



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:21 PM UTC

PDB ID : 6O9M / pdb_00006o9m
EMDB ID : EMD-3802
Title : Structure of the human apo TFIIH
Authors : Yan, C.L.; Dodd, T.; He, Y.; Tainer, J.A.; Tsutakawa, S.E.; Ivanov, I.
Deposited on : 2019-03-14
Resolution : 4.40 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:

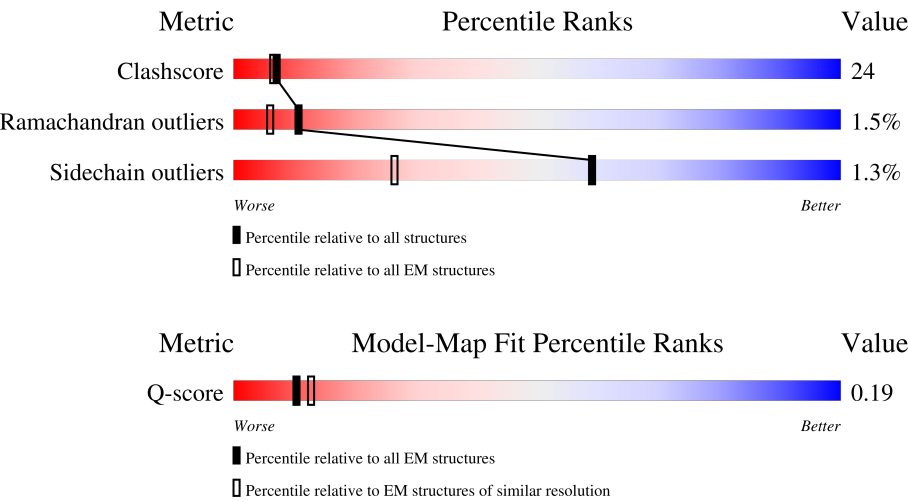
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.40 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	3132 (3.91 - 4.90)

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	0	760	16% 50% 41% . .
2	1	548	53% 49% 28% . 21%
3	2	462	30% 49% 47% . .
4	3	309	32% 42% 24% . 31%

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Mol	Chain	Length	Quality of chain
5	4	308	28% 52% 43%
6	5	71	28% 68% 25% 7%
7	6	395	33% 60% 36%
8	7	782	20% 46% 35% 17%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25785 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 TFIIF basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	732	Total	C	N	O	S	0	0
			5861	3742	1023	1068	28		

- Molecule 2 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	433	Total	C	N	O	S	0	0
			3436	2153	602	664	17		

- Molecule 3 is a protein called General transcription factor IIF subunit 4, p52.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	453	Total	C	N	O	S	0	0
			3613	2323	634	642	14		

- Molecule 4 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	212	Total	C	N	O	S	0	0
			1754	1091	309	343	11		

- Molecule 5 is a protein called General transcription factor IIF subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	295	Total	C	N	O	S	0	0
			2306	1477	384	426	19		

- Molecule 6 is a protein called General transcription factor IIF subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

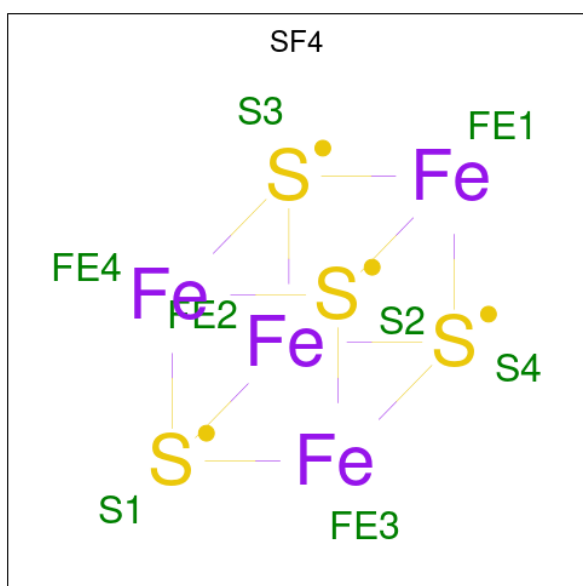
- Molecule 7 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	385	Total	C	N	O	S	0	0
			3024	1909	524	564	27		

- Molecule 8 is a protein called TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	652	Total	C	N	O	S	0	0
			5255	3345	898	980	32		

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
9	0	1	Total	Fe	S	0
			8	4	4	

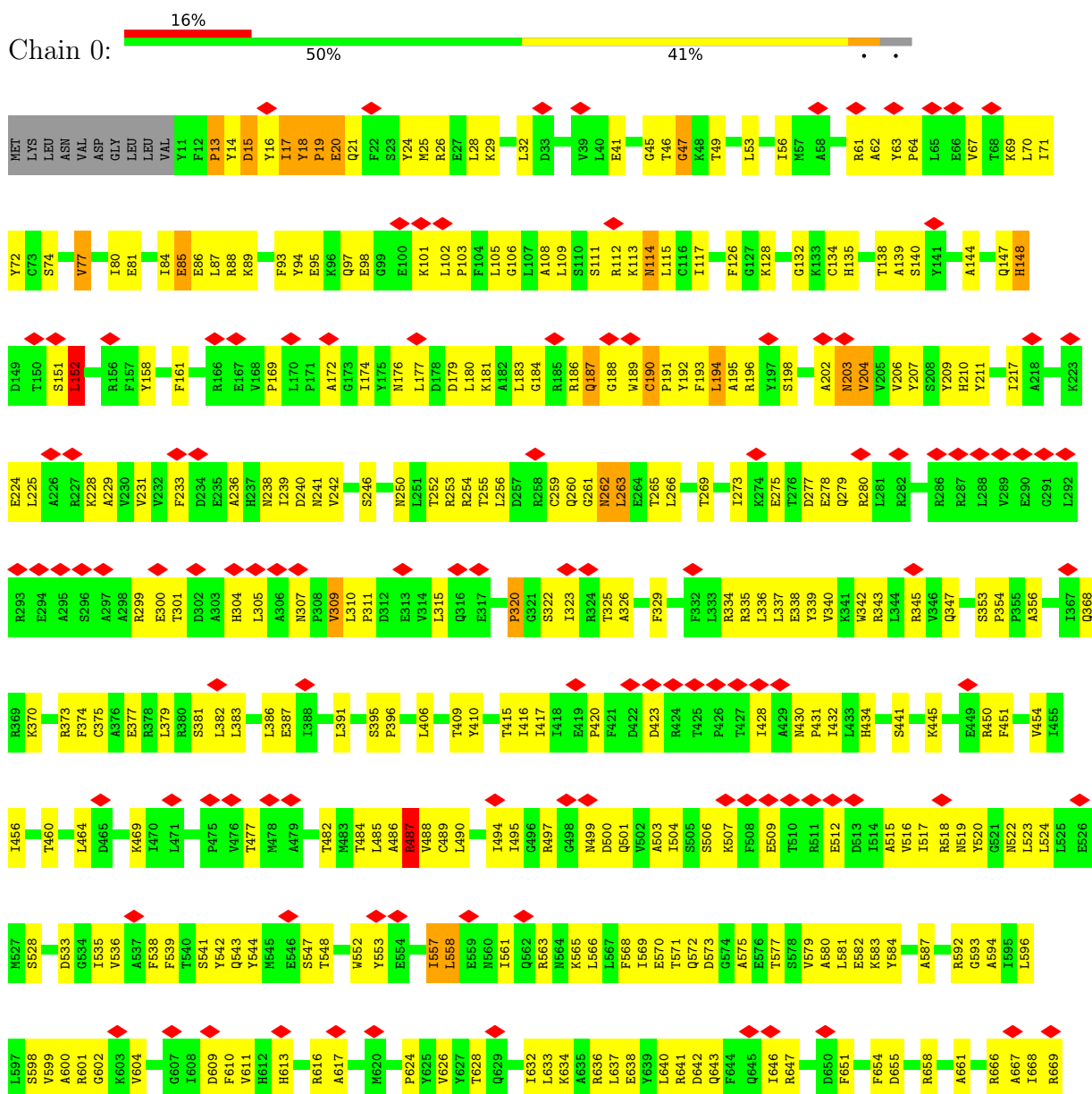
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

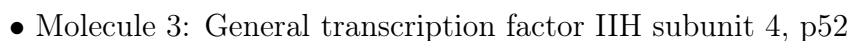
Mol	Chain	Residues	Atoms		AltConf
10	3	2	Total	Zn	0
			2	2	
10	4	1	Total	Zn	0
			1	1	
10	6	3	Total	Zn	0
			3	3	

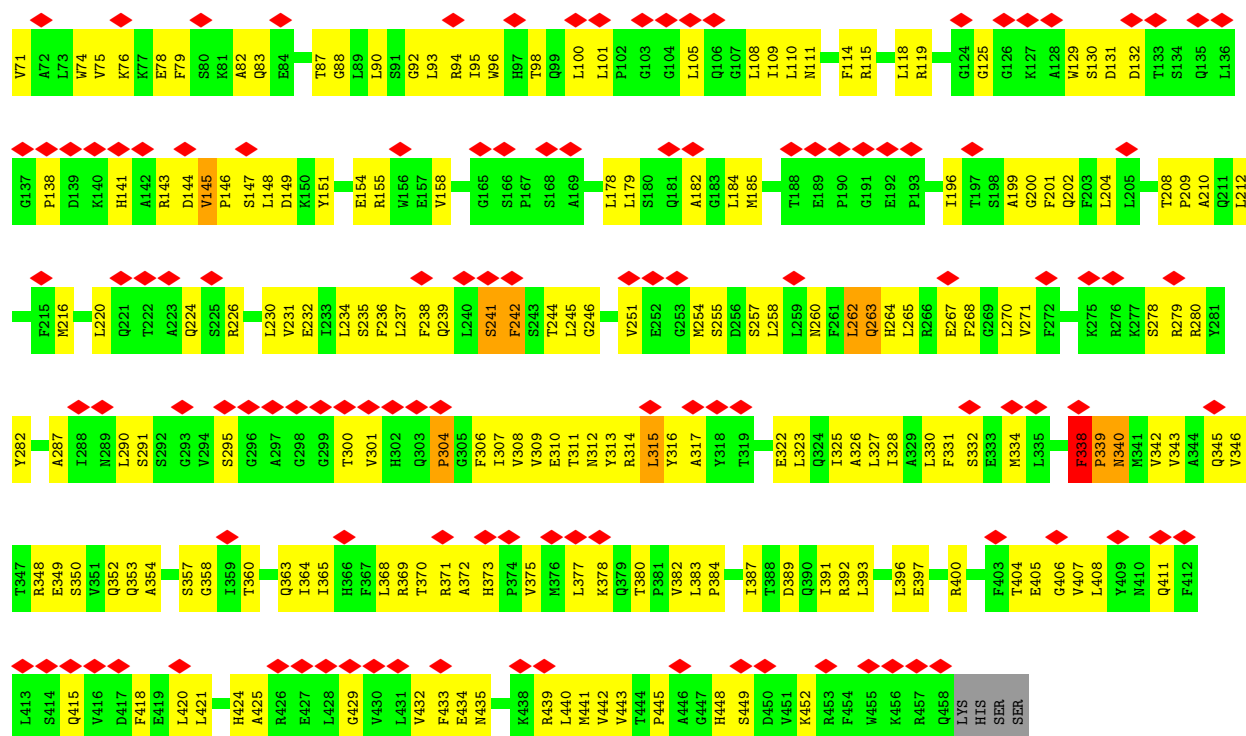
3 Residue-property plots

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.

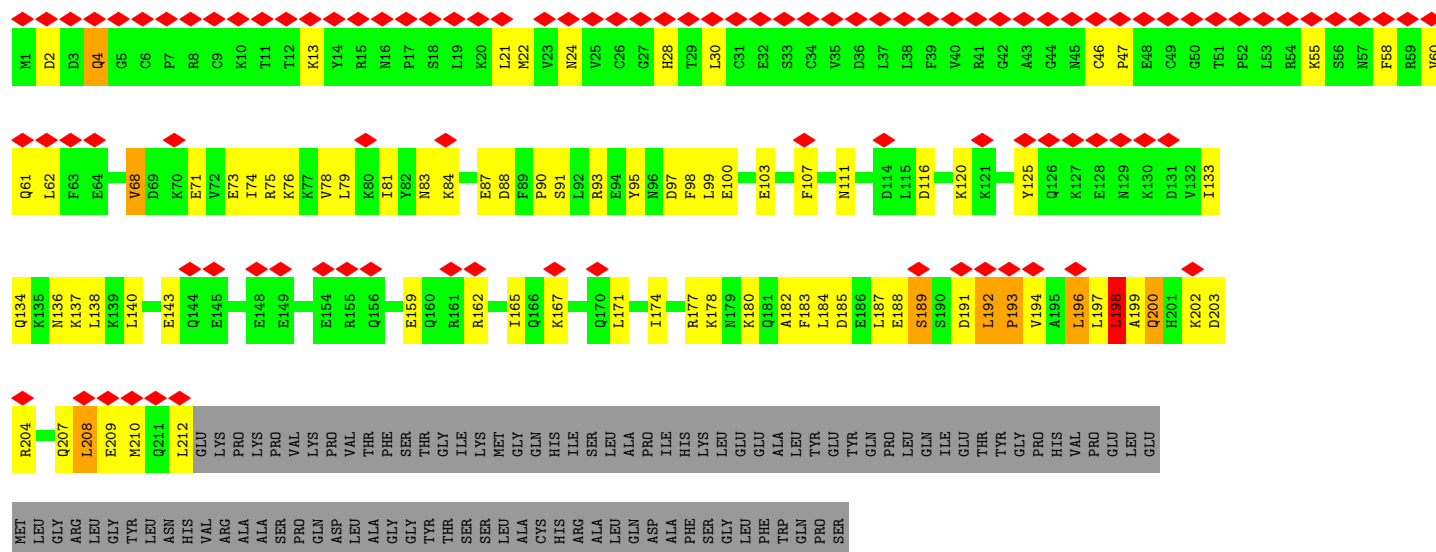
- Molecule 1: TFIIH basal transcription factor complex helicase XPD subunit





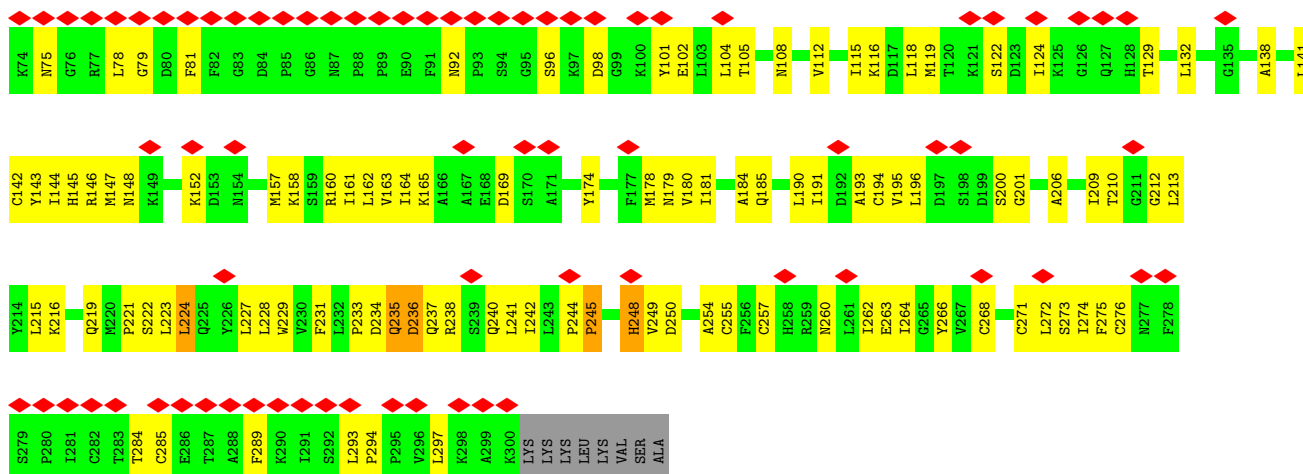


• Molecule 4: CDK-activating kinase assembly factor MAT1

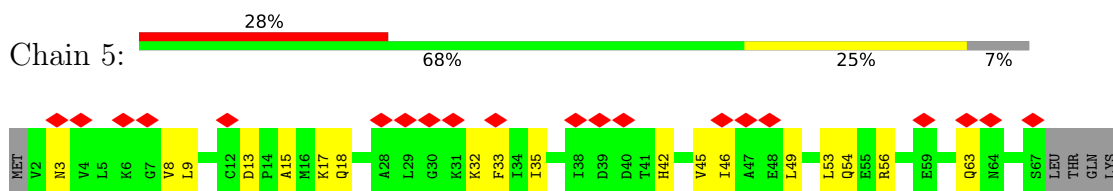


• Molecule 5: General transcription factor IIH subunit 3

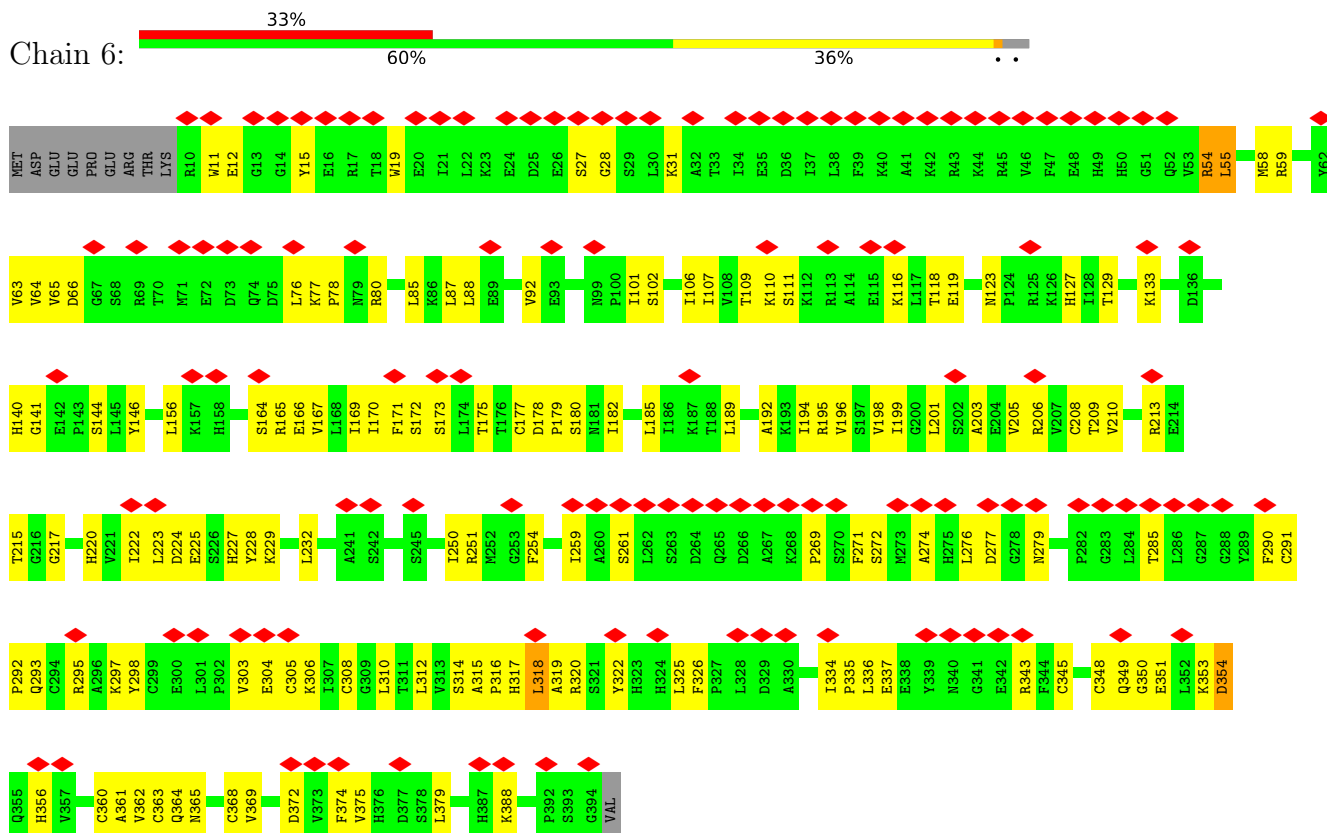




• Molecule 6: General transcription factor IIH subunit 5



• Molecule 7: General transcription factor IIH subunit 2



• Molecule 8: TFIIH basal transcription factor complex helicase XPB subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122900	Depositor
Resolution determination method	Not provided	
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4

