1.94	0.49
3:D:1304:LYS:O	3:D:1308:GLN:NE2	2.45	0.49
2:H:325:ILE:HD13	2:H:341:SER:HB3	1.94	0.49
2:H:727:ASP:OD1	2:H:799:LYS:NZ	2.44	0.49
2:B:489:ASN:ND2	2:B:591:GLY:O	2.45	0.49
3:D:826:ARG:O	3:D:827:TRP:C	2.49	0.49
1:G:417:GLU:OE2	2:H:858:ARG:NH1	2.45	0.49
3:J:1128:GLU:HA	3:J:1131:ILE:HD12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:VAL:HB	2:B:146:LEU:HB2	1.94	0.49
2:C:670:ASP:N	2:C:670:ASP:OD1	2.43	0.49
1:G:423:LEU:HB2	2:H:874:ILE:HD11	1.94	0.49
3:J:937:LEU:O	3:J:937:LEU:HG	2.11	0.49
2:B:81:LEU:HB3	2:B:92:TYR:HB2	1.94	0.49
3:D:1298:ASN:O	3:D:1302:VAL:N	2.42	0.49
1:G:103:LEU:HD23	1:G:133:LEU:HD12	1.94	0.49
2:H:452:LEU:HD22	2:H:643:ASP:HB3	1.94	0.49
2:B:325:ILE:HD13	2:B:341:SER:HB3	1.94	0.49
3:J:804:LEU:HD11	3:J:848:PHE:HZ	1.77	0.49
3:D:898:ALA:HB1	3:D:906:GLN:HB2	1.94	0.49
3:D:1087:SER:O	3:D:1091:SER:OG	2.28	0.49
1:G:646:ILE:O	1:G:673:ARG:NH2	2.45	0.49
1:G:661:ASP:OD2	1:G:693:GLN:NE2	2.45	0.49
2:I:490:THR:O	2:I:490:THR:OG1	2.30	0.49
3:J:133:THR:HG23	3:J:152:ILE:HG13	1.94	0.49
3:J:769:ILE:HG21	3:J:822:LEU:HG	1.93	0.49
3:J:826:ARG:HB3	3:J:828:GLU:HG3	1.94	0.49
2:B:502:ILE:HG12	2:B:556:THR:HG22	1.93	0.49
3:D:818:LEU:HB3	3:D:889:LEU:CD1	2.23	0.49
3:D:829:SER:HA	3:D:892:TYR:OH	2.13	0.49
2:H:137:VAL:HB	2:H:146:LEU:HB2	1.94	0.49
2:H:229:VAL:N	2:H:245:ALA:O	2.39	0.49
3:D:830:SER:N	3:D:892:TYR:OH	2.45	0.49
3:D:1368:ASN:ND2	3:D:1370:GLU:OE2	2.46	0.49
1:G:810:ASP:O	1:G:814:CYS:HA	2.13	0.49
2:H:7:PRO:HA	2:H:345:THR:HA	1.95	0.49
3:J:215:LYS:HG3	3:J:217:GLU:HG2	1.95	0.49
3:J:415:ASP:HA	3:J:417:GLN:HE21	1.77	0.49
1:A:767:PHE:HB2	1:A:782:VAL:HB	1.94	0.48
2:B:7:PRO:HA	2:B:345:THR:HA	1.95	0.48
2:B:310:ARG:NH2	4:E:471:GLY:O	2.36	0.48
1:G:734:ASN:ND2	2:I:819:ASP:OD2	2.46	0.48
3:J:723:LEU:HD23	3:J:726:ILE:HD12	1.94	0.48
3:J:1368:ASN:ND2	3:J:1370:GLU:OE2	2.46	0.48
2:C:675:ASP:O	2:C:679:GLU:N	2.46	0.48
3:J:443:ASN:HB3	3:J:589:GLN:HG2	1.93	0.48
2:H:81:LEU:HB3	2:H:92:TYR:HB2	1.94	0.48
3:J:1250:ASN:O	3:J:1254:SER:OG	2.30	0.48
3:J:1260:ASN:O	3:J:1264:SER:OG	2.28	0.48
3:J:10:ASN:O	3:J:12:GLU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1405:ARG:NH1	3:J:1425:GLU:O	2.42	0.48
3:D:1187:ILE:HG22	3:D:1191:LYS:HE3	1.95	0.48
3:D:816:SER:O	3:D:820:ALA:HB2	2.14	0.48
3:D:909:GLU:O	3:D:913:LEU:N	2.27	0.48
3:J:1187:ILE:HG22	3:J:1191:LYS:HE3	1.95	0.48
3:J:1518:LYS:HB3	3:J:1518:LYS:HE2	1.53	0.48
1:A:622:ASN:HB2	2:C:642:ASP:HB3	1.94	0.48
2:C:551:ILE:HD11	2:C:555:ILE:HD11	1.96	0.48
3:D:524:ARG:NH1	3:D:567:SER:OG	2.47	0.48
3:D:906:GLN:O	3:D:907:GLY:C	2.52	0.48
3:D:1473:ASP:O	3:D:1477:THR:OG1	2.32	0.48
1:A:406:TYR:HD1	1:A:409:ASP:OD1	1.53	0.48
3:D:10:ASN:HD22	3:D:11:ILE:HG23	1.76	0.48
3:D:884:ILE:HD12	3:D:934:PHE:HB3	1.95	0.48
3:J:721:LYS:O	3:J:733:HIS:NE2	2.47	0.48
3:J:963:HIS:NE2	3:J:978:THR:O	2.37	0.48
2:B:326:ASN:N	2:B:326:ASN:OD1	2.46	0.48
2:H:295:THR:OG1	2:H:306:TRP:NE1	2.36	0.48
3:J:412:GLY:HA3	3:J:425:THR:HG21	1.95	0.48
1:A:661:ASP:OD2	1:A:693:GLN:NE2	2.47	0.47
1:G:739:ILE:HD13	1:G:775:LEU:HD13	1.96	0.47
2:H:290:TYR:OH	2:H:356:LEU:O	2.27	0.47
2:H:326:ASN:OD1	2:H:326:ASN:N	2.46	0.47
3:J:819:THR:HG23	3:J:889:LEU:HG	1.96	0.47
3:J:1127:PHE:HA	3:J:1130:TRP:HD1	1.78	0.47
2:C:477:PRO:HB2	2:C:478:ILE:H	1.44	0.47
2:C:490:THR:O	2:C:490:THR:OG1	2.31	0.47
3:D:881:ASP:HA	3:D:929:ALA:HB1	1.97	0.47
3:D:1218:SER:HA	3:D:1244:THR:HA	1.96	0.47
3:D:1250:ASN:O	3:D:1254:SER:OG	2.30	0.47
2:B:295:THR:OG1	2:B:306:TRP:NE1	2.36	0.47
2:I:512:ASN:OD1	2:I:512:ASN:N	2.40	0.47
3:J:686:SER:OG	3:J:690:LYS:NZ	2.48	0.47
3:D:42:LYS:NZ	1:G:426:ASP:OD2	2.46	0.47
2:H:662:PRO:HD2	2:H:674:PHE:HB3	1.95	0.47
3:J:159:LYS:O	3:J:163:LEU:N	2.46	0.47
3:J:850:TYR:CE2	3:J:920:LEU:CD2	2.98	0.47
3:J:1473:ASP:O	3:J:1477:THR:OG1	2.32	0.47
4:K:444:GLU:HA	4:K:450:PRO:HB3	1.96	0.47
3:D:383:PHE:CE2	3:D:917:LEU:HD21	2.49	0.47
3:J:853:LEU:HD22	3:J:926:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1218:SER:HA	3:J:1244:THR:HA	1.96	0.47
1:A:406:TYR:CB	1:A:409:ASP:OD2	2.58	0.47
3:D:259:LYS:HE3	3:D:534:GLN:HG2	1.97	0.47
4:E:444:GLU:HA	4:E:450:PRO:HB3	1.97	0.47
1:G:357:LYS:HA	4:L:565:LEU:N	2.29	0.47
2:H:278:GLU:N	2:H:358:VAL:O	2.46	0.47
2:B:331:SER:N	2:B:336:THR:O	2.45	0.47
3:D:1127:PHE:HA	3:D:1130:TRP:HD1	1.78	0.47
3:D:1260:ASN:O	3:D:1264:SER:OG	2.28	0.47
2:H:171:ILE:N	2:H:180:THR:O	2.46	0.47
2:B:822:GLN:HB3	3:J:171:ARG:HH22	1.80	0.47
3:D:847:PHE:HA	3:D:850:TYR:HB3	1.96	0.47
3:D:1159:ASP:OD1	3:D:1242:LYS:NZ	2.45	0.47
2:H:310:ARG:NH2	4:K:471:GLY:O	2.36	0.47
3:J:880:LYS:HD2	3:J:929:ALA:HB2	1.97	0.47
3:J:1399:LYS:HD2	3:J:1399:LYS:HA	1.72	0.47
1:A:265:ARG:CD	1:A:409:ASP:OD1	2.63	0.47
2:B:495:ILE:HD11	2:B:631:TYR:HB2	1.95	0.47
2:C:488:PRO:HD2	2:C:491:SER:HB3	1.97	0.47
3:D:814:LEU:O	3:D:818:LEU:N	2.36	0.47
3:D:1634:LYS:NZ	6:N:78:LYS:HB2	2.28	0.47
1:A:420:ASN:HA	1:A:423:LEU:HD12	1.97	0.46
2:B:146:LEU:HD22	2:B:155:LYS:HE3	1.98	0.46
3:D:448:LEU:HB2	3:D:810:ALA:HB1	1.97	0.46
3:D:773:GLN:HG2	3:D:893:TYR:OH	2.15	0.46
2:H:502:ILE:HG12	2:H:556:THR:HG22	1.96	0.46
2:I:770:GLU:HB2	3:J:239:MET:HE1	1.97	0.46
2:B:20:ALA:HA	2:B:25:ILE:HA	1.98	0.46
3:D:50:ASP:OD1	3:D:88:ARG:NH2	2.48	0.46
3:D:1634:LYS:NZ	6:N:78:LYS:O	2.48	0.46
2:H:271:VAL:HB	2:H:330:TRP:CD1	2.50	0.46
3:J:968:SER:HB3	3:J:971:PHE:HB2	1.98	0.46
2:C:662:PRO:HD2	2:C:674:PHE:HB3	1.98	0.46
3:D:1405:ARG:NH1	3:D:1425:GLU:O	2.42	0.46
2:C:505:THR:HG22	2:C:521:LYS:HG3	1.98	0.46
3:D:898:ALA:CB	3:D:906:GLN:HB2	2.46	0.46
3:J:394:ILE:HB	3:J:901:ARG:HH11	1.81	0.46
2:B:662:PRO:HD2	2:B:674:PHE:HB3	1.97	0.46
2:H:146:LEU:HD22	2:H:155:LYS:HE3	1.98	0.46
3:J:773:GLN:NE2	3:J:822:LEU:HD11	2.31	0.46
1:A:785:LEU:HD23	2:C:486:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:769:ILE:HB	3:D:830:SER:HB3	1.98	0.46
3:D:968:SER:HB3	3:D:971:PHE:HB2	1.98	0.46
2:H:20:ALA:HA	2:H:25:ILE:HA	1.98	0.46
2:H:281:ASN:N	2:H:286:THR:O	2.48	0.46
2:H:577:TYR:OH	2:H:583:LYS:NZ	2.49	0.46
3:J:1363:GLU:HA	3:J:1366:TRP:CD1	2.51	0.46
2:B:290:TYR:OH	2:B:356:LEU:O	2.27	0.46
3:D:802:GLN:O	3:D:806:THR:OG1	2.33	0.46
3:D:939:GLU:O	3:D:942:LEU:N	2.49	0.46
3:D:1399:LYS:HD2	3:D:1399:LYS:HA	1.72	0.46
3:J:167:LEU:HD12	3:J:206:TYR:HE2	1.80	0.46
3:J:721:LYS:HA	3:J:724:LEU:HB2	1.98	0.46
3:J:827:TRP:NE1	3:J:937:LEU:HB2	2.31	0.46
3:J:1143:ASP:HA	3:J:1147:TRP:HD1	1.81	0.46
2:H:183:THR:OG1	2:H:187:SER:OG	2.27	0.46
2:H:223:GLN:O	2:H:372:ASN:ND2	2.47	0.46
3:J:718:THR:OG1	3:J:735:ASN:ND2	2.48	0.46
2:B:149:ARG:HB2	2:B:156:LEU:HD21	1.97	0.46
2:B:271:VAL:HB	2:B:330:TRP:CD1	2.50	0.46
2:B:670:ASP:OD1	2:B:670:ASP:N	2.49	0.46
3:D:414:SER:O	3:D:417:GLN:NE2	2.49	0.46
3:D:773:GLN:HG3	3:D:818:LEU:HD11	1.97	0.46
3:D:858:SER:O	3:D:862:ASP:N	2.49	0.46
3:D:1040:SER:O	3:D:1044:ASN:ND2	2.49	0.46
2:I:841:ASP:OD1	2:I:841:ASP:N	2.49	0.46
3:J:146:VAL:HG13	3:J:188:LEU:HD11	1.97	0.46
3:J:448:LEU:HB2	3:J:810:ALA:HB1	1.98	0.46
2:B:278:GLU:N	2:B:358:VAL:O	2.46	0.45
3:D:1143:ASP:HA	3:D:1147:TRP:HD1	1.81	0.45
2:H:22:GLY:O	2:H:39:GLN:NE2	2.50	0.45
2:H:310:ARG:HH21	2:H:312:LYS:HB2	1.81	0.45
2:H:448:VAL:HG23	2:I:476:GLN:HE21	1.81	0.45
3:J:380:HIS:NE2	3:J:857:SER:OG	2.39	0.45
3:J:946:ILE:HA	3:J:994:TYR:HE2	1.81	0.45
2:B:171:ILE:N	2:B:180:THR:O	2.46	0.45
2:B:641:SER:HB2	2:B:644:ILE:HG23	1.98	0.45
2:C:771:ASN:OD1	2:C:771:ASN:N	2.50	0.45
3:D:1444:LYS:HG3	3:D:1448:GLU:HB3	1.97	0.45
2:I:830:ILE:HB	2:I:837:PHE:HB3	1.99	0.45
1:A:806:CYS:O	1:A:819:GLU:HB3	2.16	0.45
