Full wwPDB EM Validation Report (i)

Jul 25, 2024 – 02:34 PM JST

PDB ID	:	8YWW
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 (i) 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 (i)) were used in the production of this report:
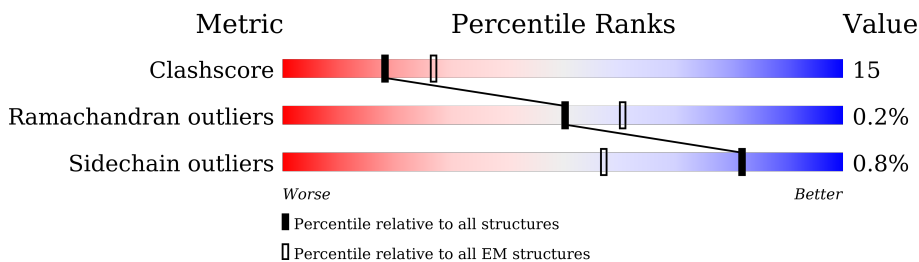
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 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	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		0.2%
Sidechain outliers		0.8%

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures

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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	• / 69% 14% • 15%
1	B	1210	• / 67% 16% • 15%
1	C	1210	11% / 68% 16% 15%
2	E	218	66% / 66% 28% 6%
2	G	218	70% / 64% 29% 6% •
3	D	212	68% / 67% 29% 5%
3	F	212	75% / 67% 28% 5%
4	H	245	94% / 58% 42%

WORLDWIDE PROTEIN DATA BANK

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 1619	C 1015	N 278	O 320	S 6	0	0
2	G	218	Total 1619	C 1015	N 278	O 320	S 6	0	0

- Molecule 3 is a protein called H4B6 light chain.

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

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

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

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 A:

● Molecule 1: Spike glycoprotein

Chain B:

• Molecule 1: Spike glycoprotein

Chain C:

11%

68% 16% 15%

• Molecule 2: H4B6 heavy chain

Chain E:

66%

66%　　28%　　6%

• Molecule 2: H4B6 heavy chain

Chain G:

70%

64%　　29%　　6%

E1 V2 Q3 L4 V5 E6 S7 G8 G9 D10 L11 V12 Q13 P14 G15 G16 S17 L18 R19 L20 S21 C22 A23 A24 S25 G26 F27 I28 V29 S30 R31 N32 Y33 W36 V37 R38 Q39 A40 P41 G42 K43 G44 L45 E46 W47 Y52 S53 G54 G55 G61 S62 V63 K64 G65 R66 F67 T68

I69 S70 R71 D72 N73 S74 K75 N76 I77 L78 Y79 M82 N83 S84 L85 R86 A87 E88 D89 T90 A91 I92 A96 R97 D98 I99 P100 R101 H102 G103 G104 D105 S106 W107 G108 Q109 G110 T111 L112 V113 T114 V115 S116 S117 A118 S119 T120 K121 G122 P123 S124 V125 F126 P127 L128 A129 P130 S131

S132 K133 S134 T135 S136 G137 G138 T139 A140 A141 L142 G143 C144 L145 V146 K147 D148 Y149 F150 P151 E152 P153 V154 T155 V156 S157 W158 N159 S160 G161 A162 L163 T164 S165 G166 V167 H168 T169 F170 P171 A172 V173 L174 Q175 S176 S177 G178 L179 Y180 S181 L182 S183 S184 V185 V186 T187 V188 P189 S190 S191

S192 L193 G194 T195 Q196 T197 Y198 I199 C200 N201 V202 N203 H204 K205 P206 S207 N208 T209 K210 V211 D212 K213 K214 V215 E216 P217 K218

● Molecule 3: H4B6 light chain

Chain D:

68%

67% 29% 5%

I2 R3 M4 T5 Q6 S7 P8 A9 S10 L11 S12 A13 S14 I15 G16 D17 R18 V19 T20 S26 Q27 N30 K31 Y32 L33 K39 P40 G41 K42 A43 P44 R45 L46 L47 D50 A51 S52 N53 L54 E55 T56 G57 V58 P59 S60 R61 F62 S63 G64 S65 G66 S67 G68 T69 D70 F71

T74 I75 S76 S77 L78 Q79 P80 E81 D82 I83 A84 C88 Q89 D92 N93 L94 Q100 G101 T102 R103 L104 E105 I106 K107 R108 T109 V110 A111 A112 P113 S114 I117 S121 D122 Q124 L125 K126 S127 G128 T129 A130 L135 L136 N137 N138 F139 Y140 P141 R142 E143 A144 K145

V146 Q147 W148 K149 V150 D151 N152 A153 L154 Q155 S156 G157 N158 S159 Q160 E161 S162 V163 T164 E165 Q166 D167 S168 K169 D170 S171 T172 Y173 S174 L175 S176 S177 T178 L179 T180 L181 S182 K183 A184 D185 Y186 E187 K188 H189 K190 V191 Y192 E195 V196 T197 H198 Q199 G200 L201 S202 S203 P204 V205 T206

K207 S208 F209 N210 R211 G212 E213

● Molecule 3: H4B6 light chain

Chain F:

75%

67% 28% 5%

I2 R3 M4 T5 Q6 S7 P8 A9 S10 L11 S12 A13 S14 I15 G16 D17 R18 V19 T20 I21 T22 A25 S26 Q27 N30 K31 Y32 L33 K39 P40 G41 K42 A43 P44 R45 L46 L47 D50 A51 S52 N53 L54 E55 T56 G57 V58 P59 S60 R61 F62 S63 G64 S65 G66 S67 G68

T69 D70 F71 T74 I75 S76 S77 L78 Q79 P80 E81 D82 I83 A84 C88 Q89 D92 N93 L94 Q100 G101 T102 R103 L104 E105 I106 K107 R108 T109 V110 A111 A112 P113 S114 V115 F116 P119 P120 S121 D122 E123 Q124 L125 K126 S127 G128 T129 A130 S131 V132 V133 C134 L135 L136 N137

N138 F139 Y140 P141 R142 E143 A144 K145 V146 Q147 W148 K149 V150 D151 N152 A153 L154 Q155 S156 G157 N158 S159 Q160 E161 S162 V163 T164 E165 Q166 D167 S168 K169 D170 S171 T172 Y173 S174 L175 S176 S177 T178 L179 T180 L181 S182 K183 A184 D185 Y186 E187 K188 H189 K190 V191 Y192 A193 C194 E195 V196 T197

H198 Q199 G200 L201 S202 S203 P204 V205 T206 K207 S208 F209 N210 R211 G212 E213

• Molecule 4: the scfv of H4D12

94%

Chain H:

58% 42%

E1 V2 Q3 L4 V5 E6 S7 G8 G9 G10 L11 V12 Q13 P14 G15 W16 S17 L18 R19 L20 S21 C22 V23 V24 S25 G26 L27 K28 F29 D30 D31 F32 A33 M34 H35 W36 V37 R38 Q39 V40 P41 G42 K43 G44 L45 E46 W47 V48 S49 G50 L51 N52 W53 N54 G55 D56 N57 V58 A59 F60

A61 D62 S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 N74 A75 E76 N77 S78 L79 Y80 L81 Q82 M83 N84 N85 L86 R87 P88 E89 D90 T91 A92 F93 Y94 Y95 C96 A97 K98 D99 S100 Y101 Y102 D103 I104 L105 T106 G107 Y108 S109 G110 A111 F112 D113 M114 W115 G116 Q117 G118 T119 M120

V121 T122 V123 S124 S125 G126 G127 G128 G129 S130 G131 G132 G133 G134 S135 G136 G137 G138 G139 A140 I141 R142 M143 T144 Q145 S146 P147 A148 T149 L150 S151 L152 S153 P154 G155 E156 R157 A158 T159 L160 S161 C162 R163 A164 S165 Q166 S167 V168 H169 N170 Y171 L172 A173 W174 Y175 Q176 Q177 K178 P179 G180

Q181 A182 P183 R184 L185 L186 F187 Y188 S191 N192 R193 A194 T195 G196 I197 P198 A199 R200 F201 S202 A203 S204 A205 S206 G207 T208 D209 S210 T211 L212 T213 I214 S215 S216 L217 E218 P219 E220 D221 F222 A223 V224 Y225 Y226 C227 Q228 Q229 R230 R231 N232 G233 Y234 S235 F236 G237 Q238 G239 T240 K241