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	0	0.52	5/5984 (0.1%)	0.96	30/8104 (0.4%)
2	1	0.33	1/3502 (0.0%)	0.82	5/4731 (0.1%)
3	2	0.40	0/3697	0.96	9/5011 (0.2%)
4	3	0.42	4/1774 (0.2%)	0.90	11/2378 (0.5%)
5	4	0.44	0/2353	0.94	7/3187 (0.2%)
6	5	0.34	0/528	0.79	2/713 (0.3%)
7	6	0.42	0/3094	0.85	4/4188 (0.1%)
8	7	0.39	0/5365	0.88	10/7247 (0.1%)
All	All	0.43	10/26297 (0.0%)	0.91	78/35559 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	673	ASP	CA-C	8.74	1.64	1.52
1	0	109	LEU	CA-C	-8.13	1.44	1.53
4	3	189	SER	CA-C	6.33	1.61	1.52
2	1	417	LYS	CA-C	6.19	1.58	1.52
1	0	109	LEU	N-CA	5.97	1.54	1.46
1	0	686	ARG	CA-C	5.77	1.59	1.52
4	3	196	LEU	CA-C	5.59	1.60	1.52
4	3	197	LEU	CA-C	5.20	1.59	1.52
4	3	200	GLN	CA-C	5.04	1.59	1.52
1	0	262	ASN	CA-C	5.03	1.60	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	338	PHE	CA-C-N	14.57	138.05	119.84
3	2	338	PHE	C-N-CA	14.57	138.05	119.84
1	0	152	LEU	CA-C-N	-12.42	104.31	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	152	LEU	C-N-CA	-12.42	104.31	119.84
1	0	726	GLN	CA-C-N	10.66	133.16	119.84
1	0	726	GLN	C-N-CA	10.66	133.16	119.84
1	0	18	TYR	CA-C-N	9.85	132.15	119.84
1	0	18	TYR	C-N-CA	9.85	132.15	119.84
6	5	63	GLN	N-CA-C	9.18	121.29	111.28
1	0	687	GLY	N-CA-C	8.85	122.77	112.50
4	3	197	LEU	N-CA-C	8.72	124.23	113.50
8	7	634	ARG	N-CA-C	8.38	121.47	111.33
5	4	245	PRO	N-CA-C	-8.16	100.75	110.70
2	1	417	LYS	N-CA-C	8.09	123.69	112.93
1	0	686	ARG	N-CA-C	7.91	123.51	113.55
1	0	261	GLY	N-CA-C	7.76	123.41	113.24
3	2	50	SER	N-CA-C	-7.74	103.86	113.38
8	7	61	TYR	N-CA-C	7.63	122.41	113.18
5	4	245	PRO	CA-C-N	-7.57	110.38	119.84
5	4	245	PRO	C-N-CA	-7.57	110.38	119.84
8	7	477	ILE	N-CA-C	-7.36	104.68	111.67
8	7	313	THR	N-CA-C	7.34	121.28	111.30
4	3	208	LEU	N-CA-C	7.33	120.33	111.82
4	3	197	LEU	CA-C-O	7.29	127.16	119.14
8	7	277	ILE	N-CA-C	-7.24	106.84	113.71
4	3	189	SER	N-CA-C	7.14	123.48	113.56
2	1	165	GLY	N-CA-C	-6.97	101.21	113.76
1	0	109	LEU	CB-CA-C	-6.95	101.48	112.05
8	7	309	ASP	N-CA-C	-6.87	99.50	110.14
4	3	196	LEU	CA-C-O	6.83	127.79	120.55
8	7	159	CYS	N-CA-C	-6.81	105.10	113.41
1	0	673	ASP	CA-C-O	6.52	129.83	120.51
1	0	85	GLU	N-CA-C	6.44	117.97	111.07
1	0	87	LEU	N-CA-C	-6.43	104.92	112.89
4	3	125	TYR	N-CA-C	-6.40	106.68	114.75
2	1	338	ASN	N-CA-C	-6.33	105.38	113.23
1	0	262	ASN	CA-C-O	6.29	127.04	119.43
4	3	55	LYS	CA-C-N	6.28	133.53	121.54
4	3	55	LYS	C-N-CA	6.28	133.53	121.54
1	0	673	ASP	N-CA-C	6.23	124.07	110.80
7	6	325	LEU	N-CA-C	-6.14	107.02	114.75
4	3	189	SER	CA-C-O	6.13	127.62	119.59
5	4	236	ASP	N-CA-C	-6.04	105.57	113.12
7	6	55	LEU	N-CA-C	5.93	119.30	110.52
3	2	334	MET	CA-C-N	5.90	132.81	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	334	MET	C-N-CA	5.90	132.81	121.54
4	3	197	LEU	N-CA-CB	-5.84	101.95	110.53
1	0	512	GLU	N-CA-C	-5.69	108.14	114.62
2	1	418	LEU	N-CA-C	5.65	122.83	110.80
3	2	132	ASP	N-CA-C	5.59	122.70	110.80
1	0	686	ARG	CA-C-O	5.55	126.05	119.67
5	4	233	PRO	CA-C-N	5.49	132.03	121.54
5	4	233	PRO	C-N-CA	5.49	132.03	121.54
1	0	262	ASN	CB-CA-C	-5.45	100.66	110.37
1	0	558	LEU	CA-C-N	5.44	128.32	120.38
1	0	558	LEU	C-N-CA	5.44	128.32	120.38
3	2	432	VAL	N-CA-C	-5.44	107.50	111.90
6	5	35	ILE	N-CA-C	-5.41	106.40	111.48
8	7	151	GLY	N-CA-C	-5.39	107.58	114.37
1	0	13	PRO	CA-C-N	5.38	131.81	121.54
1	0	13	PRO	C-N-CA	5.38	131.81	121.54
1	0	87	LEU	N-CA-CB	5.36	119.14	110.40
1	0	368	GLN	CA-C-N	5.31	131.68	121.54
1	0	368	GLN	C-N-CA	5.31	131.68	121.54
1	0	685	ALA	N-CA-C	5.29	116.73	111.07
7	6	354	ASP	CA-C-N	5.29	129.63	122.07
7	6	354	ASP	C-N-CA	5.29	129.63	122.07
8	7	263	GLU	CA-C-N	5.26	131.59	121.54
8	7	263	GLU	C-N-CA	5.26	131.59	121.54
3	2	263	GLN	N-CA-C	-5.23	105.69	111.71
1	0	20	GLU	CA-C-N	-5.22	112.76	120.28
1	0	20	GLU	C-N-CA	-5.22	112.76	120.28
1	0	632	ILE	N-CA-C	-5.21	105.25	112.50
5	4	152	LYS	N-CA-C	-5.20	106.73	114.64
3	2	315	LEU	N-CA-C	5.18	121.83	110.80
2	1	324	ALA	N-CA-C	5.15	118.43	111.17
4	3	198	LEU	N-CA-C	5.14	121.75	110.80
1	0	263	LEU	N-CA-C	-5.03	100.09	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	5861	0	5869	381	0
2	1	3436	0	3403	167	0
3	2	3613	0	3657	200	0
4	3	1754	0	1771	79	0
5	4	2306	0	2332	116	0
6	5	522	0	528	14	0
7	6	3024	0	2991	119	0
8	7	5255	0	5247	280	0
9	0	8	0	0	1	0
10	3	2	0	0	0	0
10	4	1	0	0	0	0
10	6	3	0	0	0	0
All	All	25785	0	25798	1231	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 24.

