



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 10:25 AM UTC

PDB ID : 8YWW / pdb_00008yww
EMDB ID : EMD-39645
Title : The structure of HKU1-B S protein with bsAb1
Authors : Xia, L.Y.; Zhang, Y.Y.; Zhou, Q.
Deposited on : 2024-04-01
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

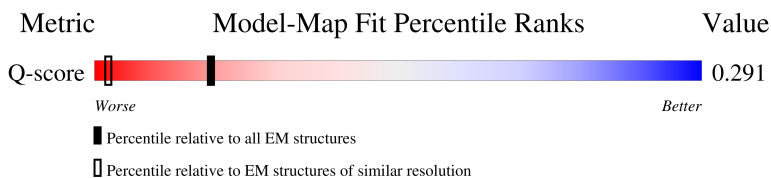
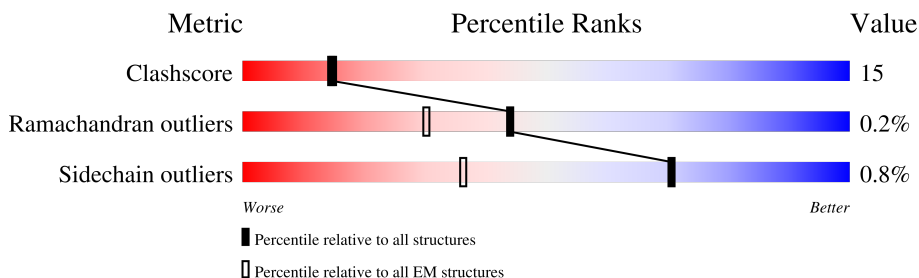
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	1210	
1	B	1210	
1	C	1210	
2	E	218	

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Mol	Chain	Length	Quality of chain
2	G	218	70% 60% 31% 9%
3	D	212	68% 67% 27% 6%
3	F	212	75% 67% 27% 6%
4	H	245	94% 57% 43%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31649 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0
			7754	4980	1288	1451	35		
1	B	1024	Total	C	N	O	S	0	0
			7754	4980	1288	1451	35		
1	C	1024	Total	C	N	O	S	0	0
			7754	4980	1288	1451	35		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	78	HIS	ARG	conflict	UNP P0DTC2
A	79	VAL	PHE	conflict	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	658	SER	ASN	conflict	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	TYR	conflict	UNP P0DTC2
A	1210	SER	ILE	conflict	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	78	HIS	ARG	conflict	UNP P0DTC2
B	79	VAL	PHE	conflict	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	658	SER	ASN	conflict	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	TYR	conflict	UNP P0DTC2
B	1210	SER	ILE	conflict	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	78	HIS	ARG	conflict	UNP P0DTC2
C	79	VAL	PHE	conflict	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	658	SER	ASN	conflict	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	TYR	conflict	UNP P0DTC2
C	1210	SER	ILE	conflict	UNP P0DTC2

- Molecule 2 is a protein called H4B6 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	218	Total	C	N	O	S	0	0
			1619	1015	278	320	6		
2	G	218	Total	C	N	O	S	0	0
			1619	1015	278	320	6		

- Molecule 3 is a protein called H4B6 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	212	Total	C	N	O	S	0	0
			1646	1028	278	335	5		
3	F	212	Total	C	N	O	S	0	0
			1646	1028	278	335	5		

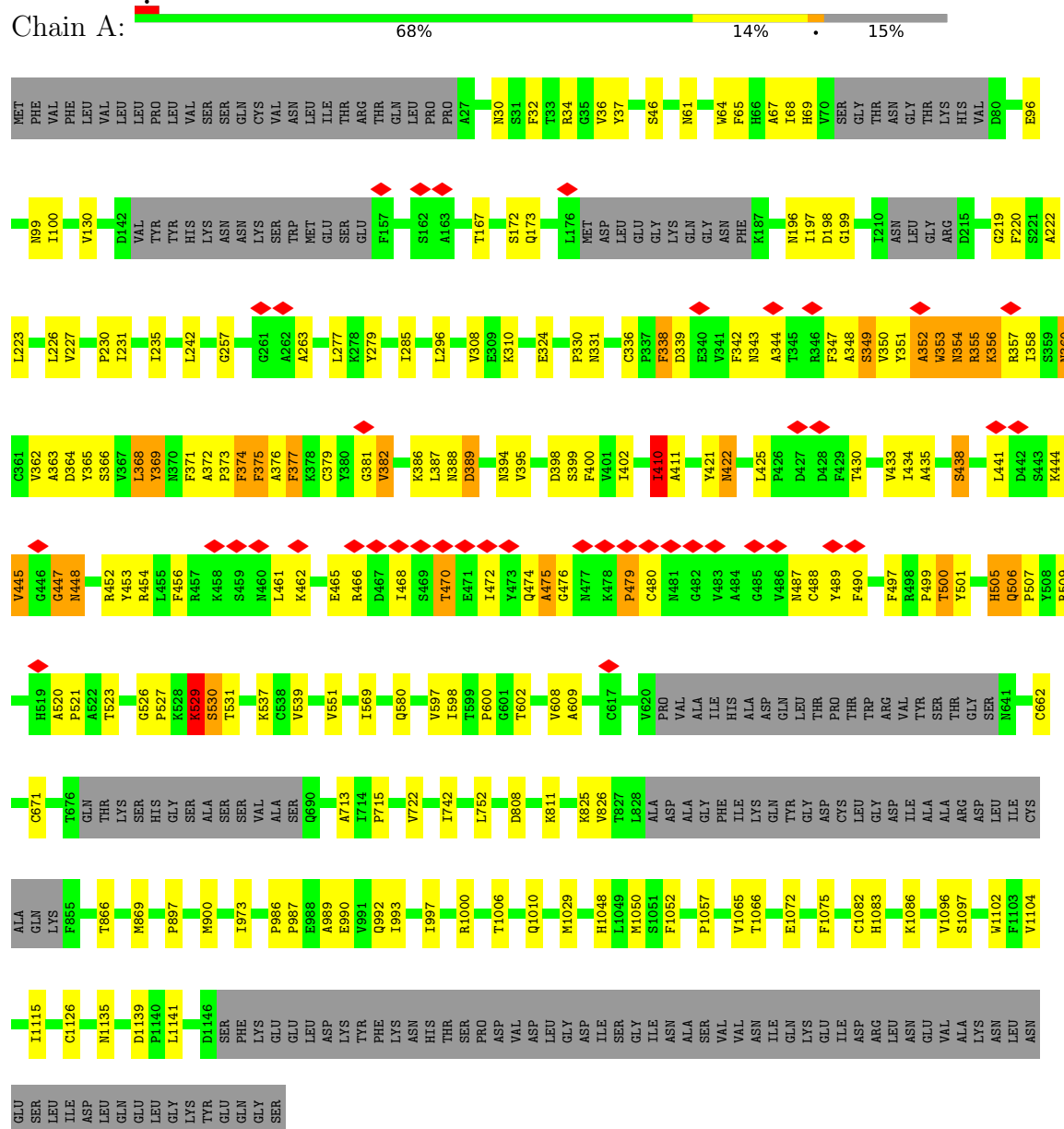
- Molecule 4 is a protein called the scfv of H4D12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	245	Total	C	N	O	S	0	0
			1857	1160	324	364	9		

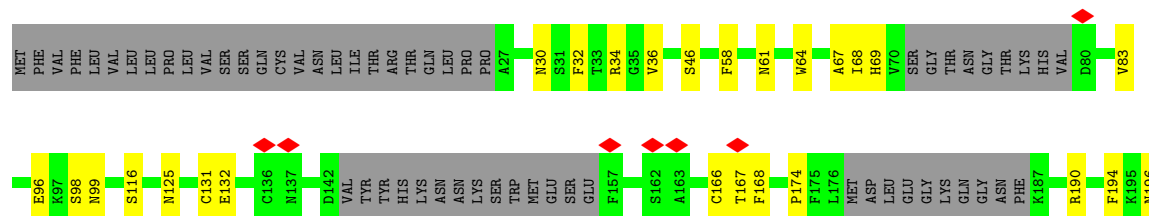
3 Residue-property plots

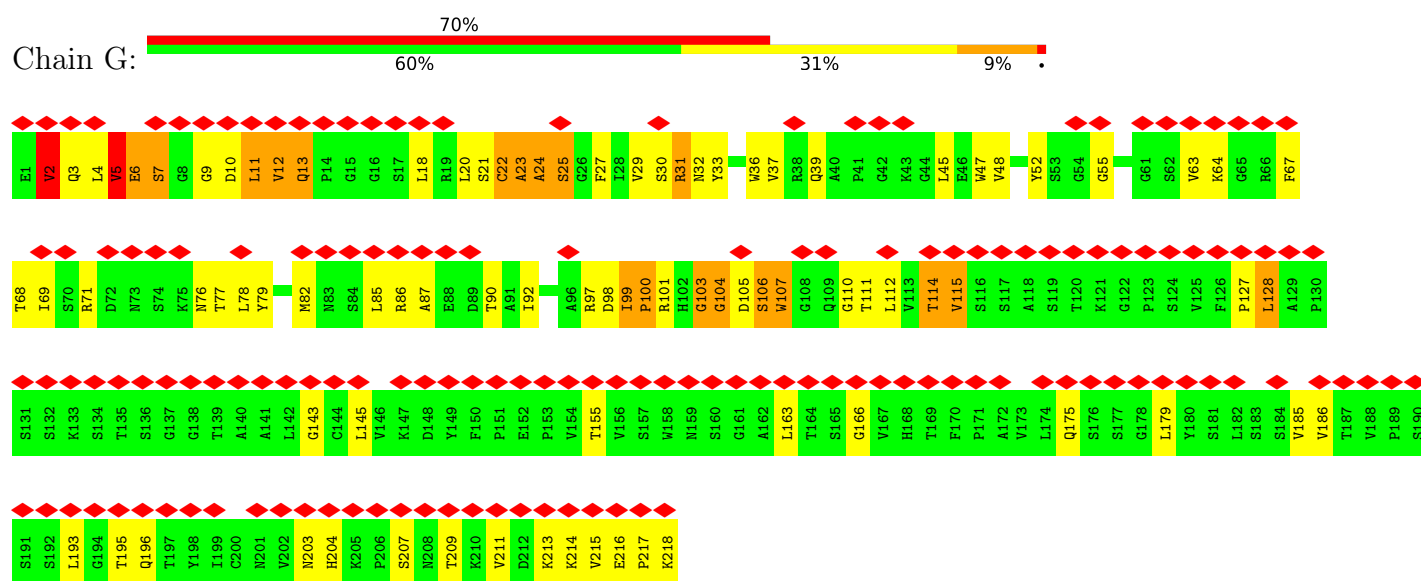
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

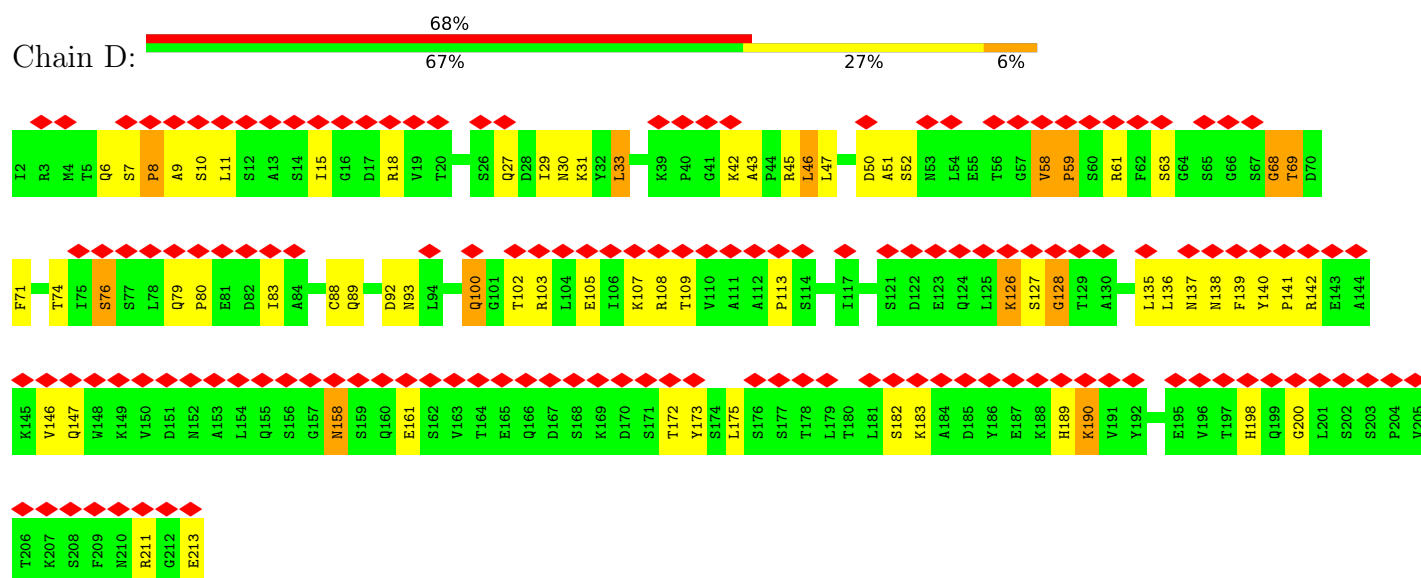


Chain B: 67% 15% • 15%

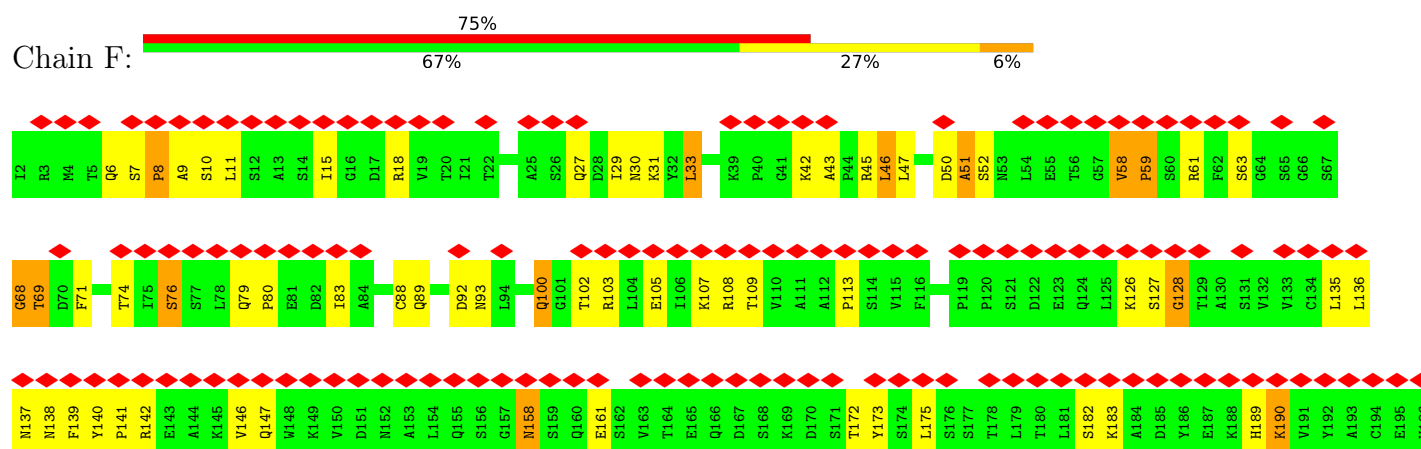




• Molecule 3: H4B6 light chain

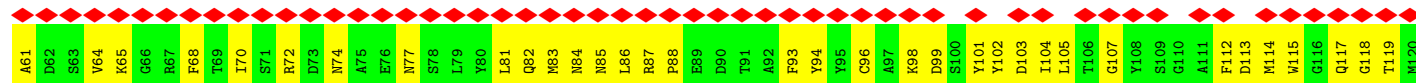


• Molecule 3: H4B6 light chain





- Molecule 4: the scfv of H4D12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	368678	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.941	Depositor
Minimum map value	-3.183	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.097	Depositor
Recommended contour level	0.31	Depositor
Map size ($\text{\AA}$)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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	0.42	2/7937 (0.0%)	1.01	55/10832 (0.5%)
1	B	0.45	4/7939 (0.1%)	1.14	59/10839 (0.5%)
1	C	0.75	2/7939 (0.0%)	0.79	5/10839 (0.0%)
2	E	0.53	2/1656 (0.1%)	1.88	62/2251 (2.8%)
2	G	0.53	2/1656 (0.1%)	1.88	62/2251 (2.8%)
3	D	0.34	1/1680 (0.1%)	1.25	35/2280 (1.5%)
3	F	0.34	1/1680 (0.1%)	1.25	34/2280 (1.5%)
4	H	0.18	0/1901	0.51	0/2573
All	All	0.52	14/32388 (0.0%)	1.12	312/44145 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	1
2	E	0	3
2	G	0	3
All	All	0	13

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	PRO	C-N	48.34	1.98	1.33
1	C	529	LYS	C-N	-44.24	0.71	1.33
1	B	529	LYS	C-N	10.81	1.48	1.33
2	E	103	GLY	C-N	-9.22	1.12	1.33
2	G	103	GLY	C-N	-9.21	1.12	1.33
2	G	2	VAL	C-N	-8.52	1.20	1.33
2	E	2	VAL	C-N	-8.51	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	330	PRO	C-N	-8.28	1.22	1.33
1	A	438	SER	CA-CB	-6.36	1.45	1.52
1	B	438	SER	CA-CB	-6.34	1.45	1.52
1	A	349	SER	CA-CB	-5.55	1.44	1.53
1	B	349	SER	CA-CB	-5.53	1.44	1.53
3	F	59	PRO	N-CD	5.05	1.54	1.47
3	D	59	PRO	N-CD	5.01	1.54	1.47