2:B:22:GLY:O	2:B:39:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:GLN:HB3	2:B:231:ASN:HB3	1.99	0.45
2:B:262:PRO:HG3	4:E:594:PHE:HD1	1.80	0.45
3:D:884:ILE:HG22	3:D:930:SER:OG	2.16	0.45
3:D:1363:GLU:HA	3:D:1366:TRP:CD1	2.51	0.45
2:H:210:GLN:HB3	2:H:231:ASN:HB3	1.99	0.45
3:J:787:LEU:HD11	3:J:807:VAL:HG11	1.98	0.45
3:J:1040:SER:O	3:J:1044:ASN:ND2	2.49	0.45
3:D:946:ILE:HA	3:D:994:TYR:HE2	1.81	0.45
3:D:963:HIS:NE2	3:D:978:THR:O	2.38	0.45
2:H:262:PRO:HG3	4:K:594:PHE:HD1	1.80	0.45
3:J:152:ILE:HD12	3:J:152:ILE:HA	1.90	0.45
3:J:823:ASN:HA	3:J:827:TRP:CG	2.52	0.45
1:A:813:SER:OG	1:A:815:ASP:OD2	2.34	0.45
2:C:637:SER:O	2:C:639:ARG:N	2.49	0.45
3:D:446:ASP:HB3	3:D:447:TYR:H	1.55	0.45
3:D:915:TRP:O	3:D:919:THR:N	2.41	0.45
3:D:1247:SER:OG	3:D:1250:ASN:ND2	2.50	0.45
2:H:149:ARG:HB2	2:H:156:LEU:HD21	1.97	0.45
2:B:281:ASN:N	2:B:286:THR:O	2.48	0.45
2:B:517:ILE:HG23	2:B:536:THR:HB	1.98	0.45
3:D:723:LEU:HA	3:D:726:ILE:HD12	1.98	0.45
4:E:437:PRO:HB3	4:E:456:VAL:HG13	1.98	0.45
3:J:574:ASN:O	3:J:578:ASN:ND2	2.43	0.45
3:J:1444:LYS:HG3	3:J:1448:GLU:HB3	1.97	0.45
1:A:357:LYS:HZ1	1:A:487:VAL:CG2	2.29	0.45
2:B:310:ARG:HH21	2:B:312:LYS:HB2	1.81	0.45
2:B:727:ASP:OD2	2:B:799:LYS:NZ	2.42	0.45
2:B:771:ASN:OD1	2:B:771:ASN:N	2.39	0.45
3:D:518:ASP:OD2	3:D:521:ASN:N	2.49	0.45
3:J:7:LEU:O	3:J:8:ASN:C	2.55	0.45
3:J:853:LEU:HD13	3:J:920:LEU:HD21	1.99	0.45
1:A:662:ILE:HG23	3:D:504:GLN:HG2	1.99	0.45
2:C:748:ASN:OD1	2:C:748:ASN:N	2.47	0.45
3:D:390:LEU:CD2	3:D:909:GLU:HA	2.47	0.45
3:D:1006:TYR:HE2	3:D:1132:LEU:HD21	1.82	0.45
1:G:727:SER:HA	1:G:742:ILE:O	2.17	0.45
3:J:9:SER:HB2	3:J:12:GLU:CB	2.47	0.45
3:J:1006:TYR:HE2	3:J:1132:LEU:HD21	1.82	0.45
3:J:1247:SER:OG	3:J:1250:ASN:ND2	2.50	0.45
2:C:574:ILE:HB	2:C:588:LEU:HB2	1.98	0.45
2:C:700:ASN:ND2	2:C:737:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:ILE:HG12	1:G:132:ARG:NH1	2.32	0.45
2:H:858:ARG:O	2:H:861:GLN:NE2	2.50	0.45
2:C:846:LEU:O	2:C:850:ILE:HD12	2.16	0.45
3:D:884:ILE:HG13	3:D:929:ALA:O	2.17	0.45
3:D:886:LEU:O	3:D:890:ILE:HB	2.17	0.45
3:D:939:GLU:HG3	3:D:954:LEU:HD11	1.99	0.45
3:J:383:PHE:CD2	3:J:916:SER:CB	3.00	0.45
3:J:383:PHE:CE2	3:J:916:SER:CB	3.00	0.45
3:J:881:ASP:N	3:J:929:ALA:HB1	2.31	0.45
2:B:750:LYS:O	2:B:750:LYS:NZ	2.40	0.44
3:D:827:TRP:CE3	3:D:937:LEU:HD22	2.51	0.44
3:D:925:HIS:HA	3:D:976:HIS:HA	1.99	0.44
3:D:1198:ASP:O	3:D:1202:SER:OG	2.32	0.44
3:D:1248:ASP:HA	3:D:1251:ILE:HD12	1.99	0.44
3:J:491:PHE:HE1	3:J:508:LYS:HG2	1.82	0.44
2:B:223:GLN:O	2:B:372:ASN:ND2	2.47	0.44
2:B:507:LYS:HD3	2:B:517:ILE:HD11	1.99	0.44
2:C:512:ASN:OD1	2:C:512:ASN:N	2.38	0.44
3:J:925:HIS:HA	3:J:976:HIS:HA	1.99	0.44
1:A:102:ILE:CG1	1:A:132:ARG:HH11	2.30	0.44
2:B:215:HIS:O	2:B:268:ARG:NE	2.50	0.44
3:D:769:ILE:HG23	3:D:821:ILE:HD12	2.00	0.44
3:D:902:THR:HB	3:D:905:GLU:CB	2.21	0.44
1:G:102:ILE:CG1	1:G:132:ARG:HH11	2.30	0.44
2:H:215:HIS:O	2:H:268:ARG:NE	2.50	0.44
2:H:596:PHE:HB2	2:H:607:LEU:HB3	2.00	0.44
3:J:819:THR:HB	3:J:933:LYS:HD2	1.98	0.44
3:J:891:LEU:CD1	3:J:914:ILE:HD11	2.48	0.44
2:B:301:GLY:HA3	2:B:321:SER:H	1.83	0.44
3:D:459:PHE:HB2	3:D:462:ASN:HB3	1.99	0.44
2:H:75:THR:OG1	2:H:76:GLY:N	2.51	0.44
2:H:80:THR:HA	2:H:93:SER:HA	2.00	0.44
2:I:764:LEU:HB2	3:J:113:LEU:HD22	1.99	0.44
3:J:850:TYR:CE2	3:J:920:LEU:HD21	2.53	0.44
3:J:1159:ASP:OD1	3:J:1242:LYS:NZ	2.45	0.44
2:B:194:ASN:ND2	2:B:196:THR:OG1	2.48	0.44
1:G:687:THR:OG1	1:G:703:ILE:O	2.32	0.44
3:J:23:ARG:NH2	3:J:26:GLN:OE1	2.50	0.44
1:A:102:ILE:CD1	1:A:132:ARG:HH11	2.31	0.44
2:B:13:GLU:OE2	2:B:33:HIS:ND1	2.51	0.44
2:H:194:ASN:ND2	2:H:196:THR:OG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:301:GLY:HA3	2:H:321:SER:H	1.83	0.44
2:H:450:ARG:NH1	2:I:477:PRO:O	2.50	0.44
4:K:437:PRO:HB3	4:K:456:VAL:HG13	1.98	0.44
2:B:37:TRP:HZ3	2:B:55:LEU:HG	1.83	0.44
2:B:493:SER:OG	2:B:495:ILE:O	2.33	0.44
2:H:13:GLU:OE2	2:H:33:HIS:ND1	2.51	0.44
2:H:658:LYS:HB3	2:H:658:LYS:HE2	1.64	0.44
4:L:478:SER:CB	4:L:572:GLU:HG2	2.48	0.44
2:B:75:THR:OG1	2:B:76:GLY:N	2.51	0.44
2:B:360:LEU:HD13	2:B:364:GLU:HG2	2.00	0.44
3:D:112:ILE:HD13	3:D:112:ILE:HA	1.92	0.44
1:G:680:GLU:OE1	2:I:758:ARG:NH2	2.51	0.44
1:G:748:VAL:HG13	1:G:760:VAL:HG13	1.99	0.44
3:J:1074:GLU:H	3:J:1074:GLU:HG3	1.59	0.44
1:A:764:ARG:HA	1:A:764:ARG:HD3	1.81	0.44
2:B:80:THR:HA	2:B:93:SER:HA	2.00	0.44
2:B:166:LYS:O	2:B:184:SER:N	2.51	0.44
3:D:862:ASP:HB3	3:D:865:ASN:HD22	1.83	0.44
3:D:1150:ASP:OD1	3:D:1150:ASP:N	2.42	0.44
2:H:37:TRP:HZ3	2:H:55:LEU:HG	1.83	0.44
2:H:452:LEU:HD23	2:H:452:LEU:HA	1.89	0.44
2:B:569:SER:OG	2:B:571:ASP:OD1	2.34	0.43
1:G:177:VAL:O	1:G:204:LYS:HE3	2.18	0.43
1:G:335:LYS:HD2	4:L:565:LEU:HD12	1.99	0.43
1:G:785:LEU:HD13	2:I:486:LEU:HD23	2.00	0.43
2:H:307:ASN:ND2	4:K:466:TYR:OH	2.50	0.43
3:J:99:ASN:OD1	3:J:102:ARG:NH1	2.51	0.43
3:J:112:ILE:HD13	3:J:112:ILE:HA	1.91	0.43
3:J:755:LEU:HA	3:J:758:VAL:HG22	1.99	0.43
3:J:891:LEU:HD23	3:J:937:LEU:HD23	2.00	0.43
3:J:895:ASP:OD1	3:J:941:LEU:HD13	2.18	0.43
3:J:906:GLN:HG2	3:J:907:GLY:N	2.32	0.43
3:J:1248:ASP:HA	3:J:1251:ILE:HD12	1.99	0.43
1:A:1:MET:H1	1:A:389:GLU:CD	2.21	0.43
2:B:218:ILE:HG23	2:B:270:LEU:HD22	2.00	0.43
2:C:592:VAL:HG11	2:C:610:ILE:HG23	2.00	0.43
3:D:582:GLU:O	3:D:586:LYS:HB2	2.18	0.43
3:D:1634:LYS:CB	6:N:78:LYS:CD	2.82	0.43
1:G:179:GLN:HB2	2:H:765:MET:HB2	2.00	0.43
2:H:360:LEU:HD13	2:H:364:GLU:HG2	2.00	0.43
2:C:522:ASN:HA	2:C:531:THR:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:959:TRP:NE1	3:D:973:PRO:HB3	2.33	0.43
2:B:307:ASN:ND2	4:E:466:TYR:OH	2.50	0.43
3:D:464:LEU:HD22	3:D:751:LEU:HD22	2.01	0.43
3:D:1250:ASN:ND2	4:E:580:GLU:OE2	2.51	0.43
2:I:683:LEU:HD11	2:I:686:ASP:HB3	2.00	0.43
3:J:880:LYS:CB	3:J:926:PHE:HD1	2.23	0.43
3:J:939:GLU:CB	3:J:957:ILE:HG21	2.46	0.43
3:J:959:TRP:NE1	3:J:973:PRO:HB3	2.33	0.43
3:D:485:SER:HB2	3:D:489:ARG:HH22	1.83	0.43
3:D:722:VAL:HA	3:D:725:HIS:HB3	2.01	0.43
3:D:1349:LEU:HD12	3:D:1368:ASN:HA	2.01	0.43
2:H:218:ILE:HG23	2:H:270:LEU:HD22	2.00	0.43
2:H:230:ILE:HA	2:H:244:THR:HA	2.00	0.43
3:J:1250:ASN:ND2	4:K:580:GLU:OE2	2.51	0.43
3:D:706:THR:HA	3:D:766:LYS:HA	2.00	0.43
2:H:166:LYS:O	2:H:184:SER:N	2.51	0.43
2:C:841:ASP:O	2:C:845:ASN:ND2	2.42	0.43
3:D:1072:ASN:N	3:D:1076:GLN:OE1	2.51	0.43
3:D:1427:ASP:OD1	3:D:1464:TYR:OH	2.34	0.43
2:H:310:ARG:HE	2:H:310:ARG:HB3	1.64	0.43
3:J:853:LEU:CD1	3:J:920:LEU:HD21	2.48	0.43
3:J:1072:ASN:N	3:J:1076:GLN:OE1	2.51	0.43
3:J:1349:LEU:HD12	3:J:1368:ASN:HA	2.00	0.43
3:J:1449:ARG:H	3:J:1449:ARG:HG3	1.38	0.43
3:J:1510:LYS:HA	3:J:1515:LEU:HB3	2.01	0.43
1:A:102:ILE:HG12	1:A:132:ARG:NH1	2.32	0.43
1:A:159:ARG:HH12	2:B:761:ARG:HB3	1.83	0.43
1:A:777:LEU:HD21	1:A:780:ARG:HB2	2.01	0.43
2:B:230:ILE:HA	2:B:244:THR:HA	2.00	0.43
3:D:686:SER:OG	3:D:690:LYS:NZ	2.52	0.43
3:D:1047:LEU:HA	3:D:1170:LEU:HD13	2.00	0.43
2:I:543:ASP:N	2:I:543:ASP:OD1	2.50	0.43
3:J:275:GLY:O	3:J:602:LYS:NZ	2.43	0.43
3:J:910:THR:CG2	3:J:945:PHE:CE2	2.99	0.43
1:A:133:LEU:HD13	1:A:164:TRP:CE3	2.54	0.43
2:B:505:THR:HA	2:B:520:VAL:O	2.19	0.43
2:C:815:ASP:OD2	2:C:815:ASP:N	2.51	0.43
2:C:844:ARG:HA	2:C:844:ARG:HD2	1.85	0.43
3:D:727:LEU:HD11	3:D:785:GLY:HA3	2.01	0.43
1:G:102:ILE:CD1	1:G:132:ARG:HH11	2.31	0.43
3:J:11:ILE:O	3:J:15:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:933:LYS:HE3	3:J:933:LYS:HB2	1.86	0.43
3:J:1346:ASN:O	3:J:1350:THR:OG1	2.29	0.43
3:J:1518:LYS:H	3:J:1518:LYS:HG2	1.49	0.43
3:D:894:TYR:HA	3:D:897:GLN:HB2	2.01	0.43
1:G:133:LEU:HD13	1:G:164:TRP:CE3	2.54	0.43
1:G:629:LYS:O	1:G:633:GLU:CB	2.65	0.43