V242 E243 I244 K245

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 $(e^-/Å^2)$	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 (Å)	434.80002, 434.80002, 434.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.36	2/7937 (0.0%)	0.80	30/10832 (0.3%)
1	B	0.37	4/7939 (0.1%)	0.84	34/10839 (0.3%)
1	C	0.52	2/7939 (0.0%)	0.77	3/10839 (0.0%)
2	E	0.48	2/1656 (0.1%)	1.43	33/2251 (1.5%)
2	G	0.48	2/1656 (0.1%)	1.43	33/2251 (1.5%)
3	D	0.32	0/1680	0.98	24/2280 (1.1%)
3	F	0.32	0/1680	0.98	24/2280 (1.1%)
4	H	0.27	0/1901	0.55	0/2573
All	All	0.41	12/32388 (0.0%)	0.89	181/44145 (0.4%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	PRO	C-N	27.88	1.98	1.34
1	C	529	LYS	C-N	-27.09	0.71	1.34
2	E	103	GLY	C-N	-11.18	1.12	1.33
2	G	103	GLY	C-N	-11.16	1.12	1.33
1	B	529	LYS	C-N	6.42	1.48	1.34
2	G	2	VAL	C-N	-5.96	1.20	1.34
2	E	2	VAL	C-N	-5.95	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	SER	CA-CB	-5.75	1.44	1.52
1	B	349	SER	CA-CB	-5.74	1.44	1.52
1	A	438	SER	CA-CB	-5.25	1.45	1.52
1	B	438	SER	CA-CB	-5.24	1.45	1.52
1	B	330	PRO	C-N	-5.07	1.22	1.34