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	529	LYS	CA-C-N	-50.73	24.66	121.54
1	C	529	LYS	C-N-CA	-50.73	24.66	121.54
1	B	529	LYS	O-C-N	-43.95	64.14	122.59
1	A	529	LYS	O-C-N	-39.07	70.62	122.59
1	B	333	THR	CA-C-N	-38.21	69.11	122.99
1	B	333	THR	C-N-CA	-38.21	69.11	122.99
2	G	24	ALA	CB-CA-C	-22.62	77.59	110.62
2	E	24	ALA	CB-CA-C	-22.61	77.60	110.62
2	E	11	LEU	N-CA-C	21.35	144.54	110.17
2	G	11	LEU	N-CA-C	21.33	144.52	110.17
2	E	10	ASP	N-CA-C	-20.64	80.07	107.73
2	G	10	ASP	N-CA-C	-20.62	80.10	107.73
1	A	529	LYS	CA-C-N	18.19	156.28	121.54
1	A	529	LYS	C-N-CA	18.19	156.28	121.54
2	G	11	LEU	CB-CA-C	-17.29	80.27	109.50
2	E	11	LEU	CB-CA-C	-17.29	80.28	109.50
2	G	11	LEU	N-CA-CB	-17.11	82.75	110.63
2	E	11	LEU	N-CA-CB	-17.10	82.76	110.63
1	A	422	ASN	N-CA-C	16.65	133.93	113.12
1	B	422	ASN	N-CA-C	16.64	133.92	113.12
2	E	5	VAL	N-CA-C	-16.57	79.39	107.24
2	G	5	VAL	N-CA-C	-16.57	79.40	107.24
2	G	103	GLY	N-CA-C	16.31	137.82	115.32
2	E	103	GLY	N-CA-C	16.28	137.78	115.32
1	B	382	VAL	N-CA-C	-15.47	98.25	111.56
1	A	382	VAL	N-CA-C	-15.46	98.26	111.56
2	G	25	SER	N-CA-CB	-13.97	88.53	110.19
2	E	25	SER	N-CA-CB	-13.96	88.55	110.19
3	D	69	THR	N-CA-C	13.93	125.98	111.07
3	F	69	THR	N-CA-C	13.93	125.98	111.07
1	B	344	ALA	N-CA-C	-13.92	86.98	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ALA	N-CA-C	-13.91	86.99	108.14
2	E	25	SER	N-CA-C	13.59	131.60	112.04
2	G	25	SER	N-CA-C	13.58	131.60	112.04
2	E	103	GLY	O-C-N	-13.46	105.34	122.43
2	G	103	GLY	O-C-N	-13.44	105.36	122.43
2	G	106	SER	N-CA-C	-13.28	84.58	108.48
2	E	106	SER	N-CA-C	-13.25	84.64	108.48
2	E	114	THR	N-CA-C	-13.05	86.60	108.26
2	G	128	LEU	N-CA-C	-13.04	85.90	108.20
2	E	128	LEU	N-CA-C	-13.03	85.91	108.20
2	G	114	THR	N-CA-C	-13.03	86.64	108.26
2	E	48	VAL	N-CA-C	12.95	123.38	110.82
2	G	48	VAL	N-CA-C	12.93	123.36	110.82
1	B	343	ASN	N-CA-C	-12.88	86.72	108.75
3	D	127	SER	CB-CA-C	-12.88	90.39	111.13
3	F	127	SER	CB-CA-C	-12.88	90.39	111.13
1	A	343	ASN	N-CA-C	-12.86	86.75	108.75
2	E	23	ALA	CB-CA-C	-12.86	86.69	110.62
2	G	23	ALA	CB-CA-C	-12.86	86.70	110.62
2	E	2	VAL	N-CA-C	-12.79	85.75	107.24
2	G	2	VAL	N-CA-C	-12.79	85.76	107.24
2	E	2	VAL	O-C-N	-12.69	110.72	123.03
2	G	2	VAL	O-C-N	-12.66	110.75	123.03
1	A	501	TYR	N-CA-C	-12.65	89.43	108.79
1	B	501	TYR	N-CA-C	-12.65	89.44	108.79
3	F	190	LYS	N-CA-C	12.55	128.99	113.17
3	D	190	LYS	N-CA-C	12.54	128.97	113.17
1	B	470	THR	CB-CA-C	12.53	129.53	110.62
1	A	470	THR	CB-CA-C	12.52	129.53	110.62
3	D	10	SER	N-CA-C	-12.49	87.53	108.26
3	F	10	SER	N-CA-C	-12.49	87.53	108.26
1	A	501	TYR	N-CA-CB	12.33	130.67	111.56
1	B	501	TYR	N-CA-CB	12.32	130.66	111.56
1	B	339	ASP	N-CA-C	12.27	128.11	112.89
1	A	339	ASP	N-CA-C	12.27	128.10	112.89
1	A	470	THR	N-CA-C	-12.06	86.56	108.02
1	B	470	THR	N-CA-C	-12.05	86.57	108.02
3	D	59	PRO	N-CA-C	-11.77	94.75	111.22
3	F	59	PRO	N-CA-C	-11.77	94.75	111.22
1	B	529	LYS	CA-C-N	11.29	143.11	121.54
1	B	529	LYS	C-N-CA	11.29	143.11	121.54
2	E	115	VAL	N-CA-C	-11.08	92.17	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	115	VAL	N-CA-C	-11.06	92.20	108.12
2	E	24	ALA	N-CA-C	11.03	126.89	107.80
2	G	24	ALA	N-CA-C	11.03	126.88	107.80
2	E	31	ARG	N-CA-C	10.97	126.66	113.28
2	G	31	ARG	N-CA-C	10.96	126.65	113.28
1	B	343	ASN	CB-CA-C	10.94	131.34	109.68
1	A	343	ASN	CB-CA-C	10.92	131.30	109.68
3	D	182	SER	CB-CA-C	-10.82	91.73	110.45
3	F	182	SER	CB-CA-C	-10.81	91.74	110.45
3	F	11	LEU	N-CA-CB	10.68	128.44	110.71
3	D	11	LEU	N-CA-CB	10.67	128.42	110.71
2	G	47	TRP	N-CA-C	10.53	124.99	108.67
2	E	47	TRP	N-CA-C	10.50	124.94	108.67
2	E	99	ILE	N-CA-C	-10.40	99.68	108.63
1	B	330	PRO	CA-C-N	-10.38	106.19	122.49
1	B	330	PRO	C-N-CA	-10.38	106.19	122.49
2	G	99	ILE	N-CA-C	-10.37	99.71	108.63
1	A	344	ALA	N-CA-CB	10.30	128.87	111.57
1	B	344	ALA	N-CA-CB	10.29	128.85	111.57
3	D	11	LEU	N-CA-C	-10.25	90.03	108.48
3	F	59	PRO	CB-CA-C	10.25	126.70	111.22
3	F	11	LEU	N-CA-C	-10.24	90.05	108.48
3	D	59	PRO	CB-CA-C	10.23	126.67	111.22
1	B	375	PHE	N-CA-C	-10.18	94.62	109.59
1	A	375	PHE	N-CA-C	-10.17	94.64	109.59
1	B	448	ASN	N-CA-C	-10.16	90.23	108.02
1	A	448	ASN	N-CA-C	-10.15	90.25	108.02
1	B	373	PRO	N-CA-C	-10.06	93.52	112.33
2	E	47	TRP	CB-CA-C	-10.05	93.98	110.77
2	G	47	TRP	CB-CA-C	-10.05	93.99	110.77
1	A	373	PRO	N-CA-C	-10.04	93.56	112.33
3	F	190	LYS	CB-CA-C	-9.56	94.12	110.09
3	D	190	LYS	CB-CA-C	-9.56	94.13	110.09
3	F	100	GLN	N-CA-C	9.26	123.83	112.54
3	D	100	GLN	N-CA-C	9.23	123.81	112.54
2	G	3	GLN	N-CA-C	-9.19	93.90	109.24
2	E	3	GLN	N-CA-C	-9.16	93.93	109.24
2	E	6	GLU	N-CA-C	-8.94	89.72	107.69
2	G	6	GLU	N-CA-C	-8.94	89.73	107.69
3	D	47	LEU	N-CA-C	8.77	124.64	112.45
3	F	47	LEU	N-CA-C	8.75	124.61	112.45
2	G	13	GLN	N-CA-C	-8.66	100.17	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	13	GLN	N-CA-C	-8.65	100.19	110.13
1	A	353	TRP	N-CA-C	-8.42	94.80	108.52
3	D	189	HIS	N-CA-C	8.40	122.72	108.02
3	F	189	HIS	N-CA-C	8.40	122.72	108.02
1	B	353	TRP	N-CA-C	-8.39	94.84	108.52
2	G	7	SER	N-CA-CB	8.38	123.97	110.90
2	E	7	SER	N-CA-CB	8.37	123.96	110.90
2	G	195	THR	CB-CA-C	-8.29	95.62	109.55
2	E	195	THR	CB-CA-C	-8.28	95.64	109.55
3	D	189	HIS	CB-CA-C	-8.20	97.55	110.74
3	F	189	HIS	CB-CA-C	-8.18	97.56	110.74
2	E	106	SER	CB-CA-C	8.05	123.48	109.80
2	E	27	PHE	N-CA-CB	-8.04	98.38	110.60
2	G	106	SER	CB-CA-C	8.04	123.47	109.80
2	G	27	PHE	N-CA-CB	-8.02	98.41	110.60
2	E	27	PHE	N-CA-C	8.02	121.49	109.95
2	G	27	PHE	N-CA-C	8.00	121.47	109.95
1	B	448	ASN	N-CA-CB	7.95	123.21	110.65
1	A	448	ASN	N-CA-CB	7.94	123.19	110.65
1	B	389	ASP	N-CA-C	7.80	119.86	111.36
1	A	389	ASP	N-CA-C	7.78	119.84	111.36
1	A	500	THR	CB-CA-C	-7.71	98.73	111.68
1	B	500	THR	CB-CA-C	-7.71	98.73	111.68
2	G	9	GLY	N-CA-C	-7.69	101.87	112.18
2	E	9	GLY	N-CA-C	-7.68	101.89	112.18
2	G	68	THR	CB-CA-C	7.67	126.95	110.07
2	E	68	THR	CB-CA-C	7.66	126.93	110.07
1	A	369	TYR	N-CA-C	-7.64	102.94	113.56
1	B	369	TYR	N-CA-C	-7.63	102.95	113.56
1	B	422	ASN	N-CA-CB	-7.56	98.86	110.42
1	A	422	ASN	N-CA-CB	-7.54	98.89	110.42
3	D	127	SER	N-CA-C	-7.52	102.33	112.26
3	F	127	SER	N-CA-C	-7.50	102.37	112.26
3	F	8	PRO	CB-CA-C	-7.44	99.29	111.56
3	D	8	PRO	CB-CA-C	-7.43	99.29	111.56
1	B	375	PHE	CB-CA-C	7.42	121.39	110.26
3	D	68	GLY	N-CA-C	-7.41	99.33	112.22
3	F	68	GLY	N-CA-C	-7.40	99.35	112.22
1	A	375	PHE	CB-CA-C	7.39	121.35	110.26
1	B	388	ASN	N-CA-C	-7.33	103.29	111.28
2	G	100	PRO	CB-CA-C	-7.31	101.44	113.06
1	A	388	ASN	N-CA-C	-7.30	103.32	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	100	PRO	CB-CA-C	-7.30	101.45	113.06
3	F	29	ILE	N-CA-C	-7.17	105.55	112.29
1	C	564	GLN	CA-C-N	7.16	135.21	121.54
1	C	564	GLN	C-N-CA	7.16	135.21	121.54
3	D	29	ILE	N-CA-C	-7.15	105.57	112.29
1	B	475	ALA	N-CA-C	-7.13	105.20	114.04
1	A	475	ALA	N-CA-C	-7.12	105.22	114.04
2	E	30	SER	N-CA-C	7.12	121.55	113.01
2	G	30	SER	N-CA-C	7.11	121.54	113.01
1	A	410	ILE	N-CA-C	-7.07	98.65	106.21
2	E	69	ILE	N-CA-C	-7.07	97.29	108.95
2	G	69	ILE	N-CA-C	-7.06	97.30	108.95
1	B	410	ILE	N-CA-C	-7.06	98.66	106.21
1	A	388	ASN	CB-CA-C	7.05	122.50	110.79
1	B	388	ASN	CB-CA-C	7.04	122.48	110.79
2	E	2	VAL	CB-CA-C	6.96	119.02	110.73
2	G	2	VAL	CB-CA-C	6.95	119.00	110.73
3	F	52	SER	N-CA-CB	-6.91	99.80	111.27
3	D	52	SER	N-CA-CB	-6.90	99.82	111.27
2	E	115	VAL	N-CA-CB	6.89	121.58	111.52
2	E	103	GLY	CA-C-N	6.89	131.66	121.05
2	E	103	GLY	C-N-CA	6.89	131.66	121.05
2	G	103	GLY	CA-C-N	6.89	131.66	121.05
2	G	103	GLY	C-N-CA	6.89	131.66	121.05
1	A	381	GLY	N-CA-C	6.88	124.48	115.40
2	G	115	VAL	N-CA-CB	6.88	121.56	111.52
1	B	381	GLY	N-CA-C	6.84	124.43	115.40
3	F	51	ALA	CB-CA-C	6.83	119.90	110.06
3	D	51	ALA	CB-CA-C	6.83	119.89	110.06
3	F	46	LEU	N-CA-C	6.83	119.41	108.41
3	D	46	LEU	N-CA-C	6.82	119.38	108.41
1	B	382	VAL	N-CA-CB	6.77	118.86	111.41
1	B	506	GLN	N-CA-CB	6.75	123.20	110.65
1	A	506	GLN	N-CA-CB	6.73	123.17	110.65
1	A	382	VAL	N-CA-CB	6.71	118.79	111.41
1	A	352	ALA	N-CA-C	-6.67	97.67	108.41
3	D	9	ALA	N-CA-C	6.67	121.59	113.38
1	B	352	ALA	N-CA-C	-6.67	97.68	108.41
3	F	128	GLY	N-CA-C	6.66	125.16	114.90
3	F	9	ALA	N-CA-C	6.65	121.56	113.38
2	G	68	THR	N-CA-C	-6.63	99.22	109.24
3	D	128	GLY	N-CA-C	6.63	125.11	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	68	THR	N-CA-C	-6.62	99.24	109.24
1	A	366	SER	N-CA-C	-6.55	104.89	114.39
1	B	366	SER	N-CA-C	-6.54	104.91	114.39
1	B	376	ALA	N-CA-C	6.52	118.54	110.91
1	A	376	ALA	N-CA-C	6.52	118.54	110.91
1	A	421	TYR	CB-CA-C	6.51	119.58	109.03
1	B	421	TYR	CB-CA-C	6.49	119.55	109.03
2	G	128	LEU	CB-CA-C	6.48	121.15	110.78
2	E	128	LEU	CB-CA-C	6.47	121.12	110.78
3	F	92	ASP	CB-CA-C	-6.35	98.72	109.38
3	D	92	ASP	CB-CA-C	-6.34	98.72	109.38
2	E	11	LEU	CA-C-N	6.18	133.09	121.97
2	E	11	LEU	C-N-CA	6.18	133.09	121.97
2	G	11	LEU	CA-C-N	6.16	133.06	121.97
2	G	11	LEU	C-N-CA	6.16	133.06	121.97
1	B	353	TRP	N-CA-CB	6.15	120.20	110.55
3	D	93	ASN	N-CA-C	-6.15	99.22	109.24
3	F	93	ASN	N-CA-C	-6.14	99.22	109.24
1	A	353	TRP	N-CA-CB	6.12	120.17	110.55
3	D	46	LEU	CB-CA-C	-6.12	100.71	110.81
2	E	196	GLN	N-CA-C	-6.11	99.03	109.24
3	F	46	LEU	CB-CA-C	-6.11	100.73	110.81
2	G	196	GLN	N-CA-C	-6.10	99.05	109.24
1	B	430	THR	N-CA-C	-6.10	94.96	107.70
1	A	430	THR	N-CA-C	-6.09	94.97	107.70
2	E	22	CYS	N-CA-C	-6.05	100.98	109.69
1	A	354	ASN	CB-CA-C	-6.02	101.47	111.41
2	G	22	CYS	N-CA-C	-6.02	101.02	109.69
1	B	354	ASN	CB-CA-C	-6.00	101.51	111.41
3	F	69	THR	N-CA-CB	-5.98	101.34	110.01
3	D	69	THR	N-CA-CB	-5.97	101.36	110.01
1	B	411	ALA	CB-CA-C	5.96	121.91	110.17
1	A	411	ALA	CB-CA-C	5.96	121.90	110.17
3	D	190	LYS	N-CA-CB	-5.92	101.73	110.49
3	F	190	LYS	N-CA-CB	-5.92	101.73	110.49
2	E	48	VAL	N-CA-CB	-5.90	102.03	110.52
1	B	339	ASP	N-CA-CB	-5.87	100.83	110.40
2	G	48	VAL	N-CA-CB	-5.87	102.06	110.52
2	E	21	SER	CB-CA-C	5.86	121.29	109.68
1	A	339	ASP	N-CA-CB	-5.86	100.86	110.40
2	G	21	SER	CB-CA-C	5.85	121.27	109.68
1	B	400	PHE	CA-C-O	-5.80	115.21	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	58	VAL	CB-CA-C	5.80	121.91	111.36
3	F	58	VAL	CB-CA-C	5.80	121.92	111.36
3	F	76	SER	N-CA-C	5.79	119.53	112.23
2	G	3	GLN	N-CA-CB	5.79	121.48	111.00
1	A	400	PHE	CA-C-O	-5.79	115.23	121.36
2	E	3	GLN	N-CA-CB	5.77	121.45	111.00
3	D	76	SER	N-CA-C	5.77	119.50	112.23
1	B	374	PHE	CB-CA-C	-5.76	101.86	110.16
1	A	374	PHE	CB-CA-C	-5.76	101.86	110.16
1	B	500	THR	N-CA-C	-5.75	97.17	107.98
1	A	500	THR	N-CA-C	-5.73	97.21	107.98
1	A	377	PHE	N-CA-C	-5.71	105.05	111.28
2	G	100	PRO	N-CA-C	5.71	121.64	113.47
2	E	100	PRO	N-CA-C	5.70	121.62	113.47
1	B	377	PHE	N-CA-C	-5.70	105.07	111.28
1	B	362	VAL	N-CA-C	-5.67	102.21	109.30
2	G	55	GLY	N-CA-C	5.67	123.15	115.32
2	E	55	GLY	N-CA-C	5.67	123.14	115.32
1	A	362	VAL	N-CA-C	-5.64	102.24	109.30
2	E	31	ARG	N-CA-CB	-5.56	101.73	110.46
1	B	400	PHE	CB-CA-C	-5.55	98.75	111.95
1	B	505	HIS	N-CA-C	-5.54	95.52	107.49
2	G	5	VAL	CB-CA-C	5.54	117.33	110.73
2	G	31	ARG	N-CA-CB	-5.54	101.77	110.46
1	A	505	HIS	N-CA-C	-5.53	95.54	107.49
1	A	400	PHE	CB-CA-C	-5.53	98.79	111.95
2	E	5	VAL	CB-CA-C	5.52	117.30	110.73
1	B	447	GLY	N-CA-C	-5.51	100.12	113.18
1	A	447	GLY	N-CA-C	-5.50	100.14	113.18
3	D	9	ALA	N-CA-CB	-5.49	102.35	110.53
3	F	9	ALA	N-CA-CB	-5.46	102.39	110.53
3	F	100	GLN	N-CA-CB	-5.42	101.40	110.39
2	E	163	LEU	CB-CA-C	-5.41	102.14	111.23
3	D	100	GLN	N-CA-CB	-5.40	101.42	110.39
2	G	163	LEU	CB-CA-C	-5.39	102.17	111.23
1	A	479	PRO	N-CA-C	-5.38	106.05	113.53
1	B	338	PHE	N-CA-C	5.36	119.45	113.01
2	E	12	VAL	CB-CA-C	5.36	120.08	111.29
1	B	479	PRO	N-CA-C	-5.36	106.09	113.53
1	A	338	PHE	N-CA-C	5.35	119.43	113.01
2	G	12	VAL	CB-CA-C	5.34	120.05	111.29
2	E	110	GLY	CA-C-O	-5.34	117.97	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	110	GLY	CA-C-O	-5.30	118.00	122.29
2	E	114	THR	CB-CA-C	5.30	118.30	110.14
2	E	107	TRP	N-CA-C	-5.29	99.66	108.34
1	C	330	PRO	O-C-N	-5.29	115.50	122.64
3	D	158	ASN	CB-CA-C	5.29	118.84	109.75
2	G	107	TRP	N-CA-C	-5.28	99.68	108.34
2	G	114	THR	CB-CA-C	5.28	118.27	110.14
3	F	158	ASN	CB-CA-C	5.27	118.81	109.75
1	A	352	ALA	CA-C-N	-5.23	115.72	123.05
1	A	352	ALA	C-N-CA	-5.23	115.72	123.05
2	G	104	GLY	N-CA-C	5.23	121.26	112.85
2	E	104	GLY	N-CA-C	5.22	121.26	112.85
1	B	352	ALA	CA-C-N	-5.21	115.75	123.05
1	B	352	ALA	C-N-CA	-5.21	115.75	123.05
1	A	445	VAL	N-CA-C	-5.18	105.33	110.62
1	B	445	VAL	N-CA-C	-5.18	105.33	110.62
1	A	400	PHE	CA-CB-CG	5.17	118.97	113.80
2	E	6	GLU	CA-C-N	-5.14	114.98	122.44
2	E	6	GLU	C-N-CA	-5.14	114.98	122.44
1	B	400	PHE	CA-CB-CG	5.13	118.93	113.80
2	G	6	GLU	CA-C-N	-5.12	115.01	122.44
2	G	6	GLU	C-N-CA	-5.12	115.01	122.44
1	A	360	ASN	CB-CA-C	-5.11	104.47	111.73
2	E	163	LEU	N-CA-C	5.11	117.96	107.69
2	G	163	LEU	N-CA-C	5.10	117.94	107.69
3	D	76	SER	CB-CA-C	-5.09	99.99	110.38
3	F	76	SER	CB-CA-C	-5.09	99.99	110.38
1	B	360	ASN	CB-CA-C	-5.08	104.52	111.73
3	D	126	LYS	CB-CA-C	-5.00	100.61	110.11

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	529	LYS	Mainchain,Peptide
1	B	330	PRO	Mainchain
1	B	333	THR	Mainchain,Peptide
1	B	529	LYS	Mainchain
1	C	529	LYS	Mainchain
2	E	103	GLY	Mainchain
2	E	2	VAL	Mainchain
2	E	5	VAL	Mainchain

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Mol	Chain	Res	Type	Group
2	G	103	GLY	Mainchain
2	G	2	VAL	Mainchain
2	G	5	VAL	Mainchain

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	7754	0	7363	230	0
1	B	7754	0	7366	216	0
1	C	7754	0	7361	250	0
2	E	1619	0	1593	73	0
2	G	1619	0	1593	80	0
3	D	1646	0	1596	52	0
3	F	1646	0	1596	52	0
4	H	1857	0	1759	135	0
All	All	31649	0	30227	934	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 15.