2:B:596:PHE:HB2	2:B:607:LEU:HB3	2.00	0.42
3:D:278:MET:SD	3:D:278:MET:N	2.91	0.42
3:D:940:LYS:O	3:D:944:GLN:NE2	2.52	0.42
3:D:1028:PRO:HG2	3:D:1118:ASN:HB3	2.01	0.42
3:J:83:LEU:O	3:J:87:ASN:ND2	2.52	0.42
3:J:382:ARG:HH12	3:J:916:SER:HB3	1.84	0.42
3:J:827:TRP:CE2	3:J:937:LEU:HB2	2.54	0.42
3:J:849:PHE:CE1	3:J:882:ILE:HG21	2.54	0.42
3:J:1427:ASP:OD1	3:J:1464:TYR:OH	2.35	0.42
2:B:81:LEU:O	2:B:92:TYR:N	2.51	0.42
3:J:1198:ASP:O	3:J:1202:SER:OG	2.32	0.42
3:J:1373:ALA:HB3	3:J:1376:TYR:HD2	1.84	0.42
4:L:568:LYS:HA	4:L:568:LYS:HD3	1.74	0.42
1:A:178:HIS:ND1	1:A:204:LYS:HE2	2.34	0.42
1:A:687:THR:OG1	1:A:703:ILE:O	2.31	0.42
2:B:758:ARG:O	2:B:762:THR:OG1	2.31	0.42
3:J:383:PHE:HE2	3:J:916:SER:HB2	1.82	0.42
3:J:583:ILE:O	3:J:588:ILE:N	2.51	0.42
3:J:857:SER:HG	3:J:924:PHE:HZ	1.64	0.42
2:B:577:TYR:OH	2:B:583:LYS:NZ	2.52	0.42
2:C:742:LYS:HD3	2:C:742:LYS:HA	1.81	0.42
3:D:408:LYS:HA	3:D:411:ILE:HG12	2.01	0.42
3:D:697:ILE:O	3:D:715:HIS:ND1	2.51	0.42
3:D:899:LYS:NZ	3:D:906:GLN:OE1	2.51	0.42
3:D:1550:PRO:HD2	3:D:1553:ILE:HD12	2.01	0.42
2:H:82:TYR:HA	2:H:91:GLY:HA2	2.01	0.42
2:I:670:ASP:OD1	2:I:670:ASP:N	2.52	0.42
3:J:858:SER:HA	3:J:861:ASN:HB2	2.01	0.42
3:J:880:LYS:H	3:J:880:LYS:HG3	1.61	0.42
3:D:715:HIS:CD2	3:D:718:THR:HB	2.54	0.42
3:D:721:LYS:O	3:D:733:HIS:NE2	2.53	0.42
3:D:1634:LYS:HD3	6:N:78:LYS:O	2.19	0.42
2:H:765:MET:SD	2:H:765:MET:N	2.93	0.42
3:J:724:LEU:O	3:J:728:HIS:N	2.42	0.42
3:J:1148:THR:HG21	3:J:1151:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:819:THR:HG22	3:D:827:TRP:CZ3	2.54	0.42
3:D:1299:CYS:HA	3:D:1302:VAL:HB	2.01	0.42
2:B:781:LEU:HD23	2:B:781:LEU:HA	1.92	0.42
2:I:675:ASP:O	2:I:679:GLU:N	2.52	0.42
3:J:1028:PRO:HG2	3:J:1118:ASN:HB3	2.01	0.42
3:D:1346:ASN:O	3:D:1350:THR:OG1	2.28	0.42
3:D:1449:ARG:H	3:D:1449:ARG:HG3	1.38	0.42
1:G:799:ARG:HA	1:G:799:ARG:HD3	1.92	0.42
3:J:1047:LEU:HA	3:J:1170:LEU:HD13	2.00	0.42
4:K:584:GLU:HG3	4:K:587:ARG:NH2	2.34	0.42
2:B:82:TYR:HA	2:B:91:GLY:HA2	2.01	0.42
3:D:602:LYS:HA	3:D:605:LYS:HD2	2.01	0.42
3:D:1074:GLU:H	3:D:1074:GLU:HG3	1.59	0.42
3:J:614:LEU:HD23	3:J:614:LEU:HA	1.91	0.42
3:J:721:LYS:HG2	3:J:724:LEU:HD12	2.02	0.42
3:J:808:LEU:HA	3:J:811:ILE:HD12	2.02	0.42
2:C:639:ARG:H	2:C:639:ARG:HG2	1.59	0.42
3:D:908:ILE:O	3:D:911:THR:N	2.53	0.42
3:D:1373:ALA:HB3	3:D:1376:TYR:HD2	1.84	0.42
3:J:202:ILE:HG23	3:J:205:ARG:HH21	1.85	0.42
3:J:802:GLN:O	3:J:806:THR:HG23	2.20	0.42
3:J:809:THR:HG23	3:J:882:ILE:HD11	2.02	0.42
3:J:868:PHE:HE2	3:J:879:MET:CG	2.32	0.42
3:J:886:LEU:HB3	3:J:890:ILE:HD12	2.02	0.42
3:J:948:ASN:HA	3:J:951:PHE:HB3	2.02	0.42
3:J:1299:CYS:HA	3:J:1302:VAL:HB	2.01	0.42
1:A:357:LYS:NZ	1:A:487:VAL:HG23	2.28	0.41
2:C:641:SER:OG	2:C:643:ASP:OD2	2.33	0.41
1:G:1:MET:H1	1:G:389:GLU:CD	2.22	0.41
3:J:891:LEU:HD11	3:J:914:ILE:CD1	2.50	0.41
3:J:905:GLU:HB3	3:J:909:GLU:OE2	2.20	0.41
3:J:1015:LYS:NZ	3:J:1019:ASP:OD2	2.51	0.41
3:J:1550:PRO:HD2	3:J:1553:ILE:HD12	2.01	0.41
1:A:798:VAL:HB	2:C:480:PHE:HA	2.01	0.41
2:C:694:GLN:OE1	2:C:807:ARG:NH2	2.53	0.41
3:D:1148:THR:HG21	3:D:1151:LYS:HE3	2.01	0.41
1:G:180:SER:HB3	1:G:199:ASP:CB	2.49	0.41
2:H:679:GLU:HG2	2:I:623:LEU:HD12	2.01	0.41
3:J:812:GLY:HA3	3:J:882:ILE:CG2	2.45	0.41
3:J:1334:CYS:O	3:J:1338:VAL:HB	2.20	0.41
1:A:646:ILE:HG13	1:A:652:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:SER:HB3	2:B:529:ARG:HE	1.84	0.41
4:E:584:GLU:HG3	4:E:587:ARG:NH2	2.34	0.41
3:J:891:LEU:HD11	3:J:914:ILE:HD11	2.00	0.41
3:D:1035:ILE:HG23	3:D:1038:ARG:HH22	1.84	0.41
2:H:75:THR:HG23	2:H:82:TYR:HB2	2.02	0.41
3:D:3:MET:SD	3:D:13:GLY:HA3	2.61	0.41
3:D:124:GLN:H	3:D:124:GLN:HG2	1.66	0.41
3:D:881:ASP:CB	3:D:930:SER:H	2.33	0.41
2:H:686:ASP:OD1	2:H:686:ASP:N	2.53	0.41
3:J:423:PRO:HA	3:J:426:ASP:HB2	2.02	0.41
3:J:989:LEU:O	3:J:993:THR:OG1	2.32	0.41
3:J:1150:ASP:OD1	3:J:1150:ASP:N	2.42	0.41
1:A:749:ILE:HG22	1:A:750:LYS:HB3	2.02	0.41
2:C:568:CYS:HB3	2:C:597:LEU:HD22	2.03	0.41
3:J:903:PRO:O	3:J:906:GLN:HB3	2.20	0.41
3:J:905:GLU:O	3:J:906:GLN:C	2.59	0.41
3:J:910:THR:CG2	3:J:945:PHE:HE2	2.25	0.41
3:J:1584:LEU:HD13	3:J:1643:LEU:HD13	2.03	0.41
1:A:410:LYS:HE3	3:J:24:GLU:HB3	2.02	0.41
3:D:948:ASN:HA	3:D:951:PHE:HB3	2.02	0.41
2:H:447:THR:HB	2:I:478:ILE:HD13	2.03	0.41
2:I:830:ILE:O	2:I:833:THR:OG1	2.30	0.41
2:B:213:PRO:HB2	3:D:1038:ARG:HB2	2.02	0.41
2:B:246:LEU:HD12	2:B:257:LYS:HB2	2.03	0.41
2:B:686:ASP:OD1	2:B:686:ASP:N	2.53	0.41
2:H:88:ARG:HG2	2:H:116:GLU:HG3	2.03	0.41
2:I:503:ARG:O	2:I:522:ASN:ND2	2.48	0.41
3:J:136:LEU:HD12	3:J:136:LEU:HA	1.88	0.41
3:J:884:ILE:O	3:J:885:ASP:C	2.59	0.41
2:B:75:THR:HG23	2:B:82:TYR:HB2	2.02	0.41
2:B:307:ASN:HB3	2:B:310:ARG:HB2	2.03	0.41
3:D:136:LEU:HD23	3:D:136:LEU:HA	1.92	0.41
3:D:819:THR:HG22	3:D:827:TRP:CH2	2.56	0.41
3:D:1046:TYR:OH	3:D:1170:LEU:O	2.31	0.41
2:H:213:PRO:HB2	3:J:1038:ARG:HB2	2.02	0.41
2:H:528:GLN:H	2:H:528:GLN:HG3	1.73	0.41
3:J:784:LYS:HZ3	3:J:841:LYS:HG2	1.86	0.41
2:C:808:LEU:HD22	2:C:813:TYR:HB2	2.03	0.41
3:D:517:TYR:N	3:D:523:ARG:O	2.53	0.41
3:D:942:LEU:HD22	3:D:950:SER:HB2	2.02	0.41
3:D:1006:TYR:OH	3:D:1135:LYS:NZ	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1334:CYS:O	3:D:1338:VAL:HB	2.20	0.41
3:D:1433:LYS:HA	3:D:1479:LEU:HD13	2.03	0.41
3:J:880:LYS:CD	3:J:926:PHE:HB2	2.51	0.41
3:J:922:GLY:N	3:J:976:HIS:HD1	2.18	0.41
1:A:202:THR:HG22	1:A:223:THR:HG22	2.03	0.40
2:B:88:ARG:HG2	2:B:116:GLU:HG3	2.03	0.40
2:C:809:SER:HA	2:C:860:VAL:HG11	2.02	0.40
3:D:378:ASP:HA	3:D:381:LYS:HD2	2.03	0.40
3:D:450:SER:O	3:D:817:GLN:NE2	2.54	0.40
3:D:815:SER:O	3:D:819:THR:OG1	2.31	0.40
3:D:1584:LEU:HD13	3:D:1643:LEU:HD13	2.03	0.40
1:G:202:THR:HG22	1:G:223:THR:HG22	2.03	0.40
2:H:246:LEU:HD12	2:H:257:LYS:HB2	2.03	0.40
3:D:119:LEU:HD22	3:D:132:VAL:HG13	2.04	0.40
3:J:1006:TYR:OH	3:J:1135:LYS:NZ	2.42	0.40
3:J:1035:ILE:HG23	3:J:1038:ARG:HH22	1.84	0.40
4:K:439:ILE:HD12	4:K:484:LYS:HD2	2.03	0.40
2:C:503:ARG:O	2:C:522:ASN:ND2	2.51	0.40
3:D:376:VAL:HG11	3:D:924:PHE:CE1	2.57	0.40
2:H:331:SER:N	2:H:336:THR:O	2.45	0.40
3:J:942:LEU:HD12	3:J:957:ILE:HD12	2.03	0.40
3:J:1361:GLU:OE1	3:J:1387:ARG:NE	2.49	0.40
3:J:1433:LYS:HA	3:J:1479:LEU:HD13	2.03	0.40
4:K:577:ASP:O	4:K:581:LEU:N	2.47	0.40
2:B:341:SER:OG	2:B:343:ASP:OD1	2.35	0.40
3:D:693:ILE:O	3:D:697:ILE:HG12	2.21	0.40
3:D:1228:ARG:O	3:D:1236:VAL:N	2.45	0.40
2:H:307:ASN:HB3	2:H:310:ARG:HB2	2.03	0.40
2:B:151:LYS:HE3	2:B:151:LYS:HB2	1.95	0.40
3:D:510:LEU:HD23	3:D:510:LEU:HA	1.94	0.40
2:H:495:ILE:HD11	2:H:631:TYR:HB2	2.04	0.40
2:H:808:LEU:HD22	2:H:813:TYR:HB2	2.03	0.40
3:J:888:THR:HG21	3:J:933:LYS:HG3	2.04	0.40
3:J:1288:LYS:HA	3:J:1288:LYS:HD2	1.88	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	A	655/840 (78%)	620 (95%)	32 (5%)	3 (0%)	29	64
1	G	641/840 (76%)	600 (94%)	38 (6%)	3 (0%)	29	64
2	B	794/875 (91%)	768 (97%)	26 (3%)	0	100	100
2	C	373/875 (43%)	353 (95%)	15 (4%)	5 (1%)	12	41
2	H	794/875 (91%)	764 (96%)	29 (4%)	1 (0%)	51	83
2	I	373/875 (43%)	357 (96%)	14 (4%)	2 (0%)	29	64
3	D	1527/1648 (93%)	1445 (95%)	72 (5%)	10 (1%)	22	56
3	J	1527/1648 (93%)	1455 (95%)	59 (4%)	13 (1%)	17	51
4	E	122/625 (20%)	118 (97%)	4 (3%)	0	100	100
4	F	39/625 (6%)	39 (100%)	0	0	100	100
4	K	122/625 (20%)	118 (97%)	4 (3%)	0	100	100
4	L	58/625 (9%)	55 (95%)	3 (5%)	0	100	100
5	M	70/136 (52%)	68 (97%)	2 (3%)	0	100	100
6	N	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
7	O	152/279 (54%)	148 (97%)	4 (3%)	0	100	100
All	All	7323/11494 (64%)	6982 (95%)	304 (4%)	37 (0%)	32	64