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	529	LYS	CA-C-N	-47.33	13.09	117.20
1	C	529	LYS	C-N-CA	-38.82	24.66	121.70
1	B	529	LYS	O-C-N	-36.60	64.14	122.70
1	A	529	LYS	O-C-N	-32.55	70.62	122.70
2	G	24	ALA	CB-CA-C	-21.67	77.59	110.10
2	E	24	ALA	CB-CA-C	-21.66	77.60	110.10
1	B	333	THR	C-N-CA	-21.04	69.11	121.70
1	A	529	LYS	CA-C-N	19.62	160.37	117.20
2	G	11	LEU	CB-CA-C	-15.75	80.27	110.20
2	E	11	LEU	CB-CA-C	-15.74	80.28	110.20
2	E	23	ALA	CB-CA-C	-15.60	86.69	110.10
2	G	23	ALA	CB-CA-C	-15.60	86.70	110.10
1	B	529	LYS	CA-C-N	14.74	149.64	117.20
2	G	25	SER	N-CA-CB	-14.64	88.53	110.50
2	E	25	SER	N-CA-CB	-14.63	88.55	110.50
1	A	529	LYS	C-N-CA	13.83	156.28	121.70
2	G	11	LEU	N-CA-CB	-13.83	82.75	110.40
2	E	11	LEU	N-CA-CB	-13.82	82.76	110.40
1	A	344	ALA	N-CA-CB	13.41	128.87	110.10
1	B	344	ALA	N-CA-CB	13.40	128.85	110.10
2	E	11	LEU	N-CA-C	12.42	144.54	111.00
2	G	11	LEU	N-CA-C	12.41	144.52	111.00
2	E	5	VAL	N-CA-C	-11.71	79.39	111.00
2	G	5	VAL	N-CA-C	-11.70	79.40	111.00
2	E	10	ASP	N-CA-C	-11.46	80.07	111.00
2	G	10	ASP	N-CA-C	-11.45	80.10	111.00
1	A	501	TYR	N-CA-CB	11.15	130.67	110.60
1	B	501	TYR	N-CA-CB	11.14	130.66	110.60
2	E	103	GLY	O-C-N	-10.51	105.34	123.20
2	G	103	GLY	O-C-N	-10.49	105.36	123.20
1	B	343	ASN	CB-CA-C	10.47	131.34	110.40
1	A	343	ASN	CB-CA-C	10.45	131.30	110.40
3	D	127	SER	CB-CA-C	-10.37	90.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	127	SER	CB-CA-C	-10.37	90.39	110.10
2	G	103	GLY	N-CA-C	9.89	137.82	113.10
2	E	103	GLY	N-CA-C	9.87	137.78	113.10
2	G	106	SER	N-CA-C	-9.79	84.58	111.00
2	E	106	SER	N-CA-C	-9.77	84.64	111.00
3	D	182	SER	CB-CA-C	-9.67	91.73	110.10
3	F	182	SER	CB-CA-C	-9.66	91.74	110.10
2	E	2	VAL	N-CA-C	-9.35	85.75	111.00
2	G	2	VAL	N-CA-C	-9.35	85.76	111.00
2	G	128	LEU	N-CA-C	-9.29	85.90	111.00
2	E	128	LEU	N-CA-C	-9.29	85.91	111.00
2	E	103	GLY	CA-C-N	9.06	134.33	116.20
1	A	470	THR	N-CA-C	-9.05	86.56	111.00
1	B	470	THR	N-CA-C	-9.05	86.57	111.00
2	G	103	GLY	CA-C-N	9.04	134.29	116.20
2	E	114	THR	N-CA-C	-9.04	86.60	111.00
2	G	114	THR	N-CA-C	-9.02	86.64	111.00
3	F	11	LEU	N-CA-CB	9.02	128.44	110.40
3	D	11	LEU	N-CA-CB	9.01	128.42	110.40
1	B	343	ASN	N-CA-C	-8.99	86.72	111.00
1	A	343	ASN	N-CA-C	-8.98	86.75	111.00
2	G	7	SER	N-CA-CB	8.98	123.97	110.50
2	E	7	SER	N-CA-CB	8.97	123.96	110.50
1	B	344	ALA	N-CA-C	-8.90	86.98	111.00
1	A	344	ALA	N-CA-C	-8.89	86.99	111.00
3	D	10	SER	N-CA-C	-8.69	87.53	111.00
3	F	10	SER	N-CA-C	-8.69	87.53	111.00
1	B	529	LYS	C-N-CA	8.56	143.11	121.70
1	A	422	ASN	N-CA-C	8.49	133.93	111.00
1	B	422	ASN	N-CA-C	8.49	133.92	111.00
1	B	330	PRO	CA-C-N	-8.43	98.66	117.20
2	E	47	TRP	CB-CA-C	-8.21	93.98	110.40
2	G	47	TRP	CB-CA-C	-8.21	93.99	110.40
3	F	190	LYS	CB-CA-C	-8.14	94.12	110.40
3	D	190	LYS	CB-CA-C	-8.13	94.13	110.40
1	A	501	TYR	N-CA-C	-7.99	89.43	111.00
1	B	501	TYR	N-CA-C	-7.99	89.44	111.00
2	E	6	GLU	N-CA-C	-7.88	89.72	111.00
2	G	6	GLU	N-CA-C	-7.88	89.73	111.00
1	B	411	ALA	CB-CA-C	7.88	121.91	110.10
1	A	411	ALA	CB-CA-C	7.87	121.90	110.10
3	D	11	LEU	N-CA-C	-7.77	90.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	11	LEU	N-CA-C	-7.76	90.05	111.00
1	B	448	ASN	N-CA-C	-7.69	90.23	111.00
1	A	448	ASN	N-CA-C	-7.68	90.25	111.00
2	E	25	SER	N-CA-C	7.63	131.60	111.00
2	G	25	SER	N-CA-C	7.63	131.60	111.00
2	E	2	VAL	O-C-N	-7.49	110.72	122.70
2	G	2	VAL	O-C-N	-7.47	110.75	122.70
1	B	373	PRO	N-CA-C	-7.15	93.52	112.10
1	A	373	PRO	N-CA-C	-7.13	93.56	112.10
3	F	52	SER	N-CA-CB	-7.13	99.80	110.50
3	D	52	SER	N-CA-CB	-7.12	99.82	110.50
2	E	106	SER	CB-CA-C	7.04	123.48	110.10
2	G	106	SER	CB-CA-C	7.04	123.47	110.10
1	B	448	ASN	N-CA-CB	7.00	123.21	110.60
1	B	506	GLN	N-CA-CB	7.00	123.20	110.60
1	A	448	ASN	N-CA-CB	7.00	123.19	110.60
1	A	506	GLN	N-CA-CB	6.98	123.17	110.60
2	E	115	VAL	N-CA-C	-6.97	92.17	111.00
2	G	115	VAL	N-CA-C	-6.96	92.20	111.00
2	E	27	PHE	N-CA-CB	-6.79	98.38	110.60
1	B	333	THR	CA-C-N	-6.78	102.28	117.20
2	G	27	PHE	N-CA-CB	-6.78	98.41	110.60
3	D	59	PRO	N-CA-C	-6.67	94.75	112.10
3	F	59	PRO	N-CA-C	-6.67	94.75	112.10
3	F	190	LYS	N-CA-C	6.66	128.99	111.00
3	D	190	LYS	N-CA-C	6.66	128.97	111.00
1	B	470	THR	CB-CA-C	6.64	129.53	111.60
1	A	470	THR	CB-CA-C	6.64	129.53	111.60
3	F	51	ALA	CB-CA-C	6.53	119.90	110.10
3	D	51	ALA	CB-CA-C	6.53	119.89	110.10
1	B	422	ASN	N-CA-CB	-6.52	98.86	110.60
1	A	422	ASN	N-CA-CB	-6.51	98.89	110.60
3	D	189	HIS	CB-CA-C	-6.43	97.55	110.40
3	F	189	HIS	CB-CA-C	-6.42	97.56	110.40
1	B	339	ASP	N-CA-C	6.34	128.11	111.00
2	G	3	GLN	N-CA-C	-6.33	93.90	111.00
1	A	339	ASP	N-CA-C	6.33	128.10	111.00
2	E	3	GLN	N-CA-C	-6.32	93.93	111.00
1	B	330	PRO	C-N-CA	-6.20	106.19	121.70
1	B	375	PHE	N-CA-C	-6.07	94.62	111.00
1	A	375	PHE	N-CA-C	-6.06	94.64	111.00
1	A	388	ASN	CB-CA-C	6.05	122.50	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	3	GLN	N-CA-CB	6.04	121.48	110.60
1	B	388	ASN	CB-CA-C	6.04	122.48	110.40
2	E	3	GLN	N-CA-CB	6.03	121.45	110.60
1	A	353	TRP	N-CA-C	-6.00	94.80	111.00
1	B	353	TRP	N-CA-C	-5.99	94.84	111.00
1	B	430	THR	N-CA-C	-5.94	94.96	111.00
1	A	430	THR	N-CA-C	-5.94	94.97	111.00
2	G	195	THR	CB-CA-C	-5.92	95.62	111.60
2	E	195	THR	CB-CA-C	-5.91	95.64	111.60
2	E	21	SER	CB-CA-C	5.89	121.29	110.10
2	E	24	ALA	N-CA-C	5.88	126.89	111.00
2	G	24	ALA	N-CA-C	5.88	126.88	111.00
3	F	59	PRO	CB-CA-C	5.88	126.70	112.00
2	G	21	SER	CB-CA-C	5.88	121.27	110.10
3	D	59	PRO	CB-CA-C	5.87	126.67	112.00
3	F	92	ASP	CB-CA-C	-5.84	98.72	110.40
3	D	92	ASP	CB-CA-C	-5.84	98.72	110.40
3	D	60	SER	N-CA-CB	5.83	119.25	110.50
1	B	400	PHE	CB-CA-C	-5.82	98.75	110.40
3	F	60	SER	N-CA-CB	5.82	119.23	110.50
1	A	400	PHE	CB-CA-C	-5.80	98.79	110.40
2	E	31	ARG	N-CA-C	5.80	126.66	111.00
2	G	31	ARG	N-CA-C	5.79	126.65	111.00
2	G	128	LEU	CB-CA-C	5.76	121.15	110.20
2	E	128	LEU	CB-CA-C	5.75	121.12	110.20
1	B	505	HIS	N-CA-C	-5.74	95.52	111.00
1	A	505	HIS	N-CA-C	-5.73	95.54	111.00
2	G	68	THR	CB-CA-C	5.69	126.95	111.60
2	E	68	THR	CB-CA-C	5.68	126.93	111.60
3	D	69	THR	N-CA-C	5.55	125.98	111.00
3	F	69	THR	N-CA-C	5.55	125.98	111.00
3	D	9	ALA	N-CA-CB	-5.54	102.35	110.10
3	F	58	VAL	CB-CA-C	5.54	121.92	111.40
3	D	58	VAL	CB-CA-C	5.53	121.91	111.40
3	D	68	GLY	N-CA-C	-5.51	99.33	113.10
3	F	9	ALA	N-CA-CB	-5.50	102.39	110.10
3	F	68	GLY	N-CA-C	-5.50	99.35	113.10
1	B	375	PHE	CB-CA-C	5.50	121.39	110.40
1	A	375	PHE	CB-CA-C	5.47	121.35	110.40
1	B	339	ASP	N-CA-CB	-5.43	100.83	110.60
1	A	339	ASP	N-CA-CB	-5.41	100.86	110.60
1	C	564	GLN	C-N-CA	5.40	135.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	77	SER	N-CA-CB	5.40	118.61	110.50
3	D	77	SER	N-CA-CB	5.39	118.59	110.50
1	B	353	TRP	N-CA-CB	5.33	120.20	110.60
3	D	76	SER	CB-CA-C	-5.32	99.99	110.10
3	F	76	SER	CB-CA-C	-5.32	99.99	110.10
1	A	353	TRP	N-CA-CB	5.32	120.17	110.60
1	B	447	GLY	N-CA-C	-5.19	100.12	113.10
1	A	447	GLY	N-CA-C	-5.18	100.14	113.10
2	G	47	TRP	N-CA-C	5.18	124.99	111.00
2	E	47	TRP	N-CA-C	5.16	124.94	111.00
1	B	500	THR	N-CA-C	-5.12	97.17	111.00
3	F	100	GLN	N-CA-CB	-5.11	101.40	110.60
1	A	500	THR	N-CA-C	-5.11	97.21	111.00
3	D	7	SER	CB-CA-C	-5.11	100.40	110.10
3	D	100	GLN	N-CA-CB	-5.10	101.42	110.60
3	F	7	SER	CB-CA-C	-5.10	100.41	110.10
3	F	8	PRO	CB-CA-C	-5.08	99.29	112.00
3	D	8	PRO	CB-CA-C	-5.08	99.29	112.00
2	E	69	ILE	N-CA-C	-5.08	97.29	111.00
2	G	69	ILE	N-CA-C	-5.08	97.30	111.00
3	D	47	LEU	N-CA-C	5.05	124.64	111.00
3	F	47	LEU	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7754	0	7362	223	0
1	B	7754	0	7366	215	0
1	C	7754	0	7361	243	0
2	E	1619	0	1592	70	0
2	G	1619	0	1592	77	0
3	D	1646	0	1596	49	0
3	F	1646	0	1596	50	0
4	H	1857	0	1759	130	0
All	All	31649	0	30224	907	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 (907) 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:382:VAL:HG11	1:B:387:LEU:CD2	1.41	1.45
1:B:364:ASP:CG	1:B:527:PRO:HG3	1.09	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
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
2:G:4:LEU:HD22	2:G:23:ALA:O	1.32	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:364:ASP:CG	1:B:527:PRO:CD	2.05	1.17
1:C:330:PRO:C	1:C:331:ASN:N	1.98	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:364:ASP:CG	1:B:527:PRO:CG	1.76	1.04
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
1:A:330:PRO:C	1:A:331:ASN:N	2.11	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:382:VAL:CG1	1:B:387:LEU:HG	1.89	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:B:364:ASP:CG	1:B:527:PRO:HD3	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:ASN:HD21	4:H:56:ASP:CG	1.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:2:VAL:HA	2:G:25:SER:HG	1.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:THR:C	1:B:357:ARG:HH12	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:460:ASN:ND2	4:H:56:ASP:CG	2.53	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:B:444:LYS:HB2	1:B:447:GLY:C	2.25	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: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:A:444:LYS:HB2	1:A:447:GLY:C	2.25	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
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:B:364:ASP:CG	1:B:527:PRO:N	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:350:VAL:HG21	1:A:402:ILE:HG22	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:866:THR:H	1:A:869:MET:HE3	1.73	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: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
4:H:37:VAL:HG11	4:H:112:PHE:HZ	1.74	0.52
1:A:521:PRO:HD2	1:C:231:ILE:C	2.31	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
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
1:A:422:ASN:HD21	1:A:454:ARG:N	2.05	0.51
1:B:355:ARG:HG3	1:B:356:LYS:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:418:ILE:HD11	4:H:105:LEU:C	2.30	0.49
1:C:498:ARG:HB2	1:C:501:TYR:CE1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:357:ARG:NH2	1:C:166:CYS:C	2.56	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:B:91:TYR:OH	1:B:191:GLU:OE2	2.24	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:480:CYS:SG	1:B:480:CYS:O	2.74	0.46
1:B:763:LEU:HG	1:B:1008:VAL:HG21	1.97	0.46
1:C:669:GLY:HA2	1:C:697:MET:HE2	1.97	0.46
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: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:C:440:LYS:HA	1:C:440:LYS:HD2	1.75	0.45
1:A:480:CYS:O	1:A:480:CYS:SG	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:213:LYS:HZ2	2:E:215:VAL:HG22	1.82	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:G:127:PRO:HA	2:G:213:LYS:HZ1	1.84	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:172:SER:OG	1:A:173:GLN:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:G:213:LYS:HZ2	2:G:215:VAL:HG22	1.83	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
1:B:501:TYR:HD1	1:B:501:TYR:HA	1.67	0.42
1:C:442:ASP:C	1:C:448:ASN:HD22	2.22	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: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
3:F:42:LYS:HG2	3:F:43:ALA:N	2.35	0.41
2:G:45:LEU:CD2	2:G:107:TRP:HZ3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:D:63:SER:OG	3:D:74:THR:OG1	2.29	0.41
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:B:537:LYS:C	1:B:551:VAL:HG12	2.40	0.41
1:C:1083:HIS:O	1:C:1086:LYS:HG2	2.21	0.41
1:A:521:PRO:CG	1:C:199:GLY:C	2.82	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
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:C:46:SER:CA	1:C:279:TYR:O	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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: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%)	47	73
1	B	1004/1210 (83%)	973 (97%)	28 (3%)	3 (0%)	41	66
1	C	1004/1210 (83%)	934 (93%)	67 (7%)	3 (0%)	41	66
2	E	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
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%)	50	73