All (934) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:TYR:CE1	4:H:105:LEU:HD11	1.46	1.50
1:C:495:TYR:CZ	4:H:105:LEU:HD11	1.46	1.50
1:B:364:ASP:CG	1:B:527:PRO:HG3	1.09	1.50
1:B:382:VAL:HG11	1:B:387:LEU:CD2	1.41	1.45
1:A:382:VAL:HG11	1:A:387:LEU:CD2	1.41	1.45
1:A:382:VAL:CG1	1:A:387:LEU:HD21	1.49	1.42
1:B:382:VAL:CG1	1:B:387:LEU:HD21	1.48	1.40
1:C:495:TYR:CE1	4:H:105:LEU:CD1	2.05	1.37
1:C:529:LYS:CB	1:C:530:SER:N	1.86	1.37
1:A:523:THR:HG22	1:C:230:PRO:CG	1.54	1.36
1:B:364:ASP:OD2	1:B:527:PRO:CD	1.71	1.34
1:B:364:ASP:OD2	1:B:527:PRO:CB	1.75	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ALA:HB3	1:B:374:PHE:CE1	1.62	1.33
1:A:372:ALA:HB3	1:A:374:PHE:CE1	1.62	1.33
1:B:374:PHE:CD2	1:B:377:PHE:HD2	1.47	1.32
1:A:374:PHE:CD2	1:A:377:PHE:HD2	1.46	1.31
1:A:523:THR:CG2	1:C:230:PRO:HG2	1.59	1.30
1:A:382:VAL:CG1	1:A:387:LEU:CD2	2.07	1.29
1:B:364:ASP:CG	1:B:527:PRO:CD	2.05	1.28
2:G:4:LEU:HD22	2:G:23:ALA:O	1.32	1.27
2:E:4:LEU:HD22	2:E:23:ALA:O	1.32	1.27
1:A:382:VAL:HG11	1:A:387:LEU:CG	1.66	1.25
1:B:382:VAL:HG11	1:B:387:LEU:CG	1.66	1.25
1:C:495:TYR:HE1	4:H:105:LEU:CG	1.51	1.24
2:G:97:ARG:NH2	2:G:99:ILE:HD11	1.53	1.23
1:B:382:VAL:CG1	1:B:387:LEU:CD2	2.07	1.22
1:A:382:VAL:CG1	1:A:387:LEU:CG	2.17	1.22
1:C:330:PRO:C	1:C:331:ASN:N	1.98	1.22
2:E:97:ARG:NH2	2:E:99:ILE:HD11	1.53	1.21
1:B:382:VAL:CG1	1:B:387:LEU:CG	2.17	1.20
1:B:372:ALA:CB	1:B:374:PHE:CE1	2.25	1.20
1:C:495:TYR:CE1	4:H:105:LEU:CG	2.24	1.19
1:B:374:PHE:CE2	1:B:377:PHE:HD2	1.61	1.19
1:A:372:ALA:CB	1:A:374:PHE:CE1	2.25	1.18
1:A:521:PRO:CG	1:C:199:GLY:O	1.92	1.17
1:A:374:PHE:CE2	1:A:377:PHE:HD2	1.61	1.17
1:C:529:LYS:HA	1:C:530:SER:N	1.54	1.14
2:E:11:LEU:O	2:E:11:LEU:HG	1.48	1.13
1:A:374:PHE:CE2	1:A:377:PHE:CD2	2.36	1.13
1:C:495:TYR:HE1	4:H:105:LEU:HG	1.14	1.13
1:B:374:PHE:CE2	1:B:377:PHE:CD2	2.36	1.12
1:A:382:VAL:HG12	1:A:387:LEU:HG	1.32	1.11
1:B:374:PHE:CD2	1:B:377:PHE:CD2	2.39	1.11
1:C:364:ASP:OD1	1:C:527:PRO:HD3	1.51	1.11
1:C:529:LYS:N	1:C:530:SER:N	1.97	1.11
1:A:374:PHE:CD2	1:A:377:PHE:CD2	2.39	1.10
1:C:495:TYR:CZ	4:H:105:LEU:CD1	2.29	1.10
1:B:364:ASP:CG	1:B:527:PRO:CG	1.76	1.09
1:C:417:ASN:HB2	4:H:107:GLY:HA2	1.35	1.09
2:G:2:VAL:HA	2:G:25:SER:OG	1.52	1.09
2:E:7:SER:HA	2:E:111:THR:HG21	1.29	1.09
2:E:2:VAL:HA	2:E:25:SER:OG	1.52	1.09
3:D:142:ARG:HG3	3:D:173:TYR:CE2	1.87	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PRO:C	1:A:331:ASN:N	2.11	1.08
3:F:142:ARG:HG3	3:F:173:TYR:CE2	1.87	1.08
1:A:521:PRO:HG2	1:C:199:GLY:O	1.49	1.08
1:A:523:THR:HG21	1:C:230:PRO:HG2	1.34	1.08
2:G:11:LEU:HG	2:G:11:LEU:O	1.48	1.07
1:C:495:TYR:CZ	4:H:105:LEU:HD21	1.90	1.07
2:G:7:SER:HA	2:G:111:THR:HG21	1.30	1.06
1:B:364:ASP:OD2	1:B:527:PRO:HG2	1.39	1.06
1:B:382:VAL:HG12	1:B:387:LEU:HG	1.32	1.06
1:A:520:ALA:HA	1:C:232:GLY:HA3	1.38	1.05
1:C:495:TYR:OH	4:H:105:LEU:CD1	2.05	1.05
1:A:230:PRO:O	1:B:521:PRO:HD2	1.57	1.04
1:B:374:PHE:CD1	1:B:434:ILE:HG23	1.92	1.04
2:E:7:SER:HA	2:E:111:THR:CG2	1.87	1.03
1:A:374:PHE:CD1	1:A:434:ILE:HG23	1.93	1.03
1:B:456:PHE:HZ	2:G:100:PRO:HD2	1.21	1.03
1:C:495:TYR:OH	4:H:105:LEU:CD2	2.06	1.02
1:A:167:THR:HA	1:B:357:ARG:HH12	1.16	1.02
1:C:495:TYR:HE1	4:H:105:LEU:CD1	1.54	1.02
1:A:456:PHE:HZ	2:E:100:PRO:HD2	1.21	1.02
2:E:6:GLU:O	2:E:111:THR:HG23	1.59	1.02
2:G:7:SER:HA	2:G:111:THR:CG2	1.87	1.02
2:G:6:GLU:O	2:G:111:THR:HG23	1.59	1.01
1:A:523:THR:CG2	1:C:230:PRO:CG	2.26	1.00
1:B:333:THR:HG23	1:B:335:LEU:HD12	1.40	1.00
1:C:529:LYS:CA	1:C:530:SER:N	0.85	1.00
1:C:495:TYR:CE1	4:H:105:LEU:HG	1.90	0.99
1:B:364:ASP:CG	1:B:527:PRO:HD3	1.85	0.98
1:B:382:VAL:CG1	1:B:387:LEU:HG	1.89	0.98
1:C:460:ASN:HD21	4:H:56:ASP:CG	1.72	0.98
2:E:4:LEU:CD2	2:E:23:ALA:O	2.12	0.98
1:C:495:TYR:OH	4:H:105:LEU:HD21	1.63	0.98
2:G:4:LEU:CD2	2:G:23:ALA:O	2.12	0.97
1:B:365:TYR:OH	1:B:395:VAL:HG21	1.65	0.97
1:A:382:VAL:HG11	1:A:387:LEU:CD1	1.95	0.96
2:E:6:GLU:O	2:E:6:GLU:HG2	1.65	0.96
1:C:505:HIS:NE2	4:H:167:SER:OG	1.98	0.96
1:B:382:VAL:HG11	1:B:387:LEU:CD1	1.95	0.96
1:C:495:TYR:OH	4:H:105:LEU:HD11	1.64	0.96
1:A:365:TYR:OH	1:A:395:VAL:HG21	1.65	0.95
1:A:372:ALA:CB	1:A:374:PHE:CD1	2.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ALA:CB	1:A:374:PHE:HE1	1.72	0.95
1:B:333:THR:HG23	1:B:335:LEU:CD1	1.95	0.95
1:C:364:ASP:OD1	1:C:527:PRO:CD	2.13	0.95
1:A:374:PHE:HE2	1:A:377:PHE:CD2	1.85	0.95
1:A:357:ARG:CZ	1:C:166:CYS:O	2.06	0.94
1:B:372:ALA:CB	1:B:374:PHE:CD1	2.49	0.94
1:B:456:PHE:CE1	2:G:33:TYR:CE1	2.56	0.94
1:A:372:ALA:HB1	1:A:374:PHE:CD1	2.03	0.94
1:A:456:PHE:CE1	2:E:33:TYR:CE1	2.56	0.94
2:G:6:GLU:O	2:G:6:GLU:HG2	1.65	0.93
1:A:382:VAL:CG1	1:A:387:LEU:HG	1.89	0.93
1:B:333:THR:CG2	1:B:335:LEU:HD12	1.98	0.93
1:A:167:THR:CA	1:B:357:ARG:HH12	1.80	0.93
1:B:372:ALA:HB1	1:B:374:PHE:CD1	2.03	0.93
1:B:374:PHE:HE2	1:B:377:PHE:CD2	1.85	0.93
2:E:97:ARG:HH22	2:E:99:ILE:HD11	1.13	0.93
1:A:374:PHE:HE2	1:A:377:PHE:CE2	1.88	0.92
1:A:382:VAL:HG13	1:A:387:LEU:HD21	1.51	0.92
2:G:97:ARG:HH22	2:G:99:ILE:HD11	1.13	0.92
1:A:374:PHE:HD2	1:A:377:PHE:HD2	1.16	0.92
1:A:520:ALA:HB1	1:C:232:GLY:N	1.84	0.91
1:C:458:LYS:HA	4:H:53:TRP:HZ2	1.32	0.91
1:A:357:ARG:CD	1:C:167:THR:HA	2.00	0.91
1:A:46:SER:HA	1:A:279:TYR:O	1.71	0.91
1:C:418:ILE:HD11	4:H:105:LEU:O	1.69	0.91
1:B:382:VAL:HG13	1:B:387:LEU:HD21	1.51	0.91
1:B:374:PHE:HE2	1:B:377:PHE:CE2	1.88	0.90
1:B:364:ASP:OD2	1:B:527:PRO:CG	0.60	0.90
1:A:382:VAL:HG11	1:A:387:LEU:HD21	0.92	0.89
1:A:523:THR:HG22	1:C:230:PRO:HG3	1.53	0.89
1:B:382:VAL:HG11	1:B:387:LEU:HD21	0.92	0.89
2:E:104:GLY:O	2:E:105:ASP:OD1	1.90	0.89
1:A:521:PRO:CD	1:C:199:GLY:O	2.19	0.89
1:A:521:PRO:HD2	1:C:230:PRO:O	1.71	0.89
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.55	0.89
3:D:8:PRO:O	3:D:102:THR:HG23	1.73	0.88
1:C:418:ILE:CD1	4:H:105:LEU:O	2.21	0.88
1:B:456:PHE:CZ	2:G:100:PRO:HD2	2.09	0.88
3:F:8:PRO:O	3:F:102:THR:HG23	1.73	0.88
3:D:190:LYS:O	3:D:190:LYS:HG3	1.72	0.88
1:B:374:PHE:HD2	1:B:377:PHE:HD2	1.16	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:52:TYR:O	2:G:71:ARG:NH1	2.07	0.88
4:H:146:SER:HG	4:H:161:SER:HG	1.15	0.88
1:B:374:PHE:CZ	1:B:434:ILE:HD13	2.09	0.87
2:E:128:LEU:HB2	2:E:143:GLY:O	1.73	0.87
1:A:456:PHE:CZ	2:E:100:PRO:HD2	2.09	0.87
2:G:104:GLY:O	2:G:105:ASP:OD1	1.90	0.87
2:G:128:LEU:HB2	2:G:143:GLY:O	1.73	0.87
1:A:374:PHE:CZ	1:A:434:ILE:HD13	2.09	0.87
1:B:372:ALA:CB	1:B:374:PHE:HE1	1.72	0.87
2:E:52:TYR:O	2:E:71:ARG:NH1	2.07	0.86
1:A:394:ASN:ND2	1:C:167:THR:HB	1.90	0.86
3:F:190:LYS:O	3:F:190:LYS:HG3	1.72	0.86
1:C:131:CYS:HB3	1:C:166:CYS:HA	1.57	0.86
1:A:520:ALA:HB1	1:C:232:GLY:H	1.37	0.86
1:A:520:ALA:CB	1:C:232:GLY:H	1.90	0.85
1:C:489:TYR:HD2	4:H:101:TYR:CE2	1.95	0.85
3:F:128:GLY:HA2	3:F:183:LYS:HB3	1.58	0.85
1:A:349:SER:O	1:A:352:ALA:O	1.95	0.84
1:B:349:SER:O	1:B:352:ALA:O	1.95	0.84
2:G:2:VAL:HA	2:G:25:SER:HG	1.43	0.84
1:B:364:ASP:CB	1:B:527:PRO:HG3	2.07	0.84
1:A:374:PHE:CE1	1:A:434:ILE:CG2	2.61	0.83
1:A:374:PHE:CD1	1:A:434:ILE:CG2	2.61	0.83
1:C:458:LYS:HA	4:H:53:TRP:CZ2	2.14	0.83
1:B:46:SER:HA	1:B:279:TYR:O	1.79	0.83
1:B:374:PHE:CD1	1:B:434:ILE:CG2	2.61	0.83
1:A:360:ASN:ND2	1:C:168:PHE:CE1	2.47	0.82
3:D:128:GLY:HA2	3:D:183:LYS:HB3	1.58	0.82
2:G:97:ARG:NH2	2:G:99:ILE:CD1	2.40	0.82
1:A:523:THR:HG22	1:C:230:PRO:CB	2.08	0.82
1:B:374:PHE:CE1	1:B:434:ILE:CG2	2.61	0.82
1:C:495:TYR:CZ	4:H:105:LEU:CD2	2.60	0.82
1:A:372:ALA:HB3	1:A:374:PHE:HE1	1.29	0.82
1:B:342:PHE:HB3	1:B:371:PHE:HZ	1.45	0.82
1:B:456:PHE:CD1	2:G:33:TYR:HE1	1.98	0.81
1:A:342:PHE:HB3	1:A:371:PHE:HZ	1.45	0.81
3:D:31:LYS:O	3:D:50:ASP:O	1.98	0.81
1:A:167:THR:HA	1:B:357:ARG:NH1	1.93	0.81
1:A:456:PHE:CD1	2:E:33:TYR:HE1	1.98	0.81
2:E:6:GLU:O	2:E:111:THR:CG2	2.29	0.81
3:F:31:LYS:O	3:F:50:ASP:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:PRO:CD	1:C:230:PRO:O	2.29	0.81
2:E:97:ARG:NH2	2:E:99:ILE:CD1	2.40	0.81
2:G:6:GLU:O	2:G:6:GLU:CG	2.28	0.81
1:C:364:ASP:OD2	1:C:527:PRO:HB3	1.79	0.81
2:G:6:GLU:O	2:G:111:THR:CG2	2.29	0.80
2:E:7:SER:CA	2:E:111:THR:HG21	2.11	0.80
1:A:372:ALA:HB3	1:A:374:PHE:CD1	2.13	0.80
1:B:374:PHE:CE1	1:B:434:ILE:HG21	2.17	0.80
1:A:374:PHE:CE1	1:A:434:ILE:HG21	2.17	0.80
1:B:372:ALA:HB3	1:B:374:PHE:CD1	2.13	0.80
1:B:422:ASN:HD21	1:B:454:ARG:H	1.30	0.80
2:G:11:LEU:O	2:G:11:LEU:CG	2.06	0.80
1:A:372:ALA:HB1	1:A:374:PHE:HD1	1.45	0.79
1:B:382:VAL:HG11	1:B:387:LEU:HD11	1.64	0.79
1:A:422:ASN:HD21	1:A:454:ARG:H	1.30	0.79
1:A:526:GLY:O	1:A:527:PRO:N	2.14	0.79
2:E:6:GLU:O	2:E:6:GLU:CG	2.28	0.79
4:H:20:LEU:HG	4:H:83:MET:HE1	1.64	0.79
2:E:11:LEU:O	2:E:11:LEU:CG	2.06	0.79
1:A:382:VAL:HG11	1:A:387:LEU:HD11	1.64	0.78
1:B:374:PHE:HD2	1:B:377:PHE:CD2	1.92	0.78
1:C:353:TRP:O	1:C:466:ARG:NH2	2.16	0.78
2:E:2:VAL:HA	2:E:25:SER:HG	1.46	0.78
1:A:374:PHE:HD2	1:A:377:PHE:CD2	1.92	0.78
1:B:444:LYS:HE2	1:B:448:ASN:HA	1.66	0.78
1:A:374:PHE:CG	1:A:434:ILE:HG23	2.17	0.78
1:B:374:PHE:CG	1:B:434:ILE:HG23	2.17	0.78
2:G:7:SER:CA	2:G:111:THR:HG21	2.11	0.78
4:H:163:ARG:NH1	4:H:164:ALA:O	2.17	0.78
1:A:520:ALA:CB	1:C:232:GLY:N	2.46	0.77
1:B:333:THR:CG2	1:B:335:LEU:CD1	2.61	0.77
1:C:403:ARG:HB2	4:H:105:LEU:HD12	1.66	0.77
1:B:456:PHE:HE1	2:G:100:PRO:HG2	1.50	0.77
2:G:32:ASN:HD22	2:G:97:ARG:HE	1.33	0.77
1:B:372:ALA:HB1	1:B:374:PHE:HD1	1.45	0.77
1:B:382:VAL:CG1	1:B:387:LEU:HD11	2.16	0.76
1:A:357:ARG:HD2	1:A:394:ASN:ND2	2.01	0.76
1:A:444:LYS:HE2	1:A:448:ASN:HA	1.66	0.76
1:A:382:VAL:HG13	1:A:387:LEU:CD2	2.12	0.76
1:A:456:PHE:HE1	2:E:100:PRO:HG2	1.50	0.75
1:A:167:THR:O	1:B:357:ARG:NH1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:HIS:CD2	4:H:167:SER:OG	2.40	0.75
1:A:382:VAL:CG1	1:A:387:LEU:CD1	2.60	0.75
1:C:458:LYS:CA	4:H:53:TRP:HZ2	1.99	0.75
1:A:364:ASP:OD1	1:A:527:PRO:N	2.18	0.75
1:B:357:ARG:HD2	1:B:394:ASN:ND2	2.01	0.75
1:A:382:VAL:CG1	1:A:387:LEU:HD11	2.16	0.74
4:H:83:MET:HG3	4:H:86:LEU:HD21	1.69	0.74
4:H:174:TRP:HB2	4:H:187:PHE:HB2	1.70	0.74
1:A:520:ALA:CA	1:C:232:GLY:HA3	2.16	0.74
3:D:8:PRO:O	3:D:102:THR:CG2	2.35	0.74
4:H:104:ILE:HG22	4:H:105:LEU:H	1.53	0.74
1:B:382:VAL:CG1	1:B:387:LEU:CD1	2.60	0.73
1:A:350:VAL:CG1	1:A:422:ASN:HB3	2.19	0.73
2:E:32:ASN:HD22	2:E:97:ARG:HE	1.33	0.73
3:F:8:PRO:O	3:F:102:THR:CG2	2.35	0.73
1:A:357:ARG:HD2	1:C:167:THR:O	1.89	0.73
1:B:350:VAL:CG1	1:B:422:ASN:HB3	2.19	0.72
1:A:167:THR:C	1:B:357:ARG:HH12	1.97	0.72
1:A:456:PHE:CE1	2:E:33:TYR:HE1	2.05	0.72
1:C:406:GLU:OE2	4:H:105:LEU:CD1	2.38	0.72
2:G:22:CYS:O	2:G:77:THR:HA	1.90	0.72
3:F:142:ARG:CG	3:F:173:TYR:CE2	2.70	0.72
1:C:417:ASN:CB	4:H:107:GLY:HA2	2.16	0.72
2:E:22:CYS:O	2:E:77:THR:HA	1.90	0.71
3:D:142:ARG:HG3	3:D:173:TYR:CZ	2.24	0.71
1:A:1104:VAL:HG23	1:A:1115:ILE:HG12	1.73	0.71
1:B:456:PHE:CE1	2:G:33:TYR:HE1	2.05	0.71
1:A:69:HIS:HB2	1:A:257:GLY:HA3	1.73	0.70
1:A:342:PHE:HB3	1:A:371:PHE:CZ	2.26	0.70
1:A:402:ILE:HD13	1:A:410:ILE:HG13	1.73	0.70
3:F:142:ARG:HG3	3:F:173:TYR:CZ	2.24	0.70
1:C:46:SER:HA	1:C:279:TYR:O	1.90	0.70
1:C:489:TYR:HD2	4:H:101:TYR:CZ	2.09	0.70
3:F:126:LYS:O	3:F:126:LYS:HG3	1.91	0.70
1:B:447:GLY:HA2	1:B:497:PHE:O	1.92	0.70
3:D:142:ARG:CG	3:D:173:TYR:CE2	2.70	0.70
1:A:394:ASN:HD21	1:C:167:THR:HB	1.54	0.70
1:C:406:GLU:OE2	4:H:105:LEU:HD13	1.89	0.70
3:D:126:LYS:O	3:D:126:LYS:HG3	1.91	0.70
1:A:447:GLY:HA2	1:A:497:PHE:O	1.91	0.69
1:B:372:ALA:HB3	1:B:374:PHE:HE1	1.29	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASP:OD1	1:B:527:PRO:CD	2.40	0.69
1:B:402:ILE:HD13	1:B:410:ILE:HG13	1.73	0.69
1:C:489:TYR:CD2	4:H:101:TYR:OH	2.46	0.69
1:A:357:ARG:HD3	1:C:167:THR:HA	1.73	0.69
1:B:190:ARG:HH11	1:B:207:HIS:HD2	1.41	0.69
1:B:342:PHE:HB3	1:B:371:PHE:CZ	2.26	0.69
1:A:230:PRO:O	1:B:521:PRO:CD	2.38	0.68
4:H:39:GLN:HB3	4:H:93:PHE:HB2	1.74	0.68
1:B:348:ALA:HB2	1:B:354:ASN:HB2	1.74	0.68
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.59	0.68
1:A:360:ASN:ND2	1:C:168:PHE:HE1	1.92	0.67
2:E:97:ARG:HH22	2:E:99:ILE:CD1	2.00	0.67
1:A:348:ALA:HB2	1:A:354:ASN:HB2	1.74	0.67
3:D:190:LYS:O	3:D:190:LYS:CG	2.43	0.67
3:F:190:LYS:O	3:F:190:LYS:CG	2.43	0.67
1:B:374:PHE:CE2	1:B:377:PHE:CE2	2.74	0.67
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.28	0.67
4:H:230:ARG:HA	4:H:234:TYR:HB3	1.76	0.67
1:B:489:TYR:OH	2:G:99:ILE:HD13	1.95	0.67
3:D:42:LYS:NZ	3:D:43:ALA:O	2.28	0.67
4:H:2:VAL:HA	4:H:25:SER:O	1.94	0.67
1:B:474:GLN:HB2	2:G:31:ARG:HH22	1.60	0.67
3:F:42:LYS:NZ	3:F:43:ALA:O	2.28	0.67
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.27	0.66
4:H:15:GLY:H	4:H:86:LEU:HB2	1.59	0.66
1:A:330:PRO:CA	1:A:331:ASN:N	2.58	0.66
1:C:495:TYR:CE1	4:H:105:LEU:CD2	2.76	0.66
1:A:425:LEU:HD21	1:A:512:VAL:HG11	1.77	0.66
1:C:489:TYR:CD2	4:H:101:TYR:CZ	2.84	0.66
1:B:425:LEU:HD21	1:B:512:VAL:HG11	1.77	0.66
1:C:363:ALA:HB2	1:C:524:VAL:HG12	1.78	0.66
1:C:374:PHE:HD1	1:C:377:PHE:H	1.42	0.66
1:B:456:PHE:CD1	2:G:33:TYR:CE1	2.82	0.66
1:C:401:VAL:HG23	1:C:509:ARG:HH11	1.60	0.66
1:A:474:GLN:HB2	2:E:31:ARG:HH22	1.60	0.66
1:A:489:TYR:OH	2:E:99:ILE:HD13	1.95	0.66
1:C:363:ALA:N	1:C:525:CYS:O	2.27	0.66
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.79	0.65
1:B:456:PHE:CE1	2:G:100:PRO:HG2	2.31	0.65
2:G:97:ARG:HH22	2:G:99:ILE:CD1	2.00	0.65
1:A:456:PHE:CE1	2:E:100:PRO:HG2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:PRO:HB3	1:C:200:TYR:CE2	2.33	0.64
4:H:52:ASN:HB2	4:H:57:ASN:HB3	1.79	0.64
1:A:374:PHE:CE1	1:A:434:ILE:HG23	2.30	0.64
1:B:364:ASP:OD1	1:B:527:PRO:N	2.30	0.64
1:C:457:ARG:NH1	1:C:467:ASP:OD2	2.30	0.64
1:C:478:LYS:HE3	1:C:479:PRO:HD2	1.79	0.64
1:A:456:PHE:CD1	2:E:33:TYR:CE1	2.82	0.64
1:B:986:PRO:HG2	1:B:987:PRO:HD3	1.79	0.63
1:B:336:CYS:SG	1:B:363:ALA:HB2	2.38	0.63
1:A:347:PHE:HD1	1:A:399:SER:HB3	1.63	0.63
1:B:347:PHE:HD1	1:B:399:SER:HB3	1.63	0.63
1:B:323:THR:N	1:B:538:CYS:O	2.32	0.63
1:C:381:GLY:O	1:C:383:SER:N	2.32	0.63
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.38	0.63
4:H:61:ALA:HB3	4:H:64:VAL:HG22	1.82	0.62
1:C:417:ASN:HB2	4:H:107:GLY:CA	2.23	0.62
1:B:106:PHE:HD2	1:B:117:LEU:HD22	1.64	0.62
1:C:403:ARG:H	4:H:105:LEU:CD1	2.12	0.62
1:A:226:LEU:HG	1:A:227:VAL:HG23	1.80	0.62
1:B:308:VAL:HG22	1:B:602:THR:HG23	1.81	0.62
1:C:453:TYR:HE2	1:C:455:LEU:HD22	1.65	0.62
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.82	0.62
3:F:6:GLN:NE2	3:F:88:CYS:SG	2.65	0.62
2:E:92:ILE:HG13	2:E:112:LEU:HD13	1.81	0.62
1:B:444:LYS:HB2	1:B:447:GLY:O	1.99	0.62
3:D:6:GLN:NE2	3:D:88:CYS:SG	2.65	0.62
4:H:17:SER:HA	4:H:83:MET:O	2.00	0.61
1:B:444:LYS:HB2	1:B:447:GLY:C	2.25	0.61
1:C:460:ASN:ND2	4:H:56:ASP:CG	2.53	0.61
1:A:444:LYS:HB2	1:A:447:GLY:O	1.99	0.61
1:C:364:ASP:OD1	1:C:527:PRO:CG	2.48	0.61
1:B:382:VAL:HG13	1:B:387:LEU:CD2	2.13	0.61
2:G:92:ILE:HG13	2:G:112:LEU:HD13	1.81	0.61
1:A:357:ARG:NE	1:C:166:CYS:O	2.33	0.61
1:A:444:LYS:HB2	1:A:447:GLY:C	2.25	0.61
1:B:364:ASP:OD2	1:B:527:PRO:CA	2.47	0.61
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.01	0.61
1:C:495:TYR:OH	4:H:105:LEU:CG	2.49	0.61
3:D:68:GLY:O	3:D:71:PHE:CE1	2.54	0.61
4:H:177:GLN:HG3	4:H:183:PRO:HG3	1.82	0.61
1:B:617:CYS:HA	1:B:620:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:LYS:CA	4:H:53:TRP:CZ2	2.81	0.61
1:C:67:ALA:HB3	1:C:263:ALA:HB3	1.83	0.61
1:C:496:GLY:O	1:C:501:TYR:OH	2.17	0.61
1:C:591:SER:HB2	1:C:615:VAL:HG12	1.82	0.61
3:F:190:LYS:HE2	3:F:211:ARG:HB2	1.83	0.60
3:F:68:GLY:O	3:F:71:PHE:CE1	2.54	0.60
1:C:418:ILE:HD12	4:H:105:LEU:O	1.99	0.60
3:F:161:GLU:HB2	3:F:175:LEU:HD11	1.82	0.60
3:F:198:HIS:HD1	3:F:200:GLY:H	1.49	0.60
4:H:33:ALA:HA	4:H:72:ARG:HH12	1.65	0.60
1:A:37:TYR:HB3	1:A:223:LEU:HB2	1.83	0.60
1:C:458:LYS:NZ	4:H:31:ASP:OD1	2.35	0.60
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.83	0.60
3:D:161:GLU:HB2	3:D:175:LEU:HD11	1.82	0.60
4:H:102:TYR:HB3	4:H:171:TYR:CZ	2.36	0.60
1:A:350:VAL:HG12	1:A:422:ASN:HB3	1.84	0.60
1:B:364:ASP:CG	1:B:527:PRO:N	2.58	0.60
4:H:113:ASP:O	4:H:114:MET:HE2	2.00	0.60
1:C:495:TYR:CZ	4:H:105:LEU:CG	2.71	0.60
4:H:222:PHE:HB3	4:H:243:GLU:HA	1.83	0.60
1:A:374:PHE:CE2	1:A:377:PHE:CE2	2.74	0.59
1:C:453:TYR:HE1	1:C:495:TYR:HA	1.66	0.59
1:C:394:ASN:HB2	1:C:516:GLU:HB2	1.85	0.59
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.84	0.59
1:C:448:ASN:HB3	1:C:497:PHE:HD2	1.66	0.59
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.85	0.59
3:D:190:LYS:HE2	3:D:211:ARG:HB2	1.83	0.59
1:A:46:SER:CA	1:A:279:TYR:O	2.49	0.59
1:A:569:ILE:HD12	1:A:569:ILE:H	1.66	0.59
1:C:308:VAL:HG22	1:C:602:THR:HG23	1.84	0.59
3:D:198:HIS:HD1	3:D:200:GLY:H	1.49	0.59
3:F:108:ARG:O	3:F:140:TYR:HE2	1.86	0.59
1:B:347:PHE:CD1	1:B:399:SER:HB3	2.38	0.59
1:C:83:VAL:HG11	1:C:237:ARG:HE	1.67	0.59
3:D:108:ARG:O	3:D:140:TYR:HE2	1.86	0.59
3:D:146:VAL:O	3:D:147:GLN:NE2	2.35	0.59
1:A:347:PHE:CD1	1:A:399:SER:HB3	2.38	0.58
1:C:495:TYR:CE1	4:H:105:LEU:HD21	2.36	0.58
4:H:17:SER:OG	4:H:84:ASN:OD1	2.16	0.58
2:E:218:LYS:NZ	3:D:213:GLU:OXT	2.32	0.58
1:A:374:PHE:CE2	1:A:434:ILE:HD13	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:146:VAL:O	3:F:147:GLN:NE2	2.35	0.58
4:H:173:ALA:HB2	4:H:230:ARG:HH12	1.67	0.58
1:C:495:TYR:OH	4:H:105:LEU:HD13	2.02	0.58
4:H:112:PHE:HB2	4:H:175:TYR:CZ	2.39	0.58
1:A:199:GLY:O	1:B:521:PRO:HG2	2.04	0.58
1:B:364:ASP:OD2	1:B:527:PRO:N	2.36	0.58
1:B:350:VAL:HG12	1:B:422:ASN:HB3	1.84	0.58
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.31	0.58
1:B:372:ALA:HB1	1:B:374:PHE:CE1	2.26	0.58
3:F:213:GLU:OXT	2:G:218:LYS:NZ	2.32	0.58
2:G:106:SER:O	2:G:107:TRP:HD1	1.87	0.58
1:A:456:PHE:CZ	2:E:100:PRO:CD	2.85	0.57
1:B:374:PHE:CE2	1:B:434:ILE:HD13	2.38	0.57
1:C:96:GLU:OE1	1:C:99:ASN:N	2.36	0.57
1:C:564:GLN:O	1:C:565:PHE:CD1	2.57	0.57
4:H:94:TYR:O	4:H:118:GLY:HA2	2.03	0.57
4:H:178:LYS:HD2	4:H:223:ALA:HB2	1.86	0.57
1:A:530:SER:OG	1:A:531:THR:N	2.37	0.57
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.86	0.57
3:D:58:VAL:HG12	3:D:59:PRO:O	2.04	0.57
1:A:521:PRO:HB2	1:C:230:PRO:O	2.04	0.57
2:E:106:SER:O	2:E:107:TRP:HD1	1.87	0.57
1:C:455:LEU:HD21	4:H:103:ASP:HA	1.87	0.57
1:A:521:PRO:CB	1:C:230:PRO:O	2.53	0.57
1:C:418:ILE:HD11	4:H:105:LEU:C	2.30	0.57
4:H:24:VAL:HB	4:H:77:ASN:HB3	1.86	0.57
4:H:88:PRO:HG2	4:H:128:GLY:HA2	1.87	0.57
1:C:454:ARG:HH11	1:C:457:ARG:NH2	2.02	0.57
3:D:27:GLN:O	3:D:69:THR:HG22	2.05	0.57
1:C:421:TYR:HD1	1:C:457:ARG:HB3	1.68	0.56
2:E:175:GLN:NE2	2:E:179:LEU:O	2.38	0.56
3:F:83:ILE:HD12	3:F:105:GLU:HA	1.86	0.56
4:H:200:ARG:HG3	4:H:201:PHE:HD1	1.70	0.56
1:A:521:PRO:HD2	1:C:231:ILE:C	2.31	0.56
1:A:521:PRO:HB3	1:C:200:TYR:CZ	2.40	0.56
3:D:83:ILE:HD12	3:D:105:GLU:HA	1.86	0.56
3:F:27:GLN:O	3:F:69:THR:HG22	2.05	0.56
1:B:438:SER:OG	1:B:507:PRO:HB2	2.05	0.56
1:C:403:ARG:CB	4:H:105:LEU:HD12	2.33	0.56
1:C:505:HIS:CD2	4:H:167:SER:HG	2.12	0.56
1:A:438:SER:OG	1:A:507:PRO:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:108:ARG:O	3:F:140:TYR:CE2	2.58	0.56
2:G:175:GLN:NE2	2:G:179:LEU:O	2.38	0.56
1:B:46:SER:CA	1:B:279:TYR:O	2.53	0.56
1:B:374:PHE:HE2	1:B:377:PHE:HE2	1.52	0.56
1:C:358:ILE:HB	1:C:395:VAL:HB	1.88	0.56
1:C:412:PRO:HG3	1:C:425:LEU:HD22	1.86	0.56
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.40	0.56
3:D:61:ARG:HH12	3:D:79:GLN:HG2	1.70	0.56
1:C:460:ASN:OD1	4:H:56:ASP:OD2	2.23	0.56
3:F:58:VAL:HG12	3:F:59:PRO:O	2.04	0.56
1:A:435:ALA:HA	1:A:509:ARG:O	2.06	0.56
1:B:435:ALA:HA	1:B:509:ARG:O	2.06	0.56
1:B:979:ASP:HB3	1:B:983:ARG:HH12	1.71	0.56
1:C:413:GLY:HA2	1:C:424:LYS:HE2	1.88	0.56
3:D:108:ARG:O	3:D:140:TYR:CE2	2.58	0.56
1:A:866:THR:H	1:A:869:MET:HE3	1.71	0.56
1:B:130:VAL:HG21	1:B:231:ILE:HG12	1.88	0.56
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.88	0.56
1:B:350:VAL:HG11	1:B:422:ASN:HB3	1.87	0.55
1:C:83:VAL:HG22	1:C:239:GLN:HE21	1.72	0.55
1:C:454:ARG:HD3	1:C:457:ARG:HH22	1.70	0.55
1:A:277:LEU:HD23	1:A:285:ILE:HD13	1.89	0.55
1:A:365:TYR:HH	1:A:395:VAL:HG21	1.72	0.55
1:C:116:SER:HB3	1:C:132:GLU:HA	1.89	0.55
1:C:190:ARG:HG2	1:C:207:HIS:CD2	2.42	0.55
1:A:350:VAL:HG11	1:A:422:ASN:HB3	1.87	0.55
1:B:100:ILE:HD12	1:B:100:ILE:H	1.72	0.55
4:H:147:PRO:HG2	4:H:150:LEU:HB2	1.87	0.55
1:B:333:THR:HG22	1:B:335:LEU:HD12	1.89	0.55
2:E:22:CYS:SG	2:E:23:ALA:N	2.80	0.55
3:F:61:ARG:HH12	3:F:79:GLN:HG2	1.70	0.55
1:C:215:ASP:OD2	1:C:266:TYR:OH	2.21	0.54
4:H:221:ASP:O	4:H:225:TYR:OH	2.25	0.54
2:G:22:CYS:SG	2:G:23:ALA:N	2.80	0.54
4:H:112:PHE:HB2	4:H:175:TYR:CE2	2.42	0.54
1:C:346:ARG:HE	1:C:347:PHE:H	1.55	0.54
1:A:505:HIS:O	1:A:506:GLN:HG3	2.08	0.54
1:B:456:PHE:CZ	2:G:100:PRO:CD	2.85	0.54
2:G:37:VAL:HG11	2:G:107:TRP:CH2	2.43	0.54
1:A:500:THR:O	1:A:500:THR:OG1	2.17	0.53
1:C:396:TYR:HB2	1:C:514:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:HG21	1:A:402:ILE:HG22	1.90	0.53
1:A:357:ARG:NH2	1:C:166:CYS:C	2.56	0.53
1:A:470:THR:HG23	1:A:490:PHE:HE1	1.73	0.53
1:B:456:PHE:HE1	2:G:33:TYR:CE1	2.19	0.53
1:B:716:THR:HG21	1:B:1073:LYS:HD3	1.89	0.53
1:B:505:HIS:O	1:B:506:GLN:HG3	2.08	0.53
1:C:96:GLU:OE1	1:C:98:SER:N	2.41	0.53
1:A:357:ARG:CD	1:C:167:THR:O	2.56	0.53
1:B:470:THR:HG23	1:B:490:PHE:HE1	1.73	0.53
1:A:520:ALA:CB	1:C:232:GLY:CA	2.87	0.53