All (1231) 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)
3:2:338:PHE:CZ	8:7:79:ALA:HB2	1.35	1.60
1:0:111:SER:HB2	1:0:192:TYR:CE1	1.40	1.52
3:2:338:PHE:HB2	3:2:339:PRO:CD	1.20	1.50
1:0:111:SER:CB	1:0:192:TYR:CE1	1.91	1.50
1:0:111:SER:CB	1:0:192:TYR:HE1	1.26	1.44
1:0:726:GLN:CB	1:0:727:PRO:CD	1.99	1.40
1:0:135:HIS:CE1	1:0:299:ARG:HG3	1.57	1.36
1:0:111:SER:HB2	1:0:192:TYR:CZ	1.58	1.35
3:2:338:PHE:CB	3:2:339:PRO:HD2	1.55	1.35
1:0:726:GLN:CB	1:0:727:PRO:HD2	1.42	1.31
2:1:187:ASN:HB2	2:1:191:ASP:CB	1.63	1.29
1:0:62:ALA:O	1:0:64:PRO:HD3	1.20	1.27
1:0:189:TRP:O	1:0:194:LEU:HB2	1.22	1.25
4:3:209:GLU:OE1	4:3:210:MET:HE2	1.37	1.24
1:0:134:CYS:SG	1:0:299:ARG:NH2	2.09	1.23
2:1:483:THR:OG1	2:1:484:PRO:HD3	1.38	1.22
1:0:726:GLN:HB3	1:0:727:PRO:CD	1.62	1.22
1:0:158:TYR:CE1	1:0:193:PHE:CZ	2.28	1.21
1:0:20:GLU:OE1	1:0:482:THR:HG22	1.41	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:158:TYR:CD1	1:0:193:PHE:CZ	2.30	1.19
3:2:338:PHE:CZ	8:7:79:ALA:CB	2.26	1.18
3:2:338:PHE:CB	3:2:339:PRO:CD	2.00	1.18
8:7:289:TYR:H	8:7:290:PRO:HD3	1.07	1.18
8:7:472:ARG:HG3	8:7:473:GLU:HG3	1.27	1.14
8:7:314:ALA:CB	8:7:381:TRP:HD1	1.60	1.14
1:0:189:TRP:O	1:0:194:LEU:CB	1.97	1.13
1:0:158:TYR:HE1	1:0:193:PHE:CE1	1.67	1.11
1:0:112:ARG:CD	2:1:271:ALA:HB1	1.81	1.11
1:0:111:SER:HB3	1:0:192:TYR:CE1	1.87	1.10
1:0:112:ARG:HD3	2:1:271:ALA:HB1	1.13	1.09
1:0:135:HIS:CE1	1:0:299:ARG:C	2.30	1.09
3:2:338:PHE:HB2	3:2:339:PRO:HD3	1.09	1.08
8:7:359:LYS:NZ	8:7:436:GLY:HA2	1.68	1.08
1:0:726:GLN:HB3	1:0:727:PRO:HD3	1.21	1.08
2:1:187:ASN:HB2	2:1:191:ASP:HB3	1.06	1.06
1:0:45:GLY:O	1:0:670:GLY:O	1.73	1.05
2:1:187:ASN:CB	2:1:191:ASP:HB3	1.86	1.05
3:2:49:PRO:O	3:2:53:LYS:HG3	1.58	1.04
3:2:338:PHE:CG	3:2:339:PRO:HD2	1.92	1.04
1:0:158:TYR:CE1	1:0:193:PHE:CE1	2.46	1.03
1:0:183:LEU:HB3	1:0:188:GLY:H	1.18	1.03
8:7:62:ARG:HA	8:7:73:SER:HB2	1.34	1.03
3:2:317:ALA:HA	3:2:340:ASN:O	1.60	1.02
1:0:111:SER:CA	1:0:192:TYR:HE1	1.73	1.02
1:0:62:ALA:O	1:0:64:PRO:CD	2.07	1.01
3:2:338:PHE:CD2	3:2:339:PRO:HD2	1.96	1.01
1:0:135:HIS:HE1	1:0:299:ARG:C	1.67	1.00
8:7:314:ALA:CB	8:7:381:TRP:CD1	2.45	0.99
4:3:209:GLU:OE1	4:3:210:MET:CE	2.09	0.99
1:0:668:ILE:HG13	1:0:673:ASP:HB2	1.42	0.99
1:0:135:HIS:ND1	1:0:299:ARG:HG3	1.77	0.98
1:0:726:GLN:HB2	1:0:727:PRO:CD	1.73	0.98
8:7:314:ALA:HB1	8:7:381:TRP:CD1	1.98	0.98
1:0:158:TYR:HD1	1:0:193:PHE:CE2	1.81	0.98
1:0:16:TYR:CE1	1:0:18:TYR:HE1	1.82	0.97
1:0:183:LEU:HB3	1:0:188:GLY:N	1.77	0.97
8:7:359:LYS:HZ1	8:7:436:GLY:CA	1.79	0.96
1:0:135:HIS:NE2	1:0:300:GLU:HA	1.78	0.96
1:0:111:SER:HB3	1:0:192:TYR:HE1	1.25	0.94
1:0:581:LEU:HD21	2:1:263:LYS:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:483:THR:OG1	2:1:484:PRO:CD	2.15	0.94
8:7:359:LYS:HZ1	8:7:436:GLY:HA2	1.31	0.94
1:0:487:ARG:HH22	1:0:728:PHE:HB3	1.31	0.94
1:0:705:ASN:HB2	1:0:708:LEU:HD11	1.48	0.94
1:0:126:PHE:HB3	2:1:274:ASP:OD2	1.66	0.93
1:0:16:TYR:HE1	1:0:18:TYR:CE1	1.86	0.92
1:0:112:ARG:HD3	2:1:271:ALA:CB	2.00	0.92
1:0:16:TYR:CE1	1:0:18:TYR:CE1	2.58	0.91
3:2:100:LEU:C	3:2:101:LEU:HD12	1.93	0.91
1:0:203:ASN:O	1:0:204:VAL:HG23	1.70	0.91
8:7:289:TYR:H	8:7:290:PRO:CD	1.82	0.91
8:7:62:ARG:HD3	8:7:75:PRO:CD	2.00	0.91
1:0:111:SER:O	1:0:192:TYR:OH	1.86	0.91
8:7:62:ARG:HD3	8:7:75:PRO:HD2	1.51	0.90
1:0:135:HIS:CE1	1:0:299:ARG:CG	2.52	0.90
3:2:338:PHE:HZ	8:7:79:ALA:HB2	1.20	0.90
8:7:289:TYR:N	8:7:290:PRO:HD3	1.86	0.90
1:0:114:ASN:ND2	1:0:177:LEU:HD13	1.88	0.89
8:7:35:GLN:CD	8:7:159:CYS:HB3	1.98	0.89
2:1:414:TYR:C	2:1:416:PRO:HD3	1.98	0.89
8:7:314:ALA:HB2	8:7:381:TRP:HD1	1.37	0.88
4:3:194:VAL:HG12	4:3:198:LEU:HD13	1.56	0.88
1:0:135:HIS:CE1	1:0:299:ARG:O	2.24	0.87
3:2:338:PHE:HB2	3:2:339:PRO:HD2	0.91	0.87
8:7:91:PRO:HB2	8:7:96:ALA:HB2	1.56	0.86
3:2:100:LEU:O	3:2:101:LEU:HD12	1.73	0.86
4:3:192:LEU:HD22	4:3:196:LEU:O	1.75	0.86
1:0:18:TYR:CE2	1:0:671:LYS:HB3	2.11	0.85
1:0:487:ARG:NH2	1:0:728:PHE:HB3	1.91	0.85
1:0:135:HIS:HE2	1:0:300:GLU:HA	1.40	0.85
1:0:158:TYR:HE1	1:0:193:PHE:CZ	1.80	0.85
4:3:188:GLU:HB2	8:7:188:LEU:CD2	2.05	0.85
8:7:289:TYR:N	8:7:290:PRO:CD	2.40	0.84
1:0:111:SER:HB2	1:0:192:TYR:OH	1.76	0.84
1:0:611:VAL:HG22	1:0:669:ARG:HD2	1.58	0.84
1:0:519:ASN:HA	1:0:522:ASN:HD22	1.44	0.82
3:2:314:ARG:O	3:2:316:TYR:HD2	1.63	0.82
8:7:472:ARG:CG	8:7:473:GLU:HG3	2.07	0.82
1:0:114:ASN:HD22	1:0:177:LEU:HD13	1.42	0.81
8:7:309:ASP:O	8:7:310:LEU:HG	1.80	0.81
1:0:726:GLN:HB2	1:0:727:PRO:HD2	0.82	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:187:ASN:CB	2:1:191:ASP:CB	2.51	0.81
1:0:111:SER:CA	1:0:192:TYR:CE1	2.56	0.81
1:0:158:TYR:HD1	1:0:193:PHE:CZ	1.86	0.81
4:3:183:PHE:CZ	4:3:200:GLN:HG3	2.16	0.81
1:0:193:PHE:C	1:0:195:ALA:H	1.87	0.80
1:0:616:ARG:NH2	1:0:674:TYR:CD2	2.49	0.80
3:2:339:PRO:O	8:7:77:TRP:CZ3	2.34	0.80
5:4:237:GLN:O	5:4:241:LEU:HB3	1.80	0.80
1:0:20:GLU:OE1	1:0:482:THR:CG2	2.26	0.80
1:0:189:TRP:O	1:0:190:CYS:O	2.00	0.79
1:0:106:GLY:HA3	1:0:174:ILE:HD12	1.65	0.79
1:0:190:CYS:O	1:0:194:LEU:HB3	1.83	0.79
1:0:135:HIS:CE1	1:0:300:GLU:N	2.51	0.79
1:0:135:HIS:HE1	1:0:299:ARG:HG3	1.36	0.79
3:2:338:PHE:CE2	8:7:79:ALA:HB2	2.15	0.79
8:7:359:LYS:NZ	8:7:436:GLY:CA	2.40	0.79
1:0:16:TYR:HE1	1:0:18:TYR:HE1	1.18	0.78
4:3:185:ASP:OD1	4:3:188:GLU:HB3	1.82	0.78
1:0:183:LEU:HB3	1:0:188:GLY:CA	2.12	0.78
5:4:224:LEU:O	5:4:228:LEU:HG	1.84	0.78
2:1:166:ILE:HD11	2:1:170:PHE:H	1.49	0.78
1:0:183:LEU:O	1:0:187:GLN:N	2.17	0.77
1:0:139:ALA:HB1	1:0:300:GLU:OE2	1.85	0.77
1:0:106:GLY:O	1:0:174:ILE:HG13	1.85	0.77
2:1:163:ASP:OD2	7:6:179:PRO:CD	2.33	0.77
1:0:518:ARG:NH2	8:7:310:LEU:HD22	2.01	0.76
1:0:147:GLN:O	1:0:148:HIS:HB2	1.86	0.76
3:2:262:LEU:CD2	3:2:265:LEU:HD12	2.15	0.76
3:2:245:LEU:HG	3:2:280:ARG:HE	1.50	0.75
1:0:180:LEU:C	1:0:180:LEU:HD12	2.11	0.75
1:0:563:ARG:HA	2:1:172:ALA:HB1	1.68	0.75
3:2:338:PHE:CB	3:2:339:PRO:HD3	1.86	0.75
1:0:61:ARG:HH12	1:0:98:GLU:HG3	1.50	0.75
2:1:475:PHE:HE1	2:1:484:PRO:O	1.70	0.75
1:0:135:HIS:HE1	1:0:300:GLU:N	1.83	0.75
1:0:106:GLY:C	1:0:174:ILE:HD12	2.11	0.75
2:1:483:THR:H	2:1:484:PRO:HD2	1.52	0.75
3:2:338:PHE:CE1	8:7:79:ALA:HB2	2.16	0.75
4:3:183:PHE:CE1	4:3:200:GLN:HG3	2.23	0.74
7:6:291:CYS:O	7:6:295:ARG:HA	1.87	0.74
1:0:486:ALA:O	1:0:487:ARG:HB2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:472:ARG:HG3	8:7:473:GLU:CG	2.14	0.73
4:3:192:LEU:HD21	4:3:200:GLN:CB	2.18	0.73
2:1:483:THR:HG1	2:1:484:PRO:HD3	1.53	0.73
3:2:262:LEU:HD22	3:2:265:LEU:HD12	1.70	0.72
4:3:188:GLU:HB2	8:7:188:LEU:HD21	1.72	0.72
2:1:181:CYS:SG	2:1:182:ASN:N	2.63	0.71
3:2:307:ILE:HG22	3:2:316:TYR:CB	2.21	0.71
1:0:69:LYS:HD2	1:0:229:ALA:HA	1.71	0.71
1:0:158:TYR:CD1	1:0:193:PHE:CE2	2.66	0.71
1:0:738:LEU:O	1:0:738:LEU:HD12	1.90	0.71
3:2:338:PHE:HD1	3:2:338:PHE:H	1.36	0.71
1:0:114:ASN:ND2	1:0:177:LEU:HD22	2.06	0.71
1:0:106:GLY:CA	1:0:174:ILE:HD12	2.20	0.71
1:0:132:GLY:HA2	1:0:391:LEU:HD12	1.73	0.71
3:2:208:THR:HG23	3:2:210:ALA:H	1.56	0.70
8:7:35:GLN:HB3	8:7:159:CYS:SG	2.31	0.70
1:0:739:LEU:C	1:0:741:LEU:H	1.99	0.70
3:2:317:ALA:CA	3:2:340:ASN:O	2.38	0.70
8:7:312:PRO:HG3	8:7:383:THR:HG23	1.74	0.70
4:3:187:LEU:HD22	8:7:188:LEU:HB3	1.74	0.70
8:7:35:GLN:OE1	8:7:159:CYS:HB3	1.92	0.69
3:2:314:ARG:O	3:2:316:TYR:CD2	2.45	0.69
5:4:257:CYS:HB2	5:4:275:PHE:HB3	1.74	0.69
1:0:88:ARG:HH11	1:0:174:ILE:HG22	1.57	0.69
7:6:272:SER:HB3	7:6:285:THR:HG22	1.75	0.69
3:2:316:TYR:CE2	3:2:371:ARG:HD3	2.28	0.69
8:7:472:ARG:HH11	8:7:473:GLU:H	1.36	0.69
8:7:158:LEU:HD11	8:7:161:VAL:HG22	1.75	0.69
1:0:111:SER:HA	1:0:192:TYR:CE1	2.27	0.68
7:6:54:ARG:HG2	7:6:55:LEU:HD12	1.76	0.68
1:0:102:LEU:HB3	1:0:103:PRO:HD2	1.75	0.68
1:0:135:HIS:CE1	1:0:300:GLU:HA	2.27	0.68
8:7:633:ARG:HD2	8:7:679:PHE:CD1	2.28	0.68
2:1:458:GLN:HA	2:1:461:LEU:HB3	1.75	0.68
3:2:339:PRO:O	8:7:77:TRP:HZ3	1.76	0.68
1:0:111:SER:HA	1:0:192:TYR:HE1	1.57	0.68
8:7:435:TRP:HB3	8:7:461:HIS:ND1	2.08	0.68
8:7:314:ALA:HB2	8:7:381:TRP:CD1	2.21	0.68
1:0:487:ARG:NH1	1:0:487:ARG:HG3	2.08	0.68
1:0:611:VAL:HG22	1:0:669:ARG:CD	2.23	0.67
3:2:304:PRO:CG	3:2:372:ALA:HA	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:135:HIS:ND1	1:0:299:ARG:CG	2.54	0.67
1:0:106:GLY:O	1:0:174:ILE:CG1	2.43	0.67
8:7:415:HIS:HB2	8:7:418:LYS:HB2	1.76	0.67
8:7:472:ARG:NH1	8:7:473:GLU:HA	2.09	0.67
1:0:158:TYR:CE1	1:0:193:PHE:HZ	2.11	0.66
1:0:183:LEU:HB3	1:0:188:GLY:HA3	1.75	0.66
1:0:726:GLN:O	1:0:728:PHE:HD1	1.78	0.66
7:6:182:ILE:HG13	7:6:185:LEU:HD12	1.78	0.66
1:0:487:ARG:HG3	1:0:487:ARG:HH11	1.60	0.66
3:2:49:PRO:O	3:2:53:LYS:CG	2.41	0.66
1:0:114:ASN:HD21	1:0:177:LEU:HD22	1.61	0.66
2:1:444:GLY:HA2	7:6:269:PRO:HB3	1.77	0.66
4:3:208:LEU:HD12	4:3:209:GLU:N	2.10	0.66
1:0:739:LEU:O	1:0:741:LEU:N	2.22	0.66
2:1:187:ASN:HD22	2:1:191:ASP:HB2	1.59	0.66
5:4:248:HIS:O	5:4:248:HIS:ND1	2.29	0.66
5:4:297:LEU:HB2	7:6:250:ILE:HD13	1.76	0.65
8:7:504:LYS:HB2	8:7:655:TYR:HA	1.76	0.65
8:7:326:LYS:HD2	8:7:489:TYR:HB2	1.79	0.65
8:7:330:ASN:HD21	8:7:334:ARG:HB2	1.60	0.65
1:0:128:LYS:HD2	2:1:274:ASP:O	1.95	0.65
4:3:4:GLN:O	4:3:4:GLN:HG2	1.96	0.65
7:6:343:ARG:HG3	7:6:351:GLU:HG3	1.79	0.65
3:2:58:ARG:NH1	3:2:59:MET:SD	2.70	0.65
4:3:192:LEU:HD21	4:3:200:GLN:HB2	1.76	0.65
3:2:44:VAL:O	3:2:53:LYS:NZ	2.30	0.65
8:7:285:ILE:O	8:7:290:PRO:HG2	1.96	0.65
1:0:18:TYR:CD2	1:0:671:LYS:HB3	2.32	0.64
1:0:193:PHE:C	1:0:195:ALA:N	2.52	0.64
3:2:300:THR:HG23	3:2:373:HIS:HB3	1.77	0.64
8:7:361:CYS:SG	8:7:362:LEU:N	2.70	0.64
1:0:203:ASN:O	1:0:204:VAL:CG2	2.43	0.64
3:2:338:PHE:CE1	8:7:79:ALA:CB	2.79	0.64
5:4:165:LYS:HE2	5:4:200:SER:HB2	1.78	0.64
1:0:191:PRO:O	1:0:195:ALA:HB2	1.98	0.64
3:2:262:LEU:HD13	3:2:271:VAL:HG11	1.78	0.64
4:3:2:ASP:HB2	4:3:13:LYS:HZ1	1.62	0.64
8:7:79:ALA:H	8:7:84:ILE:HG22	1.62	0.64
2:1:461:LEU:HD21	2:1:504:LYS:CD	2.28	0.64
1:0:88:ARG:HD3	1:0:174:ILE:CG2	2.27	0.64
5:4:266:TYR:HB2	7:6:250:ILE:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:180:LEU:O	1:0:184:GLY:N	2.30	0.64
8:7:359:LYS:HZ2	8:7:436:GLY:HA2	1.62	0.64
1:0:88:ARG:NH1	1:0:174:ILE:HG22	2.12	0.64
8:7:419:ARG:HB3	8:7:422:GLU:HB3	1.79	0.64
1:0:523:LEU:HD12	1:0:523:LEU:C	2.23	0.63
2:1:497:LEU:HD11	2:1:536:LEU:HD22	1.79	0.63
8:7:309:ASP:O	8:7:310:LEU:CG	2.46	0.63
2:1:513:ARG:HG3	2:1:514:ARG:HG3	1.81	0.63
5:4:12:VAL:HB	5:4:161:ILE:HA	1.79	0.63
3:2:239:GLN:HA	3:2:287:ALA:HB1	1.80	0.63
5:4:174:TYR:OH	7:6:320:ARG:NH2	2.31	0.63
8:7:372:GLU:HA	8:7:375:LYS:HE3	1.81	0.63
1:0:152:LEU:O	1:0:152:LEU:HD23	1.98	0.63
3:2:304:PRO:HG2	3:2:372:ALA:HA	1.80	0.63
7:6:304:GLU:HA	7:6:312:LEU:H	1.63	0.63
8:7:62:ARG:HB2	8:7:75:PRO:HD3	1.81	0.63
1:0:15:ASP:O	1:0:17:ILE:HG13	1.97	0.63
2:1:415:THR:N	2:1:416:PRO:HD3	2.14	0.63
1:0:334:ARG:HE	4:3:74:ILE:HD13	1.63	0.63
2:1:417:LYS:HG2	5:4:224:LEU:HD21	1.80	0.63
4:3:204:ARG:HD2	8:7:266:GLN:CG	2.29	0.62
7:6:195:ARG:HE	7:6:217:GLY:HA2	1.62	0.62
8:7:507:CYS:HA	8:7:659:PHE:HB3	1.82	0.62
2:1:478:CYS:CB	2:1:484:PRO:HG3	2.29	0.62
5:4:15:VAL:HA	5:4:164:ILE:HB	1.79	0.62
2:1:161:LYS:O	2:1:162:GLN:HB2	1.99	0.62
5:4:48:HIS:O	5:4:55:ASN:ND2	2.32	0.62
7:6:224:ASP:H	7:6:227:HIS:HB3	1.63	0.62
8:7:514:MET:HG2	8:7:665:GLN:HE21	1.63	0.62
4:3:192:LEU:HD21	4:3:200:GLN:HB3	1.80	0.62
5:4:146:ARG:NH2	7:6:348:CYS:O	2.32	0.62
5:4:289:PHE:HB2	5:4:294:PRO:HG2	1.82	0.62
3:2:411:GLN:OE1	6:5:3:ASN:ND2	2.32	0.62
5:4:196:LEU:HD21	5:4:223:LEU:HD22	1.82	0.62
1:0:460:THR:HG23	1:0:661:ALA:HB3	1.81	0.62
2:1:454:PRO:HB2	7:6:274:ALA:HB3	1.80	0.62
3:2:377:LEU:HD23	3:2:378:LYS:HG3	1.82	0.62
5:4:60:ILE:HG12	5:4:69:PHE:HA	1.82	0.62
1:0:705:ASN:HA	1:0:708:LEU:HD21	1.82	0.61
1:0:18:TYR:CE2	1:0:671:LYS:CB	2.83	0.61
1:0:489:CYS:SG	1:0:490:LEU:N	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:175:ARG:HH21	2:1:310:HIS:HB2	1.65	0.61
2:1:369:VAL:HA	2:1:374:LEU:HB2	1.82	0.61
8:7:76:LEU:HD23	8:7:87:GLU:HG2	1.81	0.61
1:0:16:TYR:OH	2:1:339:SER:HA	1.99	0.61
1:0:581:LEU:HD23	2:1:264:ASN:OD1	2.00	0.61
3:2:15:GLN:OE1	3:2:46:ARG:NH1	2.32	0.61
8:7:164:GLY:HA2	8:7:293:ALA:HB3	1.83	0.61
7:6:363:CYS:SG	7:6:365:ASN:ND2	2.73	0.61
1:0:497:ARG:HH11	1:0:710:VAL:HB	1.64	0.61
3:2:364:ILE:HG21	3:2:391:ILE:HD13	1.82	0.61
5:4:237:GLN:O	5:4:241:LEU:CB	2.48	0.61
8:7:472:ARG:HH11	8:7:473:GLU:N	1.97	0.61
3:2:415:GLN:HG2	3:2:439:ARG:HD3	1.82	0.61
6:5:15:ALA:HA	8:7:516:PRO:HB3	1.81	0.61
8:7:688:LYS:NZ	8:7:689:VAL:O	2.33	0.61
4:3:183:PHE:CZ	4:3:200:GLN:CG	2.83	0.61
1:0:18:TYR:CD2	1:0:671:LYS:CB	2.83	0.61
8:7:425:ARG:HA	8:7:428:GLU:HG2	1.81	0.61
1:0:315:LEU:HD23	1:0:373:ARG:HH21	1.65	0.60
2:1:187:ASN:HB2	2:1:191:ASP:HB2	1.72	0.60
3:2:304:PRO:HG2	3:2:373:HIS:H	1.64	0.60
3:2:307:ILE:HG22	3:2:316:TYR:HB3	1.83	0.60
3:2:338:PHE:HD2	3:2:339:PRO:HD2	1.60	0.60
4:3:199:ALA:HA	4:3:202:LYS:HB2	1.83	0.60
8:7:62:ARG:HD3	8:7:75:PRO:HD3	1.80	0.60
8:7:198:ARG:HB2	8:7:271:GLU:HB3	1.83	0.60
1:0:229:ALA:HB3	1:0:451:PHE:HA	1.83	0.60
2:1:187:ASN:CA	2:1:191:ASP:HB3	2.30	0.60
3:2:46:ARG:NH2	3:2:290:LEU:O	2.34	0.60
4:3:193:PRO:HG2	4:3:199:ALA:HB2	1.82	0.60
5:4:190:LEU:HB2	5:4:235:GLN:HE21	1.66	0.60
8:7:158:LEU:HD11	8:7:161:VAL:HA	1.83	0.60
8:7:538:PRO:HA	8:7:541:PHE:HB3	1.83	0.60
1:0:67:VAL:HB	1:0:228:LYS:HD2	1.83	0.60
3:2:406:GLY:HA2	3:2:445:PRO:HD3	1.82	0.60
8:7:184:VAL:HA	8:7:187:HIS:HB3	1.84	0.60
1:0:16:TYR:CD1	1:0:18:TYR:CE1	2.89	0.60
1:0:482:THR:OG1	1:0:695:ARG:NE	2.35	0.60
1:0:495:ILE:O	1:0:708:LEU:N	2.35	0.60
4:3:198:LEU:HD23	4:3:199:ALA:N	2.17	0.60
7:6:63:VAL:HB	7:6:106:ILE:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:52:LYS:O	8:7:56:TYR:N	2.33	0.60
1:0:726:GLN:O	1:0:728:PHE:CD1	2.55	0.60
2:1:483:THR:N	2:1:484:PRO:HD2	2.17	0.60
4:3:200:GLN:O	4:3:204:ARG:NH1	2.34	0.60
1:0:70:LEU:HD23	1:0:204:VAL:HG13	1.84	0.60
1:0:566:LEU:H	1:0:594:ALA:HA	1.65	0.60
1:0:582:GLU:HB2	2:1:257:MET:SD	2.42	0.60
8:7:62:ARG:CA	8:7:73:SER:HB2	2.22	0.60
5:4:12:VAL:HA	5:4:58:ALA:HB3	1.83	0.60
8:7:625:GLN:NE2	8:7:627:SER:O	2.35	0.59
1:0:180:LEU:HD12	1:0:181:LYS:N	2.17	0.59
2:1:491:VAL:HG23	2:1:494:LYS:HD2	1.84	0.59
8:7:497:GLN:HE21	8:7:504:LYS:HA	1.68	0.59
4:3:188:GLU:HB2	8:7:188:LEU:HD22	1.83	0.59
3:2:364:ILE:O	3:2:368:LEU:N	2.33	0.59
2:1:188:LEU:H	2:1:191:ASP:HB3	1.66	0.59
3:2:15:GLN:OE1	3:2:18:ASN:ND2	2.36	0.59
3:2:224:GLN:OE1	3:2:226:ARG:NH2	2.35	0.59
8:7:266:GLN:O	8:7:268:VAL:N	2.33	0.59
1:0:135:HIS:CE1	1:0:300:GLU:CA	2.85	0.59
1:0:599:VAL:HG12	1:0:602:GLY:H	1.67	0.59
2:1:481:VAL:HG12	2:1:483:THR:HG23	1.85	0.59
7:6:335:PRO:O	7:6:353:LYS:NZ	2.35	0.59
1:0:106:GLY:O	1:0:174:ILE:CD1	2.51	0.59
1:0:112:ARG:HD2	2:1:271:ALA:HB1	1.79	0.59
2:1:360:TYR:O	2:1:364:GLY:N	2.36	0.59
3:2:71:VAL:HA	3:2:74:TRP:HB2	1.84	0.59
3:2:346:VAL:HG12	3:2:348:ARG:H	1.68	0.59
5:4:104:LEU:O	5:4:108:ASN:N	2.36	0.59
8:7:633:ARG:HD2	8:7:679:PHE:CG	2.38	0.58
2:1:166:ILE:HG23	2:1:166:ILE:O	2.03	0.58
5:4:213:LEU:HD11	5:4:245:PRO:HG2	1.84	0.58
1:0:273:ILE:HG22	1:0:278:GLU:HG2	1.85	0.58
2:1:417:LYS:NZ	5:4:43:VAL:HG21	2.18	0.58
7:6:111:SER:HA	7:6:141:GLY:HA3	1.86	0.58
8:7:76:LEU:HD22	8:7:86:LEU:HA	1.85	0.58
1:0:183:LEU:CB	1:0:188:GLY:H	2.06	0.58
1:0:487:ARG:HH22	1:0:728:PHE:CB	2.10	0.58
4:3:78:VAL:O	4:3:83:ASN:N	2.33	0.58
1:0:53:LEU:HA	1:0:56:ILE:HB	1.84	0.58
2:1:478:CYS:HB3	2:1:484:PRO:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:496:ASN:HA	2:1:499:ARG:HB2	1.84	0.58
3:2:392:ARG:O	3:2:396:LEU:N	2.34	0.58
7:6:334:ILE:HG12	7:6:336:LEU:H	1.69	0.58
8:7:91:PRO:O	8:7:94:LYS:HG2	2.04	0.58
2:1:410:GLU:HA	2:1:413:ALA:HB3	1.86	0.58
3:2:384:PRO:HB3	3:2:387:ILE:HB	1.85	0.58
4:3:81:ILE:HD12	4:3:84:LYS:HD3	1.86	0.58
1:0:705:ASN:CB	1:0:708:LEU:HD11	2.27	0.58
2:1:387:THR:OG1	2:1:393:GLN:NE2	2.37	0.57
8:7:153:MET:O	8:7:156:ILE:HG22	2.03	0.57
8:7:481:ASN:OD1	8:7:487:LYS:NZ	2.37	0.57
1:0:616:ARG:CZ	1:0:674:TYR:HD2	2.17	0.57
3:2:278:SER:OG	3:2:279:ARG:N	2.37	0.57
5:4:263:GLU:HG3	5:4:264:ILE:HG12	1.86	0.57
2:1:163:ASP:OD2	7:6:179:PRO:HD3	2.04	0.57
1:0:13:PRO:O	1:0:17:ILE:HG12	2.04	0.57
7:6:305:CYS:SG	7:6:306:LYS:N	2.76	0.57
8:7:343:GLY:H	8:7:346:LYS:HZ2	1.50	0.57
8:7:625:GLN:OE1	8:7:676:ARG:NH2	2.37	0.57
7:6:116:LYS:HE2	7:6:119:GLU:HA	1.86	0.57
8:7:337:VAL:H	8:7:488:LEU:HD13	1.69	0.57
1:0:74:SER:O	1:0:209:TYR:N	2.35	0.57
2:1:165:GLY:O	7:6:179:PRO:CB	2.52	0.57
3:2:342:VAL:HG13	3:2:342:VAL:O	2.02	0.57
1:0:193:PHE:O	1:0:195:ALA:N	2.38	0.57
5:4:293:LEU:HG	7:6:250:ILE:HD12	1.87	0.57
6:5:33:PHE:HA	6:5:45:VAL:HG13	1.86	0.57
1:0:189:TRP:O	1:0:194:LEU:HB3	2.01	0.57
5:4:31:GLN:O	5:4:36:LYS:NZ	2.33	0.57
1:0:24:TYR:OH	1:0:41:GLU:O	2.20	0.57
4:3:204:ARG:HD2	8:7:266:GLN:HG2	1.86	0.57
4:3:209:GLU:CD	4:3:209:GLU:O	2.48	0.57
1:0:111:SER:CB	1:0:192:TYR:CZ	2.49	0.57
1:0:535:ILE:HG12	1:0:617:ALA:HB3	1.86	0.57
2:1:387:THR:HG23	2:1:388:PRO:HD3	1.85	0.57
2:1:516:TYR:HA	2:1:519:THR:HG22	1.86	0.57
5:4:78:LEU:HA	5:4:81:PHE:HB3	1.86	0.57
7:6:166:GLU:HG2	7:6:195:ARG:HB3	1.86	0.57
6:5:18:GLN:HE21	8:7:520:ARG:HE	1.52	0.56
1:0:190:CYS:O	1:0:194:LEU:CB	2.51	0.56
1:0:343:ARG:NH2	1:0:431:PRO:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:165:GLY:O	7:6:179:PRO:HB2	2.05	0.56
3:2:245:LEU:HD23	3:2:246:GLY:O	2.05	0.56
4:3:21:LEU:HB2	4:3:62:LEU:HD11	1.86	0.56
8:7:59:LYS:HG3	8:7:62:ARG:NH2	2.21	0.56
1:0:111:SER:CB	1:0:192:TYR:OH	2.52	0.56
1:0:273:ILE:HG21	1:0:277:ASP:HB2	1.87	0.56
1:0:487:ARG:HH11	1:0:487:ARG:CG	2.18	0.56
2:1:314:VAL:O	2:1:318:GLY:N	2.38	0.56
2:1:408:ARG:HD3	5:4:116:LYS:HB2	1.87	0.56
5:4:255:CYS:HB2	5:4:260:ASN:HD21	1.70	0.56
7:6:77:LYS:HE3	7:6:78:PRO:HD2	1.87	0.56
3:2:200:GLY:O	3:2:204:LEU:N	2.33	0.56
4:3:187:LEU:HD21	8:7:185:ILE:HA	1.88	0.56
7:6:259:ILE:HG13	7:6:261:SER:H	1.70	0.56
4:3:199:ALA:HA	4:3:202:LYS:CB	2.36	0.56
1:0:517:ILE:HA	1:0:520:TYR:HD2	1.71	0.56
1:0:542:TYR:HB3	1:0:572:GLN:HE21	1.71	0.56
1:0:741:LEU:HD12	1:0:741:LEU:O	2.06	0.56
2:1:497:LEU:C	2:1:497:LEU:HD23	2.31	0.56
3:2:60:LEU:HA	3:2:119:ARG:HE	1.71	0.56
3:2:254:MET:HA	3:2:258:LEU:HD22	1.87	0.56
6:5:13:ASP:OD1	6:5:13:ASP:N	2.39	0.55
3:2:295:SER:OG	3:2:369:ARG:NH1	2.39	0.55
2:1:408:ARG:HG2	5:4:112:VAL:HB	1.89	0.55
3:2:63:GLU:OE1	3:2:64:GLN:NE2	2.38	0.55
4:3:194:VAL:HG22	4:3:194:VAL:O	2.06	0.55
1:0:501:GLN:OE1	8:7:299:ASN:ND2	2.40	0.55
8:7:556:ASP:OD2	8:7:647:LYS:NZ	2.34	0.55
8:7:582:GLY:O	8:7:589:ARG:NH2	2.39	0.55
1:0:739:LEU:C	1:0:741:LEU:N	2.65	0.55
5:4:25:GLN:NE2	5:4:32:PHE:O	2.38	0.55
8:7:444:HIS:HD2	8:7:467:THR:HG23	1.71	0.55
1:0:255:THR:HG23	1:0:396:PRO:HB3	1.87	0.55
7:6:196:VAL:H	7:6:215:THR:HG21	1.71	0.55
8:7:363:VAL:HA	8:7:439:ILE:HB	1.89	0.55
2:1:355:GLN:NE2	5:4:285:CYS:SG	2.80	0.55
1:0:18:TYR:CG	1:0:671:LYS:HD3	2.41	0.55
1:0:161:PHE:HD1	1:0:189:TRP:HE1	1.54	0.55
1:0:262:ASN:C	1:0:262:ASN:OD1	2.49	0.55
3:2:304:PRO:CG	3:2:373:HIS:H	2.20	0.55
8:7:693:LEU:HD12	8:7:696:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:18:TYR:CD2	1:0:671:LYS:HD3	2.42	0.55
1:0:224:GLU:HG2	1:0:450:ARG:HG3	1.89	0.55
3:2:130:SER:O	3:2:131:ASP:OD1	2.24	0.55
2:1:187:ASN:HB2	2:1:191:ASP:CA	2.35	0.55
2:1:199:THR:HG23	2:1:317:ALA:HB2	1.89	0.55
3:2:17:ARG:HA	3:2:20:GLN:HB3	1.89	0.55
5:4:14:VAL:O	5:4:164:ILE:N	2.38	0.55
1:0:538:PHE:HB3	1:0:600:ALA:HB2	1.89	0.54
3:2:155:ARG:HA	3:2:158:VAL:HG12	1.90	0.54
7:6:123:ASN:O	7:6:127:HIS:ND1	2.37	0.54
7:6:156:LEU:HD11	7:6:165:ARG:HG2	1.88	0.54
7:6:199:ILE:HG12	7:6:220:HIS:HB2	1.90	0.54
8:7:575:LEU:O	8:7:577:LYS:NZ	2.35	0.54
1:0:128:LYS:CD	2:1:274:ASP:O	2.55	0.54
1:0:582:GLU:CB	2:1:257:MET:SD	2.96	0.54
5:4:191:ILE:HB	5:4:210:THR:HG21	1.89	0.54
1:0:506:SER:HB3	1:0:509:GLU:HA	1.88	0.54
1:0:582:GLU:HG3	2:1:257:MET:SD	2.47	0.54
2:1:390:GLN:O	2:1:394:TYR:N	2.37	0.54
3:2:405:GLU:HG2	6:5:8:VAL:HG22	1.89	0.54
2:1:321:LYS:HG2	7:6:180:SER:H	1.73	0.54
3:2:59:MET:HA	3:2:62:LEU:HB2	1.89	0.54
4:3:97:ASP:OD1	4:3:97:ASP:N	2.40	0.54
1:0:242:VAL:O	1:0:246:SER:N	2.41	0.54
8:7:309:ASP:HA	8:7:384:ILE:HD11	1.88	0.54
1:0:106:GLY:O	1:0:174:ILE:HD12	2.06	0.54
1:0:277:ASP:HA	1:0:280:ARG:HD2	1.90	0.54
1:0:705:ASN:CA	1:0:708:LEU:HD21	2.38	0.54
8:7:62:ARG:HG3	8:7:74:ARG:HA	1.89	0.54
1:0:275:GLU:HA	1:0:278:GLU:HB2	1.90	0.54
1:0:507:LYS:NZ	8:7:300:ASP:O	2.40	0.54
2:1:461:LEU:HD21	2:1:504:LYS:HD2	1.90	0.54
8:7:35:GLN:OE1	8:7:159:CYS:CB	2.55	0.54
1:0:523:LEU:HB2	1:0:710:VAL:HG21	1.90	0.54
1:0:553:TYR:OH	2:1:229:TYR:O	2.23	0.54
1:0:345:ARG:NH2	4:3:61:GLN:OE1	2.41	0.54
1:0:601:ARG:HH12	1:0:626:VAL:HG22	1.73	0.54
5:4:263:GLU:O	7:6:254:PHE:N	2.39	0.54
8:7:472:ARG:HG3	8:7:473:GLU:N	2.23	0.54
1:0:49:THR:O	1:0:53:LEU:N	2.41	0.53
2:1:533:TYR:O	2:1:537:HIS:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:93:ARG:NE	4:3:95:TYR:O	2.39	0.53
8:7:413:LEU:HD22	8:7:418:LYS:HG2	1.88	0.53
8:7:472:ARG:NH1	8:7:473:GLU:CA	2.71	0.53
4:3:24:ASN:ND2	4:3:46:CYS:SG	2.82	0.53
4:3:188:GLU:CB	8:7:188:LEU:CD2	2.83	0.53
1:0:464:LEU:HD13	1:0:477:THR:HG22	1.90	0.53
2:1:359:GLU:O	2:1:363:LEU:N	2.36	0.53
3:2:338:PHE:CD1	3:2:338:PHE:N	2.77	0.53
7:6:110:LYS:HE3	7:6:140:HIS:H	1.73	0.53
2:1:132:VAL:O	2:1:135:GLN:NE2	2.41	0.53
3:2:50:SER:O	3:2:54:ASN:ND2	2.41	0.53
5:4:145:HIS:HA	5:4:148:ASN:HD22	1.72	0.53
1:0:240:ASP:OD2	1:0:636:ARG:NH2	2.31	0.53
1:0:16:TYR:CD1	1:0:18:TYR:HE1	2.24	0.53
1:0:684:PHE:O	1:0:689:LYS:NZ	2.40	0.53
5:4:180:VAL:O	5:4:184:ALA:N	2.39	0.53
5:4:250:ASP:OD1	5:4:250:ASP:N	2.39	0.53
1:0:503:ALA:HA	1:0:682:LYS:HD2	1.90	0.53
1:0:582:GLU:CG	2:1:257:MET:SD	2.97	0.53
1:0:672:THR:OG1	1:0:731:GLU:OE1	2.27	0.53
1:0:726:GLN:O	1:0:728:PHE:N	2.39	0.53
2:1:163:ASP:OD2	7:6:179:PRO:HD2	2.07	0.53
2:1:368:SER:HB3	2:1:373:ALA:HB1	1.90	0.53
3:2:408:LEU:HD11	3:2:440:LEU:HB3	1.91	0.53
8:7:175:TYR:HB2	8:7:270:PHE:HB2	1.91	0.53
8:7:324:LEU:O	8:7:328:PHE:N	2.41	0.53
1:0:579:VAL:HG22	2:1:257:MET:HG3	1.91	0.53
2:1:372:ILE:HG21	5:4:201:GLY:HA3	1.91	0.53
3:2:304:PRO:HG3	3:2:372:ALA:HA	1.91	0.53
3:2:307:ILE:HD13	3:2:371:ARG:HB3	1.91	0.53
3:2:339:PRO:HG3	8:7:52:LYS:HD3	1.91	0.53
3:2:435:ASN:HB3	3:2:440:LEU:HB2	1.91	0.53
8:7:557:LYS:HA	8:7:603:ASN:HB2	1.89	0.53
1:0:519:ASN:HD22	1:0:522:ASN:ND2	2.07	0.53
3:2:26:LEU:O	3:2:94:ARG:NH1	2.38	0.53
3:2:322:GLU:HA	3:2:325:ILE:HD12	1.91	0.53
3:2:360:THR:O	3:2:364:ILE:N	2.37	0.53
4:3:28:HIS:ND1	4:3:46:CYS:SG	2.78	0.53
7:6:167:VAL:HB	7:6:196:VAL:HA	1.91	0.53
2:1:130:ASP:HA	2:1:133:VAL:HB	1.90	0.52
3:2:308:VAL:HG11	8:7:115:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:328:ILE:HA	3:2:331:PHE:HB3	1.89	0.52
5:4:21:TRP:O	5:4:25:GLN:N	2.38	0.52
5:4:112:VAL:HA	5:4:115:ILE:HG22	1.91	0.52
8:7:153:MET:HA	8:7:156:ILE:HG22	1.91	0.52
8:7:390:CYS:HB2	8:7:406:ALA:HA	1.89	0.52
8:7:565:VAL:O	8:7:569:LYS:N	2.37	0.52
1:0:140:SER:HA	1:0:387:GLU:OE2	2.10	0.52
2:1:169:ALA:HA	7:6:177:CYS:HB3	1.92	0.52
1:0:673:ASP:O	1:0:674:TYR:HB2	2.10	0.52
2:1:483:THR:C	2:1:485:PHE:H	2.16	0.52
3:2:304:PRO:HG2	3:2:372:ALA:CA	2.39	0.52
3:2:310:GLU:HB3	3:2:315:LEU:HD22	1.91	0.52
8:7:197:CYS:SG	8:7:198:ARG:N	2.82	0.52
8:7:497:GLN:HG2	8:7:504:LYS:HG2	1.91	0.52
1:0:138:THR:CG2	1:0:299:ARG:HD3	2.40	0.52
1:0:262:ASN:HA	1:0:265:THR:HB	1.91	0.52
1:0:277:ASP:OD1	1:0:280:ARG:NH1	2.43	0.52
5:4:48:HIS:NE2	5:4:56:LYS:O	2.43	0.52
5:4:236:ASP:O	5:4:240:GLN:HB2	2.09	0.52
5:4:263:GLU:HB2	7:6:292:PRO:HB3	1.91	0.52
8:7:65:MET:HB2	8:7:73:SER:HB3	1.91	0.52
8:7:324:LEU:HD12	8:7:327:MET:HB3	1.92	0.52
3:2:145:VAL:HG13	3:2:146:PRO:HD3	1.92	0.52
3:2:231:VAL:O	3:2:235:SER:N	2.41	0.52
7:6:59:ARG:HA	7:6:164:SER:HB2	1.91	0.52
5:4:165:LYS:NZ	5:4:169:ASP:OD1	2.43	0.52
7:6:19:TRP:CG	8:7:101:VAL:HG11	2.45	0.52
7:6:87:LEU:HD13	7:6:229:LYS:HD3	1.90	0.52
1:0:81:GLU:HA	1:0:84:ILE:HD12	1.92	0.52
1:0:88:ARG:NH1	1:0:174:ILE:H	2.08	0.52
1:0:575:ALA:HA	2:1:266:LEU:HD22	1.90	0.52
8:7:672:TYR:HE2	8:7:676:ARG:HH11	1.58	0.52
1:0:420:PRO:HB2	1:0:428:ILE:HD11	1.92	0.52
3:2:209:PRO:HA	3:2:212:LEU:HD13	1.92	0.52
7:6:229:LYS:HA	7:6:232:LEU:HD12	1.92	0.52
3:2:397:GLU:OE2	3:2:400:ARG:NH2	2.43	0.52
8:7:132:GLN:HG3	8:7:134:SER:H	1.74	0.52
8:7:360:ARG:NH1	8:7:432:THR:O	2.41	0.52
1:0:203:ASN:C	1:0:204:VAL:HG23	2.33	0.52
1:0:343:ARG:HG2	1:0:347:GLN:HE21	1.75	0.52
1:0:583:LYS:O	1:0:587:ALA:N	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:245:LEU:CG	3:2:280:ARG:HE	2.21	0.52
4:3:194:VAL:CG1	4:3:198:LEU:HD13	2.36	0.52
7:6:87:LEU:HB2	7:6:228:TYR:HE2	1.74	0.52
7:6:277:ASP:N	7:6:277:ASP:OD1	2.43	0.52
1:0:391:LEU:O	1:0:395:SER:N	2.43	0.51
2:1:360:TYR:HA	2:1:363:LEU:HB3	1.92	0.51
2:1:463:HIS:HA	2:1:466:VAL:HG22	1.92	0.51
4:3:75:ARG:HA	4:3:79:LEU:HD13	1.91	0.51
8:7:105:GLU:HA	8:7:124:TYR:HB2	1.91	0.51
8:7:299:ASN:HB3	8:7:332:ARG:HD3	1.90	0.51
1:0:152:LEU:HD23	1:0:152:LEU:C	2.35	0.51
1:0:523:LEU:HA	1:0:710:VAL:HG11	1.92	0.51
2:1:260:LEU:HG	2:1:328:GLN:HB3	1.92	0.51
7:6:172:SER:HA	7:6:201:LEU:HB3	1.91	0.51
1:0:195:ALA:HA	1:0:198:SER:OG	2.10	0.51
1:0:487:ARG:HD2	1:0:724:MET:SD	2.50	0.51
3:2:48:LEU:HG	3:2:48:LEU:O	2.10	0.51
4:3:13:LYS:HD2	4:3:21:LEU:HD11	1.91	0.51
5:4:13:ILE:HA	5:4:162:LEU:HB3	1.92	0.51
8:7:55:GLU:OE2	8:7:62:ARG:NH1	2.42	0.51
8:7:194:ILE:HG22	8:7:195:ARG:HG2	1.92	0.51
8:7:359:LYS:HZ1	8:7:436:GLY:N	2.09	0.51
8:7:532:LEU:HD12	8:7:724:ALA:HB2	1.93	0.51
1:0:85:GLU:OE2	2:1:334:ASN:ND2	2.44	0.51
1:0:183:LEU:CB	1:0:188:GLY:HA3	2.40	0.51
1:0:441:SER:O	1:0:445:LYS:N	2.32	0.51
4:3:22:MET:HB3	4:3:58:PHE:HB3	1.91	0.51
5:4:13:ILE:HB	5:4:59:VAL:HG22	1.92	0.51
8:7:91:PRO:HB2	8:7:96:ALA:CB	2.33	0.51
8:7:435:TRP:CB	8:7:461:HIS:ND1	2.72	0.51
1:0:191:PRO:O	1:0:195:ALA:CB	2.58	0.51
7:6:129:THR:O	7:6:133:LYS:N	2.43	0.51
8:7:62:ARG:NH2	8:7:77:TRP:CZ3	2.79	0.51
2:1:423:SER:O	2:1:427:ALA:N	2.41	0.51
3:2:125:GLY:O	5:4:101:TYR:OH	2.27	0.51
8:7:113:VAL:O	8:7:115:GLU:N	2.44	0.51
8:7:151:GLY:HA2	8:7:154:GLN:HB2	1.93	0.51
8:7:625:GLN:N	8:7:660:TYR:O	2.39	0.51
8:7:665:GLN:O	8:7:667:THR:OG1	2.22	0.51
1:0:697:ILE:HG22	1:0:701:LEU:HD22	1.92	0.51
3:2:328:ILE:O	3:2:332:SER:N	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:316:LEU:HB3	8:7:320:GLN:HE21	1.75	0.51
8:7:360:ARG:NH2	8:7:403:CYS:SG	2.83	0.51
1:0:722:ARG:HD3	7:6:223:LEU:HA	1.92	0.51
4:3:22:MET:HG2	4:3:60:VAL:HB	1.93	0.51
8:7:137:THR:HG21	8:7:154:GLN:HE22	1.76	0.51
1:0:697:ILE:HA	1:0:701:LEU:HB3	1.92	0.51
7:6:76:LEU:HD22	7:6:225:GLU:HG3	1.92	0.51
1:0:135:HIS:ND1	1:0:299:ARG:NE	2.59	0.51
1:0:610:PHE:HB2	1:0:667:ALA:HA	1.91	0.51
5:4:146:ARG:HH12	7:6:350:GLY:HA3	1.76	0.51
8:7:175:TYR:CZ	8:7:272:VAL:HA	2.46	0.51
8:7:377:GLN:HB3	8:7:381:TRP:CZ3	2.46	0.51
1:0:309:VAL:HG11	1:0:409:THR:HB	1.93	0.50
1:0:423:ASP:HB2	2:1:285:SER:HA	1.93	0.50
4:3:107:PHE:O	4:3:111:ASN:ND2	2.43	0.50
8:7:191:ASP:O	8:7:195:ARG:N	2.37	0.50
8:7:394:SER:O	8:7:394:SER:OG	2.29	0.50
8:7:438:MET:HB2	8:7:463:LYS:HA	1.93	0.50
1:0:114:ASN:ND2	1:0:177:LEU:CD1	2.68	0.50
1:0:311:PRO:HD2	1:0:410:TYR:HE2	1.75	0.50
1:0:571:THR:HG22	1:0:573:ASP:H	1.76	0.50
8:7:165:LYS:HB2	8:7:294:GLU:HA	1.93	0.50
1:0:377:GLU:O	1:0:381:SER:N	2.37	0.50
2:1:509:GLN:HG2	2:1:512:ILE:HD11	1.91	0.50
3:2:7:ARG:NH2	6:5:54:GLN:OE1	2.44	0.50
5:4:178:MET:HE2	7:6:320:ARG:HE	1.75	0.50