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%)	811 (99%)	9 (1%)	73	90
1	B	820/1055 (78%)	811 (99%)	9 (1%)	73	90
1	C	820/1055 (78%)	820 (100%)	0	100	100
2	E	182/182 (100%)	181 (100%)	1 (0%)	88	96
2	G	182/182 (100%)	181 (100%)	1 (0%)	88	96
3	D	187/187 (100%)	185 (99%)	2 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	187/187 (100%)	185 (99%)	2 (1%)	73	90
4	H	193/193 (100%)	191 (99%)	2 (1%)	76	91
All	All	3391/4096 (83%)	3365 (99%)	26 (1%)	82	93

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

Mol	Chain	Res	Type
1	A	355	ARG
1	A	368	LEU
1	A	375	PHE
1	A	379	CYS
1	A	398	ASP
1	A	433	VAL
1	A	453	TYR
1	A	472	ILE
1	A	488	CYS
1	B	355	ARG
1	B	368	LEU
1	B	375	PHE
1	B	379	CYS
1	B	398	ASP
1	B	433	VAL
1	B	453	TYR
1	B	472	ILE
1	B	488	CYS
2	E	218	LYS
3	D	33	LEU
3	D	61	ARG
3	F	33	LEU
3	F	61	ARG
2	G	218	LYS
4	H	142	ARG
4	H	163	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	ASN
1	A	422	ASN
1	A	901	GLN

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Mol	Chain	Res	Type
1	B	207	HIS
1	B	360	ASN
1	B	422	ASN
1	C	405	ASN
1	C	439	ASN
1	C	460	ASN
2	E	32	ASN
2	E	76	ASN
3	D	27	GLN
3	F	27	GLN
2	G	32	ASN
2	G	76	ASN
4	H	229	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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
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 ⓘ

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 ⓘ
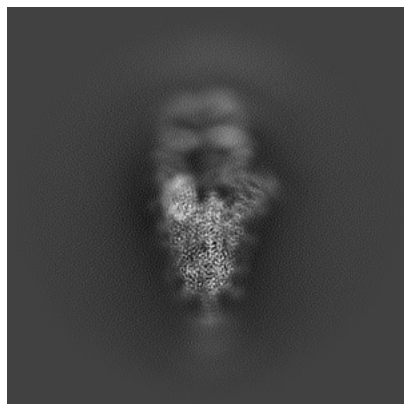
6.1.1 Primary map

X
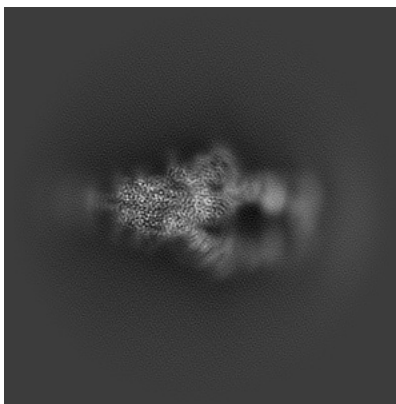
Y
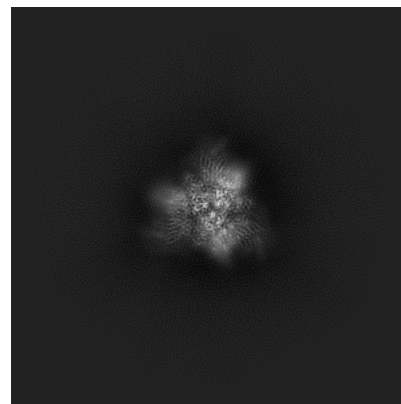
Z

6.1.2 Raw map

X

Y

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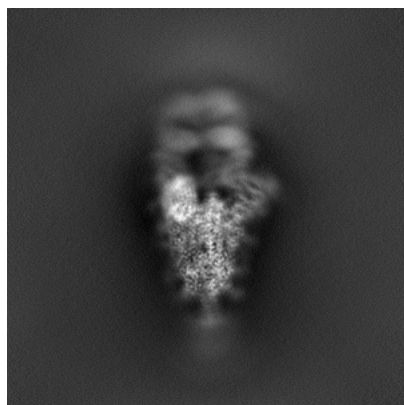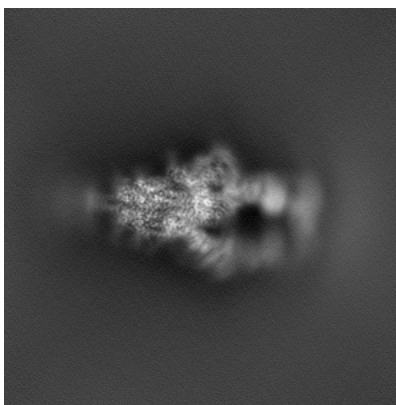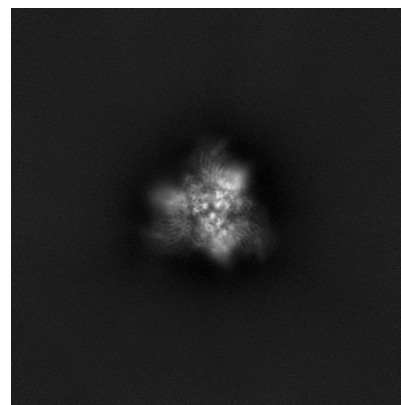
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map
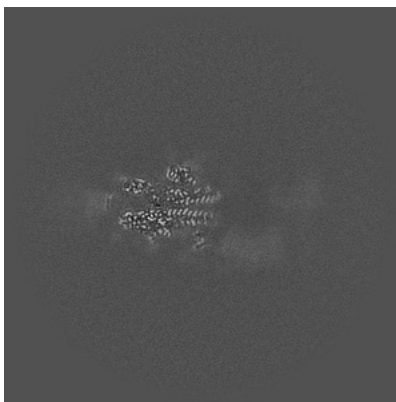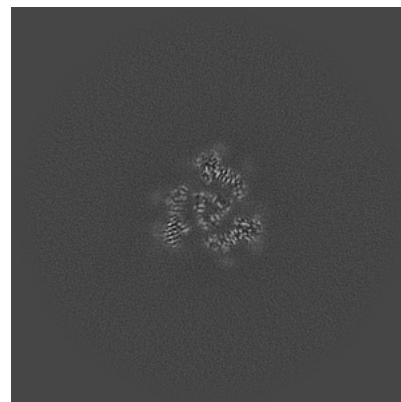
| X Index: 200 | Y Index: 200 | Z Index: 200 |