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	477	PRO
2	C	478	ILE
2	C	488	PRO
3	D	11	ILE
2	I	488	PRO
3	J	11	ILE
3	J	826	ARG
3	J	903	PRO

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	642	GLN
2	C	835	SER
3	D	173	PHE
3	D	486	ASP
3	D	828	GLU
1	G	112	GLN
2	H	449	PRO
3	J	169	ARG
3	J	174	LEU
3	J	1519	SER
2	C	638	LEU
3	D	266	PRO
3	D	831	ASP
3	D	914	ILE
3	D	916	SER
3	J	170	HIS
3	J	906	GLN
3	J	934	PHE
3	J	936	ASP
1	A	122	HIS
1	G	122	HIS
2	I	477	PRO
3	J	10	ASN
3	D	908	ILE
1	G	634	GLU
3	J	821	ILE
3	D	1445	PRO
3	J	1445	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	596/753 (79%)	572 (96%)	24 (4%)	31 64
1	G	583/753 (77%)	556 (95%)	27 (5%)	27 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	727/790 (92%)	689 (95%)	38 (5%)	23	56
2	C	343/790 (43%)	330 (96%)	13 (4%)	33	66
2	H	727/790 (92%)	692 (95%)	35 (5%)	25	59
2	I	343/790 (43%)	314 (92%)	29 (8%)	10	34
3	D	1419/1528 (93%)	1328 (94%)	91 (6%)	17	47
3	J	1420/1528 (93%)	1331 (94%)	89 (6%)	18	48
4	E	114/557 (20%)	112 (98%)	2 (2%)	59	82
4	F	40/557 (7%)	38 (95%)	2 (5%)	24	57
4	K	114/557 (20%)	112 (98%)	2 (2%)	59	82
4	L	60/557 (11%)	57 (95%)	3 (5%)	24	57
5	M	62/113 (55%)	62 (100%)	0	100	100
6	N	65/81 (80%)	65 (100%)	0	100	100
7	O	142/252 (56%)	140 (99%)	2 (1%)	67	86
All	All	6755/10396 (65%)	6398 (95%)	357 (5%)	26	55