2:1:475:PHE:CE1	2:1:484:PRO:O	2.58	0.50
2:1:478:CYS:HB2	2:1:484:PRO:HG3	1.93	0.50
3:2:71:VAL:O	3:2:83:GLN:NE2	2.45	0.50
5:4:272:LEU:HD11	7:6:319:ALA:HA	1.93	0.50
8:7:62:ARG:HH11	8:7:75:PRO:HG3	1.76	0.50
2:1:398:GLN:O	2:1:402:ASN:N	2.44	0.50
3:2:308:VAL:HG13	3:2:310:GLU:H	1.75	0.50
1:0:640:LEU:HD12	1:0:643:GLN:HB2	1.93	0.50
2:1:187:ASN:N	2:1:191:ASP:CB	2.74	0.50
5:4:8:LEU:HD11	5:4:157:MET:HG3	1.92	0.50
5:4:219:GLN:HG2	5:4:221:PRO:HD2	1.92	0.50
7:6:19:TRP:NE1	8:7:98:ASP:OD1	2.45	0.50
2:1:447:GLN:HB3	7:6:269:PRO:HB2	1.93	0.50
3:2:96:TRP:HD1	3:2:110:LEU:HA	1.77	0.50
3:2:264:HIS:ND1	3:2:267:GLU:OE1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:348:ARG:O	3:2:352:GLN:N	2.40	0.50
8:7:570:GLU:OE2	8:7:715:LYS:NZ	2.38	0.50
1:0:616:ARG:CZ	1:0:674:TYR:CD2	2.94	0.50
5:4:124:ILE:HD11	5:4:129:THR:H	1.77	0.50
1:0:354:PRO:HG3	1:0:415:THR:HA	1.94	0.49
2:1:187:ASN:H	2:1:191:ASP:HB2	1.77	0.49
2:1:262:VAL:HG11	2:1:330:SER:HB2	1.93	0.49
3:2:300:THR:HG22	3:2:300:THR:O	2.12	0.49
8:7:184:VAL:HG12	8:7:188:LEU:HB2	1.93	0.49
1:0:101:LYS:O	1:0:101:LYS:HG3	2.11	0.49
1:0:482:THR:H	1:0:695:ARG:HG3	1.77	0.49
3:2:75:VAL:HG22	5:4:241:LEU:HA	1.94	0.49
3:2:114:PHE:O	3:2:118:LEU:N	2.41	0.49
1:0:18:TYR:CD2	1:0:671:LYS:CD	2.95	0.49
2:1:237:THR:HA	2:1:240:LYS:HB3	1.94	0.49
2:1:372:ILE:HD13	5:4:201:GLY:H	1.77	0.49
3:2:332:SER:C	3:2:343:VAL:HG11	2.37	0.49
4:3:134:GLN:O	4:3:138:LEU:N	2.43	0.49
8:7:634:ARG:O	8:7:638:GLN:N	2.44	0.49
5:4:219:GLN:HB3	5:4:222:SER:HB3	1.93	0.49
8:7:339:VAL:N	8:7:489:TYR:O	2.42	0.49
8:7:508:ALA:O	8:7:661:SER:N	2.41	0.49
1:0:69:LYS:NZ	1:0:225:LEU:O	2.37	0.49
1:0:117:ILE:HD13	1:0:184:GLY:HA3	1.95	0.49
3:2:350:SER:HA	3:2:353:GLN:HB2	1.94	0.49
1:0:89:LYS:O	1:0:93:PHE:N	2.45	0.49
1:0:581:LEU:CD2	2:1:264:ASN:OD1	2.60	0.49
3:2:425:ALA:O	3:2:429:GLY:N	2.43	0.49
2:1:461:LEU:CD2	2:1:504:LYS:HE3	2.42	0.49
3:2:58:ARG:HD3	5:4:229:TRP:HZ2	1.76	0.49
4:3:116:ASP:O	4:3:120:LYS:N	2.38	0.49
8:7:103:ILE:HG23	8:7:106:PRO:HB2	1.95	0.49
8:7:667:THR:H	8:7:670:MET:HB3	1.78	0.49
8:7:62:ARG:NE	8:7:77:TRP:CH2	2.81	0.49
1:0:266:LEU:O	1:0:269:THR:OG1	2.25	0.49
1:0:552:TRP:HA	1:0:557:ILE:HD13	1.95	0.49
2:1:166:ILE:HA	7:6:179:PRO:HG3	1.95	0.49
8:7:433:GLN:O	8:7:434:GLU:HB2	2.13	0.49
3:2:309:VAL:HG22	3:2:312:ASN:HA	1.94	0.49
7:6:290:PHE:CE1	7:6:295:ARG:HB3	2.47	0.49
1:0:72:TYR:HB3	1:0:206:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:565:LYS:HE3	1:0:593:GLY:HA3	1.94	0.48
3:2:310:GLU:HG3	3:2:311:THR:HG23	1.94	0.48
5:4:14:VAL:N	5:4:162:LEU:O	2.40	0.48
6:5:49:LEU:HD13	6:5:56:ARG:HH22	1.77	0.48
1:0:194:LEU:HG	1:0:194:LEU:O	2.12	0.48
1:0:370:LYS:HD3	1:0:374:PHE:HE2	1.78	0.48
1:0:484:THR:OG1	1:0:695:ARG:NH2	2.45	0.48
1:0:539:PHE:HB2	1:0:599:VAL:HG22	1.95	0.48
3:2:260:ASN:O	3:2:263:GLN:HB2	2.13	0.48
8:7:532:LEU:HD11	8:7:723:ASP:HB2	1.95	0.48
1:0:111:SER:C	1:0:192:TYR:OH	2.54	0.48
2:1:307:PHE:O	2:1:311:SER:N	2.44	0.48
3:2:98:THR:HA	3:2:108:LEU:HG	1.95	0.48
3:2:307:ILE:HG21	3:2:371:ARG:HD2	1.95	0.48
5:4:257:CYS:HB3	5:4:276:CYS:HB2	1.94	0.48
8:7:309:ASP:O	8:7:309:ASP:OD1	2.31	0.48
8:7:375:LYS:O	8:7:379:LYS:N	2.38	0.48
8:7:664:SER:N	8:7:669:GLU:OE1	2.43	0.48
1:0:217:ILE:HG12	1:0:305:LEU:HA	1.95	0.48
2:1:396:THR:O	2:1:400:ILE:N	2.39	0.48
3:2:143:ARG:HD3	3:2:148:LEU:HD21	1.95	0.48
4:3:84:LYS:HA	4:3:136:ASN:HD21	1.78	0.48
5:4:235:GLN:HA	5:4:238:ARG:HG2	1.95	0.48
1:0:325:THR:HG23	1:0:382:LEU:HD13	1.96	0.48
1:0:375:CYS:O	1:0:379:LEU:N	2.39	0.48
2:1:302:ALA:O	2:1:306:ARG:N	2.46	0.48
5:4:13:ILE:N	5:4:58:ALA:O	2.35	0.48
8:7:128:SER:HB2	8:7:131:LEU:HD21	1.95	0.48
1:0:338:GLU:HG3	1:0:342:TRP:CD1	2.48	0.48
1:0:485:LEU:HB2	1:0:732:ASP:HB2	1.94	0.48
1:0:634:LYS:HA	1:0:637:LEU:HD12	1.96	0.48
1:0:638:GLU:O	1:0:642:ASP:N	2.46	0.48
3:2:304:PRO:HG2	3:2:373:HIS:N	2.28	0.48
7:6:360:CYS:SG	7:6:361:ALA:N	2.87	0.48
8:7:570:GLU:HA	8:7:573:ILE:HB	1.95	0.48
8:7:673:SER:HA	8:7:676:ARG:HB3	1.96	0.48
1:0:192:TYR:O	1:0:196:ARG:HG2	2.14	0.48
2:1:150:ASN:HA	2:1:153:ASP:HB2	1.94	0.48
2:1:350:LYS:HG3	2:1:353:LYS:HB3	1.96	0.48
3:2:220:LEU:HD11	3:2:226:ARG:H	1.79	0.48
4:3:188:GLU:CA	8:7:188:LEU:HD22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:75:PRO:HA	8:7:144:SER:HA	1.94	0.48
8:7:442:GLU:N	8:7:466:LEU:O	2.45	0.48
1:0:102:LEU:CB	1:0:103:PRO:HD2	2.42	0.48
1:0:337:LEU:HD13	4:3:68:VAL:HG11	1.96	0.48
1:0:516:VAL:HG12	1:0:520:TYR:HE2	1.77	0.48
1:0:646:ILE:O	1:0:647:ARG:NH1	2.43	0.48
2:1:233:ASP:OD1	2:1:233:ASP:N	2.47	0.48
3:2:48:LEU:N	3:2:49:PRO:CD	2.77	0.48
3:2:148:LEU:HA	3:2:151:TYR:HD2	1.78	0.48
3:2:300:THR:HG23	3:2:373:HIS:CB	2.43	0.48
3:2:357:SER:OG	3:2:358:GLY:O	2.32	0.48
5:4:14:VAL:HB	5:4:163:VAL:HA	1.96	0.48
8:7:288:GLU:HB2	8:7:290:PRO:HD3	1.96	0.48
1:0:132:GLY:CA	1:0:391:LEU:HD12	2.42	0.48
1:0:238:ASN:HB3	1:0:241:ASN:HD22	1.78	0.48
1:0:252:THR:HG23	1:0:430:ASN:HD21	1.79	0.48
1:0:570:GLU:HB3	1:0:577:THR:HG23	1.95	0.48
5:4:43:VAL:O	5:4:47:SER:N	2.46	0.48
5:4:266:TYR:H	5:4:274:ILE:HG23	1.78	0.48
6:5:32:LYS:HB3	6:5:46:ILE:HB	1.95	0.48
2:1:419:THR:HG22	2:1:422:LEU:H	1.79	0.48
4:3:99:LEU:O	4:3:103:GLU:N	2.47	0.48
4:3:167:LYS:O	4:3:171:LEU:N	2.46	0.48
5:4:195:VAL:HG22	5:4:216:LYS:HA	1.96	0.48
1:0:26:ARG:HD3	1:0:29:LYS:HD3	1.95	0.47
1:0:335:ARG:O	1:0:339:TYR:N	2.46	0.47
3:2:79:PHE:HB3	3:2:82:ALA:HB3	1.96	0.47
3:2:100:LEU:C	3:2:101:LEU:CD1	2.80	0.47
8:7:624:ILE:HA	8:7:660:TYR:HB2	1.96	0.47
2:1:417:LYS:HZ1	5:4:43:VAL:HG21	1.79	0.47
8:7:378:PHE:O	8:7:382:SER:OG	2.28	0.47
1:0:581:LEU:CD2	2:1:264:ASN:HA	2.44	0.47
4:3:208:LEU:HD12	4:3:208:LEU:C	2.40	0.47
7:6:171:PHE:HE2	7:6:205:VAL:HG21	1.80	0.47
8:7:296:ASP:OD1	8:7:296:ASP:N	2.44	0.47
8:7:309:ASP:OD1	8:7:309:ASP:C	2.55	0.47
8:7:410:TYR:HB3	8:7:450:MET:HE2	1.96	0.47
8:7:496:LEU:HB3	8:7:502:ILE:HD12	1.96	0.47
1:0:112:ARG:HH22	1:0:211:TYR:HB2	1.78	0.47
1:0:417:ILE:HG23	1:0:434:HIS:HB2	1.96	0.47
1:0:541:SER:H	1:0:544:TYR:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:670:GLY:HA3	2:1:338:ASN:HD22	1.79	0.47
2:1:177:GLN:C	2:1:192:ILE:HD11	2.39	0.47
7:6:205:VAL:HG12	7:6:208:CYS:H	1.80	0.47
8:7:104:ALA:H	8:7:106:PRO:HD2	1.79	0.47
8:7:105:GLU:HG2	8:7:121:TYR:HE1	1.78	0.47
1:0:499:ASN:HA	8:7:324:LEU:HD23	1.96	0.47
3:2:76:LYS:H	5:4:242:ILE:HB	1.78	0.47
3:2:230:LEU:HD21	3:2:258:LEU:HB2	1.96	0.47
8:7:309:ASP:C	8:7:310:LEU:HG	2.38	0.47
8:7:337:VAL:O	8:7:488:LEU:N	2.35	0.47
8:7:363:VAL:HG22	8:7:439:ILE:HD12	1.95	0.47
8:7:472:ARG:HH11	8:7:473:GLU:CA	2.27	0.47
8:7:554:ARG:HB3	8:7:647:LYS:HZ1	1.80	0.47
1:0:311:PRO:O	1:0:410:TYR:OH	2.32	0.47
1:0:524:LEU:O	1:0:528:SER:N	2.40	0.47
3:2:141:HIS:HD2	5:4:92:ASN:HD21	1.61	0.47
8:7:313:THR:O	8:7:313:THR:HG23	2.12	0.47
8:7:439:ILE:HG12	8:7:464:LEU:HD23	1.97	0.47
1:0:135:HIS:NE2	1:0:300:GLU:CA	2.65	0.47
1:0:692:LYS:HB3	1:0:697:ILE:HG23	1.97	0.47
2:1:493:MET:HE1	2:1:535:LYS:HG3	1.95	0.47
3:2:38:PRO:HG3	3:2:129:TRP:CD1	2.49	0.47
3:2:342:VAL:O	3:2:342:VAL:HG22	2.15	0.47
3:2:389:ASP:HA	3:2:392:ARG:HB2	1.96	0.47
4:3:193:PRO:CG	4:3:199:ALA:HB2	2.45	0.47
5:4:181:ILE:O	5:4:185:GLN:N	2.46	0.47
5:4:194:CYS:HA	5:4:215:LEU:HB3	1.95	0.47
7:6:210:VAL:HA	7:6:213:ARG:HG2	1.95	0.47
7:6:316:PRO:HD2	7:6:317:HIS:CE1	2.49	0.47
8:7:123:LEU:HD23	8:7:479:ASP:HB3	1.97	0.47
8:7:581:TYR:O	8:7:589:ARG:NH2	2.43	0.47
8:7:621:ASN:ND2	8:7:646:ALA:O	2.48	0.47
8:7:656:ASN:OD1	8:7:656:ASN:N	2.47	0.47
1:0:253:ARG:HB2	1:0:343:ARG:HH21	1.80	0.47
1:0:340:VAL:HA	1:0:343:ARG:HB3	1.97	0.47
4:3:30:LEU:HD22	4:3:47:PRO:HG3	1.95	0.47
5:4:115:ILE:HD12	5:4:118:LEU:HB2	1.96	0.47
1:0:354:PRO:HA	1:0:416:ILE:HD12	1.97	0.47
3:2:340:ASN:OD1	3:2:340:ASN:N	2.47	0.47
6:5:53:LEU:HD23	6:5:56:ARG:HB3	1.96	0.47
1:0:21:GLN:O	1:0:25:MET:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:522:VAL:HA	2:1:525:ILE:HG22	1.97	0.47
3:2:338:PHE:CE2	8:7:79:ALA:CB	2.89	0.47
5:4:249:VAL:HG13	5:4:249:VAL:O	2.14	0.47
8:7:174:ARG:HG2	8:7:269:SER:HB2	1.97	0.47
1:0:18:TYR:HA	1:0:19:PRO:HD2	1.68	0.46
3:2:262:LEU:CD1	3:2:271:VAL:HG11	2.45	0.46
4:3:174:ILE:HA	4:3:177:ARG:HB2	1.98	0.46
4:3:188:GLU:O	4:3:189:SER:OG	2.26	0.46
7:6:28:GLY:O	7:6:31:LYS:NZ	2.42	0.46
7:6:80:ARG:HD3	7:6:201:LEU:HD21	1.97	0.46
8:7:703:PHE:O	8:7:709:GLN:NE2	2.40	0.46
2:1:399:ASP:HA	2:1:402:ASN:HB2	1.97	0.46
3:2:201:PHE:HA	3:2:204:LEU:HD12	1.97	0.46
3:2:226:ARG:HD2	3:2:257:SER:HB3	1.97	0.46
3:2:239:GLN:OE1	3:2:291:SER:OG	2.22	0.46
7:6:271:PHE:N	7:6:285:THR:O	2.48	0.46
8:7:154:GLN:C	8:7:156:ILE:H	2.23	0.46
8:7:471:VAL:O	8:7:634:ARG:NH1	2.39	0.46
8:7:562:ALA:HA	8:7:626:ILE:HB	1.96	0.46
1:0:148:HIS:CE1	1:0:151:SER:H	2.33	0.46
1:0:568:PHE:HB2	1:0:596:LEU:HA	1.98	0.46
1:0:683:ARG:HH12	1:0:687:GLY:H	1.63	0.46
3:2:244:THR:HB	5:4:96:SER:OG	2.14	0.46
8:7:139:TYR:HA	8:7:142:LYS:HB3	1.97	0.46
8:7:286:HIS:HA	8:7:290:PRO:O	2.14	0.46
8:7:634:ARG:HA	8:7:637:ALA:HB3	1.97	0.46
1:0:539:PHE:N	1:0:598:SER:O	2.43	0.46
1:0:598:SER:HB2	1:0:604:VAL:HG21	1.98	0.46
2:1:188:LEU:N	2:1:191:ASP:HB3	2.31	0.46
3:2:151:TYR:HA	3:2:154:GLU:HG2	1.97	0.46
5:4:213:LEU:HD11	5:4:245:PRO:CG	2.45	0.46
7:6:189:LEU:HA	7:6:192:ALA:HB3	1.97	0.46
8:7:578:PRO:O	8:7:606:PHE:N	2.45	0.46
2:1:187:ASN:H	2:1:191:ASP:CB	2.29	0.46
3:2:12:VAL:HB	3:2:202:GLN:HE21	1.80	0.46
3:2:433:PHE:O	3:2:442:VAL:N	2.43	0.46
4:3:188:GLU:CB	8:7:188:LEU:HD22	2.45	0.46
1:0:236:ALA:HB1	1:0:239:ILE:HD11	1.97	0.46
1:0:326:ALA:HA	1:0:329:PHE:HB3	1.98	0.46
2:1:136:VAL:HG12	2:1:137:ILE:HG23	1.98	0.46
3:2:421:LEU:HA	3:2:424:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:102:GLU:HA	5:4:105:THR:HG22	1.97	0.46
7:6:279:ASN:N	7:6:298:TYR:HB3	2.31	0.46
8:7:73:SER:HA	8:7:145:LYS:HG3	1.98	0.46
3:2:307:ILE:HG22	3:2:316:TYR:HB2	1.96	0.46
3:2:330:LEU:HD12	3:2:331:PHE:HB2	1.97	0.46
3:2:354:ALA:O	3:2:358:GLY:N	2.47	0.46
4:3:87:GLU:HA	4:3:90:PRO:HD2	1.97	0.46
4:3:88:ASP:O	4:3:91:SER:OG	2.33	0.46
5:4:234:ASP:C	5:4:236:ASP:H	2.22	0.46
5:4:272:LEU:HD21	7:6:319:ALA:HB1	1.98	0.46
1:0:236:ALA:HB3	1:0:456:ILE:HG13	1.97	0.46
1:0:240:ASP:N	1:0:240:ASP:OD1	2.48	0.46
1:0:705:ASN:HB2	1:0:708:LEU:CD1	2.33	0.46
2:1:222:THR:O	2:1:226:GLN:N	2.49	0.46
3:2:280:ARG:HH12	3:2:282:TYR:HB2	1.80	0.46
4:3:178:LYS:O	4:3:182:ALA:N	2.37	0.46
5:4:32:PHE:HA	5:4:36:LYS:HD3	1.96	0.46
7:6:293:GLN:HB2	7:6:308:CYS:HB2	1.97	0.46
8:7:112:HIS:HD2	8:7:117:LYS:HG3	1.81	0.46
1:0:134:CYS:SG	1:0:299:ARG:CZ	2.98	0.46
2:1:459:SER:HA	2:1:462:LYS:HZ2	1.80	0.46
2:1:519:THR:HA	2:1:522:VAL:HG22	1.97	0.46
3:2:90:LEU:HD12	3:2:93:LEU:HD12	1.96	0.46
4:3:180:LYS:O	4:3:184:LEU:N	2.45	0.46
7:6:109:THR:HG21	7:6:144:SER:H	1.81	0.46
8:7:178:GLU:HG3	8:7:180:CYS:H	1.80	0.46
1:0:28:LEU:HG	1:0:32:LEU:HD13	1.97	0.46
1:0:544:TYR:O	1:0:548:THR:N	2.47	0.46
2:1:248:LYS:O	2:1:252:LYS:N	2.44	0.46
2:1:333:SER:O	2:1:334:ASN:C	2.58	0.46
3:2:88:GLY:O	3:2:92:GLY:N	2.46	0.46
4:3:209:GLU:CD	4:3:209:GLU:C	2.84	0.46
5:4:12:VAL:N	5:4:160:ARG:O	2.40	0.46
8:7:62:ARG:CZ	8:7:77:TRP:CZ3	2.99	0.46
8:7:360:ARG:O	8:7:433:GLN:NE2	2.49	0.46
8:7:579:TYR:HA	8:7:606:PHE:HB2	1.97	0.46
1:0:683:ARG:NH1	1:0:687:GLY:H	2.14	0.45
3:2:349:GLU:O	3:2:353:GLN:N	2.47	0.45
5:4:10:LEU:N	5:4:158:LYS:O	2.48	0.45
7:6:374:PHE:O	7:6:379:LEU:N	2.49	0.45
8:7:309:ASP:HA	8:7:384:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:696:MET:HB3	8:7:701:LEU:HD11	1.98	0.45
1:0:77:VAL:HA	1:0:80:ILE:HD12	1.97	0.45
3:2:238:PHE:CZ	3:2:270:LEU:HB2	2.50	0.45
7:6:59:ARG:N	7:6:102:SER:OG	2.49	0.45
7:6:276:LEU:HD21	7:6:297:LYS:HB2	1.97	0.45
7:6:303:VAL:HG12	7:6:304:GLU:HG2	1.98	0.45
1:0:263:LEU:HD11	1:0:336:LEU:HD23	1.97	0.45
1:0:441:SER:HB2	1:0:445:LYS:HE3	1.97	0.45
1:0:515:ALA:HA	1:0:518:ARG:HG2	1.99	0.45
2:1:304:ILE:O	2:1:308:ASN:ND2	2.50	0.45
7:6:290:PHE:HE1	7:6:295:ARG:HB3	1.81	0.45
1:0:86:GLU:O	1:0:86:GLU:HG2	2.15	0.45
1:0:613:HIS:CE1	7:6:206:ARG:HH21	2.34	0.45
2:1:187:ASN:ND2	2:1:191:ASP:HB2	2.29	0.45
3:2:144:ASP:O	3:2:147:SER:OG	2.30	0.45
7:6:375:VAL:HA	7:6:379:LEU:HB3	1.97	0.45
8:7:254:GLN:O	8:7:258:ASP:N	2.47	0.45
8:7:309:ASP:O	8:7:310:LEU:CD2	2.65	0.45
8:7:700:ASP:OD1	8:7:700:ASP:N	2.47	0.45
1:0:323:ILE:HD12	4:3:100:GLU:HB3	1.98	0.45
1:0:494:ILE:HA	1:0:679:PHE:HB2	1.98	0.45
2:1:350:LYS:HG3	2:1:353:LYS:HD3	1.99	0.45
7:6:201:LEU:HA	7:6:222:ILE:HD12	1.99	0.45
7:6:318:LEU:H	7:6:318:LEU:HG	1.61	0.45
8:7:109:ARG:HH22	8:7:471:VAL:HG23	1.82	0.45
8:7:463:LYS:HD2	8:7:484:ILE:HA	1.97	0.45
8:7:506:GLN:OE1	8:7:686:SER:OG	2.28	0.45
1:0:301:THR:HA	1:0:304:HIS:HB3	1.98	0.45
2:1:294:SER:O	2:1:298:ASN:ND2	2.49	0.45
3:2:418:PHE:CZ	3:2:441:MET:HG3	2.51	0.45
2:1:281:TYR:O	2:1:285:SER:OG	2.29	0.45
3:2:28:PRO:HA	3:2:31:LEU:HG	1.98	0.45
1:0:486:ALA:O	1:0:487:ARG:CB	2.61	0.45
1:0:670:GLY:HA3	2:1:338:ASN:ND2	2.32	0.45
2:1:296:LYS:HA	2:1:299:SER:HB2	1.99	0.45
3:2:83:GLN:O	3:2:87:THR:OG1	2.29	0.45
7:6:106:ILE:HB	7:6:118:THR:HB	1.99	0.45
1:0:353:SER:HB2	1:0:356:ALA:HB3	1.99	0.45
1:0:710:VAL:O	1:0:714:VAL:N	2.49	0.45
2:1:370:LYS:HA	5:4:254:ALA:HB3	1.98	0.45
3:2:179:LEU:HD22	3:2:184:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:156:LEU:HD21	7:6:165:ARG:HB3	1.99	0.45
8:7:51:THR:OG1	8:7:52:LYS:N	2.49	0.45
8:7:359:LYS:NZ	8:7:436:GLY:C	2.75	0.45
2:1:167:SER:OG	2:1:317:ALA:O	2.35	0.45
5:4:63:HIS:ND1	5:4:65:GLN:HG2	2.31	0.45
6:5:9:LEU:HD21	6:5:42:HIS:HD2	1.81	0.45
7:6:314:SER:H	7:6:318:LEU:HD21	1.82	0.45
8:7:66:PRO:HB3	8:7:71:HIS:HA	1.99	0.45
8:7:337:VAL:HG21	8:7:484:ILE:HB	1.99	0.45
8:7:601:LYS:HG3	8:7:602:ILE:HG13	1.98	0.45
1:0:726:GLN:HE22	7:6:223:LEU:HB2	1.82	0.44
8:7:296:ASP:OD1	8:7:334:ARG:N	2.49	0.44
8:7:350:GLY:O	8:7:354:ALA:N	2.49	0.44
1:0:580:ALA:O	1:0:583:LYS:HB2	2.17	0.44
1:0:609:ASP:OD1	1:0:666:ARG:NH1	2.46	0.44
2:1:527:GLU:OE2	2:1:531:THR:OG1	2.34	0.44
3:2:145:VAL:O	3:2:149:ASP:N	2.46	0.44
5:4:262:ILE:HG12	5:4:264:ILE:H	1.82	0.44
7:6:65:VAL:HG22	7:6:170:ILE:HD12	1.99	0.44
8:7:318:PRO:HA	8:7:321:GLU:HB2	1.99	0.44
1:0:579:VAL:HG13	2:1:257:MET:HE3	1.99	0.44
1:0:730:ARG:CZ	1:0:733:GLN:H	2.30	0.44
7:6:169:ILE:HD12	7:6:198:VAL:HG22	1.98	0.44
5:4:38:ILE:O	5:4:42:MET:N	2.41	0.44
7:6:58:MET:HG2	7:6:101:ILE:HB	1.98	0.44
7:6:107:ILE:HG12	7:6:116:LYS:HG3	2.00	0.44
7:6:337:GLU:HG3	7:6:353:LYS:HE3	1.99	0.44
1:0:114:ASN:ND2	1:0:177:LEU:CD2	2.80	0.44
1:0:210:HIS:HE1	2:1:275:LYS:HD3	1.83	0.44
1:0:497:ARG:HH12	1:0:711:ASP:CG	2.26	0.44
2:1:210:ASN:HA	2:1:213:HIS:HB3	1.99	0.44
7:6:251:ARG:HB3	7:6:310:LEU:HD13	1.98	0.44
1:0:71:ILE:HB	1:0:231:VAL:HG13	1.98	0.44
1:0:95:GLU:HG3	1:0:101:LYS:HB3	2.00	0.44
1:0:169:PRO:HG3	1:0:189:TRP:HH2	1.82	0.44
1:0:309:VAL:HG13	1:0:406:LEU:HD23	2.00	0.44
5:4:64:ILE:HD13	5:4:124:ILE:HB	1.99	0.44
5:4:75:ASN:O	5:4:79:GLY:N	2.40	0.44
5:4:147:MET:HG3	5:4:157:MET:HE1	1.99	0.44
1:0:504:ILE:HD13	1:0:680:ALA:HB1	1.99	0.44
1:0:543:GLN:O	1:0:547:SER:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:130:ASP:OD2	2:1:461:LEU:HD12	2.18	0.44
2:1:136:VAL:HG13	2:1:503:THR:HG21	1.98	0.44
4:3:204:ARG:HD2	8:7:266:GLN:HG3	2.00	0.44
1:0:176:ASN:H	1:0:179:ASP:HB2	1.83	0.44
2:1:487:GLU:HA	2:1:490:VAL:HG12	2.00	0.44
2:1:495:SER:OG	2:1:496:ASN:N	2.50	0.44
3:2:245:LEU:HG	3:2:280:ARG:NE	2.27	0.44
4:3:183:PHE:HZ	4:3:200:GLN:CG	2.30	0.44
5:4:271:CYS:SG	5:4:284:THR:OG1	2.76	0.44
7:6:88:LEU:O	7:6:92:VAL:N	2.43	0.44
8:7:156:ILE:O	8:7:156:ILE:HG23	2.16	0.44
8:7:187:HIS:O	8:7:191:ASP:N	2.39	0.44
8:7:363:VAL:O	8:7:408:SER:N	2.37	0.44
1:0:95:GLU:OE2	1:0:101:LYS:HD3	2.18	0.44
1:0:299:ARG:NH1	9:0:801:SF4:S1	2.91	0.44
3:2:314:ARG:NH2	3:2:346:VAL:H	2.15	0.44
5:4:51:MET:HB2	5:4:55:ASN:HD21	1.83	0.44
7:6:146:TYR:N	7:6:178:ASP:OD2	2.51	0.44
8:7:136:ILE:O	8:7:140:LEU:N	2.32	0.44
8:7:310:LEU:O	8:7:312:PRO:HD3	2.17	0.44
1:0:14:TYR:O	1:0:15:ASP:HB2	2.17	0.43
2:1:530:GLN:HG3	2:1:534:ASN:ND2	2.33	0.43
3:2:45:PHE:HE1	5:4:52:ASN:HA	1.82	0.43
3:2:231:VAL:HG13	3:2:232:GLU:HG3	2.00	0.43
5:4:190:LEU:HD11	5:4:212:GLY:HA2	2.00	0.43
7:6:11:TRP:O	7:6:15:TYR:N	2.38	0.43
7:6:31:LYS:HB2	8:7:145:LYS:HD2	2.00	0.43
8:7:363:VAL:HB	8:7:407:ILE:HA	2.00	0.43
8:7:504:LYS:NZ	8:7:653:GLU:O	2.42	0.43
2:1:483:THR:N	2:1:484:PRO:CD	2.81	0.43
3:2:42:LEU:HD11	3:2:236:PHE:HB2	1.99	0.43
3:2:323:LEU:O	3:2:327:LEU:N	2.48	0.43
4:3:193:PRO:HD3	4:3:199:ALA:HB3	2.00	0.43
7:6:64:VAL:HB	7:6:169:ILE:HA	1.99	0.43
8:7:472:ARG:NH1	8:7:473:GLU:CG	2.81	0.43
8:7:509:GLU:H	8:7:687:PHE:HE1	1.66	0.43
1:0:536:VAL:HG22	1:0:596:LEU:HB3	2.01	0.43
1:0:569:ILE:HG21	2:1:304:ILE:HG23	2.00	0.43
3:2:380:THR:HG22	3:2:382:VAL:H	1.83	0.43
4:3:203:ASP:O	4:3:207:GLN:HG2	2.18	0.43
5:4:144:ILE:O	5:4:148:ASN:N	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:206:ALA:HA	5:4:209:ILE:HD12	2.00	0.43
1:0:180:LEU:HA	1:0:183:LEU:HB2	2.01	0.43
1:0:210:HIS:CE1	2:1:275:LYS:HD3	2.53	0.43
2:1:335:MET:O	2:1:337:GLY:N	2.51	0.43
3:2:27:SER:HB2	3:2:30:VAL:HG23	2.01	0.43
3:2:309:VAL:HG23	3:2:314:ARG:HA	2.00	0.43
3:2:317:ALA:C	3:2:340:ASN:O	2.61	0.43
4:3:100:GLU:HA	4:3:103:GLU:HB3	2.00	0.43
1:0:180:LEU:C	1:0:180:LEU:CD1	2.84	0.43
1:0:252:THR:HG22	1:0:254:ARG:H	1.84	0.43
3:2:365:ILE:HA	3:2:368:LEU:HD12	2.00	0.43
8:7:141:ARG:HH12	8:7:148:VAL:HG23	1.83	0.43
8:7:442:GLU:HB3	8:7:444:HIS:NE2	2.33	0.43
1:0:135:HIS:CE1	1:0:139:ALA:HB3	2.54	0.43
5:4:115:ILE:O	5:4:119:MET:N	2.41	0.43
8:7:168:LEU:HD13	8:7:174:ARG:HD3	2.01	0.43
8:7:385:ASP:OD1	8:7:385:ASP:N	2.51	0.43
8:7:455:LEU:H	8:7:455:LEU:HG	1.69	0.43
1:0:250:ASN:HB2	1:0:432:ILE:HD11	1.99	0.43
2:1:461:LEU:O	2:1:464:LEU:HB2	2.18	0.43
3:2:420:LEU:O	3:2:424:HIS:N	2.42	0.43
5:4:263:GLU:HA	7:6:254:PHE:HB2	2.00	0.43
1:0:469:LYS:HD3	1:0:640:LEU:HD22	2.00	0.43
2:1:166:ILE:CD1	2:1:169:ALA:HB3	2.48	0.43
2:1:413:ALA:HA	2:1:416:PRO:HG3	2.01	0.43
3:2:75:VAL:HG13	5:4:242:ILE:HG12	2.00	0.43
3:2:78:GLU:HB3	5:4:242:ILE:HD11	2.00	0.43
4:3:162:ARG:HA	4:3:165:ILE:HD12	2.00	0.43
8:7:472:ARG:CG	8:7:473:GLU:N	2.81	0.43
1:0:638:GLU:HA	1:0:641:ARG:HB2	2.01	0.43
1:0:655:ASP:HA	1:0:658:ARG:HG2	2.01	0.43
2:1:535:LYS:HA	2:1:538:THR:HG22	2.00	0.43
3:2:17:ARG:O	3:2:21:GLU:N	2.50	0.43
8:7:95:TYR:O	8:7:99:PHE:N	2.52	0.43
8:7:375:LYS:HE2	8:7:391:ARG:HH11	1.83	0.43
1:0:144:ALA:HB2	1:0:387:GLU:CD	2.44	0.43
1:0:672:THR:O	1:0:672:THR:HG22	2.18	0.43
7:6:173:SER:HB3	7:6:203:ALA:HB3	2.00	0.43
1:0:102:LEU:HB3	1:0:103:PRO:CD	2.48	0.42
2:1:414:TYR:C	2:1:416:PRO:CD	2.83	0.42
3:2:178:LEU:O	3:2:182:ALA:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:306:PHE:CD2	3:2:375:VAL:HA	2.55	0.42
3:2:316:TYR:CZ	3:2:371:ARG:HD3	2.54	0.42
7:6:362:VAL:HG12	7:6:388:LYS:HE3	2.01	0.42
8:7:92:VAL:HB	8:7:94:LYS:NZ	2.34	0.42
1:0:207:TYR:HD2	1:0:211:TYR:HB3	1.84	0.42
1:0:320:PRO:O	1:0:322:SER:N	2.50	0.42
1:0:497:ARG:HG2	1:0:709:THR:HA	2.01	0.42
1:0:592:ARG:HA	7:6:175:THR:HG23	2.01	0.42
2:1:125:PHE:O	2:1:129:LYS:N	2.52	0.42
3:2:370:THR:HG22	3:2:373:HIS:HE2	1.83	0.42
7:6:66:ASP:HB2	7:6:171:PHE:HA	2.00	0.42
8:7:38:VAL:HB	8:7:156:ILE:HG12	2.00	0.42
8:7:113:VAL:HG23	8:7:115:GLU:HG2	2.00	0.42
8:7:183:ASP:OD1	8:7:183:ASP:N	2.50	0.42
8:7:339:VAL:HG13	8:7:468:ALA:HA	2.00	0.42
8:7:441:ASP:HA	8:7:466:LEU:HB2	2.01	0.42
1:0:533:ASP:HB2	1:0:616:ARG:HD3	2.00	0.42
2:1:404:PHE:O	2:1:408:ARG:NH1	2.52	0.42
5:4:98:ASP:HA	5:4:102:GLU:HB2	2.01	0.42
7:6:205:VAL:O	7:6:209:THR:N	2.47	0.42
7:6:363:CYS:HA	7:6:388:LYS:HE2	2.01	0.42
8:7:58:ALA:HB1	8:7:75:PRO:HG3	2.00	0.42
8:7:137:THR:OG1	8:7:157:LYS:NZ	2.49	0.42
8:7:184:VAL:HG21	8:7:268:VAL:HG11	2.01	0.42
5:4:12:VAL:O	5:4:162:LEU:N	2.40	0.42
5:4:227:LEU:HD12	5:4:231:PHE:HB2	2.01	0.42
7:6:224:ASP:O	7:6:228:TYR:N	2.44	0.42
8:7:444:HIS:HB2	8:7:472:ARG:HD3	2.00	0.42
1:0:233:PHE:HE2	1:0:454:VAL:HB	1.84	0.42
1:0:628:THR:HA	2:1:287:PRO:HG3	2.02	0.42
3:2:23:LEU:HG	3:2:31:LEU:HD22	2.02	0.42
5:4:165:LYS:HB3	5:4:195:VAL:HA	2.01	0.42
7:6:314:SER:O	7:6:317:HIS:ND1	2.32	0.42
8:7:316:LEU:HD22	8:7:348:LEU:HD13	2.01	0.42
8:7:435:TRP:HD1	8:7:460:ALA:HA	1.84	0.42
1:0:420:PRO:HA	1:0:431:PRO:HA	2.02	0.42
3:2:241:SER:C	3:2:242:PHE:CD1	2.98	0.42
7:6:27:SER:HA	7:6:31:LYS:HG2	2.02	0.42
1:0:640:LEU:HG	1:0:647:ARG:HG3	2.02	0.42
2:1:398:GLN:HG3	2:1:402:ASN:HD21	1.85	0.42
3:2:184:LEU:HA	3:2:199:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:449:SER:HA	3:2:452:LYS:HB3	2.01	0.42
5:4:181:ILE:H	5:4:181:ILE:HG13	1.59	0.42
8:7:305:ASP:OD1	8:7:305:ASP:N	2.52	0.42
1:0:233:PHE:HB2	1:0:456:ILE:HA	2.02	0.42
1:0:638:GLU:OE1	1:0:641:ARG:NH1	2.51	0.42
3:2:185:MET:HG2	3:2:196:ILE:HD13	2.01	0.42
3:2:245:LEU:HG	3:2:280:ARG:HB2	2.01	0.42
3:2:360:THR:HB	3:2:363:GLN:HB2	2.01	0.42
5:4:193:ALA:O	5:4:215:LEU:N	2.53	0.42
8:7:62:ARG:HH11	8:7:75:PRO:CG	2.33	0.42
1:0:18:TYR:HB3	1:0:671:LYS:CD	2.50	0.42
1:0:94:TYR:HA	1:0:97:GLN:HB2	2.02	0.42
1:0:580:ALA:O	1:0:584:TYR:N	2.51	0.42
3:2:109:ILE:HG12	3:2:115:ARG:HH22	1.85	0.42
6:5:49:LEU:O	6:5:53:LEU:N	2.43	0.42
8:7:365:GLY:N	8:7:408:SER:O	2.40	0.42
8:7:582:GLY:HA2	8:7:610:VAL:HG21	2.01	0.42
1:0:192:TYR:O	1:0:195:ALA:HB3	2.20	0.42
1:0:507:LYS:NZ	8:7:300:ASP:OD1	2.51	0.42
1:0:569:ILE:HD13	2:1:304:ILE:HA	2.00	0.42
1:0:668:ILE:HG13	1:0:673:ASP:CB	2.30	0.42
3:2:18:ASN:OD1	3:2:19:LEU:N	2.52	0.42
5:4:248:HIS:O	5:4:248:HIS:CG	2.73	0.42
7:6:54:ARG:HB3	7:6:55:LEU:H	1.51	0.42
2:1:211:VAL:HA	2:1:212:PRO:HA	1.82	0.41
1:0:46:THR:O	1:0:47:GLY:C	2.64	0.41
1:0:70:LEU:HB3	1:0:204:VAL:HG22	2.02	0.41
1:0:259:CYS:HA	1:0:262:ASN:ND2	2.35	0.41
2:1:404:PHE:CZ	5:4:116:LYS:HG3	2.56	0.41
3:2:328:ILE:C	3:2:331:PHE:H	2.28	0.41
7:6:64:VAL:HB	7:6:169:ILE:HG12	2.02	0.41
7:6:85:LEU:HA	7:6:88:LEU:HD12	2.03	0.41
8:7:448:ALA:HA	8:7:451:PHE:HB2	2.02	0.41
8:7:665:GLN:HA	8:7:670:MET:HE3	2.01	0.41
1:0:20:GLU:O	1:0:21:GLN:C	2.62	0.41
1:0:70:LEU:HA	1:0:70:LEU:HD12	1.82	0.41
3:2:255:SER:H	3:2:258:LEU:HB3	1.85	0.41
7:6:12:GLU:OE2	8:7:129:VAL:N	2.49	0.41
8:7:706:LYS:O	8:7:710:GLN:N	2.48	0.41
1:0:256:LEU:O	1:0:260:GLN:N	2.47	0.41
2:1:472:LEU:HD21	2:1:496:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:191:ASP:O	4:3:192:LEU:O	2.39	0.41
5:4:11:LEU:HB2	5:4:48:HIS:CE1	2.56	0.41
8:7:390:CYS:HB3	8:7:392:PHE:CE2	2.55	0.41
8:7:547:LEU:HA	8:7:550:PHE:HB3	2.02	0.41
3:2:313:TYR:HA	3:2:345:GLN:HB3	2.02	0.41
3:2:404:THR:O	6:5:9:LEU:N	2.52	0.41
3:2:434:GLU:HA	3:2:441:MET:HA	2.02	0.41
8:7:74:ARG:HB3	8:7:87:GLU:CD	2.45	0.41
1:0:105:LEU:HD21	1:0:198:SER:HB2	2.03	0.41
1:0:108:ALA:HA	1:0:206:VAL:O	2.20	0.41
1:0:198:SER:O	1:0:202:ALA:HB2	2.20	0.41
1:0:518:ARG:NH1	8:7:310:LEU:HB3	2.36	0.41
3:2:234:LEU:HA	3:2:237:LEU:HB3	2.02	0.41
8:7:338:ILE:HG23	8:7:489:TYR:HB3	2.02	0.41
1:0:115:LEU:HA	1:0:191:PRO:HG3	2.03	0.41
1:0:189:TRP:N	1:0:194:LEU:HD22	2.35	0.41
2:1:349:VAL:HB	7:6:54:ARG:NH2	2.35	0.41
2:1:422:LEU:HD23	5:4:222:SER:HB2	2.03	0.41
3:2:322:GLU:O	3:2:326:ALA:N	2.46	0.41
4:3:93:ARG:HB2	4:3:98:PHE:HB2	2.03	0.41
4:3:133:ILE:O	4:3:137:LYS:N	2.46	0.41
8:7:62:ARG:CZ	8:7:77:TRP:CH2	3.04	0.41
8:7:317:ARG:HB2	8:7:319:TYR:CE1	2.55	0.41
8:7:563:ASP:HA	8:7:627:SER:HB2	2.02	0.41
1:0:112:ARG:HD3	2:1:271:ALA:O	2.21	0.41
1:0:240:ASP:OD2	1:0:658:ARG:NH2	2.53	0.41
1:0:275:GLU:OE1	1:0:279:GLN:NE2	2.54	0.41
1:0:523:LEU:HD12	1:0:523:LEU:O	2.21	0.41
2:1:400:ILE:HG21	5:4:122:SER:HB3	2.02	0.41
2:1:417:LYS:HZ2	5:4:43:VAL:HG21	1.84	0.41
3:2:407:VAL:HG11	3:2:448:HIS:HB2	2.02	0.41
7:6:354:ASP:HB3	7:6:356:HIS:HD2	1.86	0.41
8:7:279:GLU:O	8:7:283:ARG:NE	2.51	0.41
8:7:562:ALA:HB3	8:7:568:LEU:HD22	2.02	0.41
1:0:500:ASP:OD1	8:7:311:LYS:NZ	2.54	0.41
2:1:180:GLY:HA3	2:1:184:LEU:HD13	2.03	0.41
2:1:461:LEU:HD21	2:1:504:LYS:HE3	2.03	0.41
3:2:11:ARG:O	3:2:11:ARG:HG3	2.21	0.41
3:2:52:ALA:HB1	3:2:90:LEU:HD22	2.03	0.41
3:2:130:SER:C	3:2:131:ASP:CG	2.89	0.41
3:2:304:PRO:HD2	3:2:373:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:393:LEU:HA	3:2:396:LEU:HB2	2.02	0.41
4:3:194:VAL:HG12	4:3:198:LEU:CD1	2.37	0.41
6:5:17:LYS:NZ	6:5:42:HIS:H	2.19	0.41
7:6:345:CYS:H	7:6:349:GLN:HA	1.86	0.41
8:7:62:ARG:HG3	8:7:74:ARG:H	1.85	0.41
8:7:76:LEU:HA	8:7:87:GLU:HG2	2.03	0.41
8:7:106:PRO:HB3	8:7:119:THR:HG21	2.03	0.41
8:7:112:HIS:CD2	8:7:117:LYS:HA	2.56	0.41
8:7:586:GLN:HA	8:7:589:ARG:HD2	2.02	0.41
1:0:231:VAL:H	1:0:454:VAL:HG12	1.86	0.41
1:0:539:PHE:H	1:0:599:VAL:HA	1.86	0.41
1:0:626:VAL:HG12	1:0:628:THR:H	1.86	0.41
3:2:28:PRO:O	3:2:32:ASP:N	2.52	0.41
4:3:140:LEU:HA	4:3:143:GLU:HG2	2.03	0.41
4:3:159:GLU:HA	4:3:162:ARG:HG2	2.02	0.41
8:7:133:THR:OG1	8:7:158:LEU:HB2	2.21	0.41
8:7:320:GLN:O	8:7:323:SER:OG	2.27	0.41
1:0:383:LEU:HD12	1:0:386:LEU:HD12	2.02	0.40
1:0:601:ARG:NH2	1:0:624:PRO:O	2.54	0.40
1:0:633:LEU:O	1:0:637:LEU:N	2.36	0.40
3:2:58:ARG:O	3:2:62:LEU:N	2.52	0.40
3:2:212:LEU:HD23	3:2:268:PHE:HD1	1.85	0.40
3:2:383:LEU:HA	3:2:383:LEU:HD23	1.87	0.40
5:4:223:LEU:O	5:4:223:LEU:HG	2.21	0.40
7:6:322:TYR:CZ	7:6:326:PHE:HB3	2.56	0.40
7:6:345:CYS:HB3	7:6:349:GLN:H	1.85	0.40
7:6:360:CYS:HB3	7:6:364:GLN:H	1.85	0.40
8:7:177:VAL:HG23	8:7:268:VAL:O	2.20	0.40
1:0:262:ASN:HA	1:0:265:THR:CB	2.49	0.40
1:0:651:PHE:O	1:0:654:PHE:N	2.54	0.40
2:1:497:LEU:HD21	2:1:501:GLN:NE2	2.35	0.40
4:3:68:VAL:HG22	4:3:71:GLU:H	1.86	0.40
5:4:138:ALA:HA	5:4:141:LEU:HD12	2.04	0.40
8:7:160:THR:HG21	8:7:291:LEU:HD22	2.04	0.40
1:0:307:ASN:ND2	1:0:310:LEU:HA	2.36	0.40
1:0:580:ALA:HA	1:0:583:LYS:HD2	2.03	0.40
1:0:739:LEU:C	1:0:739:LEU:HD12	2.47	0.40
2:1:491:VAL:O	2:1:495:SER:N	2.55	0.40
3:2:212:LEU:HB3	3:2:216:MET:HE2	2.03	0.40
3:2:314:ARG:NH1	3:2:345:GLN:HB2	2.37	0.40
4:3:73:GLU:HA	4:3:76:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:27:SER:OG	7:6:28:GLY:N	2.53	0.40
7:6:315:ALA:HB1	7:6:320:ARG:NH1	2.36	0.40
8:7:71:HIS:CE1	8:7:95:TYR:HE2	2.38	0.40
8:7:117:LYS:HE3	8:7:117:LYS:HB2	1.89	0.40
2:1:351:ARG:HG2	7:6:54:ARG:HG3	2.03	0.40
3:2:95:ILE:O	3:2:111:ASN:N	2.40	0.40
3:2:407:VAL:HG13	3:2:443:VAL:HB	2.03	0.40
4:3:83:ASN:N	4:3:83:ASN:OD1	2.55	0.40
5:4:22:TRP:CD2	5:4:34:LEU:HD13	2.56	0.40
5:4:268:CYS:N	5:4:273:SER:O	2.46	0.40
7:6:356:HIS:CE1	7:6:369:VAL:HG23	2.57	0.40
7:6:368:CYS:O	7:6:372:ASP:N	2.52	0.40
8:7:349:VAL:O	8:7:353:ALA:N	2.41	0.40
8:7:592:ILE:O	8:7:596:PHE:N	2.54	0.40
1:0:558:LEU:HA	1:0:561:ILE:HB	2.04	0.40
3:2:236:PHE:O	3:2:239:GLN:N	2.53	0.40
3:2:251:VAL:HA	3:2:254:MET:HB3	2.03	0.40
4:3:209:GLU:HA	4:3:212:LEU:HB2	2.03	0.40
5:4:142:CYS:SG	5:4:143:TYR:N	2.93	0.40
5:4:179:ASN:OD1	5:4:179:ASN:N	2.52	0.40
5:4:257:CYS:H	5:4:276:CYS:H	1.69	0.40
8:7:52:LYS:HB2	8:7:55:GLU:HB3	2.04	0.40
8:7:442:GLU:HA	8:7:467:THR:HA	2.03	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	0	730/760 (96%)	590 (81%)	121 (17%)	19 (3%)	4	25
2	1	431/548 (79%)	352 (82%)	72 (17%)	7 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	451/462 (98%)	371 (82%)	72 (16%)	8 (2%)	6	33
4	3	210/309 (68%)	171 (81%)	35 (17%)	4 (2%)	6	32
5	4	293/308 (95%)	239 (82%)	51 (17%)	3 (1%)	12	47
6	5	64/71 (90%)	57 (89%)	7 (11%)	0	100	100
7	6	383/395 (97%)	313 (82%)	70 (18%)	0	100	100
8	7	648/782 (83%)	518 (80%)	123 (19%)	7 (1%)	11	45
All	All	3210/3635 (88%)	2611 (81%)	551 (17%)	48 (2%)	11	38