6.2.2 Raw map
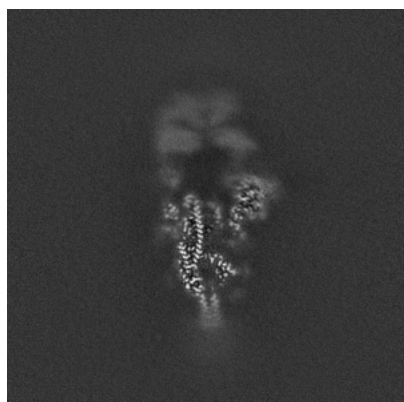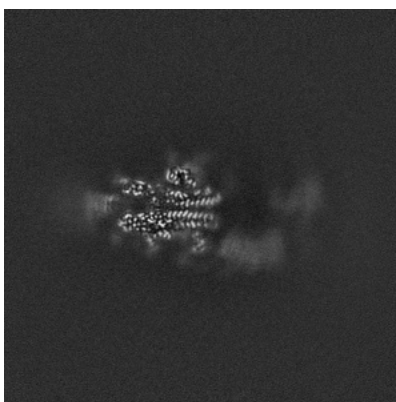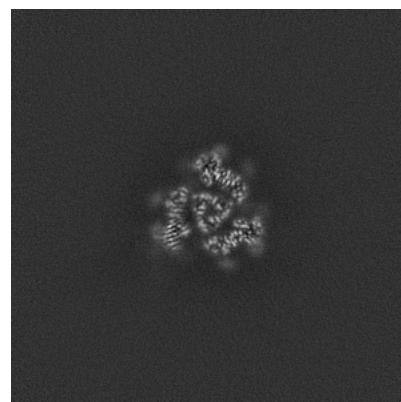
| X Index: 200 | Y Index: 200 | Z Index: 200 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
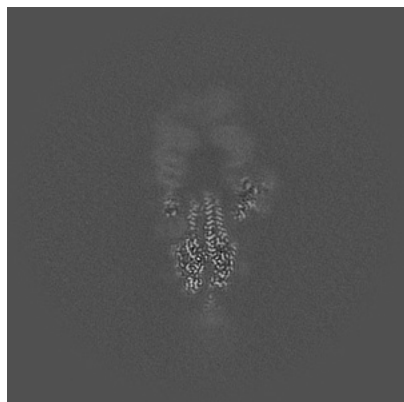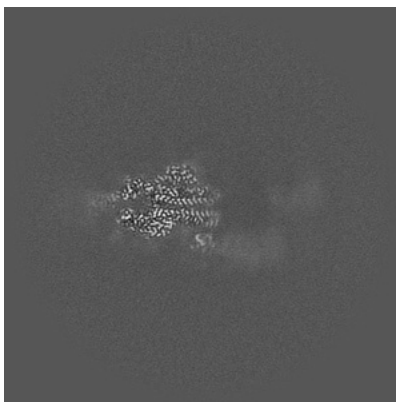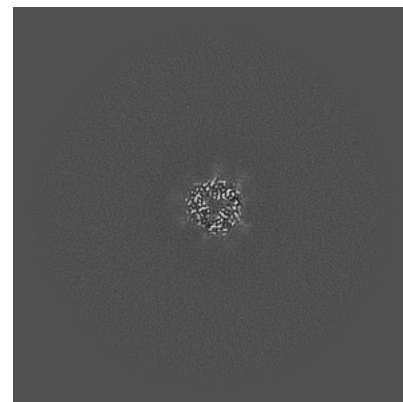
X Index: 207	Y Index: 203	Z Index: 137

6.3.2 Raw map
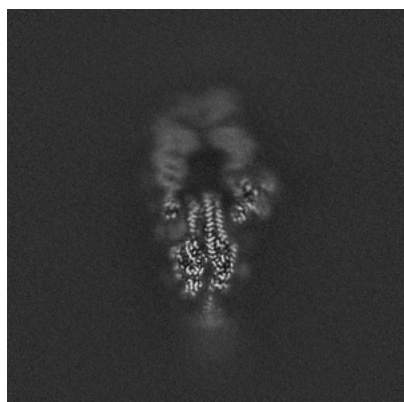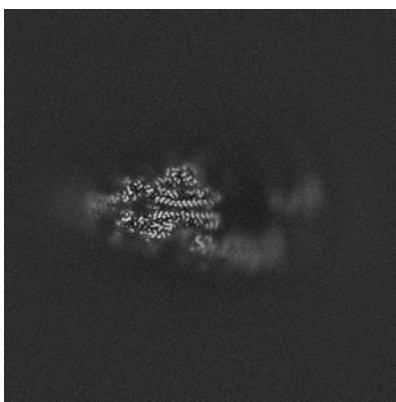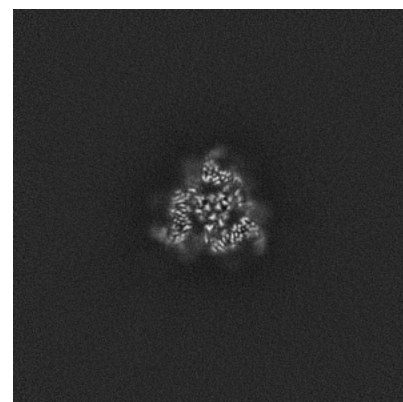
X Index: 207	Y Index: 203	Z Index: 192

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
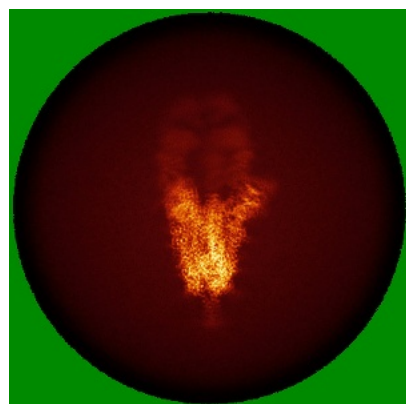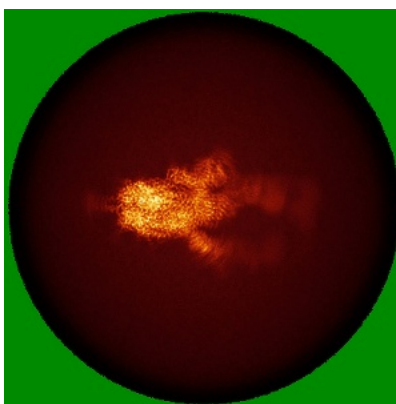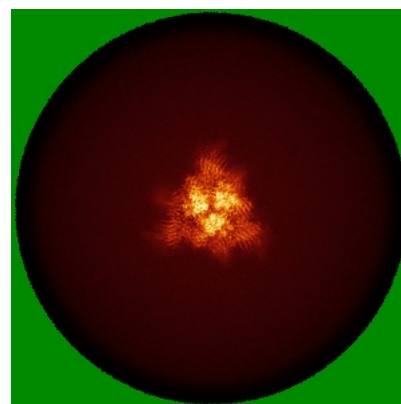
X   Y   Z

6.4.2 Raw map

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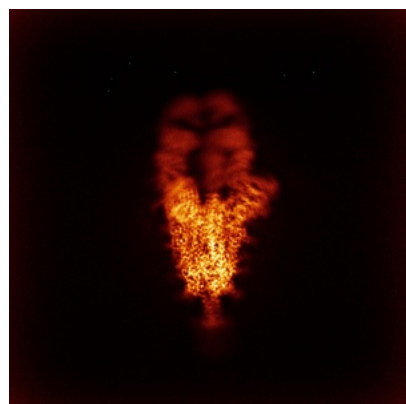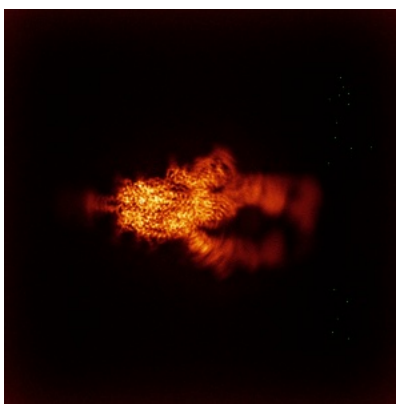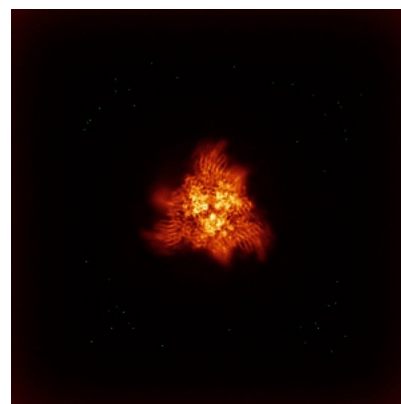
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