All (357) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	37	LEU
1	A	139	ASP
1	A	187	PHE
1	A	211	THR
1	A	240	TRP
1	A	269	ASP
1	A	415	PHE
1	A	424	LEU
1	A	499	THR
1	A	568	MET
1	A	636	THR
1	A	637	THR
1	A	639	CYS
1	A	653	VAL
1	A	697	ARG
1	A	711	ILE
1	A	715	ASP
1	A	750	LYS

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Mol	Chain	Res	Type
1	A	759	LEU
1	A	773	LEU
1	A	777	LEU
1	A	784	ILE
1	A	789	ASN
2	B	18	LEU
2	B	54	ASP
2	B	70	ASP
2	B	86	GLU
2	B	140	SER
2	B	161	ILE
2	B	220	MET
2	B	241	THR
2	B	267	CYS
2	B	270	LEU
2	B	271	VAL
2	B	299	THR
2	B	371	VAL
2	B	378	LEU
2	B	454	ARG
2	B	505	THR
2	B	515	ASN
2	B	546	LEU
2	B	553	LYS
2	B	558	CYS
2	B	562	ASP
2	B	622	LYS
2	B	629	THR
2	B	665	THR
2	B	670	ASP
2	B	673	LEU
2	B	678	MET
2	B	714	PHE
2	B	727	ASP
2	B	741	CYS
2	B	742	LYS
2	B	754	LYS
2	B	759	PHE
2	B	765	MET
2	B	771	ASN
2	B	801	MET
2	B	815	ASP

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Mol	Chain	Res	Type
2	B	819	ASP
2	C	476	GLN
2	C	490	THR
2	C	495	ILE
2	C	497	LEU
2	C	585	MET
2	C	639	ARG
2	C	653	LEU
2	C	670	ASP
2	C	673	LEU
2	C	742	LYS
2	C	771	ASN
2	C	815	ASP
2	C	841	ASP
3	D	11	ILE
3	D	12	GLU
3	D	88	ARG
3	D	90	MET
3	D	100	TYR
3	D	134	ASP
3	D	142	SER
3	D	172	LYS
3	D	191	LYS
3	D	211	TYR
3	D	233	LYS
3	D	239	MET
3	D	240	LYS
3	D	249	LEU
3	D	276	ARG
3	D	292	LYS
3	D	377	MET
3	D	384	PHE
3	D	405	PHE
3	D	470	PHE
3	D	482	ASP
3	D	486	ASP
3	D	587	ARG
3	D	672	ASN
3	D	673	TYR
3	D	692	ARG
3	D	715	HIS
3	D	735	ASN

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Mol	Chain	Res	Type
3	D	818	LEU
3	D	821	ILE
3	D	822	LEU
3	D	827	TRP
3	D	828	GLU
3	D	830	SER
3	D	831	ASP
3	D	839	PHE
3	D	848	PHE
3	D	890	ILE
3	D	895	ASP
3	D	900	LEU
3	D	906	GLN
3	D	910	THR
3	D	913	LEU
3	D	916	SER
3	D	918	HIS
3	D	927	CYS
3	D	937	LEU
3	D	944	GLN
3	D	949	ASP
3	D	969	ASP
3	D	976	HIS
3	D	981	VAL
3	D	998	LEU
3	D	1015	LYS
3	D	1016	GLN
3	D	1037	SER
3	D	1091	SER
3	D	1110	ASP
3	D	1119	ASP
3	D	1125	ASN
3	D	1148	THR
3	D	1186	THR
3	D	1188	ASP
3	D	1189	ASP
3	D	1202	SER
3	D	1214	LYS
3	D	1229	LEU
3	D	1249	PHE
3	D	1254	SER
3	D	1264	SER

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Mol	Chain	Res	Type
3	D	1275	VAL
3	D	1284	TYR
3	D	1304	LYS
3	D	1305	TYR
3	D	1332	ASN
3	D	1342	VAL
3	D	1362	GLN
3	D	1386	ILE
3	D	1387	ARG
3	D	1397	LYS
3	D	1429	LEU
3	D	1442	ILE
3	D	1446	ASP
3	D	1449	ARG
3	D	1471	ILE
3	D	1477	THR
3	D	1492	VAL
3	D	1514	GLN
3	D	1516	GLN
3	D	1543	VAL
3	D	1559	LEU
4	E	578	ASP
4	E	591	LYS
4	F	463	THR
4	F	466	TYR
1	G	19	GLU
1	G	37	LEU
1	G	139	ASP
1	G	177	VAL
1	G	187	PHE
1	G	211	THR
1	G	240	TRP
1	G	269	ASP
1	G	335	LYS
1	G	357	LYS
1	G	554	SER
1	G	555	SER
1	G	633	GLU
1	G	636	THR
1	G	637	THR
1	G	641	LEU
1	G	642	GLN