2:E:37:VAL:HG11	2:E:107:TRP:CH2	2.43	0.53
1:B:172:SER:OG	1:B:173:GLN:N	2.42	0.53
3:D:108:ARG:NE	3:D:109:THR:O	2.42	0.53
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.91	0.53
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.88	0.53
1:B:808:ASP:OD2	1:B:811:LYS:NZ	2.42	0.53
1:C:458:LYS:O	4:H:53:TRP:CZ2	2.62	0.53
4:H:98:LYS:HB3	4:H:114:MET:HB2	1.89	0.53
1:A:96:GLU:OE1	1:A:99:ASN:N	2.40	0.52
1:A:353:TRP:CE2	1:A:466:ARG:HG2	2.44	0.52
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.24	0.52
1:B:462:LYS:HG2	1:B:465:GLU:HB2	1.92	0.52
1:B:350:VAL:HG21	1:B:402:ILE:HG22	1.90	0.52
1:B:569:ILE:HD12	1:B:569:ILE:H	1.73	0.52
1:A:36:VAL:HG21	1:A:220:PHE:CZ	2.44	0.52
1:A:462:LYS:HG2	1:A:465:GLU:HB2	1.91	0.52
1:A:394:ASN:HD21	1:C:167:THR:CB	2.21	0.52
1:A:597:VAL:HG13	1:A:608:VAL:HG13	1.92	0.52
1:A:986:PRO:HG2	1:A:987:PRO:HD3	1.92	0.52
1:A:374:PHE:HE2	1:A:377:PHE:HE2	1.52	0.52
1:C:354:ASN:O	1:C:398:ASP:HA	2.09	0.52
1:C:669:GLY:HA2	1:C:697:MET:HE2	1.92	0.52
1:B:374:PHE:CE1	1:B:434:ILE:HG23	2.30	0.52
1:C:30:ASN:HA	1:C:61:ASN:HA	1.90	0.52
1:C:426:PRO:HD3	1:C:463:PRO:HB3	1.91	0.52
1:B:330:PRO:HD3	1:B:544:ASN:HD21	1.75	0.52
1:B:353:TRP:CE2	1:B:466:ARG:HG2	2.44	0.52
3:F:108:ARG:NE	3:F:109:THR:O	2.42	0.52
4:H:60:PHE:HB2	4:H:65:LYS:HD3	1.92	0.52
1:A:441:LEU:HD12	1:A:441:LEU:H	1.75	0.52
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:37:VAL:HG11	4:H:112:PHE:HZ	1.74	0.52
2:G:2:VAL:CA	2:G:25:SER:OG	2.43	0.52
4:H:229:GLN:NE2	4:H:235:SER:H	2.08	0.52
1:C:194:PHE:HD1	1:C:203:ILE:HG12	1.76	0.51
1:B:441:LEU:HD12	1:B:441:LEU:H	1.75	0.51
1:C:380:TYR:HE2	1:C:429:PHE:HB3	1.76	0.51
1:C:457:ARG:HG3	1:C:459:SER:H	1.75	0.51
3:F:18:ARG:HH12	3:F:74:THR:HB	1.75	0.51
2:E:20:LEU:HG	2:E:82:MET:HE2	1.92	0.51
1:C:68:ILE:HG13	1:C:69:HIS:H	1.75	0.51
3:F:15:ILE:HD11	3:F:80:PRO:HD3	1.93	0.51
2:G:20:LEU:HG	2:G:82:MET:HE2	1.91	0.51
2:G:213:LYS:HZ2	2:G:215:VAL:HG22	1.75	0.51
1:A:422:ASN:HD21	1:A:454:ARG:N	2.05	0.51
1:A:1050:MET:HE2	1:A:1052:PHE:CE1	2.46	0.51
1:B:355:ARG:HG3	1:B:356:LYS:N	2.26	0.51
4:H:30:ASP:OD1	4:H:30:ASP:N	2.42	0.51
1:A:355:ARG:HG3	1:A:356:LYS:N	2.25	0.51
1:A:475:ALA:HB2	2:E:32:ASN:HD21	1.75	0.51
1:C:353:TRP:HZ2	1:C:466:ARG:HA	1.75	0.51
1:A:1141:LEU:HD11	1:C:1146:ASP:HB2	1.93	0.50
1:B:475:ALA:CB	2:G:32:ASN:HD21	2.24	0.50
1:C:131:CYS:HB3	1:C:166:CYS:CA	2.34	0.50
1:A:475:ALA:CB	2:E:32:ASN:HD21	2.24	0.50
2:G:77:THR:HB	2:G:79:TYR:CE1	2.47	0.50
1:B:476:GLY:H	1:B:487:ASN:HB3	1.77	0.50
1:C:597:VAL:HG13	1:C:608:VAL:HG13	1.92	0.50
1:B:475:ALA:HB2	2:G:32:ASN:HD21	1.75	0.50
1:C:36:VAL:HG21	1:C:220:PHE:CZ	2.47	0.50
1:C:365:TYR:N	1:C:388:ASN:OD1	2.34	0.50
1:C:368:LEU:HG	1:C:369:TYR:H	1.75	0.50
1:A:382:VAL:HG12	1:A:387:LEU:CG	1.98	0.50
1:B:475:ALA:H	1:B:487:ASN:HB3	1.77	0.50
3:D:18:ARG:HH12	3:D:74:THR:HB	1.75	0.50
3:D:158:ASN:OD1	3:D:158:ASN:O	2.30	0.50
1:A:475:ALA:H	1:A:487:ASN:HB3	1.77	0.50
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.12	0.50
2:E:77:THR:HB	2:E:79:TYR:CE1	2.47	0.50
4:H:52:ASN:OD1	4:H:53:TRP:N	2.43	0.50
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.12	0.50
3:D:33:LEU:HD11	3:D:88:CYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:GLY:H	1:A:487:ASN:HB3	1.77	0.49
1:B:196:ASN:HD22	1:B:235:ILE:HD12	1.77	0.49
1:C:458:LYS:HB3	4:H:53:TRP:CH2	2.47	0.49
1:C:472:ILE:HD13	1:C:482:GLY:HA2	1.94	0.49
3:F:33:LEU:HD11	3:F:88:CYS:HB2	1.94	0.49
3:D:15:ILE:HD11	3:D:80:PRO:HD3	1.93	0.49
3:F:158:ASN:OD1	3:F:158:ASN:O	2.30	0.49
4:H:178:LYS:NZ	4:H:220:GLU:O	2.42	0.49
4:H:36:TRP:NE1	4:H:81:LEU:HB2	2.27	0.49
2:G:18:LEU:HB2	2:G:82:MET:HE3	1.94	0.49
4:H:224:VAL:HG22	4:H:241:LYS:HG3	1.93	0.49
1:B:445:VAL:HA	1:B:499:PRO:HD2	1.94	0.49
1:C:498:ARG:HB2	1:C:501:TYR:CE1	2.47	0.49
2:E:18:LEU:HB2	2:E:82:MET:HE3	1.94	0.49
4:H:86:LEU:HD13	4:H:123:VAL:HG11	1.95	0.49
1:C:480:CYS:O	1:C:483:VAL:HG22	2.13	0.49
3:F:7:SER:HB2	3:F:8:PRO:HD3	1.95	0.49
1:B:197:ILE:HG13	1:B:198:ASP:H	1.77	0.49
1:B:1139:ASP:OD1	1:B:1139:ASP:N	2.45	0.49
4:H:115:TRP:CH2	4:H:183:PRO:HB2	2.48	0.49
4:H:200:ARG:HE	4:H:201:PHE:HE1	1.60	0.49
1:A:973:ILE:HG12	1:A:992:GLN:OE1	2.13	0.49
1:B:32:PHE:O	1:B:34:ARG:N	2.46	0.49
1:C:344:ALA:HB3	1:C:347:PHE:CE1	2.47	0.49
1:A:357:ARG:HD2	1:C:167:THR:HA	1.91	0.49
1:A:445:VAL:HA	1:A:499:PRO:HD2	1.94	0.49
1:B:532:ASN:OD1	1:B:533:LEU:N	2.46	0.49
1:C:586:ASP:OD2	1:C:587:ILE:N	2.45	0.49
2:E:213:LYS:HZ2	2:E:215:VAL:HG22	1.78	0.49
2:E:214:LYS:NZ	2:E:216:GLU:HB2	2.28	0.49
4:H:14:PRO:HG3	4:H:123:VAL:HB	1.94	0.49
1:C:460:ASN:ND2	4:H:56:ASP:OD2	2.45	0.49
1:C:495:TYR:OH	4:H:105:LEU:HD22	2.05	0.49
4:H:151:SER:HB3	4:H:245:LYS:HA	1.95	0.48
1:A:523:THR:HG22	1:C:230:PRO:HB2	1.93	0.48
1:C:529:LYS:CB	1:C:530:SER:O	2.60	0.48
1:A:30:ASN:HA	1:A:61:ASN:HA	1.94	0.48
1:A:456:PHE:HE1	2:E:33:TYR:CE1	2.19	0.48
1:B:333:THR:HG23	1:B:335:LEU:HD11	1.87	0.48
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.94	0.48
1:C:489:TYR:CD2	4:H:101:TYR:CE2	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:214:LYS:NZ	2:G:216:GLU:HB2	2.28	0.48
4:H:54:ASN:ND2	4:H:56:ASP:OD2	2.47	0.48
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.96	0.48
1:A:130:VAL:HG21	1:A:231:ILE:HG12	1.95	0.48
1:B:422:ASN:HD21	1:B:454:ARG:N	2.05	0.48
1:B:474:GLN:HA	1:B:487:ASN:O	2.13	0.48
1:C:34:ARG:NH1	1:C:219:GLY:O	2.46	0.48
1:C:454:ARG:HH22	1:C:471:GLU:H	1.62	0.48
1:C:401:VAL:HG23	1:C:509:ARG:NH1	2.28	0.48
2:E:82:MET:HB3	2:E:85:LEU:HD21	1.96	0.48
4:H:113:ASP:OD1	4:H:114:MET:N	2.47	0.48
4:H:182:ALA:HB3	4:H:184:ARG:HH12	1.78	0.48
1:A:351:TYR:CE1	1:A:452:ARG:HB2	2.49	0.48
1:A:523:THR:CG2	1:C:230:PRO:HG3	2.26	0.48
1:B:669:GLY:HA2	1:B:697:MET:HE2	1.95	0.48
1:B:782:PHE:CZ	1:B:1060:VAL:HG22	2.48	0.48
1:C:399:SER:HB2	1:C:509:ARG:HH21	1.78	0.48
1:A:422:ASN:ND2	1:A:454:ARG:H	2.06	0.48
1:A:521:PRO:HD3	1:C:199:GLY:O	2.09	0.48
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.96	0.48
1:A:1075:PHE:HB3	1:A:1096:VAL:HG13	1.96	0.48
1:C:826:VAL:HG13	1:C:1057:PRO:HG2	1.96	0.48
1:A:36:VAL:HG23	1:A:222:ALA:HA	1.94	0.47
1:A:100:ILE:HG22	1:A:242:LEU:HD23	1.96	0.47
1:B:351:TYR:CE1	1:B:452:ARG:HB2	2.49	0.47
1:C:347:PHE:HB3	1:C:509:ARG:NH2	2.29	0.47
1:C:417:ASN:HA	1:C:421:TYR:CD2	2.47	0.47
1:C:505:HIS:NE2	4:H:167:SER:CB	2.76	0.47
1:C:398:ASP:HB2	1:C:512:VAL:HG12	1.96	0.47
2:E:127:PRO:HA	2:E:213:LYS:NZ	2.29	0.47
2:G:127:PRO:HA	2:G:213:LYS:NZ	2.29	0.47
1:A:897:PRO:HD2	1:A:900:MET:HE2	1.96	0.47
1:C:417:ASN:HA	1:C:421:TYR:HD2	1.79	0.47
4:H:6:GLU:HB2	4:H:119:THR:HG23	1.96	0.47
4:H:115:TRP:CZ2	4:H:183:PRO:HB2	2.48	0.47
1:B:402:ILE:CD1	1:B:410:ILE:HG13	2.43	0.47
3:D:7:SER:HB2	3:D:8:PRO:HD3	1.95	0.47
1:A:402:ILE:CD1	1:A:410:ILE:HG13	2.43	0.47
1:A:474:GLN:HA	1:A:487:ASN:O	2.13	0.47
1:B:34:ARG:NH1	1:B:219:GLY:O	2.47	0.47
1:B:612:TYR:HB2	1:B:649:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:TYR:CD1	1:C:457:ARG:HB3	2.48	0.47
1:C:363:ALA:HB2	1:C:524:VAL:CG1	2.45	0.47
3:F:136:LEU:HB3	3:F:175:LEU:HB3	1.97	0.47
3:F:140:TYR:HD1	3:F:141:PRO:HA	1.80	0.47
1:A:330:PRO:C	1:A:331:ASN:CA	2.88	0.47
1:C:406:GLU:OE2	4:H:105:LEU:CB	2.62	0.47
2:E:2:VAL:CA	2:E:25:SER:OG	2.43	0.47
2:E:39:GLN:HB2	2:E:45:LEU:HG	1.97	0.47
1:C:403:ARG:HH21	1:C:495:TYR:HB3	1.77	0.47
1:C:442:ASP:C	1:C:448:ASN:HD22	2.22	0.47
1:C:454:ARG:HH11	1:C:457:ARG:HH21	1.60	0.47
1:A:520:ALA:CB	1:C:232:GLY:HA3	2.45	0.47
1:C:813:SER:HB3	1:C:815:ARG:HG3	1.96	0.47
3:D:140:TYR:HD1	3:D:141:PRO:HA	1.79	0.47
1:B:422:ASN:ND2	1:B:454:ARG:H	2.06	0.47
2:G:63:VAL:HB	2:G:67:PHE:HB2	1.97	0.47
1:B:530:SER:OG	1:B:531:THR:N	2.48	0.46
4:H:102:TYR:HB3	4:H:171:TYR:OH	2.15	0.46
1:C:335:LEU:HA	1:C:362:VAL:H	1.80	0.46
1:B:749:CYS:HA	1:B:752:LEU:HD12	1.97	0.46
1:C:752:LEU:O	1:C:755:GLN:HG2	2.15	0.46
2:E:185:VAL:HG21	3:D:135:LEU:HD11	1.98	0.46
1:C:447:GLY:HA2	1:C:497:PHE:O	2.15	0.46
2:E:33:TYR:HB2	2:E:98:ASP:O	2.16	0.46
2:G:82:MET:HB3	2:G:85:LEU:HD21	1.96	0.46
1:B:826:VAL:HG13	1:B:1057:PRO:HG2	1.98	0.46
1:C:403:ARG:HB3	1:C:406:GLU:OE1	2.16	0.46
3:D:142:ARG:CG	3:D:173:TYR:CZ	2.97	0.46
4:H:65:LYS:HE2	4:H:65:LYS:HB2	1.84	0.46
1:A:479:PRO:O	1:A:480:CYS:HB3	2.16	0.46
1:A:825:LYS:HA	1:A:825:LYS:HD3	1.77	0.46
1:B:64:TRP:HD1	1:B:65:PHE:N	2.13	0.46
1:B:194:PHE:HD1	1:B:203:ILE:HG12	1.80	0.46
1:C:353:TRP:CD1	1:C:353:TRP:H	2.33	0.46
2:E:63:VAL:HB	2:E:67:PHE:HB2	1.97	0.46
3:D:126:LYS:O	3:D:126:LYS:CG	2.63	0.46
2:G:12:VAL:HG22	2:G:13:GLN:H	1.80	0.46
1:B:68:ILE:HG13	1:B:69:HIS:H	1.80	0.46
1:B:338:PHE:HE1	1:B:358:ILE:HG13	1.81	0.46
3:D:42:LYS:NZ	3:D:45:ARG:HG3	2.31	0.46
1:B:763:LEU:HG	1:B:1008:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:SER:O	2:E:107:TRP:CD1	2.68	0.46
2:G:106:SER:O	2:G:107:TRP:CD1	2.68	0.46
1:A:338:PHE:HE1	1:A:358:ILE:HG13	1.81	0.46
1:B:537:LYS:C	1:B:551:VAL:HG12	2.40	0.46
1:B:662:CYS:HB2	1:B:671:CYS:HB3	1.69	0.46
2:G:33:TYR:HB2	2:G:98:ASP:O	2.16	0.46
1:A:521:PRO:CG	1:C:199:GLY:C	2.82	0.45
1:C:440:LYS:HA	1:C:440:LYS:HD2	1.75	0.45
1:A:713:ALA:HB3	1:C:894:LEU:HB3	1.99	0.45
1:B:466:ARG:HE	1:B:466:ARG:HB3	1.56	0.45
1:B:470:THR:HG23	1:B:490:PHE:CE1	2.51	0.45
1:B:1093:GLY:HA3	1:B:1105:THR:O	2.16	0.45
3:F:142:ARG:CG	3:F:173:TYR:CZ	2.97	0.45
1:A:986:PRO:O	1:A:990:GLU:HG2	2.17	0.45
1:C:505:HIS:CE1	4:H:169:HIS:HB2	2.52	0.45
3:D:42:LYS:HZ1	3:D:45:ARG:HG3	1.81	0.45
1:A:199:GLY:O	1:B:521:PRO:CG	2.64	0.45
1:A:480:CYS:O	1:A:480:CYS:SG	2.74	0.45
1:C:782:PHE:CZ	1:C:1060:VAL:HG22	2.52	0.45
2:E:12:VAL:HG22	2:E:13:GLN:H	1.80	0.45
3:D:136:LEU:HB3	3:D:175:LEU:HB3	1.97	0.45
3:F:135:LEU:HD11	2:G:185:VAL:HG21	1.97	0.45
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.81	0.45
1:B:364:ASP:OD1	1:B:527:PRO:HD3	2.12	0.45
2:G:39:GLN:HB2	2:G:45:LEU:HG	1.97	0.45
2:G:90:THR:HG23	2:G:114:THR:HA	1.98	0.45
4:H:98:LYS:CB	4:H:114:MET:HB2	2.47	0.45
1:A:444:LYS:CE	1:A:447:GLY:O	2.65	0.45
1:A:1083:HIS:O	1:A:1086:LYS:HG2	2.17	0.45
1:B:456:PHE:HZ	2:G:100:PRO:CD	2.07	0.45
1:B:994:ASP:O	1:B:998:THR:HG23	2.17	0.45
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.98	0.45
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.99	0.45
4:H:33:ALA:N	4:H:99:ASP:HB2	2.31	0.45
1:B:489:TYR:OH	2:G:99:ILE:CD1	2.65	0.45
1:C:197:ILE:HG13	1:C:198:ASP:N	2.31	0.45
2:E:204:HIS:ND1	2:E:207:SER:OG	2.32	0.45
3:D:63:SER:O	3:D:74:THR:OG1	2.33	0.45
1:B:444:LYS:CE	1:B:447:GLY:O	2.65	0.45
1:B:479:PRO:O	1:B:480:CYS:HB3	2.16	0.45
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:TYR:CE2	1:C:455:LEU:HD13	2.52	0.45
3:F:42:LYS:NZ	3:F:45:ARG:HG3	2.31	0.45
3:F:46:LEU:O	3:F:46:LEU:HG	2.15	0.45
4:H:104:ILE:HG22	4:H:105:LEU:N	2.26	0.45
1:A:32:PHE:O	1:A:34:ARG:N	2.49	0.45
1:A:662:CYS:HB2	1:A:671:CYS:HB3	1.70	0.45
1:A:808:ASP:OD2	1:A:811:LYS:NZ	2.49	0.45
2:E:90:THR:HG23	2:E:114:THR:HA	1.98	0.45
2:G:29:VAL:HG22	2:G:76:ASN:HA	1.99	0.45
1:C:439:ASN:ND2	1:C:506:GLN:OE1	2.50	0.44
2:E:37:VAL:HG21	2:E:107:TRP:CZ3	2.52	0.44
3:D:46:LEU:O	3:D:46:LEU:HG	2.15	0.44
1:C:196:ASN:HD22	1:C:235:ILE:HD12	1.82	0.44
3:F:126:LYS:O	3:F:126:LYS:CG	2.63	0.44
4:H:157:ARG:NH1	4:H:159:THR:OG1	2.51	0.44
1:B:83:VAL:HG22	1:B:239:GLN:HE21	1.83	0.44
2:E:64:LYS:HA	2:E:64:LYS:HE2	1.99	0.44
4:H:6:GLU:H	4:H:117:GLN:HE22	1.64	0.44
4:H:19:ARG:HB2	4:H:82:GLN:HE22	1.82	0.44
1:B:197:ILE:HG13	1:B:198:ASP:N	2.32	0.44
1:B:330:PRO:HB2	1:B:331:ASN:H	1.30	0.44
1:B:597:VAL:HG13	1:B:608:VAL:HG13	1.99	0.44
1:C:386:LYS:HD3	1:C:386:LYS:N	2.32	0.44
2:G:64:LYS:HE2	2:G:64:LYS:HA	1.99	0.44
1:A:64:TRP:HD1	1:A:65:PHE:N	2.16	0.44
1:A:1139:ASP:OD1	1:A:1139:ASP:N	2.48	0.44
3:F:63:SER:O	3:F:74:THR:OG1	2.33	0.44
2:G:37:VAL:HG21	2:G:107:TRP:CZ3	2.52	0.44
4:H:175:TYR:O	4:H:225:TYR:HA	2.17	0.44
1:A:521:PRO:CG	1:C:230:PRO:O	2.65	0.44
1:B:480:CYS:SG	1:B:480:CYS:O	2.74	0.44
1:C:374:PHE:HB2	1:C:377:PHE:HB2	2.00	0.44
2:G:7:SER:HA	2:G:111:THR:HG22	1.91	0.44
2:E:193:LEU:HB3	2:E:217:PRO:HG2	1.99	0.44
1:A:470:THR:HG23	1:A:490:PHE:CE1	2.51	0.44
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.88	0.44
1:C:406:GLU:OE2	4:H:105:LEU:HB3	2.18	0.44
2:G:128:LEU:HD11	2:G:145:LEU:HB2	2.00	0.44
2:G:193:LEU:HB3	2:G:217:PRO:HG2	1.99	0.44
1:A:324:GLU:HB3	1:A:539:VAL:HG23	2.00	0.44
1:C:335:LEU:HG	1:C:362:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:LYS:C	1:C:551:VAL:HG12	2.43	0.44
2:E:29:VAL:HG22	2:E:76:ASN:HA	1.99	0.44
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.99	0.43
1:B:356:LYS:HE3	1:B:356:LYS:HB3	1.83	0.43
1:B:977:LEU:HD21	1:B:1000:ARG:HH12	1.82	0.43
1:C:385:THR:OG1	1:C:387:LEU:HG	2.18	0.43
1:C:460:ASN:CG	4:H:56:ASP:OD2	2.61	0.43
1:A:197:ILE:HG13	1:A:198:ASP:N	2.33	0.43
1:A:230:PRO:HB2	1:B:521:PRO:HB2	1.99	0.43
1:B:368:LEU:O	1:B:369:TYR:HB2	2.18	0.43
1:C:364:ASP:CG	1:C:527:PRO:HB3	2.43	0.43
1:C:662:CYS:HB2	1:C:671:CYS:HB3	1.75	0.43
2:E:86:ARG:HG2	2:E:87:ALA:H	1.83	0.43
1:B:365:TYR:HH	1:B:395:VAL:HG21	1.75	0.43
1:C:1093:GLY:HA3	1:C:1105:THR:O	2.19	0.43
1:A:356:LYS:HE3	1:A:356:LYS:HB3	1.82	0.43
1:C:612:TYR:HB2	1:C:649:CYS:SG	2.59	0.43
1:C:666:ILE:HD11	1:C:672:ALA:HB2	2.00	0.43
3:F:100:GLN:CD	3:F:100:GLN:H	2.27	0.43
1:A:475:ALA:CA	2:E:31:ARG:HH12	2.32	0.43
1:A:196:ASN:HD22	1:A:235:ILE:HD12	1.83	0.43
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	2.01	0.43
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	2.00	0.43
1:B:762:GLN:HG2	1:B:765:ARG:HH22	1.83	0.43
1:C:206:LYS:HB3	1:C:223:LEU:HD23	2.01	0.43
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	2.00	0.43
4:H:68:PHE:CE2	4:H:83:MET:HB2	2.54	0.43
1:A:752:LEU:HD21	1:A:990:GLU:OE1	2.19	0.43
1:B:382:VAL:CB	1:B:387:LEU:HD11	2.49	0.43
1:C:900:MET:HE2	1:C:900:MET:HB3	1.94	0.43
3:D:107:LYS:HG3	3:D:140:TYR:OH	2.19	0.43
3:D:138:ASN:HA	3:D:172:THR:HB	2.01	0.43
1:A:296:LEU:HB2	1:A:608:VAL:HG21	2.01	0.43
1:A:489:TYR:OH	2:E:99:ILE:CD1	2.65	0.43
1:B:96:GLU:OE1	1:B:99:ASN:N	2.49	0.43
1:B:993:ILE:O	1:B:997:ILE:HG12	2.19	0.43
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	2.00	0.43
1:C:815:ARG:NH1	1:C:820:ASP:OD1	2.52	0.43
3:D:33:LEU:HA	3:D:89:GLN:O	2.19	0.43
3:F:33:LEU:HA	3:F:89:GLN:O	2.19	0.43
1:A:368:LEU:O	1:A:369:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:VAL:HA	1:A:499:PRO:CD	2.49	0.43
1:B:296:LEU:HB2	1:B:608:VAL:HG21	2.01	0.43
1:B:866:THR:OG1	1:B:869:MET:HG3	2.19	0.43
1:C:426:PRO:HG2	1:C:429:PHE:HB2	2.01	0.43
1:C:448:ASN:HB3	1:C:497:PHE:CD2	2.51	0.43
3:F:69:THR:H	3:F:69:THR:HG23	1.50	0.43
2:G:86:ARG:HG2	2:G:87:ALA:H	1.83	0.43
4:H:68:PHE:CZ	4:H:83:MET:HB2	2.53	0.43
1:B:85:PRO:HD2	1:B:269:TYR:OH	2.19	0.42
1:B:168:PHE:HE2	1:B:229:LEU:HD13	1.84	0.42
1:B:445:VAL:HA	1:B:499:PRO:CD	2.49	0.42
1:C:472:ILE:HG13	1:C:490:PHE:HD1	1.84	0.42
3:F:107:LYS:HG3	3:F:140:TYR:OH	2.19	0.42
4:H:176:GLN:HB2	4:H:186:LEU:HD11	2.00	0.42
1:A:68:ILE:HG13	1:A:69:HIS:H	1.84	0.42
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.88	0.42
1:B:342:PHE:CB	1:B:371:PHE:HZ	2.26	0.42
1:B:374:PHE:HD2	1:B:377:PHE:HB2	1.84	0.42
3:D:138:ASN:N	3:D:173:TYR:O	2.49	0.42
3:F:61:ARG:HB3	3:F:76:SER:HB3	2.01	0.42
4:H:200:ARG:HG3	4:H:201:PHE:CD1	2.52	0.42
1:A:310:LYS:HG3	1:A:600:PRO:HA	2.02	0.42
1:B:475:ALA:CA	2:G:31:ARG:HH12	2.32	0.42
1:C:403:ARG:H	4:H:105:LEU:HD13	1.82	0.42
4:H:177:GLN:O	4:H:223:ALA:HB1	2.19	0.42
1:A:374:PHE:HD2	1:A:377:PHE:HB2	1.84	0.42
1:A:382:VAL:CB	1:A:387:LEU:HD11	2.49	0.42
1:A:520:ALA:HB2	1:C:232:GLY:H	1.74	0.42
3:D:100:GLN:CD	3:D:100:GLN:H	2.27	0.42
1:A:537:LYS:C	1:A:551:VAL:HG12	2.45	0.42
2:E:12:VAL:HG12	2:E:115:VAL:HG12	2.01	0.42
3:F:138:ASN:HA	3:F:172:THR:HB	2.01	0.42
4:H:47:TRP:HH2	4:H:59:ALA:HB1	1.84	0.42
4:H:177:GLN:HA	4:H:183:PRO:HB3	2.02	0.42
1:C:1082:CYS:HB2	1:C:1126:CYS:HB2	1.84	0.42
2:G:29:VAL:CG2	2:G:76:ASN:HA	2.50	0.42
2:G:204:HIS:ND1	2:G:207:SER:OG	2.32	0.42
4:H:2:VAL:HA	4:H:26:GLY:HA3	2.02	0.42
4:H:29:PHE:CD2	4:H:77:ASN:HA	2.54	0.42
4:H:51:LEU:HB2	4:H:70:ILE:HD13	2.02	0.42
1:A:993:ILE:O	1:A:997:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:TYR:HD1	1:B:501:TYR:HA	1.67	0.42
2:E:128:LEU:HD11	2:E:145:LEU:HB2	2.00	0.42
3:D:113:PRO:HB3	3:D:139:PHE:HB3	2.02	0.42
1:A:1082:CYS:HB2	1:A:1126:CYS:HB2	1.77	0.42
1:A:1097:SER:HB3	1:A:1102:TRP:CD2	2.55	0.42
1:C:32:PHE:O	1:C:34:ARG:N	2.53	0.42
1:C:449:TYR:O	1:C:452:ARG:NH1	2.52	0.42
1:C:1086:LYS:HA	1:C:1125:ASN:HA	2.02	0.42
3:D:61:ARG:HB3	3:D:76:SER:HB3	2.01	0.42
3:F:30:ASN:O	3:F:71:PHE:HZ	2.03	0.42
2:G:12:VAL:HG12	2:G:115:VAL:HG12	2.01	0.42
2:G:209:THR:HG22	2:G:211:VAL:HG23	2.02	0.42
1:B:96:GLU:OE1	1:B:98:SER:N	2.46	0.42
1:C:989:ALA:O	1:C:993:ILE:HG12	2.20	0.42
1:B:776:LYS:HE3	1:B:780:GLU:OE2	2.20	0.42
1:C:346:ARG:NE	1:C:347:PHE:H	2.16	0.42
1:A:374:PHE:CZ	1:A:434:ILE:HG21	2.54	0.41
1:B:475:ALA:C	2:G:31:ARG:HH12	2.28	0.41
1:C:399:SER:CB	1:C:509:ARG:HH21	2.33	0.41
1:B:67:ALA:HB1	1:B:242:LEU:HD21	2.02	0.41
1:C:387:LEU:HD22	1:C:390:LEU:HD13	2.01	0.41
1:C:406:GLU:OE1	1:C:406:GLU:N	2.53	0.41
2:G:45:LEU:CD2	2:G:107:TRP:HZ3	2.33	0.41
1:A:172:SER:OG	1:A:173:GLN:N	2.53	0.41
1:C:205:SER:HB3	1:C:226:LEU:CD1	2.49	0.41
1:C:351:TYR:CE1	1:C:452:ARG:HB2	2.55	0.41
1:C:433:VAL:O	1:C:434:ILE:HD13	2.19	0.41
1:C:945:LEU:HD12	1:C:948:LEU:HD12	2.01	0.41
3:F:135:LEU:HD21	3:F:137:ASN:ND2	2.35	0.41
4:H:33:ALA:H	4:H:99:ASP:HB2	1.85	0.41
1:A:1029:MET:HE2	1:A:1029:MET:HB2	1.91	0.41
3:F:42:LYS:HZ1	3:F:45:ARG:HG3	1.86	0.41
1:B:750:SER:O	1:B:754:LEU:HG	2.21	0.41
1:B:1083:HIS:O	1:B:1086:LYS:HG2	2.20	0.41
1:C:351:TYR:O	1:C:468:ILE:HG12	2.20	0.41
2:E:29:VAL:CG2	2:E:76:ASN:HA	2.50	0.41
2:E:45:LEU:CD2	2:E:107:TRP:HZ3	2.33	0.41
3:D:30:ASN:O	3:D:71:PHE:HZ	2.03	0.41
4:H:38:ARG:HB2	4:H:48:VAL:CG2	2.51	0.41
1:A:1050:MET:HE2	1:A:1052:PHE:CZ	2.56	0.41
3:D:63:SER:OG	3:D:74:THR:OG1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:ILE:HG22	3:D:103:ARG:HH12	1.86	0.41
4:H:38:ARG:HG3	4:H:94:TYR:HE1	1.85	0.41
1:B:444:LYS:HE2	1:B:447:GLY:O	2.21	0.41
1:C:58:PHE:CD2	1:C:290:ASP:HB2	2.56	0.41
1:C:348:ALA:O	1:C:400:PHE:HA	2.20	0.41
4:H:169:HIS:ND1	4:H:170:ASN:N	2.68	0.41
1:B:106:PHE:HE2	1:B:119:ILE:HD12	1.86	0.41
1:B:386:LYS:O	1:B:389:ASP:HB2	2.21	0.41
1:C:1083:HIS:O	1:C:1086:LYS:HG2	2.21	0.41
1:A:986:PRO:HA	1:A:989:ALA:HB3	2.02	0.41
1:C:355:ARG:HG3	1:C:396:TYR:CD1	2.55	0.41
1:C:473:TYR:HB2	1:C:491:PRO:HD3	2.03	0.41
3:F:42:LYS:HG2	3:F:43:ALA:N	2.35	0.41
4:H:85:ASN:O	4:H:87:ARG:NH1	2.54	0.41
1:A:34:ARG:NH1	1:A:219:GLY:O	2.54	0.41
1:A:386:LYS:O	1:A:389:ASP:HB2	2.21	0.41
1:A:475:ALA:C	2:E:31:ARG:HH12	2.28	0.41
1:C:46:SER:CA	1:C:279:TYR:O	2.63	0.41
1:C:458:LYS:C	4:H:53:TRP:HZ2	2.27	0.41
2:E:209:THR:HG22	2:E:211:VAL:HG23	2.01	0.41
2:G:101:ARG:HE	2:G:101:ARG:HB2	1.59	0.41
1:A:331:ASN:HB2	1:A:580:GLN:HA	2.03	0.40
1:B:1048:HIS:HA	1:B:1066:THR:HG22	2.03	0.40
1:C:412:PRO:HB3	1:C:426:PRO:O	2.21	0.40
1:C:424:LYS:HD2	1:C:463:PRO:HD3	2.04	0.40
3:F:108:ARG:NH2	3:F:109:THR:OG1	2.52	0.40
3:F:113:PRO:HB3	3:F:139:PHE:HB3	2.02	0.40
1:A:399:SER:HA	1:A:510:VAL:O	2.21	0.40
1:B:119:ILE:HG12	1:B:128:ILE:HG12	2.03	0.40
1:B:729:VAL:HG21	1:B:1060:VAL:HG23	2.03	0.40
1:C:68:ILE:HG13	1:C:69:HIS:N	2.36	0.40
1:C:456:PHE:H	1:C:491:PRO:HB3	1.85	0.40
3:D:135:LEU:HD21	3:D:137:ASN:ND2	2.35	0.40
4:H:72:ARG:NH2	4:H:74:ASN:OD1	2.47	0.40
1:A:444:LYS:HE2	1:A:447:GLY:O	2.21	0.40
1:B:1084:ASP:HB3	1:B:1086:LYS:HE3	2.02	0.40
1:C:168:PHE:CZ	1:C:229:LEU:HD22	2.57	0.40
1:C:197:ILE:HG13	1:C:198:ASP:H	1.85	0.40
1:C:335:LEU:C	1:C:361:CYS:HB2	2.47	0.40
1:C:644:GLN:NE2	1:C:648:GLY:O	2.53	0.40
2:E:155:THR:OG1	2:E:203:ASN:ND2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:31:LYS:O	3:D:50:ASP:C	2.64	0.40
3:D:42:LYS:HG2	3:D:43:ALA:N	2.35	0.40
3:F:33:LEU:HD23	3:F:51:ALA:HB2	2.03	0.40
2:G:24:ALA:HB3	2:G:76:ASN:ND2	2.36	0.40
4:H:188:TYR:C	4:H:190:ALA:H	2.30	0.40
1:A:338:PHE:CE1	1:A:358:ILE:HG13	2.56	0.40
1:A:382:VAL:HG21	1:A:515:PHE:CD2	2.56	0.40
1:B:312:ILE:HD12	1:B:598:ILE:HD11	2.03	0.40
1:C:502:GLY:O	1:C:506:GLN:HG2	2.22	0.40
1:C:1048:HIS:HA	1:C:1066:THR:HG22	2.02	0.40
2:E:114:THR:HG23	2:E:114:THR:O	2.22	0.40
2:G:2:VAL:CA	2:G:25:SER:HG	2.23	0.40
2:G:36:TRP:HE1	2:G:78:LEU:HG	1.87	0.40
2:G:155:THR:OG1	2:G:203:ASN:ND2	2.50	0.40
2:G:166:GLY:O	2:G:186:VAL:HA	2.22	0.40
1:B:374:PHE:CZ	1:B:434:ILE:HG21	2.54	0.40
1:B:382:VAL:HG21	1:B:515:PHE:CD2	2.56	0.40
3:F:83:ILE:HG22	3:F:103:ARG:HH12	1.86	0.40
2:G:5:VAL:O	2:G:5:VAL:CG2	2.69	0.40
4:H:36:TRP:CZ3	4:H:96:CYS:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1000/1210 (83%)	962 (96%)	36 (4%)	2 (0%)	43	68
1	B	1004/1210 (83%)	973 (97%)	28 (3%)	3 (0%)	36	60
1	C	1004/1210 (83%)	934 (93%)	67 (7%)	3 (0%)	36	60
2	E	216/218 (99%)	209 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	D	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
3	F	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
4	H	243/245 (99%)	221 (91%)	22 (9%)	0	100	100
All	All	4103/4735 (87%)	3910 (95%)	185 (4%)	8 (0%)	44	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	529	LYS
1	C	529	LYS
1	A	529	LYS
1	A	530	SER
1	B	530	SER
1	B	330	PRO
1	C	332	ILE
1	C	383	SER