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	19	PRO
1	0	63	TYR
1	0	190	CYS
1	0	726	GLN
1	0	727	PRO
2	1	191	ASP
3	2	338	PHE
8	7	267	THR
1	0	15	ASP
1	0	148	HIS
1	0	186	ARG
1	0	194	LEU
1	0	704	ALA
1	0	739	LEU
2	1	148	ASN
2	1	163	ASP
2	1	187	ASN
2	1	192	ILE
2	1	336	ASP
2	1	418	LEU
3	2	301	VAL
3	2	339	PRO
4	3	4	GLN
8	7	92	VAL
1	0	672	THR
3	2	242	PHE
3	2	340	ASN
5	4	244	PRO
8	7	289	TYR

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Mol	Chain	Res	Type
1	0	487	ARG
3	2	241	SER
4	3	198	LEU
5	4	235	GLN
5	4	248	HIS
8	7	266	GLN
8	7	397	LYS
1	0	172	ALA
1	0	740	SER
3	2	304	PRO
8	7	114	HIS
8	7	434	GLU
1	0	47	GLY
3	2	138	PRO
4	3	192	LEU
1	0	204	VAL
1	0	670	GLY
1	0	320	PRO
4	3	193	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	630/664 (95%)	615 (98%)	15 (2%)	43	63
2	1	384/484 (79%)	380 (99%)	4 (1%)	68	76
3	2	390/399 (98%)	384 (98%)	6 (2%)	57	70
4	3	202/283 (71%)	201 (100%)	1 (0%)	81	81
5	4	259/272 (95%)	257 (99%)	2 (1%)	73	77
6	5	59/64 (92%)	59 (100%)	0	100	100
7	6	342/352 (97%)	339 (99%)	3 (1%)	70	76
8	7	576/688 (84%)	571 (99%)	5 (1%)	70	76
All	All	2842/3206 (89%)	2806 (99%)	36 (1%)	59	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	17	ILE
1	0	77	VAL
1	0	113	LYS
1	0	114	ASN
1	0	152	LEU
1	0	187	GLN
1	0	203	ASN
1	0	309	VAL
1	0	487	ARG
1	0	488	VAL
1	0	557	ILE
1	0	697	ILE
1	0	705	ASN
1	0	741	LEU
1	0	742	GLU
2	1	188	LEU
2	1	189	THR
2	1	191	ASP
2	1	461	LEU
3	2	14	LEU
3	2	56	VAL
3	2	105	LEU
3	2	145	VAL
3	2	262	LEU
3	2	338	PHE
4	3	68	VAL
5	4	132	LEU
5	4	224	LEU
7	6	54	ARG
7	6	194	ILE
7	6	318	LEU
8	7	123	LEU
8	7	154	GLN
8	7	170	LEU
8	7	267	THR
8	7	580	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	114	ASN