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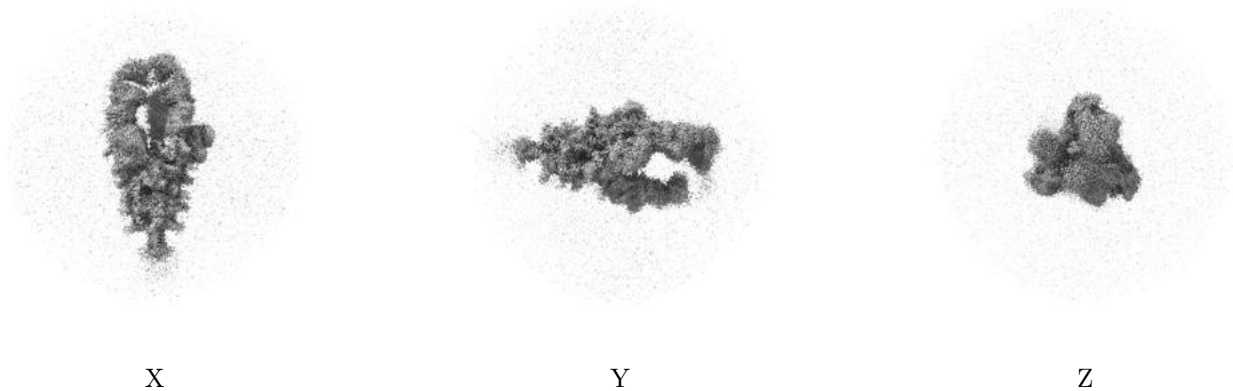
The images above show the 3D surface view of the map at the recommended contour level 0.31. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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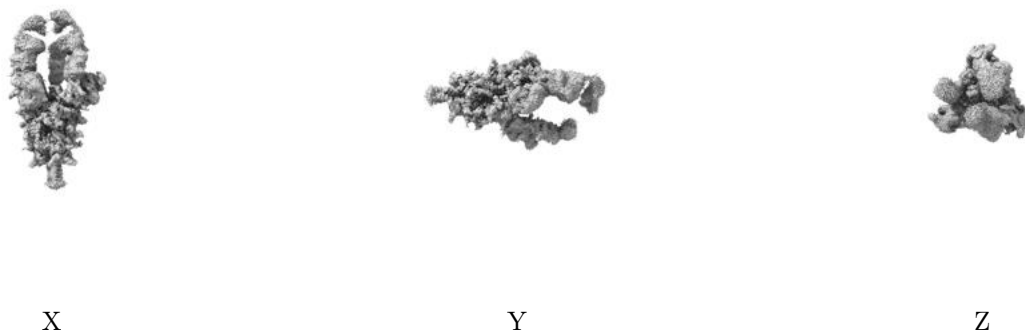
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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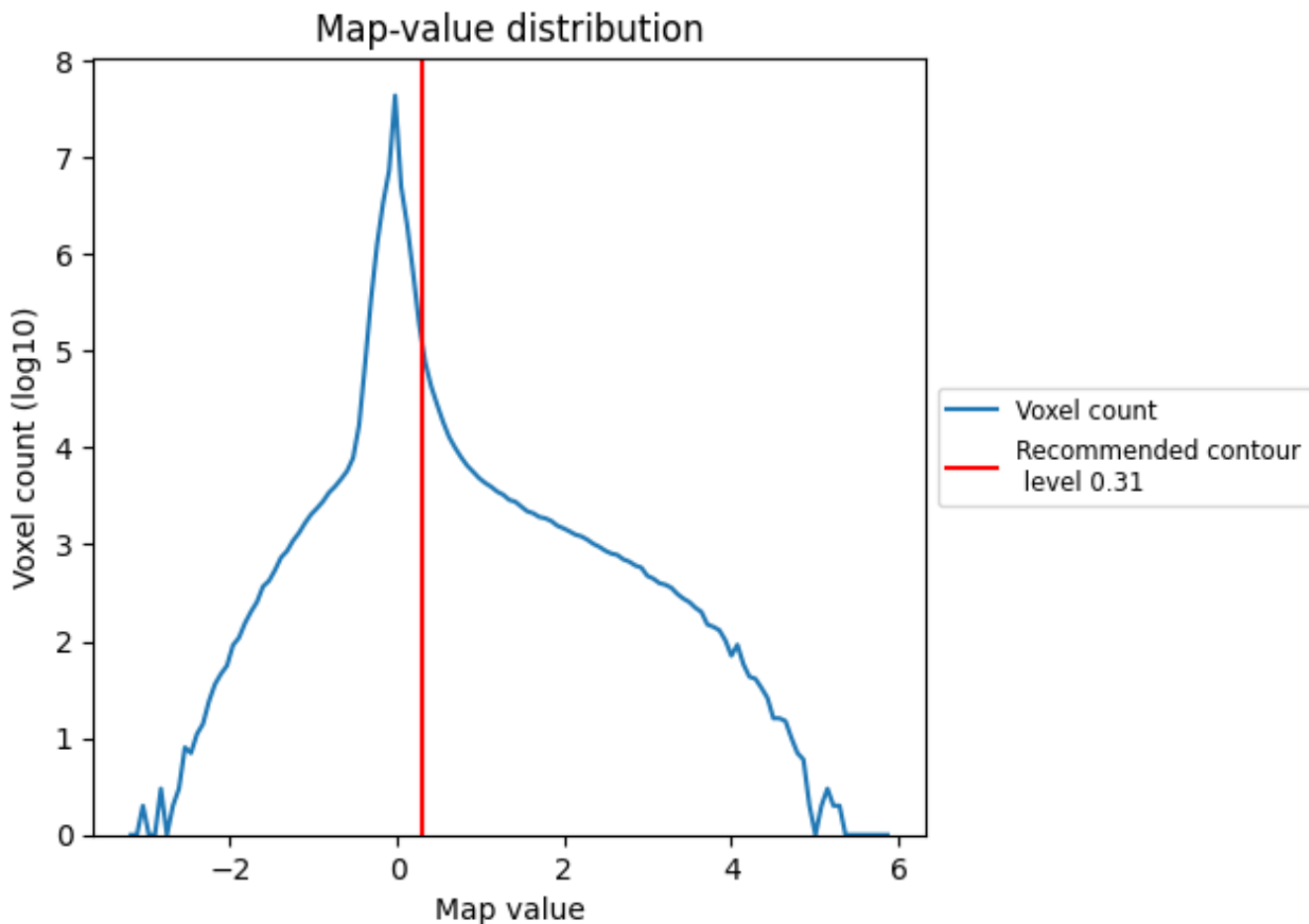
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

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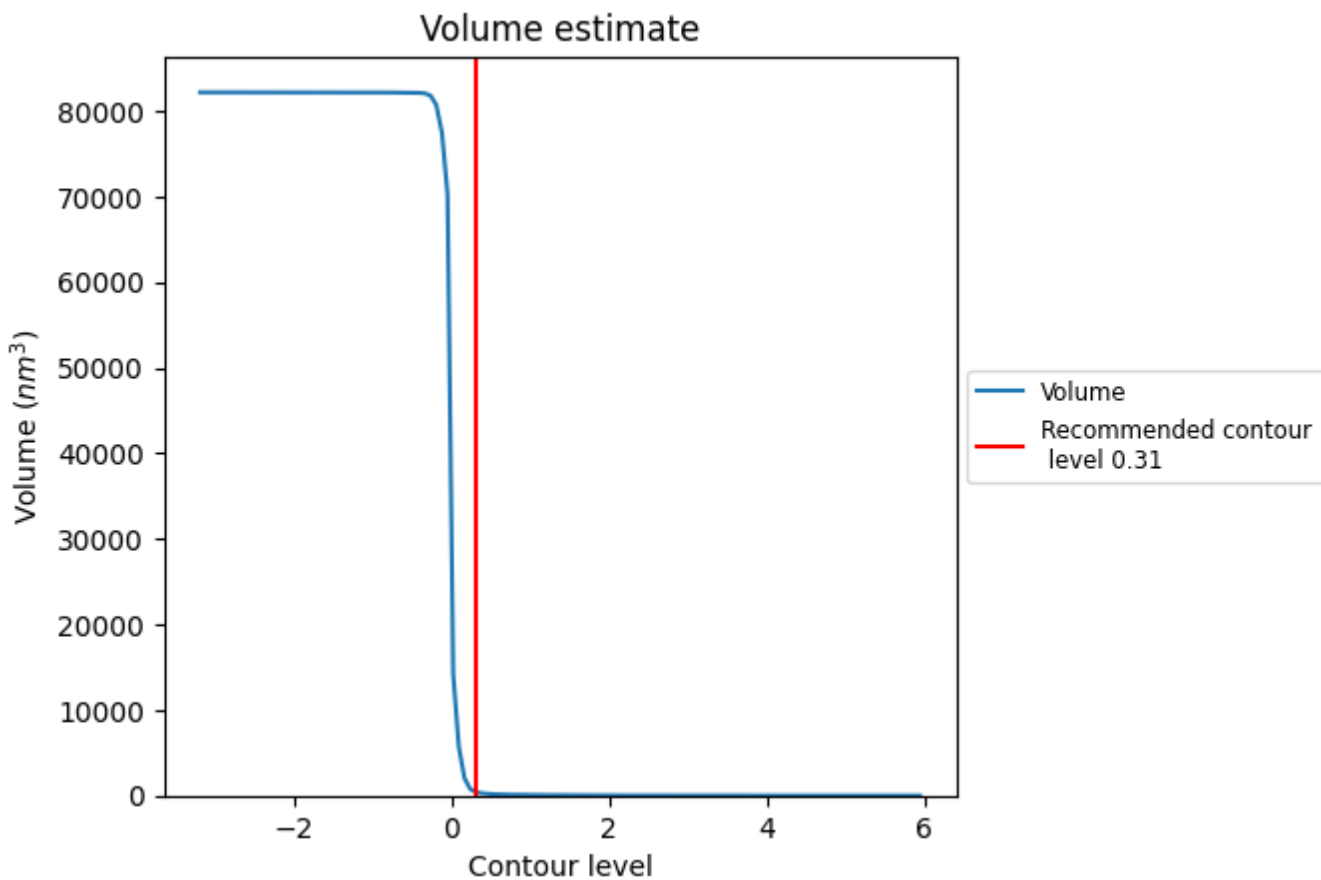
The volume at the recommended contour level is 406 nm^3; this corresponds to an approximate mass of 367 kDa.