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	A	820/1055 (78%)	808 (98%)	12 (2%)	57	81
1	B	820/1055 (78%)	808 (98%)	12 (2%)	57	81
1	C	820/1055 (78%)	820 (100%)	0	100	100
2	E	182/182 (100%)	182 (100%)	0	100	100
2	G	182/182 (100%)	182 (100%)	0	100	100
3	D	187/187 (100%)	186 (100%)	1 (0%)	81	92
3	F	187/187 (100%)	186 (100%)	1 (0%)	81	92
4	H	193/193 (100%)	193 (100%)	0	100	100
All	All	3391/4096 (83%)	3365 (99%)	26 (1%)	70	88

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ARG
1	A	356	LYS
1	A	368	LEU
1	A	375	PHE
1	A	379	CYS
1	A	398	ASP
1	A	410	ILE
1	A	433	VAL
1	A	453	TYR
1	A	468	ILE
1	A	472	ILE
1	A	488	CYS
1	B	355	ARG
1	B	356	LYS
1	B	368	LEU
1	B	375	PHE
1	B	379	CYS
1	B	398	ASP
1	B	410	ILE
1	B	433	VAL
1	B	453	TYR
1	B	468	ILE
1	B	472	ILE
1	B	488	CYS
3	D	33	LEU
3	F	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	314	GLN
1	A	321	GLN
1	A	394	ASN
1	A	414	GLN
1	A	422	ASN
1	A	481	ASN
1	A	505	HIS
1	A	607	GLN
1	A	901	GLN
1	A	914	ASN