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Mol	Chain	Res	Type
1	0	147	GLN
1	0	241	ASN
1	0	279	GLN
1	0	307	ASN
1	0	347	GLN
1	0	430	ASN
1	0	522	ASN
1	0	726	GLN
2	1	126	GLN
2	1	187	ASN
2	1	298	ASN
2	1	300	ASN
2	1	328	GLN
2	1	338	ASN
2	1	384	HIS
2	1	393	GLN
2	1	398	GLN
2	1	450	ASN
2	1	501	GLN
2	1	534	ASN
3	2	64	GLN
3	2	117	ASN
3	2	202	GLN
3	2	260	ASN
3	2	363	GLN
3	2	424	HIS
4	3	156	GLN
4	3	160	GLN
4	3	170	GLN
5	4	92	ASN
5	4	148	ASN
5	4	235	GLN
5	4	237	GLN
7	6	49	HIS
7	6	98	GLN
7	6	99	ASN
7	6	123	ASN
7	6	234	HIS
7	6	275	HIS
7	6	323	HIS
7	6	324	HIS
7	6	340	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	6	365	ASN
8	7	64	GLN
8	7	97	GLN
8	7	307	ASN
8	7	320	GLN
8	7	330	ASN
8	7	497	GLN
8	7	665	GLN

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](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SF4	0	801	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	0	801	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	0	801	SF4	1	0

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.