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 ⓘ
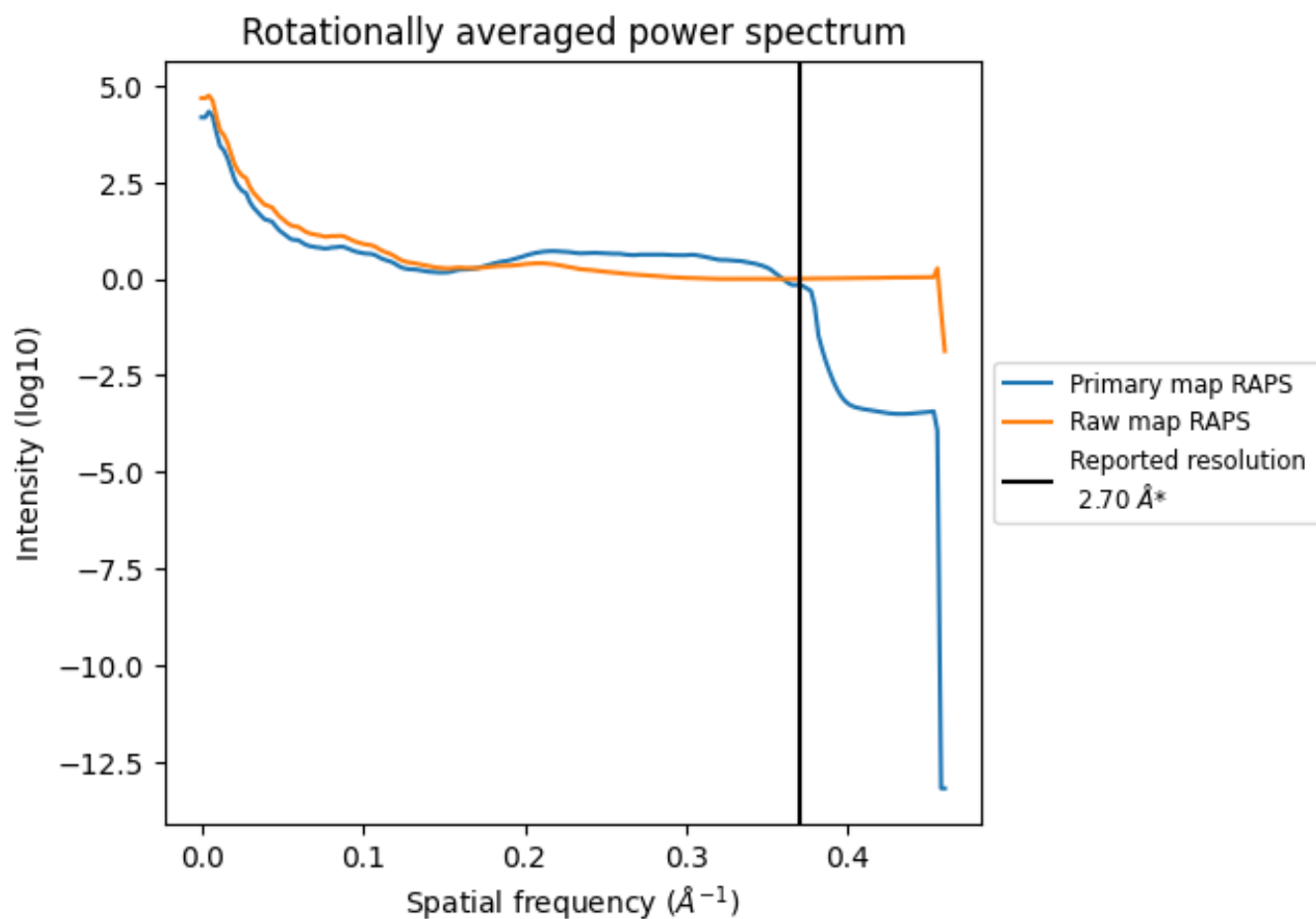
*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

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)
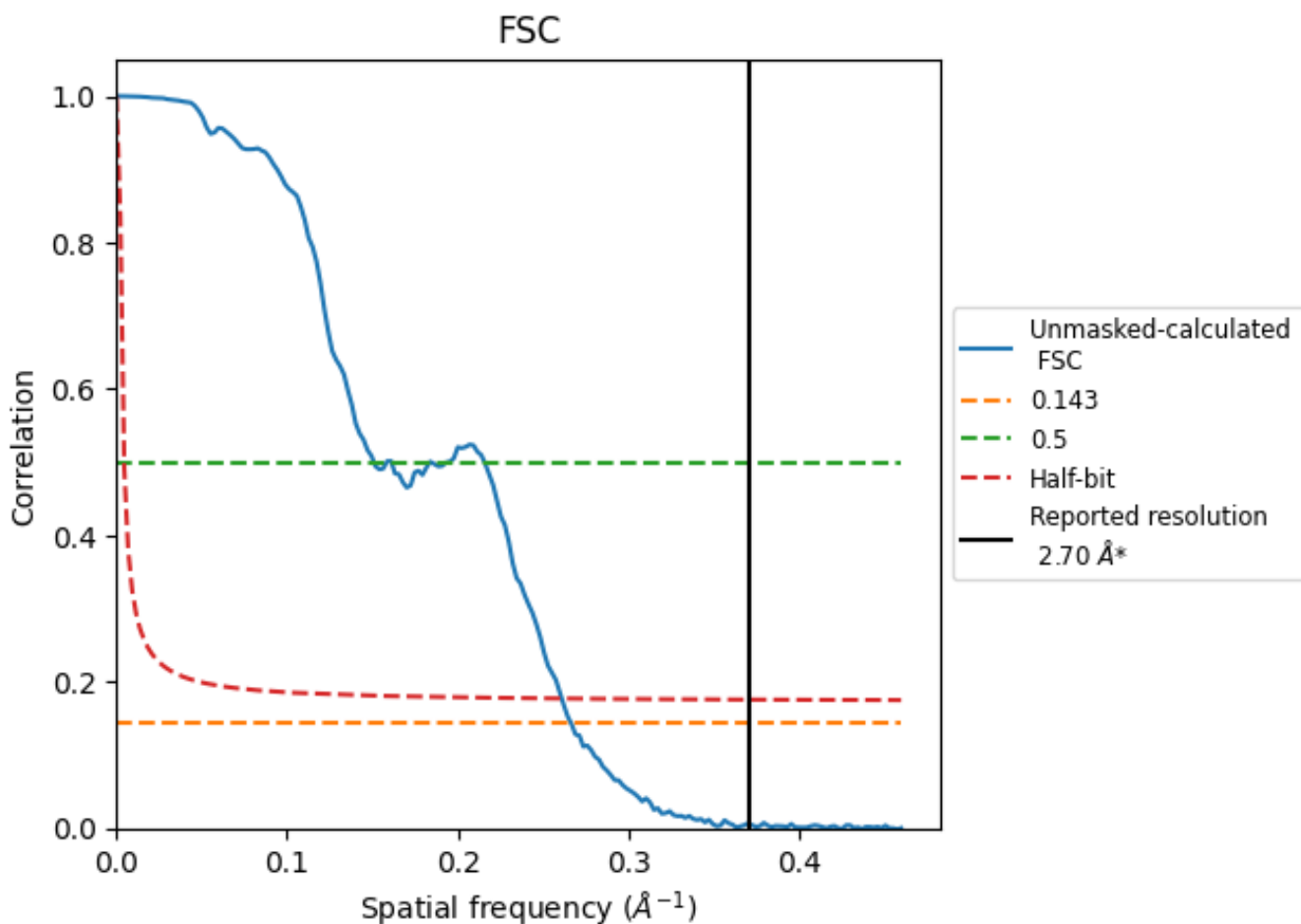
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates ⓘ

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 7.