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Mol	Chain	Res	Type
1	A	1048	HIS
1	A	1054	GLN
1	A	1083	HIS
1	A	1106	GLN
1	B	196	ASN
1	B	207	HIS
1	B	414	GLN
1	B	422	ASN
1	B	481	ASN
1	B	505	HIS
1	B	641	ASN
1	B	762	GLN
1	B	784	GLN
1	B	801	ASN
1	B	856	ASN
1	B	914	ASN
1	B	949	GLN
1	B	1054	GLN
1	B	1064	HIS
1	B	1106	GLN
1	C	196	ASN
1	C	405	ASN
1	C	439	ASN
1	C	460	ASN
1	C	477	ASN
1	C	563	GLN
1	C	644	GLN
1	C	901	GLN
1	C	1106	GLN
1	C	1134	ASN
1	C	1135	ASN
2	E	32	ASN
2	E	76	ASN
3	D	27	GLN
3	D	137	ASN
3	D	158	ASN
3	F	27	GLN
3	F	137	ASN
3	F	158	ASN
2	G	32	ASN
2	G	76	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	C	4
1	B	2
2	E	2
2	G	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	321:GLN	C	322:PRO	N	3.93
1	C	333:THR	C	334:ASN	N	3.40
1	A	526:GLY	C	527:PRO	N	3.36
1	B	322:PRO	C	323:THR	N	3.26
1	A	333:THR	C	334:ASN	N	2.99
1	B	526:GLY	C	527:PRO	N	2.75
1	C	526:GLY	C	527:PRO	N	2.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	330:PRO	C	331:ASN	N	2.11
1	C	330:PRO	C	331:ASN	N	1.98
1	E	2:VAL	C	3:GLN	N	1.20
1	G	2:VAL	C	3:GLN	N	1.20
1	G	103:GLY	C	104:GLY	N	1.13
1	E	103:GLY	C	104:GLY	N	1.12
1	C	529:LYS	C	530:SER	N	0.71

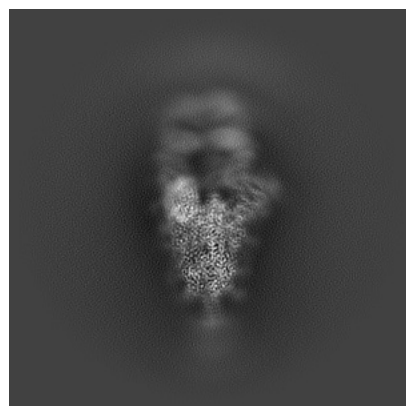
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39645. These allow visual inspection of the internal detail of the map and identification of artifacts.