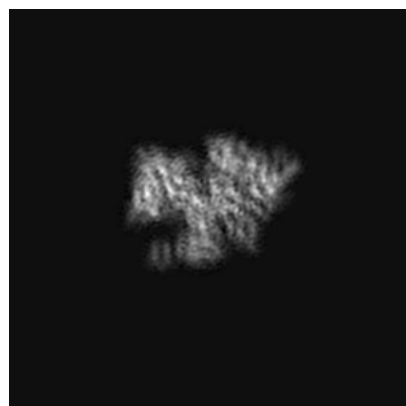
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3802. These allow visual inspection of the internal detail of the map and identification of artifacts.

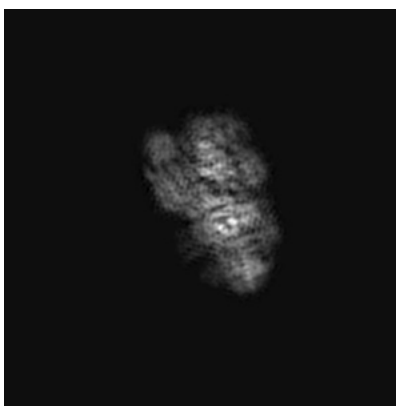
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

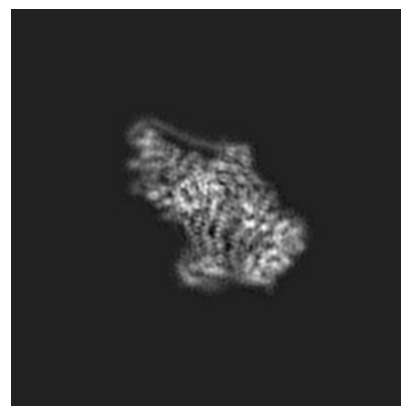
6.1.1 Primary map



X

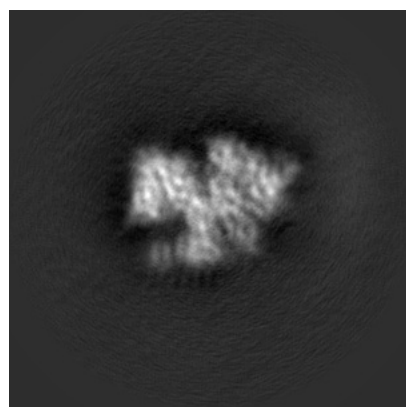


Y

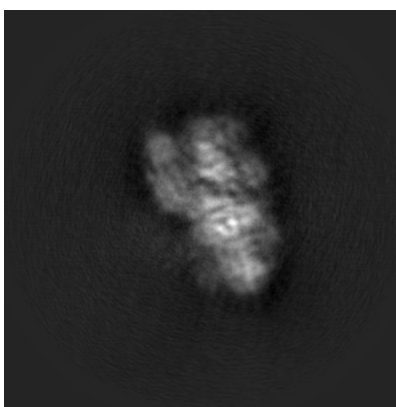


Z

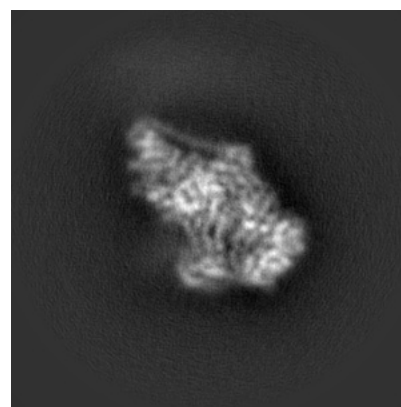
6.1.2 Raw map



X



Y

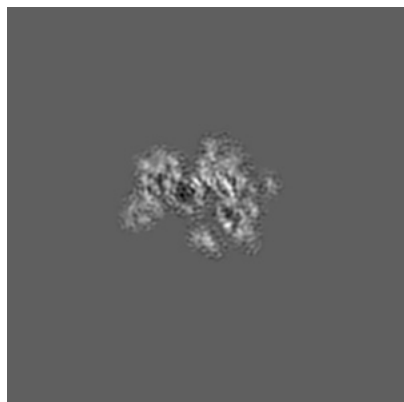


Z

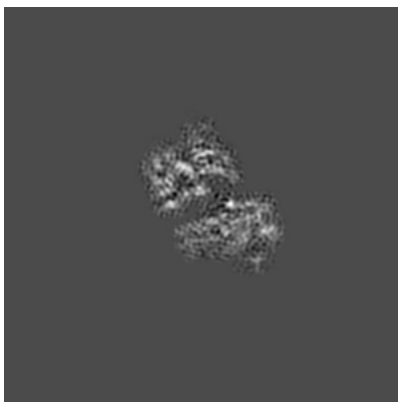
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

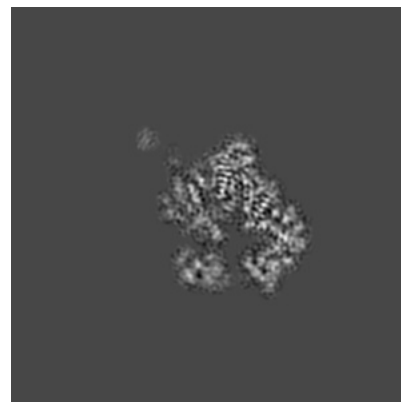
6.2.1 Primary map



X Index: 128

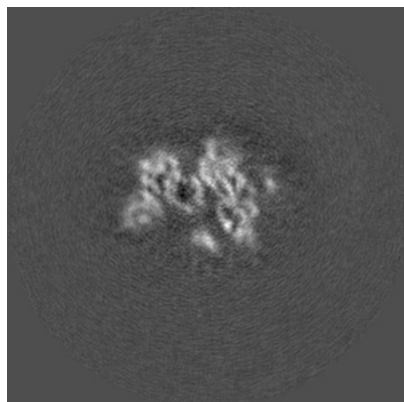


Y Index: 128

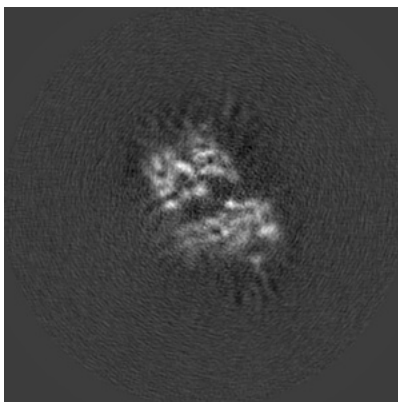


Z Index: 128

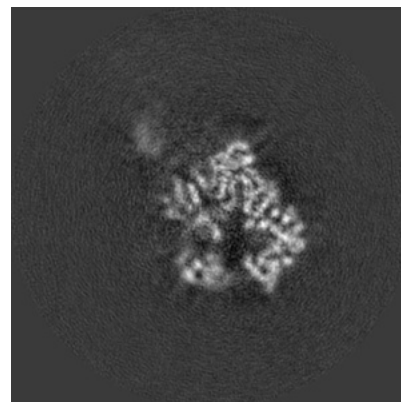
6.2.2 Raw map



X Index: 128



Y Index: 128

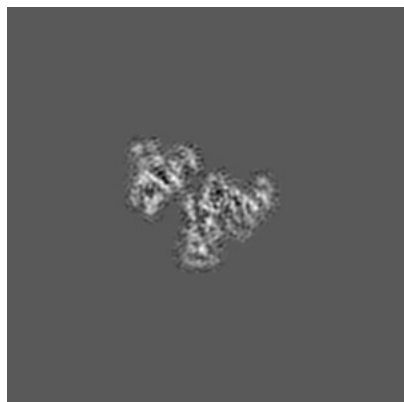


Z Index: 128

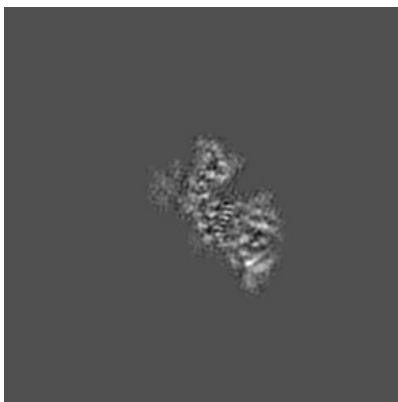
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

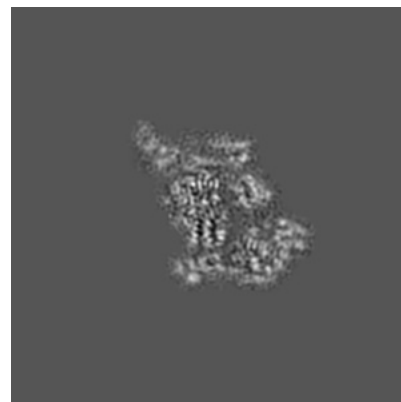
6.3.1 Primary map



X Index: 151

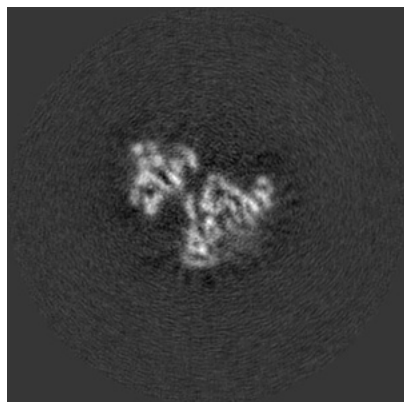


Y Index: 138

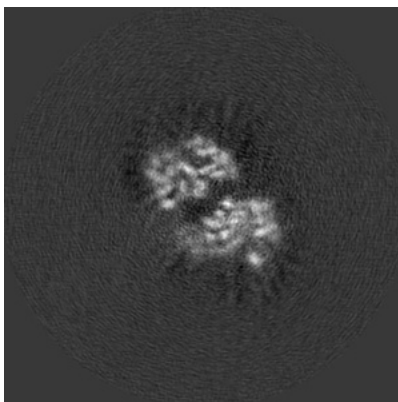


Z Index: 138

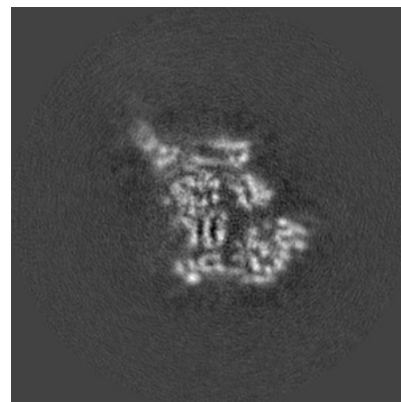
6.3.2 Raw map



X Index: 151



Y Index: 130

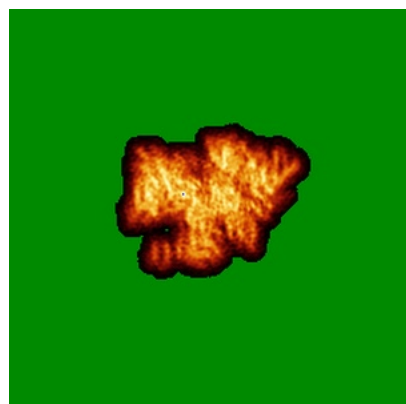


Z Index: 138

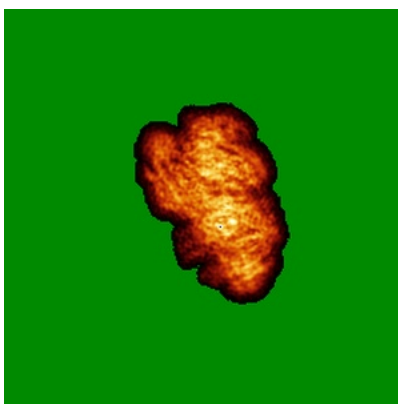
The images above show the largest variance slices of the map in three orthogonal directions.

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

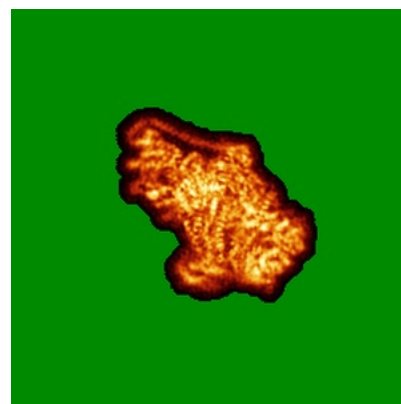
6.4.1 Primary map



X

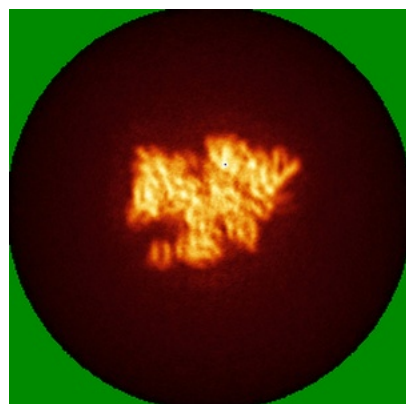


Y

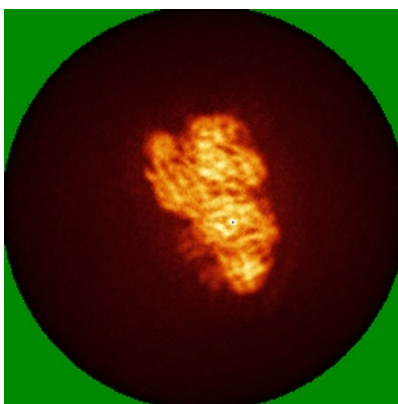


Z

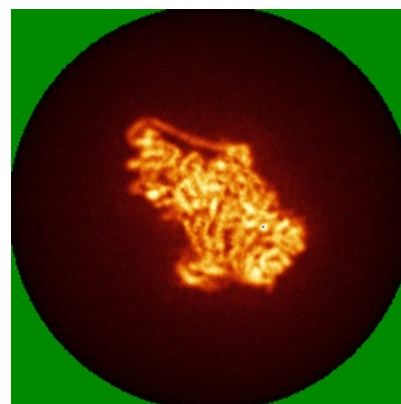
6.4.2 Raw map



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.

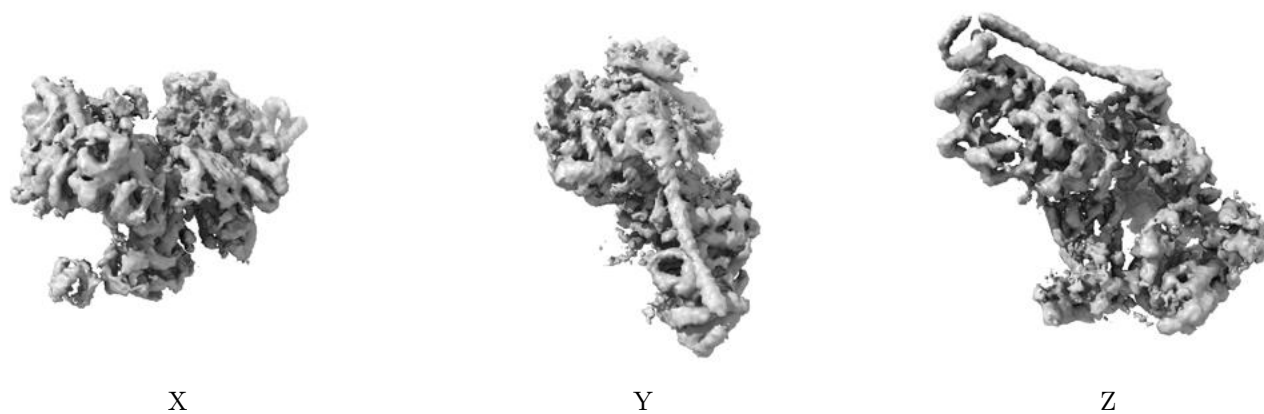
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

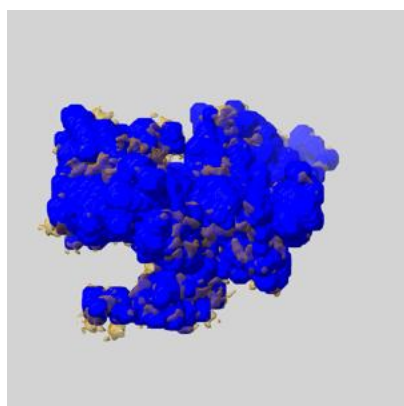
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

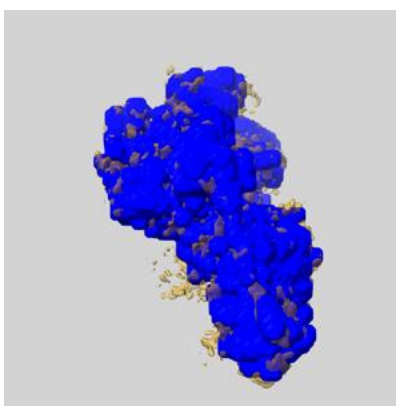
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

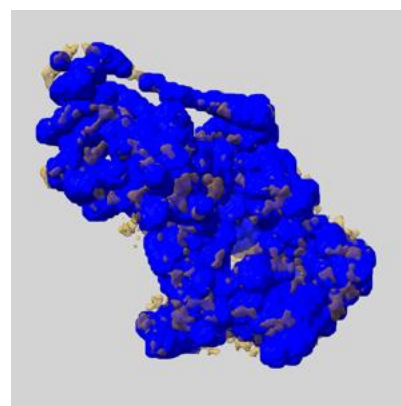
6.6.1 emd_3802_msk_1.map [i](#)