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Mol	Chain	Res	Type
1	G	660	ASP
1	G	711	ILE
1	G	713	SER
1	G	751	MET
1	G	753	THR
1	G	773	LEU
1	G	791	GLN
1	G	794	HIS
1	G	801	ASN
1	G	813	SER
2	H	18	LEU
2	H	54	ASP
2	H	70	ASP
2	H	86	GLU
2	H	140	SER
2	H	161	ILE
2	H	220	MET
2	H	241	THR
2	H	267	CYS
2	H	270	LEU
2	H	271	VAL
2	H	299	THR
2	H	371	VAL
2	H	378	LEU
2	H	454	ARG
2	H	483	THR
2	H	491	SER
2	H	509	SER
2	H	515	ASN
2	H	553	LYS
2	H	558	CYS
2	H	567	PHE
2	H	627	THR
2	H	637	SER
2	H	665	THR
2	H	754	LYS
2	H	758	ARG
2	H	759	PHE
2	H	767	GLU
2	H	790	ARG
2	H	798	SER
2	H	801	MET

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Mol	Chain	Res	Type
2	H	816	ARG
2	H	849	LYS
2	H	870	GLU
2	I	479	ASP
2	I	489	ASN
2	I	490	THR
2	I	503	ARG
2	I	537	SER
2	I	542	GLN
2	I	562	ASP
2	I	578	SER
2	I	585	MET
2	I	605	LEU
2	I	606	CYS
2	I	612	GLU
2	I	628	ASN
2	I	637	SER
2	I	639	ARG
2	I	646	THR
2	I	654	CYS
2	I	670	ASP
2	I	680	THR
2	I	683	LEU
2	I	747	LEU
2	I	754	LYS
2	I	779	SER
2	I	815	ASP
2	I	825	TYR
2	I	840	LYS
2	I	841	ASP
2	I	854	CYS
2	I	856	ASP
3	J	8	ASN
3	J	9	SER
3	J	66	ARG
3	J	71	ARG
3	J	88	ARG
3	J	105	SER
3	J	121	GLU
3	J	142	SER
3	J	182	MET
3	J	204	GLU

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Mol	Chain	Res	Type
3	J	212	LYS
3	J	213	ASP
3	J	443	ASN
3	J	470	PHE
3	J	486	ASP
3	J	553	LEU
3	J	672	ASN
3	J	783	MET
3	J	816	SER
3	J	817	GLN
3	J	818	LEU
3	J	824	SER
3	J	826	ARG
3	J	827	TRP
3	J	848	PHE
3	J	875	SER
3	J	878	LYS
3	J	879	MET
3	J	880	LYS
3	J	881	ASP
3	J	883	MET
3	J	888	THR
3	J	895	ASP
3	J	899	LYS
3	J	903	PRO
3	J	906	GLN
3	J	910	THR
3	J	916	SER
3	J	918	HIS
3	J	927	CYS
3	J	933	LYS
3	J	935	LEU
3	J	937	LEU
3	J	939	GLU
3	J	944	GLN
3	J	949	ASP
3	J	969	ASP
3	J	976	HIS
3	J	981	VAL
3	J	998	LEU
3	J	1015	LYS
3	J	1016	GLN

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Mol	Chain	Res	Type
3	J	1037	SER
3	J	1091	SER
3	J	1110	ASP
3	J	1119	ASP
3	J	1125	ASN
3	J	1148	THR
3	J	1186	THR
3	J	1188	ASP
3	J	1189	ASP
3	J	1202	SER
3	J	1214	LYS
3	J	1229	LEU
3	J	1249	PHE
3	J	1254	SER
3	J	1264	SER
3	J	1275	VAL
3	J	1284	TYR
3	J	1304	LYS
3	J	1305	TYR
3	J	1332	ASN
3	J	1342	VAL
3	J	1362	GLN
3	J	1386	ILE
3	J	1387	ARG
3	J	1397	LYS
3	J	1429	LEU
3	J	1442	ILE
3	J	1446	ASP
3	J	1449	ARG
3	J	1471	ILE
3	J	1477	THR
3	J	1492	VAL
3	J	1515	LEU
3	J	1516	GLN
3	J	1518	LYS
3	J	1543	VAL
3	J	1559	LEU
4	K	578	ASP
4	K	591	LYS
4	L	463	THR
4	L	466	TYR
4	L	568	LYS

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Mol	Chain	Res	Type
7	O	1	MET
7	O	52	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	GLN
1	A	746	HIS
1	A	789	ASN
2	B	39	GLN
2	B	65	GLN
2	B	677	ASN
2	B	783	ASN
2	C	548	GLN
2	C	744	ASN
2	C	822	GLN
3	D	10	ASN
3	D	72	ASN
3	D	118	ASN
3	D	184	ASN
3	D	585	ASN
3	D	601	ASN
3	D	735	ASN
3	D	802	GLN
3	D	825	ASN
3	D	865	ASN
3	D	1020	ASN
3	D	1044	ASN
3	D	1118	ASN
3	D	1250	ASN
3	D	1332	ASN
3	D	1377	GLN
4	E	476	ASN
2	H	39	GLN
2	H	40	GLN
2	H	65	GLN
2	H	861	GLN
2	I	476	GLN
2	I	542	GLN
3	J	43	ASN
3	J	87	ASN
3	J	110	ASN

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Mol	Chain	Res	Type
3	J	125	HIS
3	J	160	GLN
3	J	162	ASN
3	J	417	GLN
3	J	443	ASN
3	J	487	HIS
3	J	687	GLN
3	J	695	GLN
3	J	735	ASN
3	J	823	ASN
3	J	918	HIS
3	J	953	GLN
3	J	1020	ASN
3	J	1044	ASN
3	J	1118	ASN
3	J	1250	ASN
3	J	1332	ASN
3	J	1377	GLN
3	J	1516	GLN
4	K	476	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 monosaccharides 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.

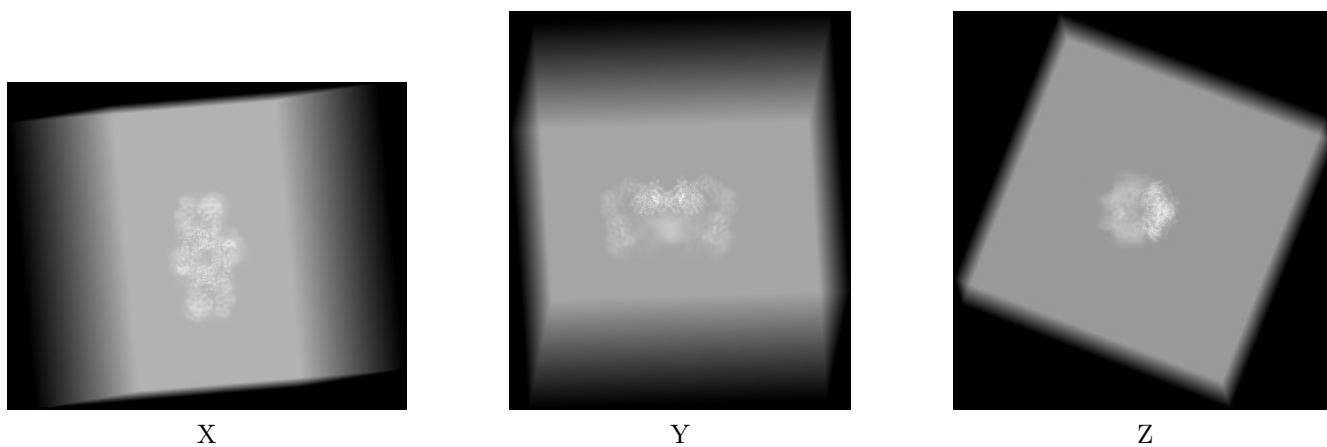
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40037. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



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

6.2 Central slices [i](#)

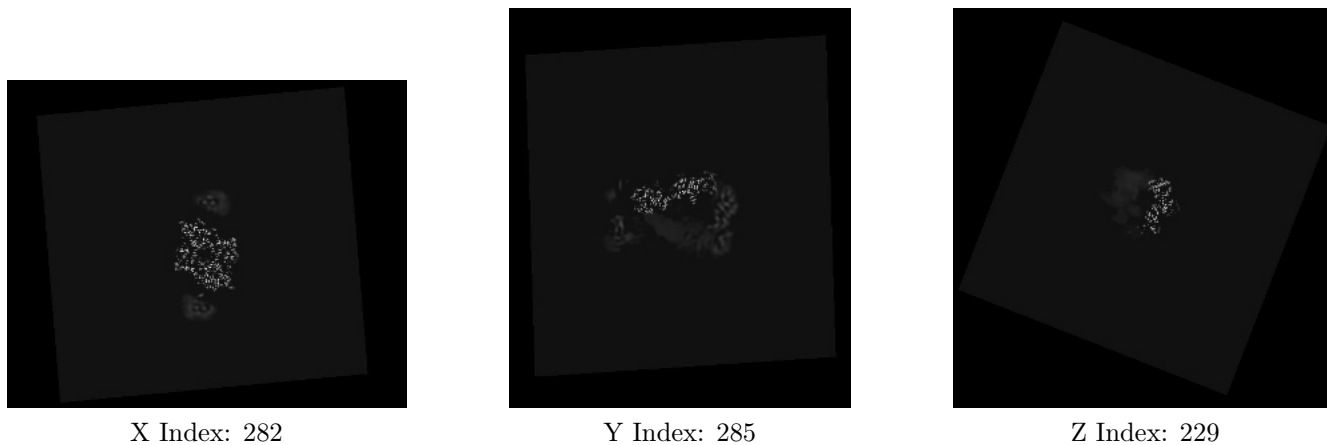
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