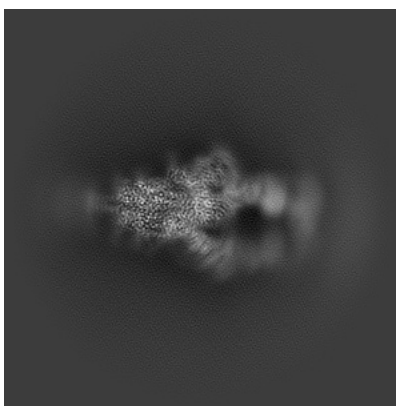
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

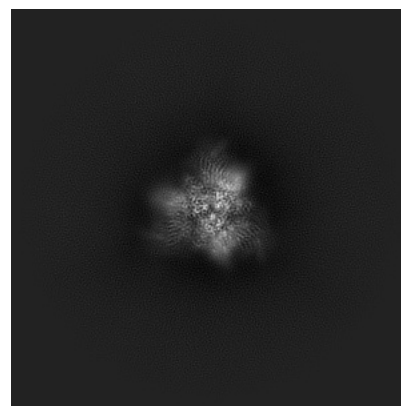
6.1.1 Primary map



X

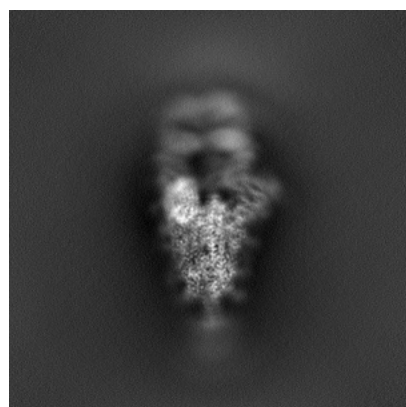


Y

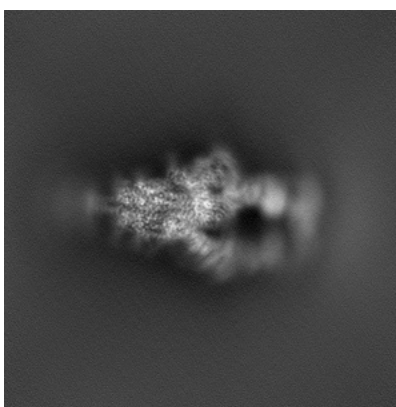


Z

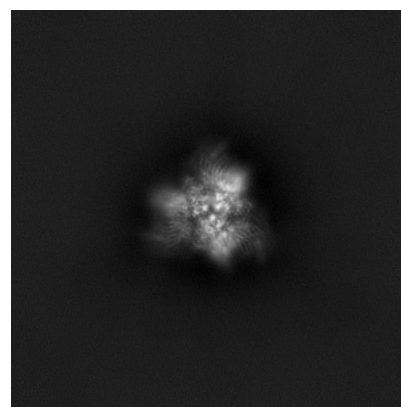
6.1.2 Raw map



X



Y



Z

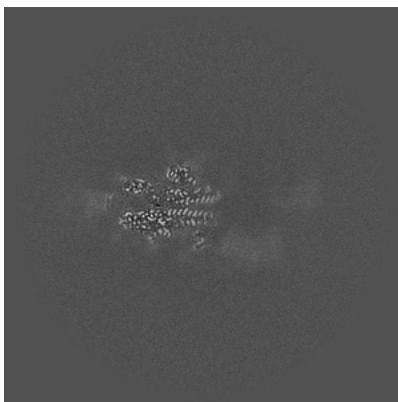
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

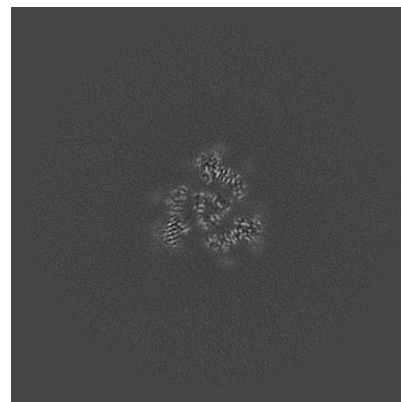
6.2.1 Primary map



X Index: 200

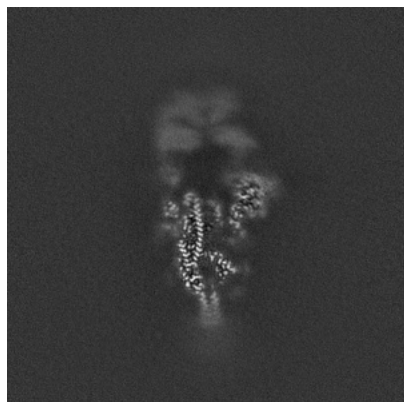


Y Index: 200

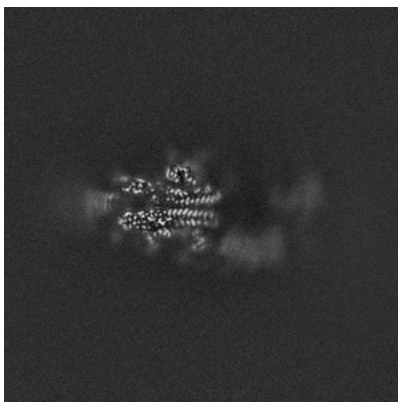


Z Index: 200

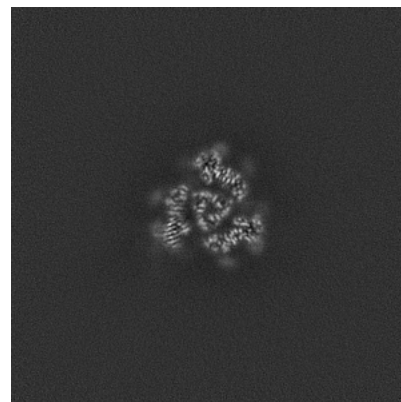
6.2.2 Raw map



X Index: 200



Y Index: 200

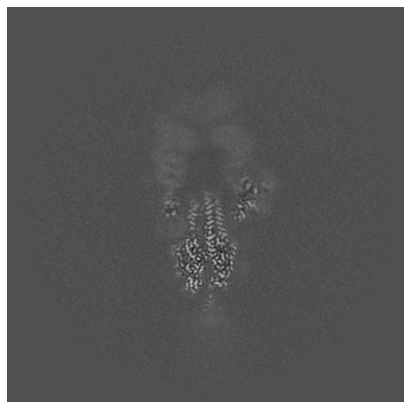


Z Index: 200

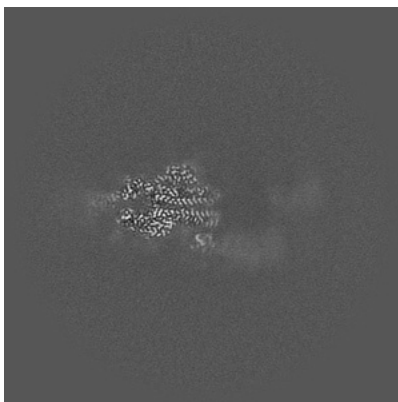
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

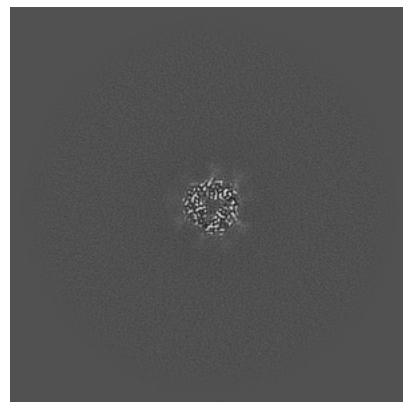
6.3.1 Primary map



X Index: 207

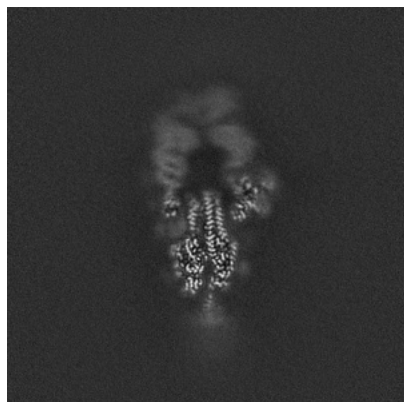


Y Index: 203

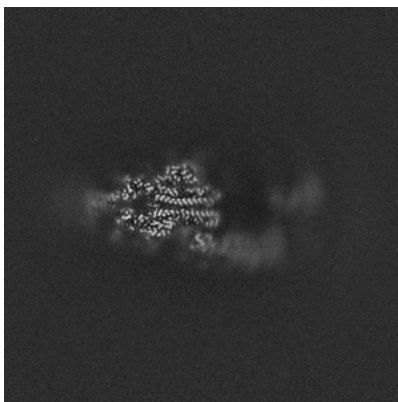


Z Index: 137

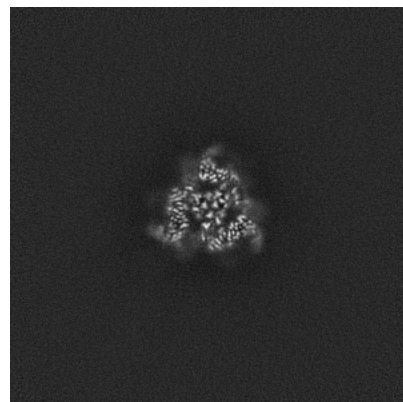
6.3.2 Raw map



X Index: 207



Y Index: 203

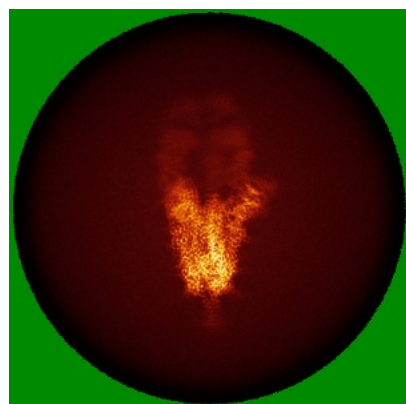


Z Index: 192

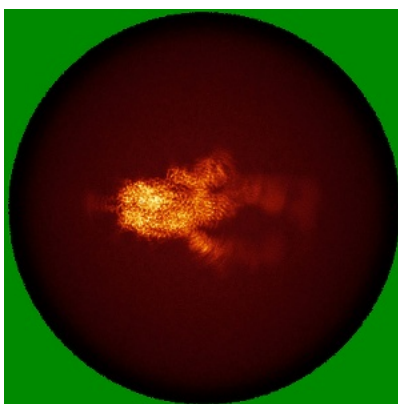
The images above show the largest variance slices of the map in three orthogonal directions.

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

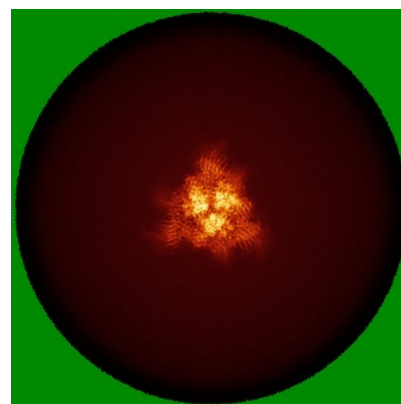
6.4.1 Primary map



X

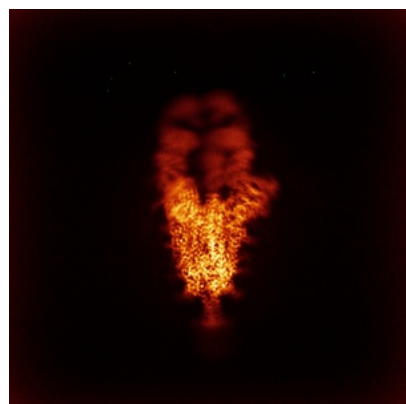


Y

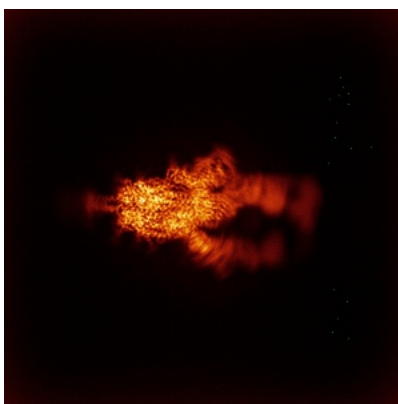


Z

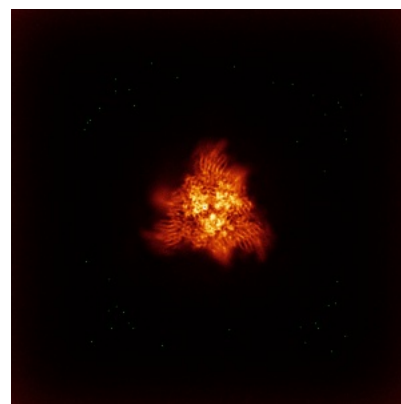
6.4.2 Raw map



X



Y

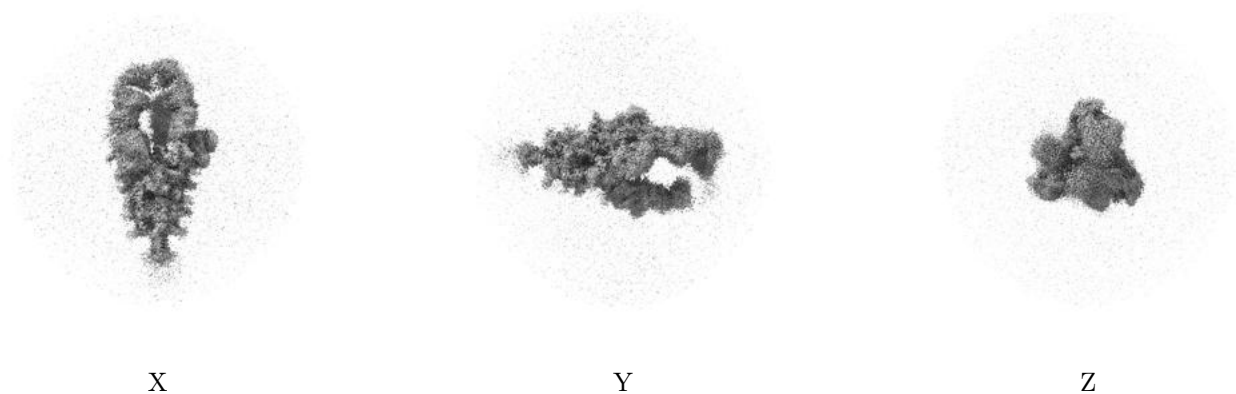


Z

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.

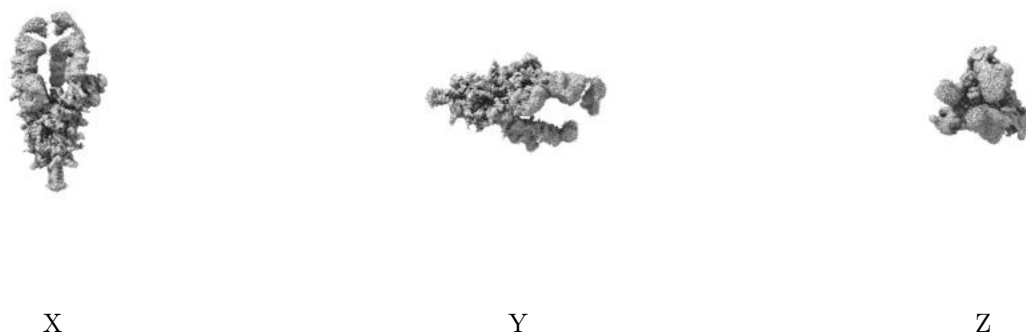
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.31. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

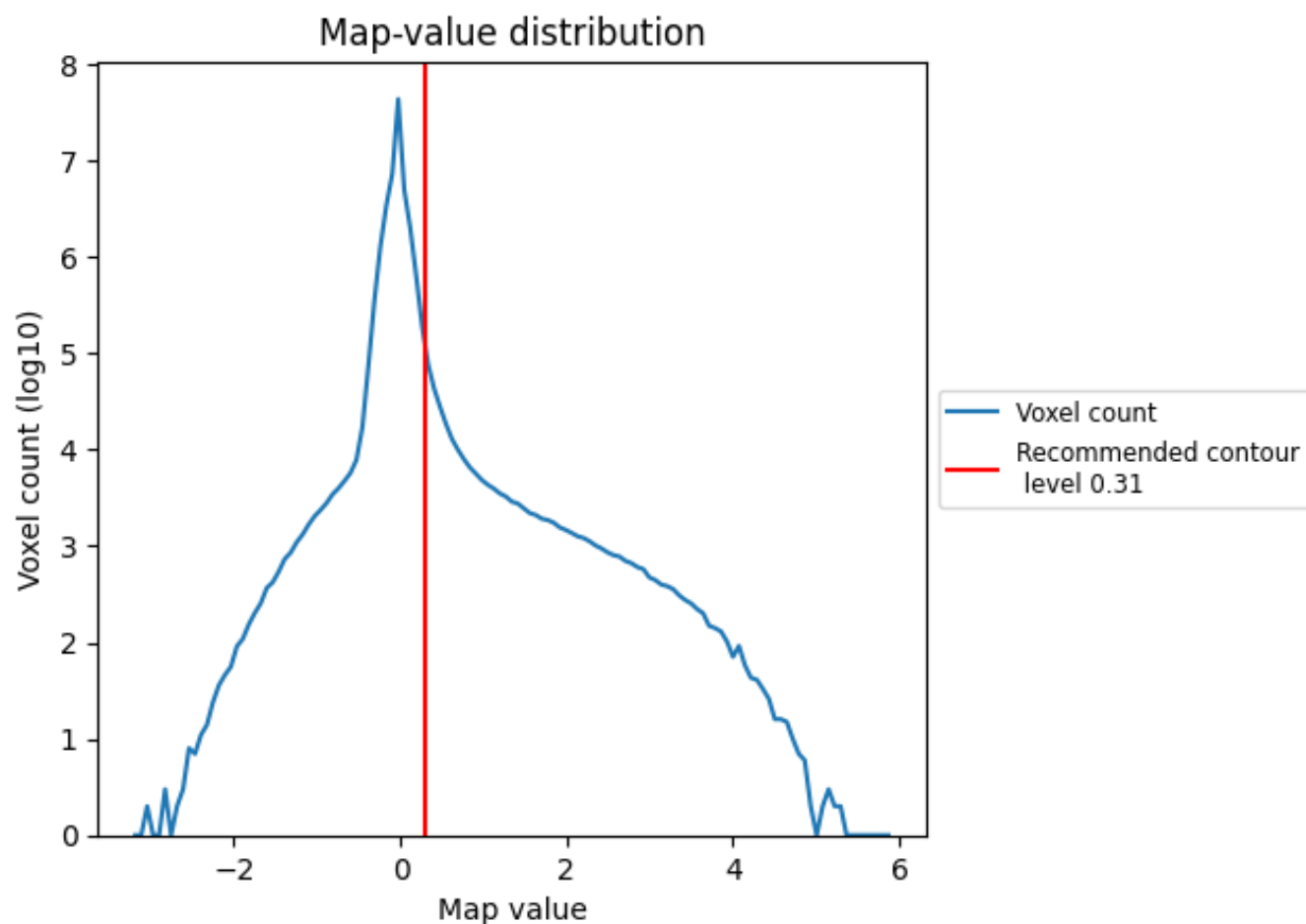
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