9.1 Map-model overlay (i)

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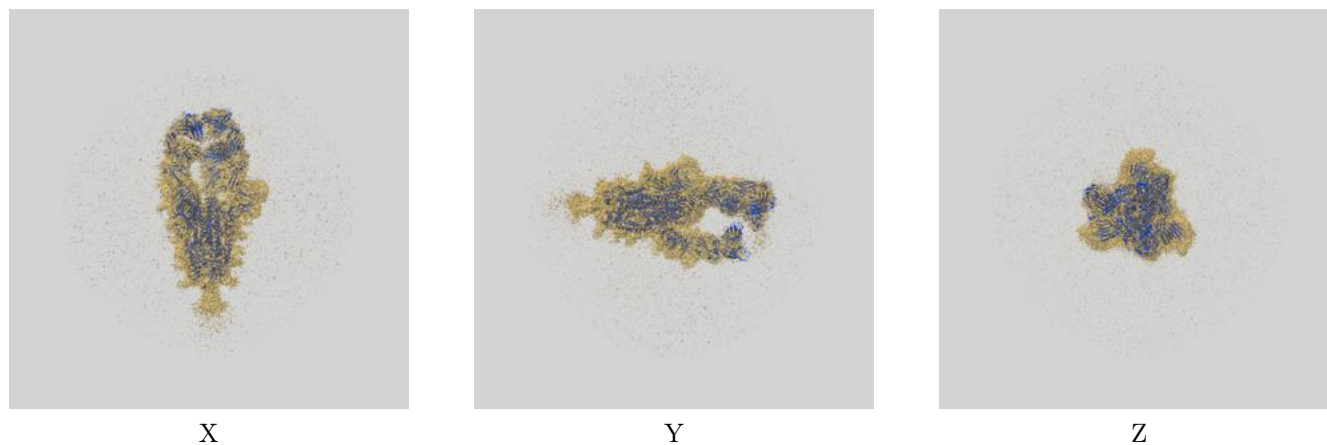
The images above show the 3D surface view of the map at the recommended contour level 0.31 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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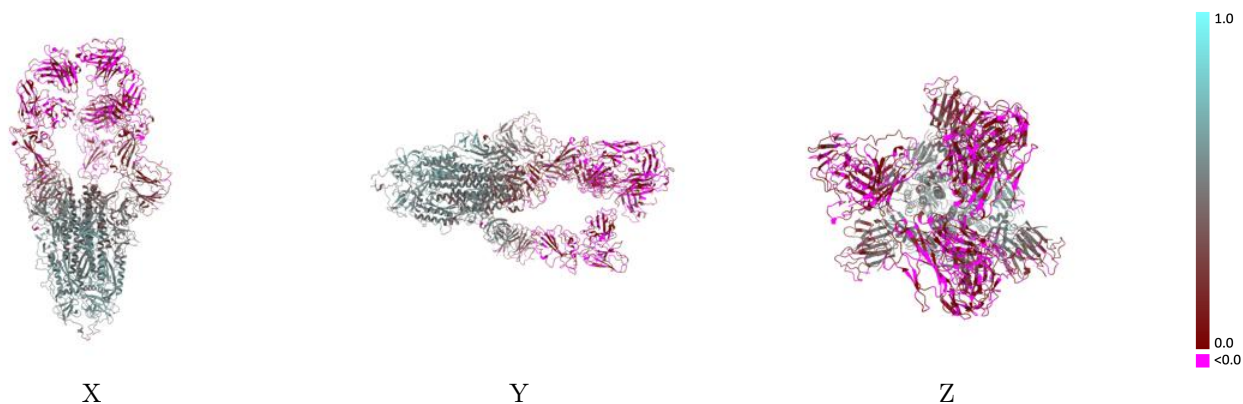
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
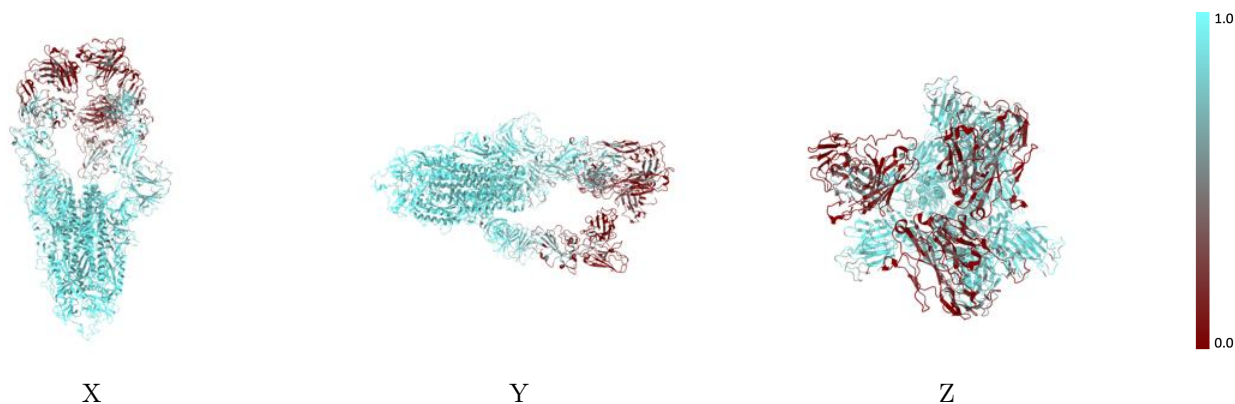
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.31).

9.4 Atom inclusion ⓘ
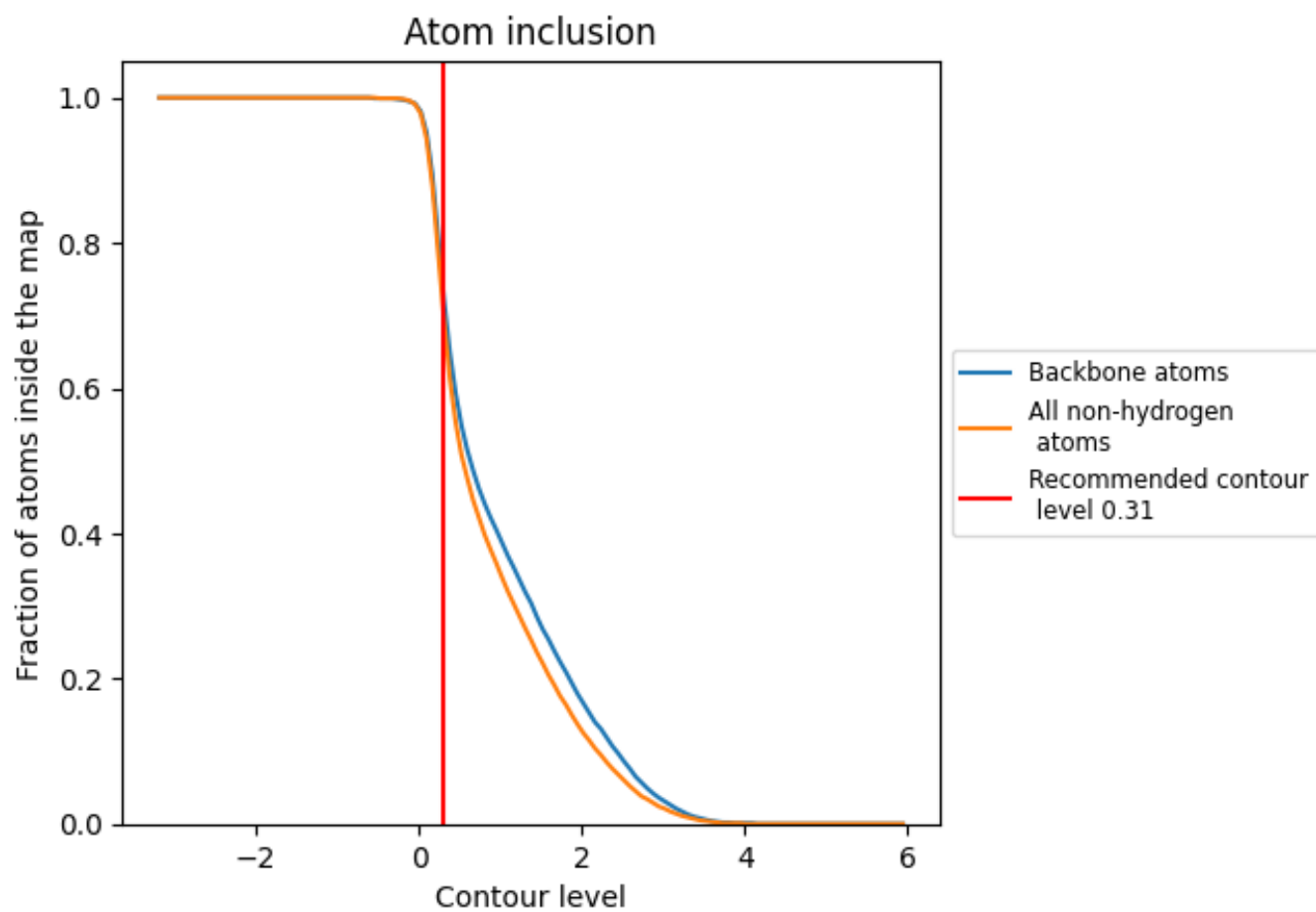
At the recommended contour level, 72% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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