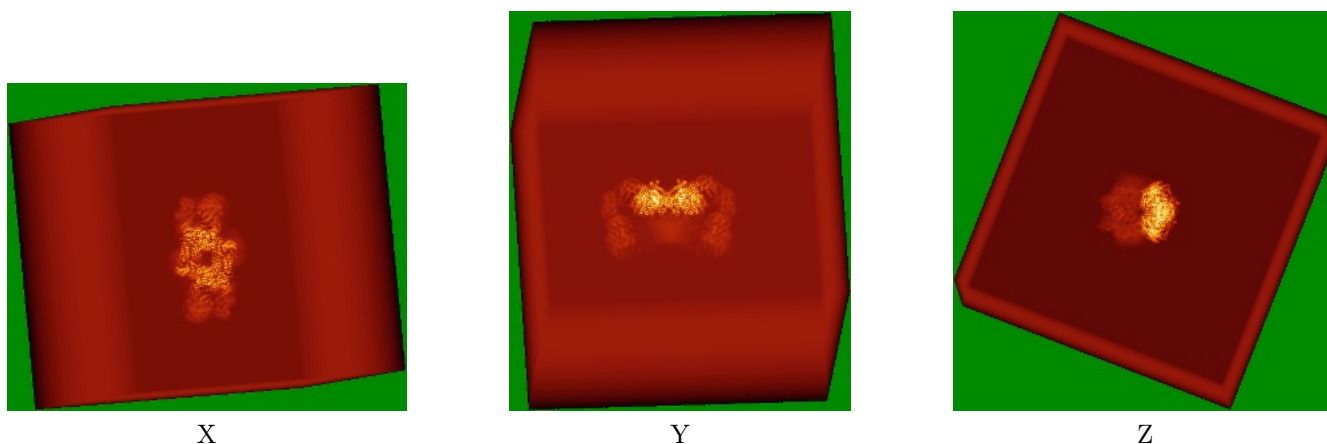
6.3.1 Primary map



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



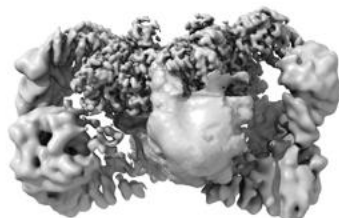
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

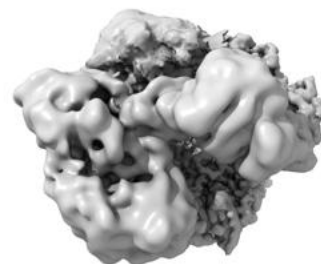
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

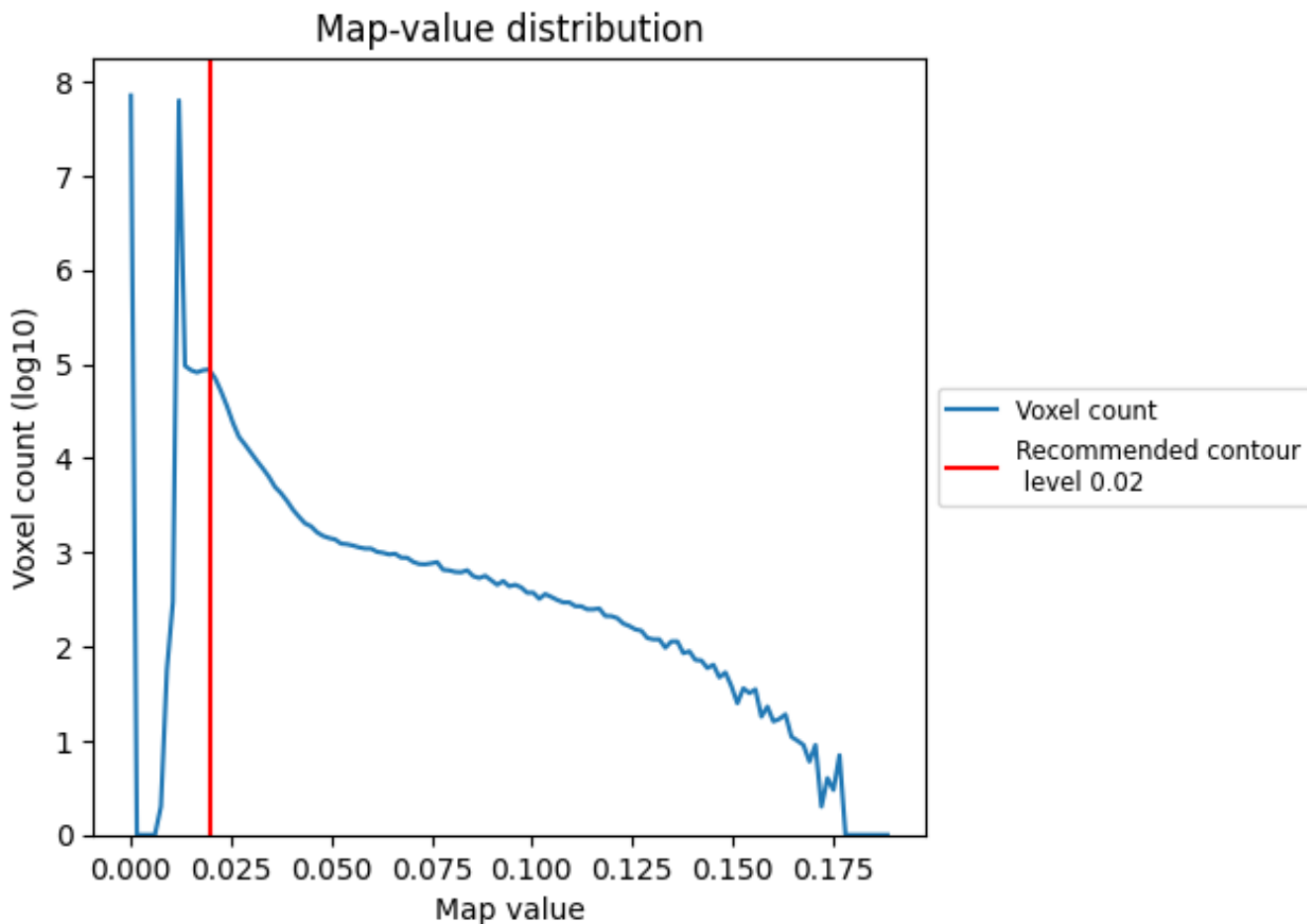
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

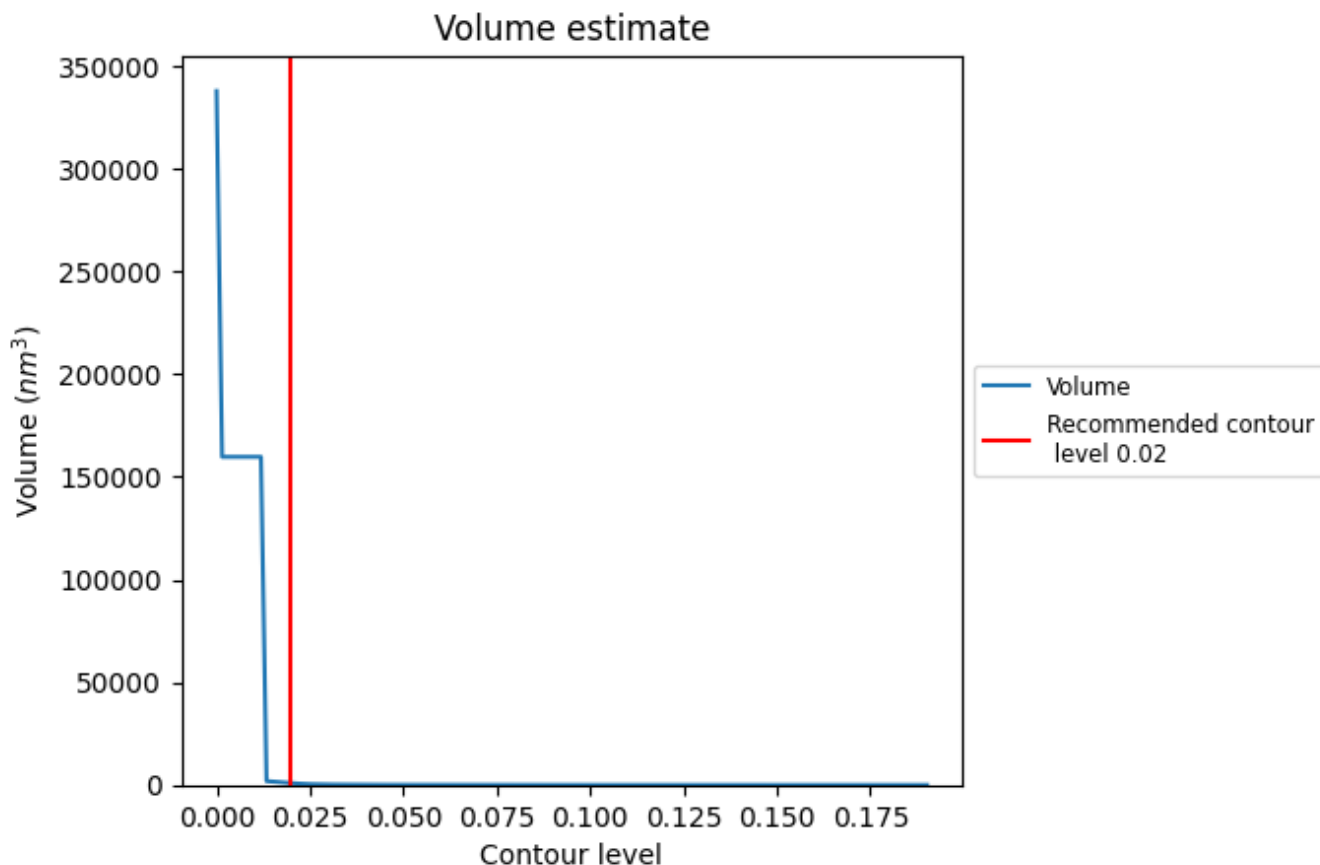
This section contains the results of statistical analysis of the map.