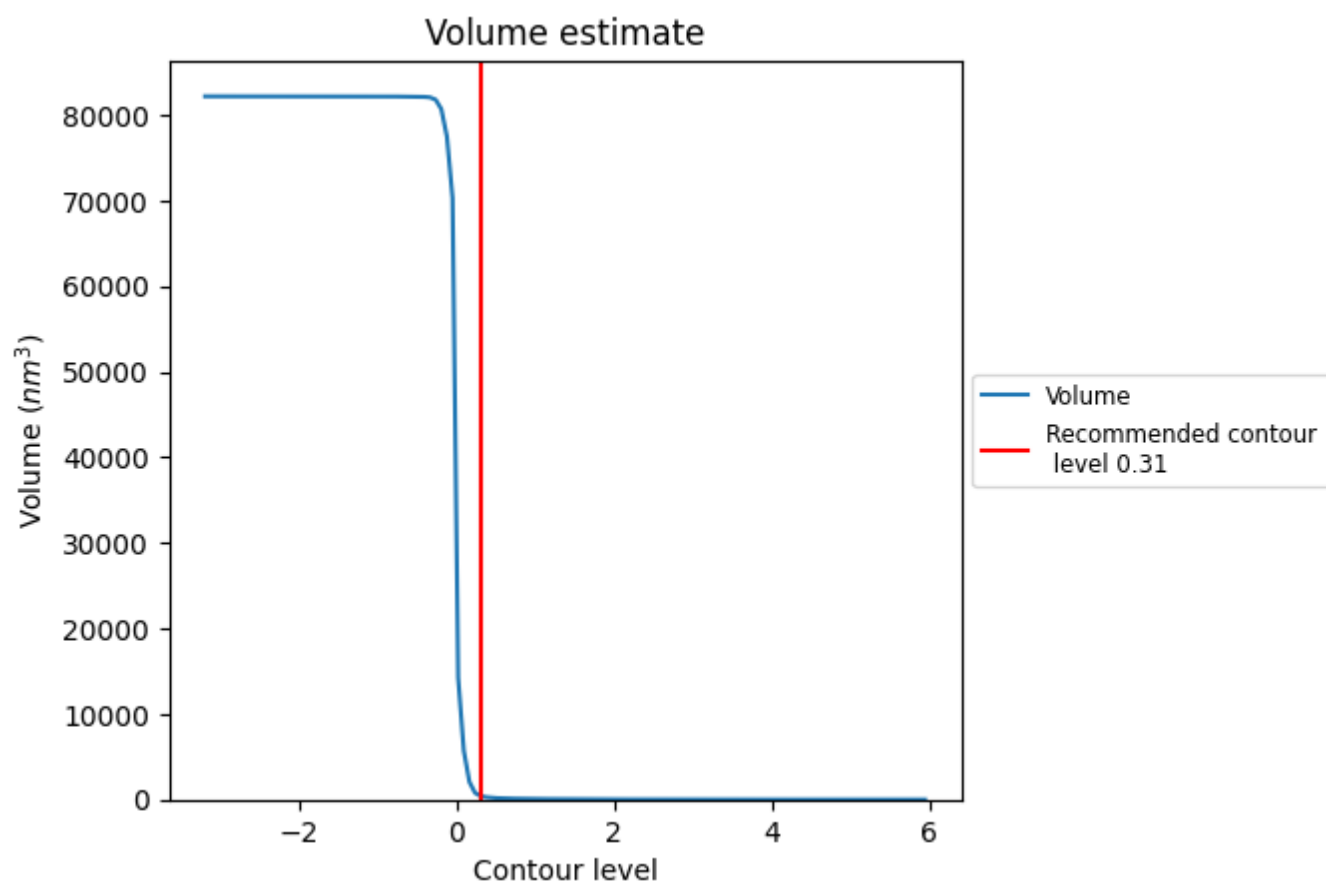
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

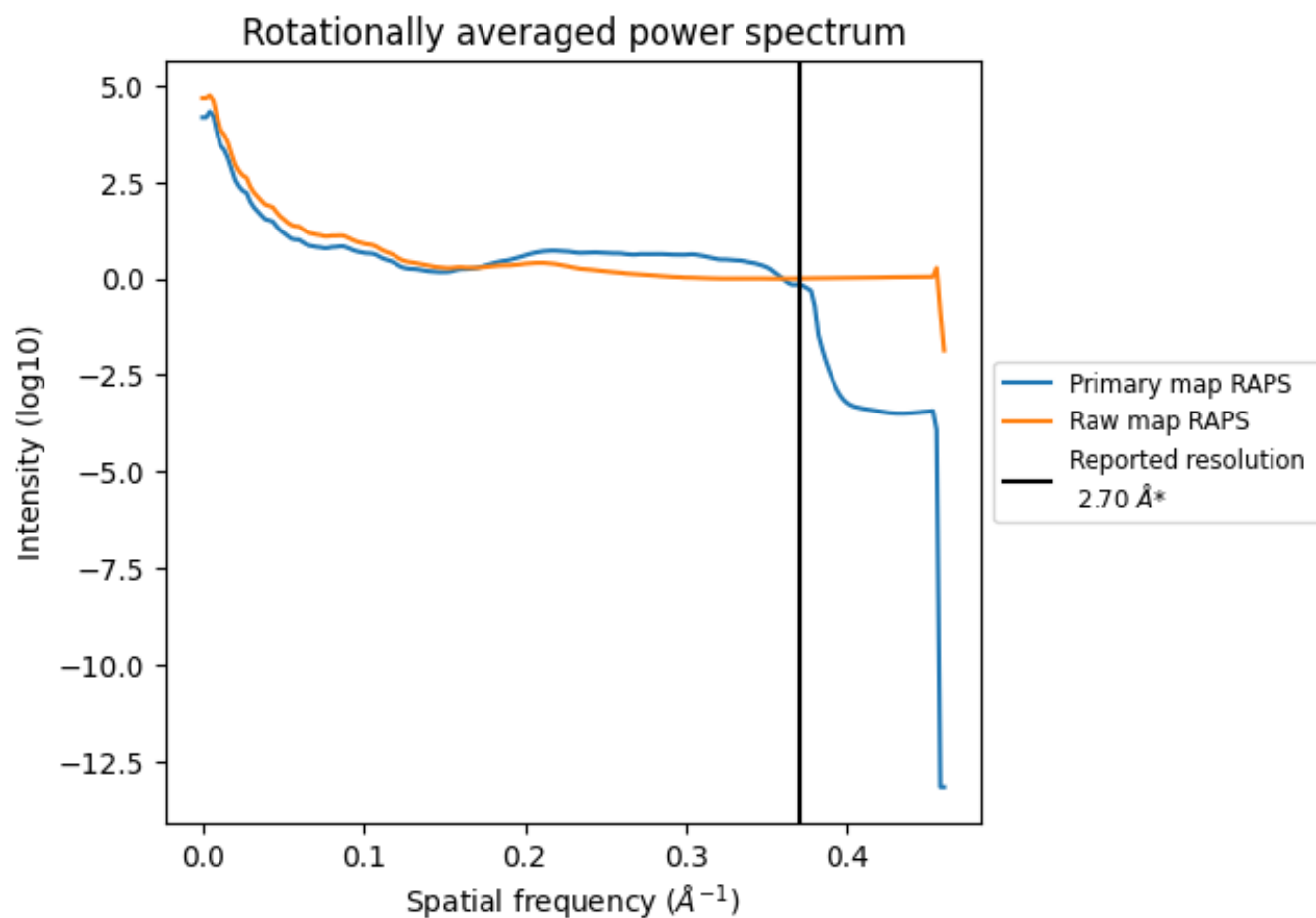
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 406 nm^3 ; this corresponds to an approximate mass of 367 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 ⓘ

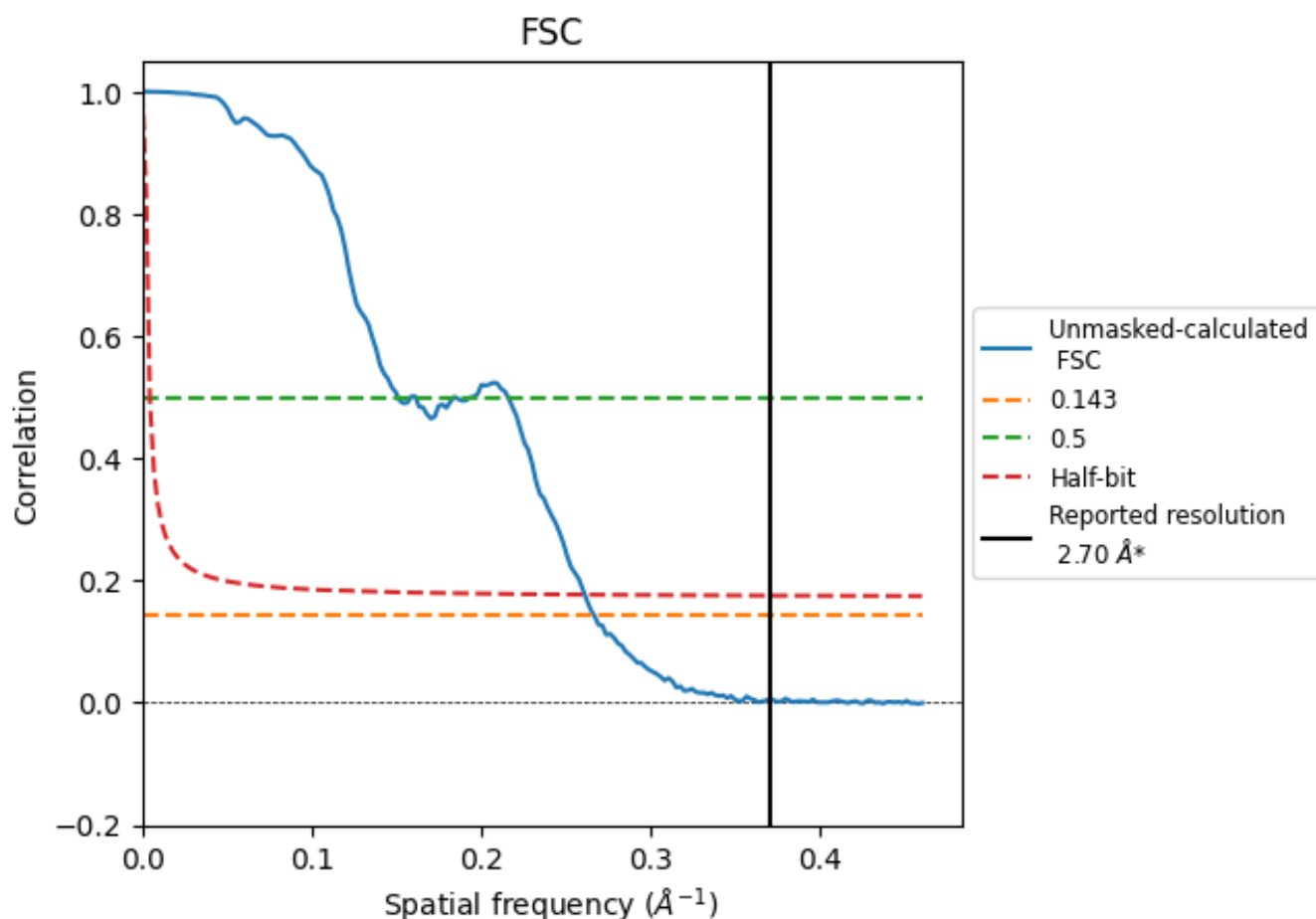


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

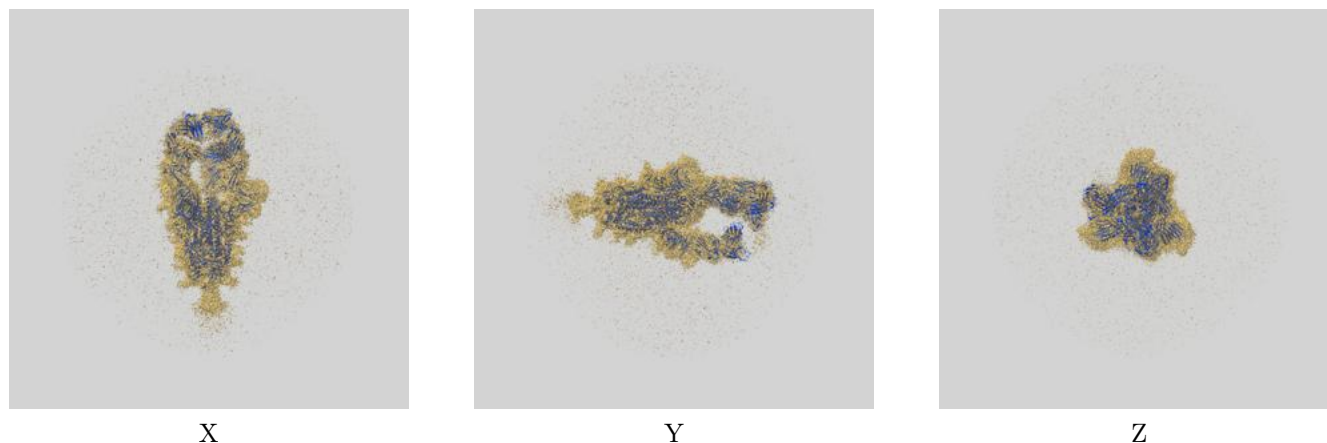
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	6.63	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

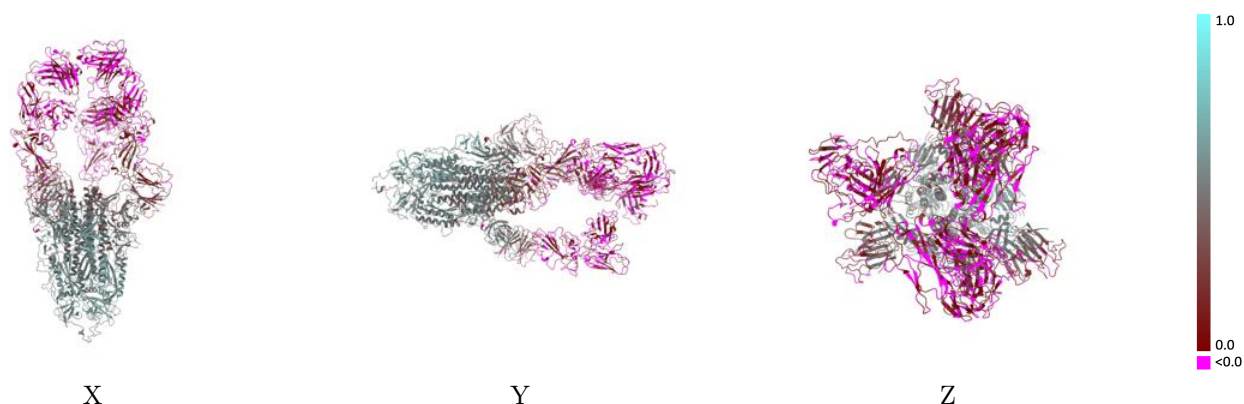
This section contains information regarding the fit between EMDB map EMD-39645 and PDB model 8YWW. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



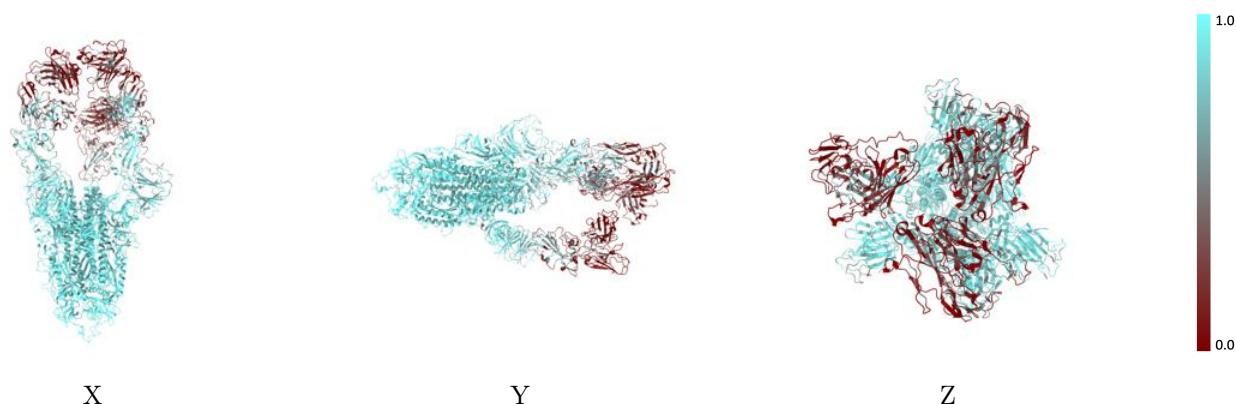
The images above show the 3D surface view of the map at the recommended contour level 0.31 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



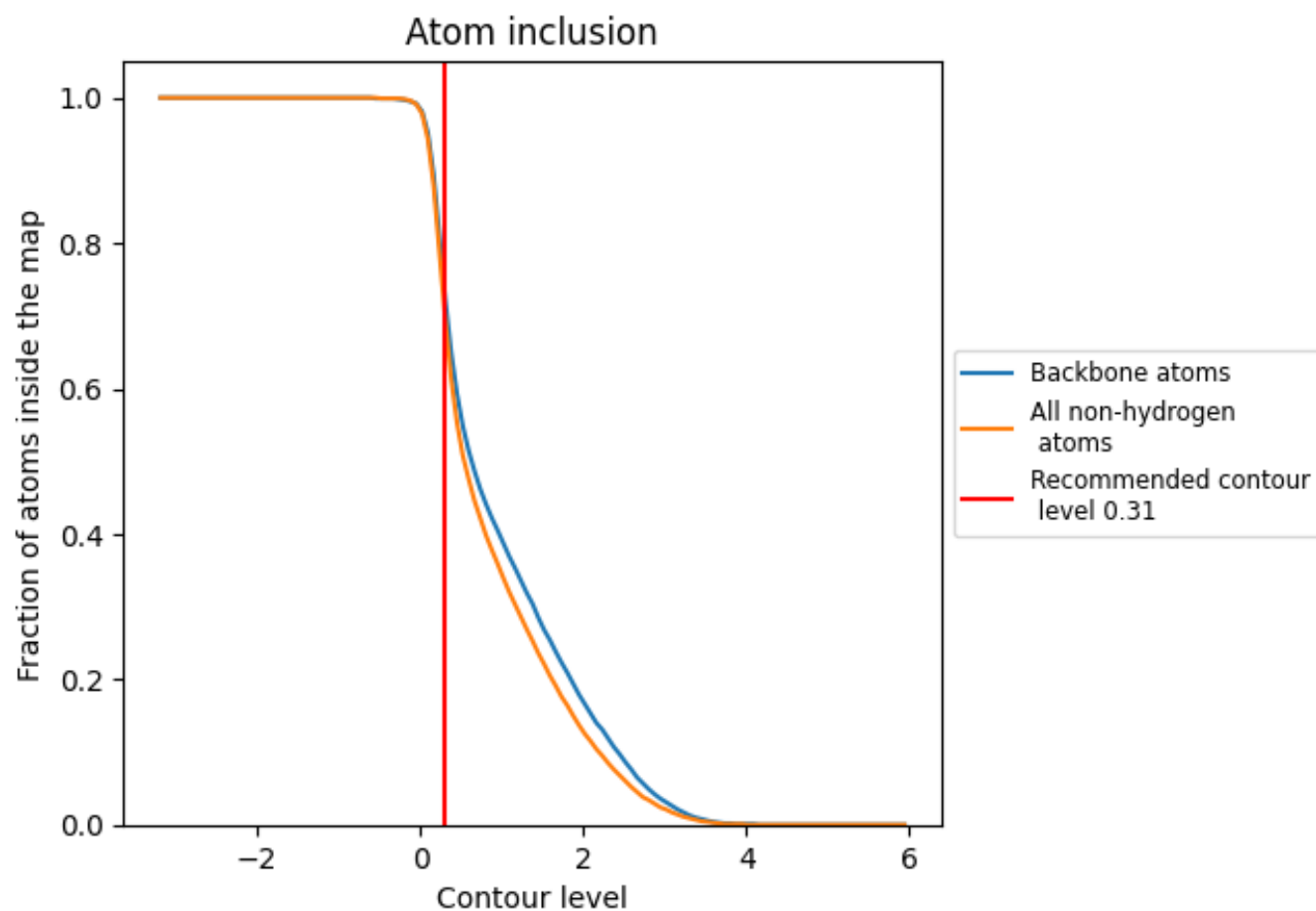
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.31).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 69% 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 (0.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.2910
A	0.8810	0.4110
B	0.8720	0.3920
C	0.7950	0.3600
D	0.3080	0.0150
E	0.3150	0.0180
F	0.2850	0.0240
G	0.2810	0.0200
H	0.1170	0.0370

1.0

0.0

<0.0