X



Y

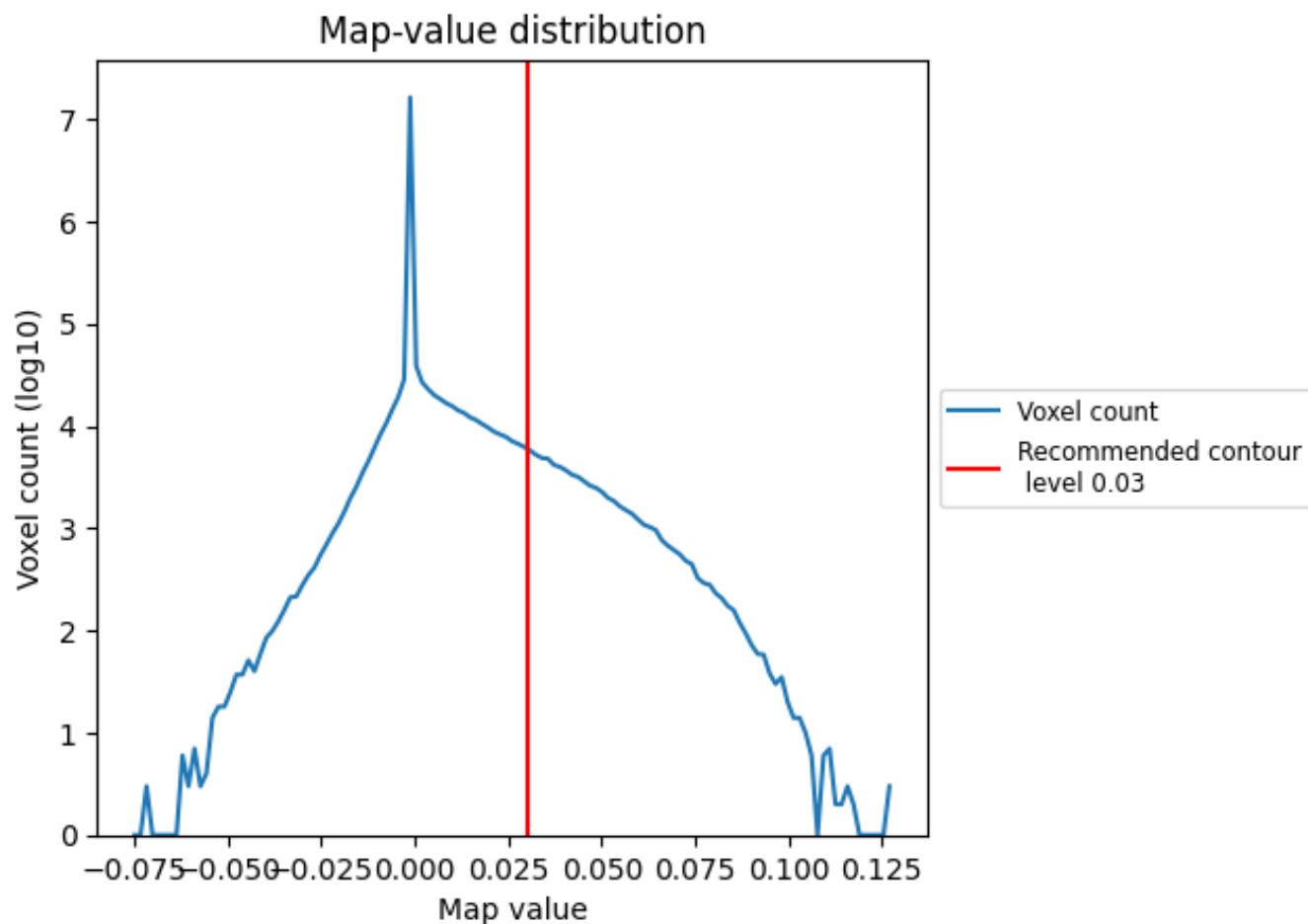


Z

7 Map analysis [i](#)

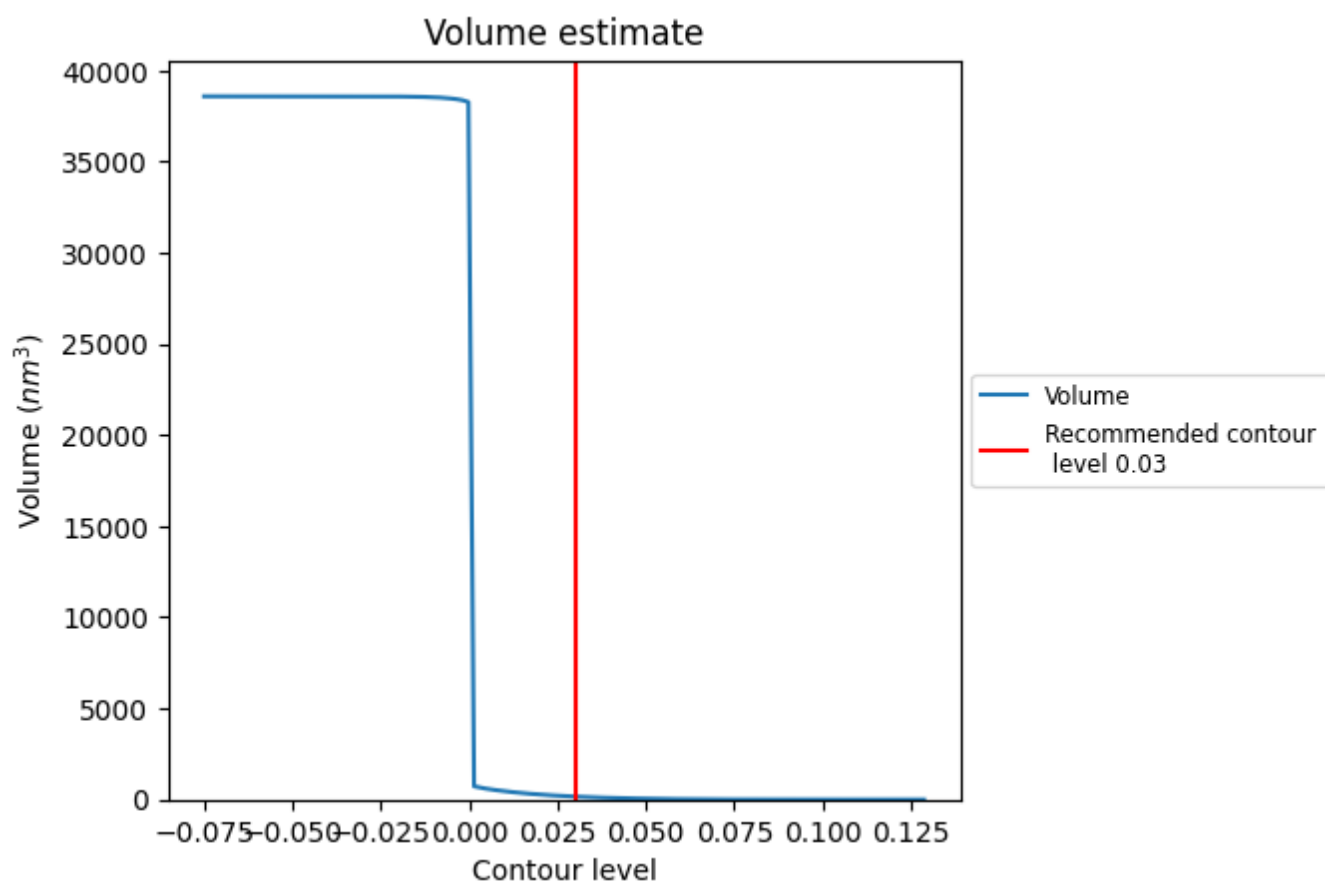
This section contains the results of statistical analysis of the map.

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.

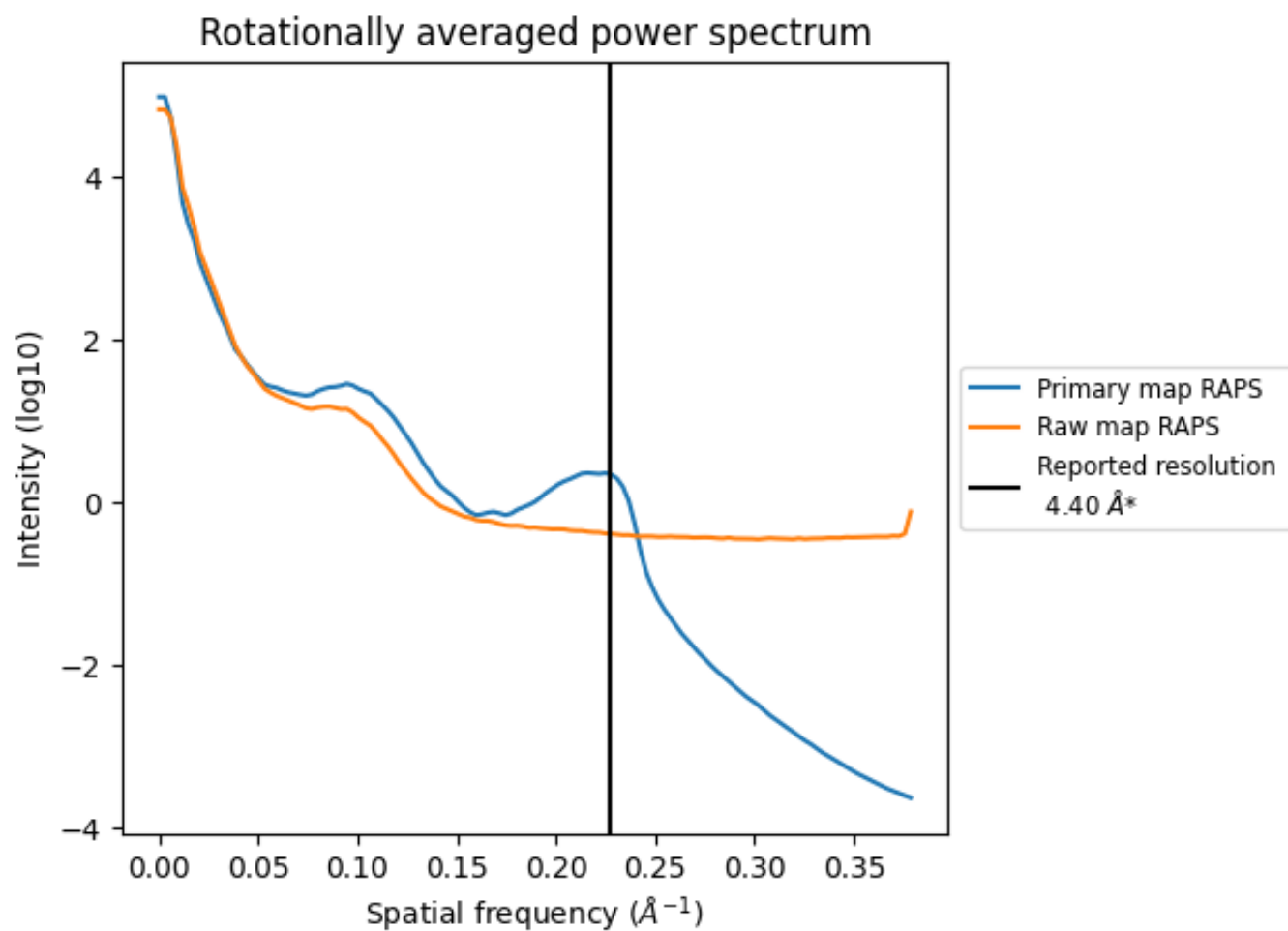
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm³; this corresponds to an approximate mass of 147 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 ⓘ

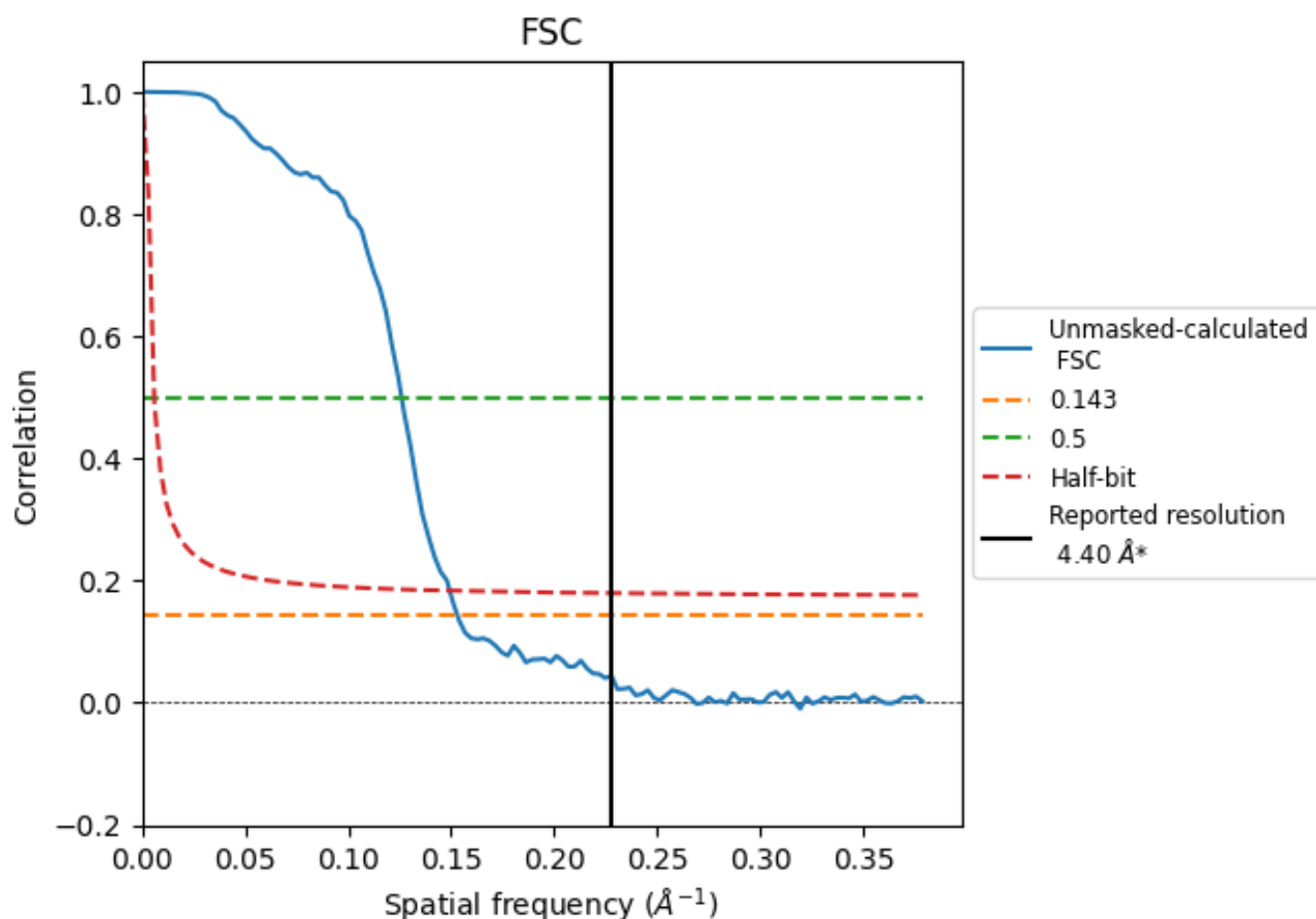


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

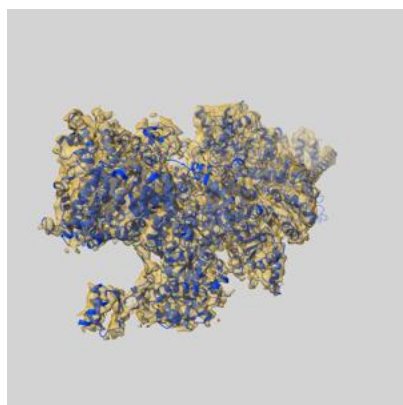
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.53	7.94	6.69

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

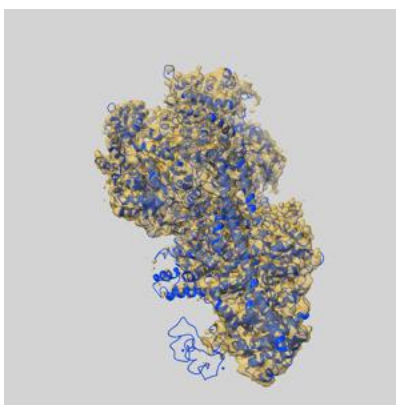
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3802 and PDB model 6O9M. Per-residue inclusion information can be found in section [3](#) on page [6](#).

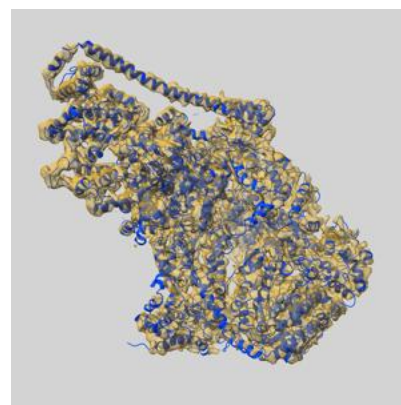
9.1 Map-model overlay [i](#)



X



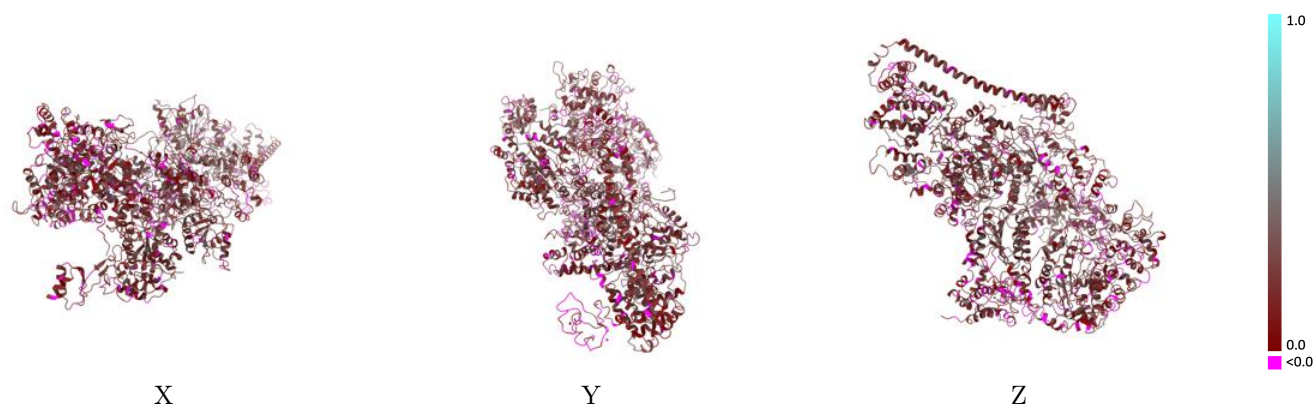
Y



Z

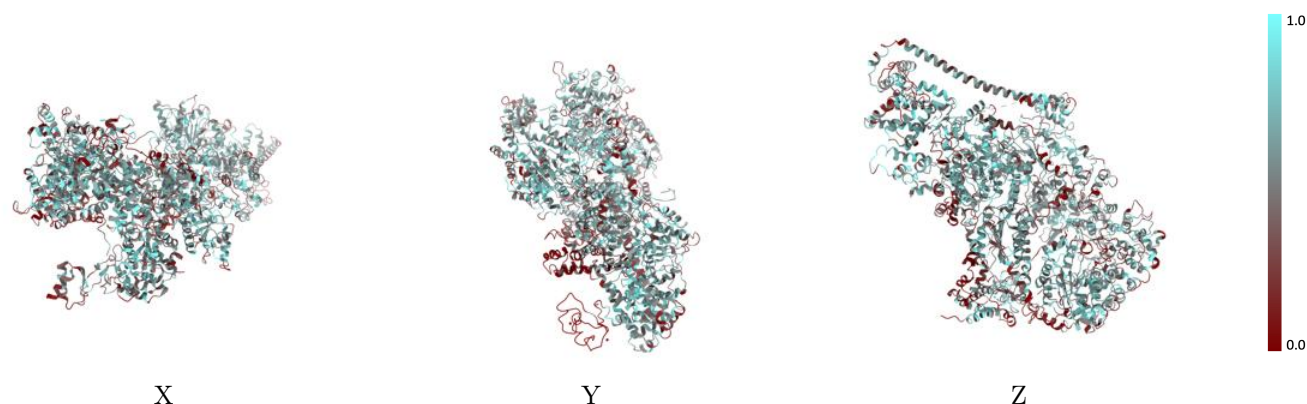
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



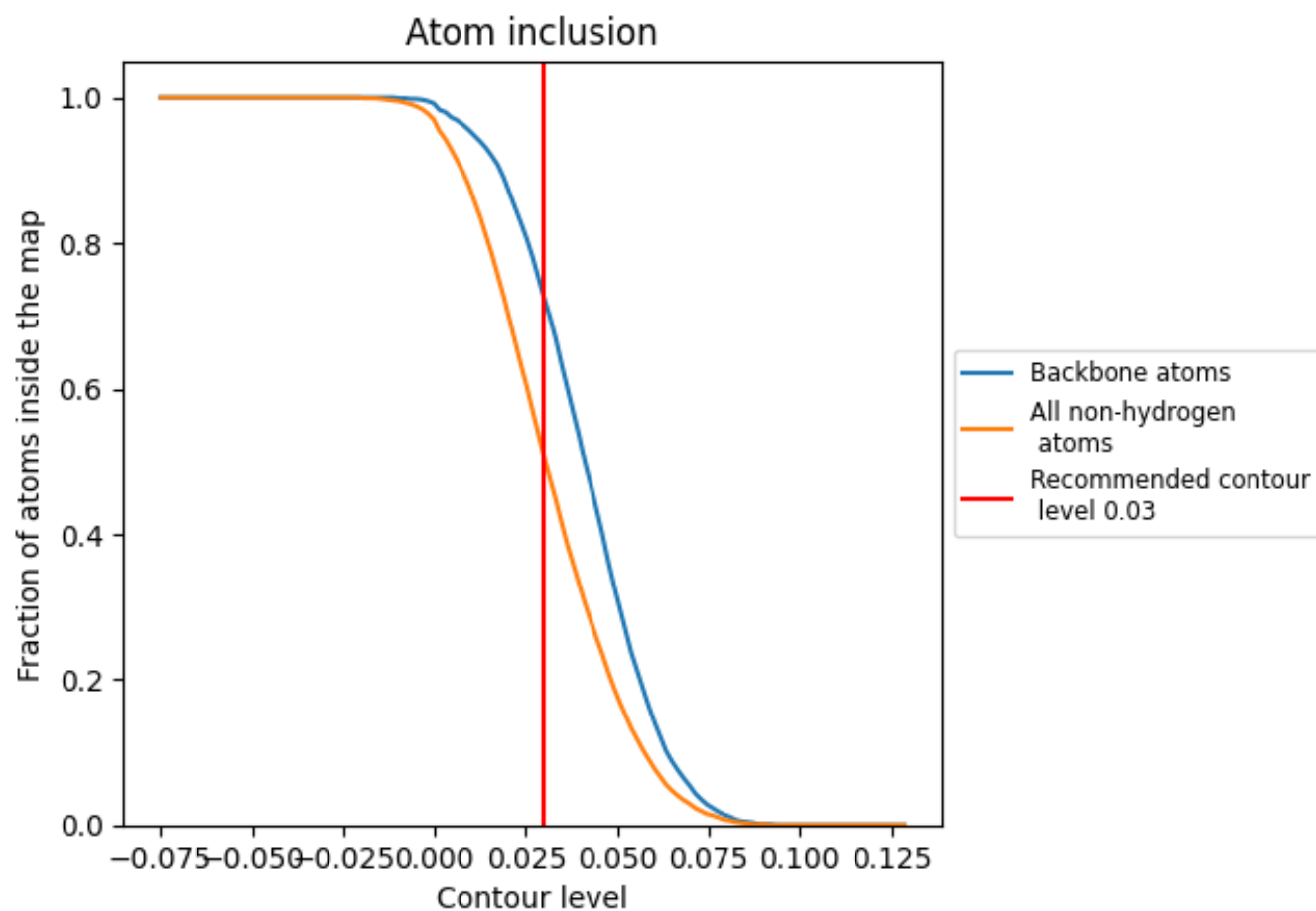
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 51% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5060	0.1900
0	0.6110	0.2310
1	0.2730	0.1260
2	0.5370	0.1740
3	0.3810	0.1340
4	0.5170	0.1730
5	0.4820	0.2010
6	0.5110	0.2190
7	0.5570	0.2040

1.0

0.0

<0.0