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 910 nm^3 ; this corresponds to an approximate mass of 822 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.

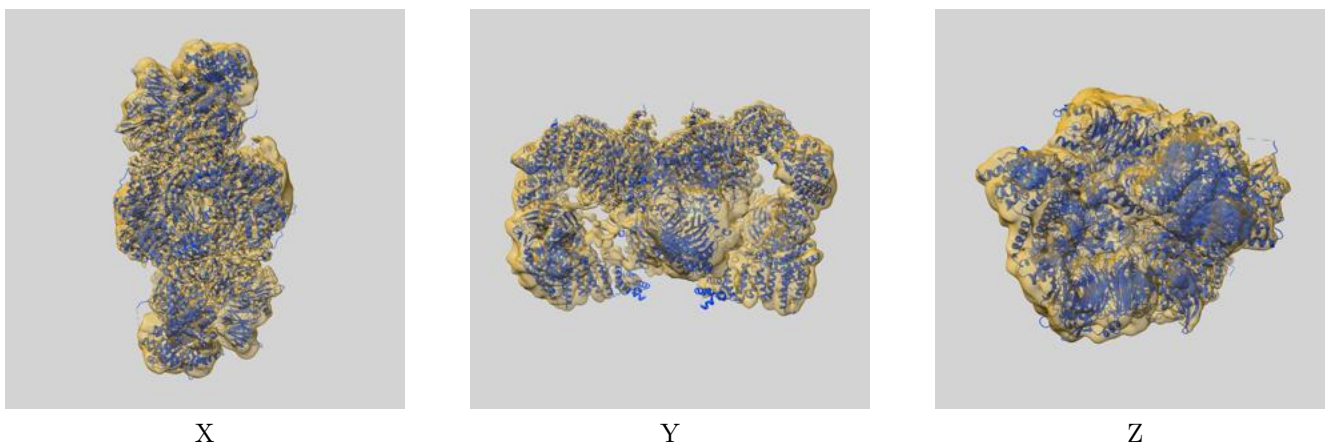
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

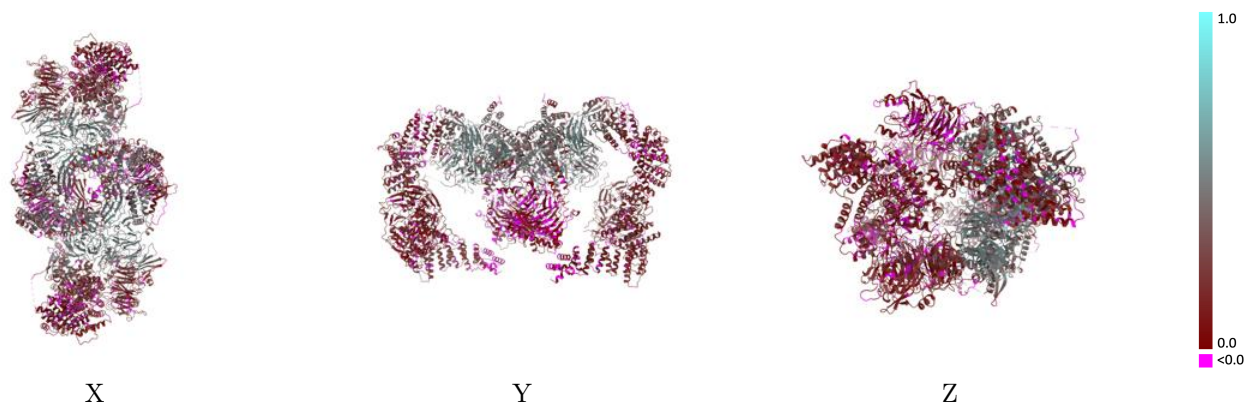
This section contains information regarding the fit between EMDB map EMD-40037 and PDB model 8GHN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



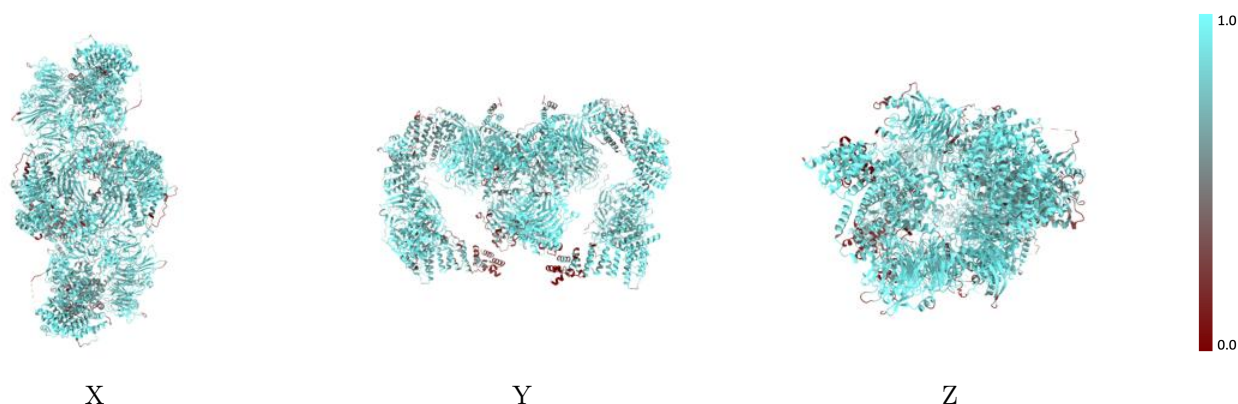
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



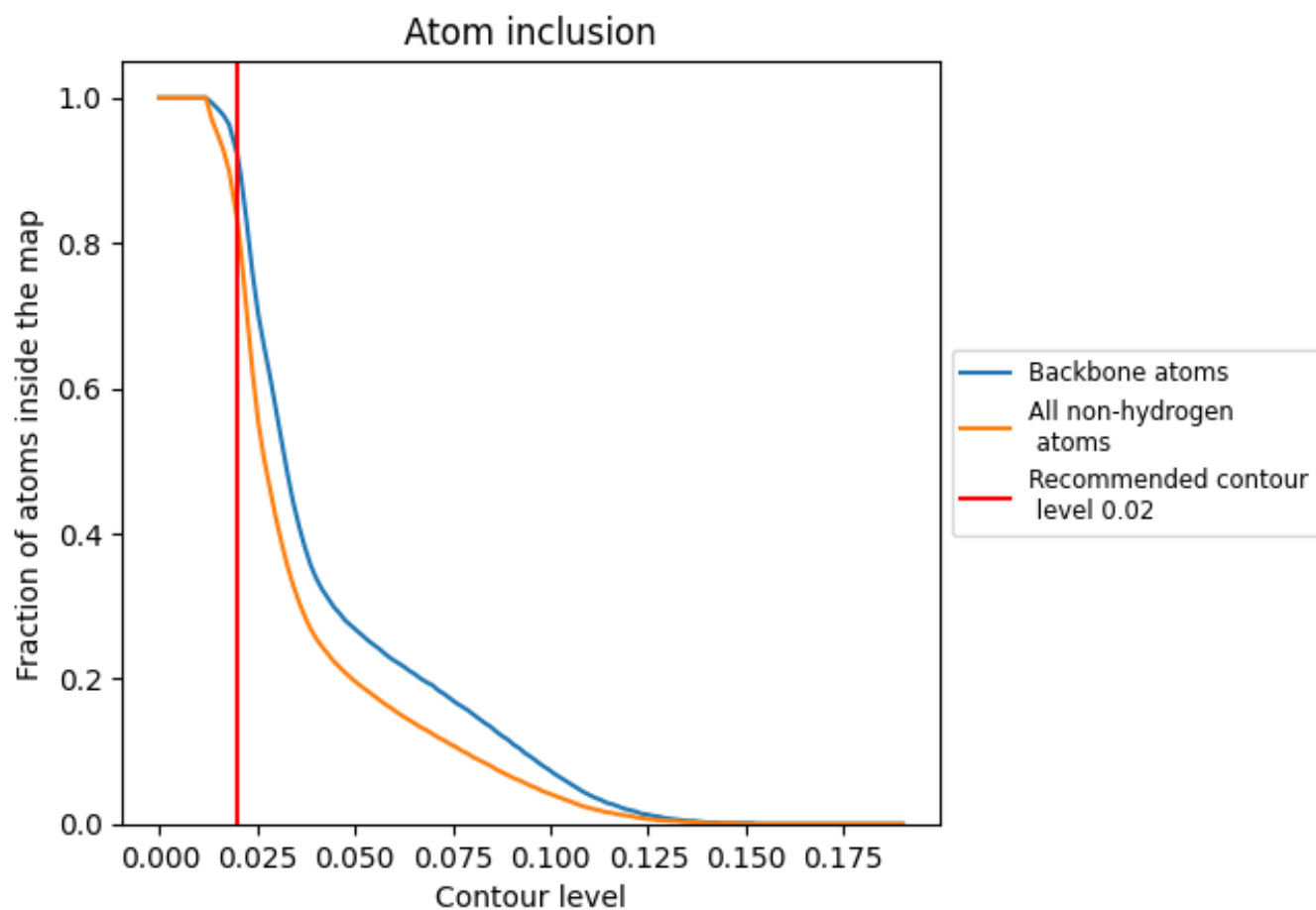
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8290	 0.2320
A	 0.8490	 0.2160
B	 0.8800	 0.3060
C	 0.8750	 0.4510
D	 0.8060	 0.1860
E	 0.8510	 0.1440
F	 0.4610	 -0.0110
G	 0.8980	 0.2180
H	 0.8720	 0.2980
I	 0.8660	 0.4540
J	 0.7590	 0.1820
K	 0.8010	 0.1290
L	 0.9060	 0.0290
M	 0.8920	 0.0190
N	 0.8910	 0.0470
O	 0.7220	 0.0400

