



## Full wwPDB EM Validation Report ⓘ

Nov 1, 2022 – 10:04 PM EDT

PDB ID : 5L1D  
EMDB ID : EMD-8303  
Title : Structure of rabbit RyR2 in complex with FKBP12.6 in a closed state (conformation C1)  
Authors : Dhindwal, S.; Lobo, J.J.; Samso, M.  
Deposited on : 2016-07-29  
Resolution : 10.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

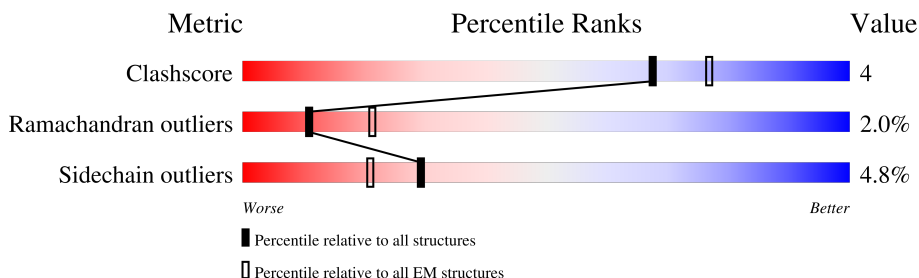
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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  $\geq 3$ , 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	4387	<div> <div>9%</div> <div>71%</div> <div>10%</div> <div>19%</div> </div>
1	C	4387	<div> <div>9%</div> <div>70%</div> <div>11%</div> <div>19%</div> </div>
1	E	4387	<div> <div>9%</div> <div>70%</div> <div>11%</div> <div>19%</div> </div>
1	G	4387	<div> <div>9%</div> <div>70%</div> <div>10%</div> <div>19%</div> </div>
2	B	158	<div> <div>8%</div> <div>58%</div> <div>10%</div> <div>32%</div> </div>
2	D	158	<div> <div>8%</div> <div>60%</div> <div>8%</div> <div>32%</div> </div>
2	F	158	<div> <div>8%</div> <div>56%</div> <div>12%</div> <div>32%</div> </div>
2	H	158	<div> <div>8%</div> <div>63%</div> <div>•</div> <div>32%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 112936 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 Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	C	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	E	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		
1	G	3570	Total	C	N	O	S	0	0
			27416	17427	4732	5102	155		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-50	MET	-	expression tag	UNP P68106
B	-49	ASN	-	expression tag	UNP P68106
B	-48	HIS	-	expression tag	UNP P68106
B	-47	LYS	-	expression tag	UNP P68106
B	-46	VAL	-	expression tag	UNP P68106
B	-45	HIS	-	expression tag	UNP P68106
B	-44	HIS	-	expression tag	UNP P68106
B	-43	HIS	-	expression tag	UNP P68106
B	-42	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-41	HIS	-	expression tag	UNP P68106
B	-40	HIS	-	expression tag	UNP P68106
B	-39	MET	-	expression tag	UNP P68106
B	-38	ASP	-	expression tag	UNP P68106
B	-37	GLU	-	expression tag	UNP P68106
B	-36	LYS	-	expression tag	UNP P68106
B	-35	THR	-	expression tag	UNP P68106
B	-34	THR	-	expression tag	UNP P68106
B	-33	GLY	-	expression tag	UNP P68106
B	-32	TRP	-	expression tag	UNP P68106
B	-31	ARG	-	expression tag	UNP P68106
B	-30	GLY	-	expression tag	UNP P68106
B	-29	GLY	-	expression tag	UNP P68106
B	-28	HIS	-	expression tag	UNP P68106
B	-27	VAL	-	expression tag	UNP P68106
B	-26	VAL	-	expression tag	UNP P68106
B	-25	GLU	-	expression tag	UNP P68106
B	-24	GLY	-	expression tag	UNP P68106
B	-23	LEU	-	expression tag	UNP P68106
B	-22	ALA	-	expression tag	UNP P68106
B	-21	GLY	-	expression tag	UNP P68106
B	-20	GLU	-	expression tag	UNP P68106
B	-19	LEU	-	expression tag	UNP P68106
B	-18	GLU	-	expression tag	UNP P68106
B	-17	GLN	-	expression tag	UNP P68106
B	-16	LEU	-	expression tag	UNP P68106
B	-15	ARG	-	expression tag	UNP P68106
B	-14	ALA	-	expression tag	UNP P68106
B	-13	ARG	-	expression tag	UNP P68106
B	-12	LEU	-	expression tag	UNP P68106
B	-11	GLU	-	expression tag	UNP P68106
B	-10	HIS	-	expression tag	UNP P68106
B	-9	HIS	-	expression tag	UNP P68106
B	-8	PRO	-	expression tag	UNP P68106
B	-7	GLN	-	expression tag	UNP P68106
B	-6	GLY	-	expression tag	UNP P68106
B	-5	GLN	-	expression tag	UNP P68106
B	-4	ARG	-	expression tag	UNP P68106
B	-3	GLU	-	expression tag	UNP P68106
B	-2	PRO	-	expression tag	UNP P68106
B	-1	GLU	-	expression tag	UNP P68106
B	0	LEU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-50	MET	-	expression tag	UNP P68106
D	-49	ASN	-	expression tag	UNP P68106
D	-48	HIS	-	expression tag	UNP P68106
D	-47	LYS	-	expression tag	UNP P68106
D	-46	VAL	-	expression tag	UNP P68106
D	-45	HIS	-	expression tag	UNP P68106
D	-44	HIS	-	expression tag	UNP P68106
D	-43	HIS	-	expression tag	UNP P68106
D	-42	HIS	-	expression tag	UNP P68106
D	-41	HIS	-	expression tag	UNP P68106
D	-40	HIS	-	expression tag	UNP P68106
D	-39	MET	-	expression tag	UNP P68106
D	-38	ASP	-	expression tag	UNP P68106
D	-37	GLU	-	expression tag	UNP P68106
D	-36	LYS	-	expression tag	UNP P68106
D	-35	THR	-	expression tag	UNP P68106
D	-34	THR	-	expression tag	UNP P68106
D	-33	GLY	-	expression tag	UNP P68106
D	-32	TRP	-	expression tag	UNP P68106
D	-31	ARG	-	expression tag	UNP P68106
D	-30	GLY	-	expression tag	UNP P68106
D	-29	GLY	-	expression tag	UNP P68106
D	-28	HIS	-	expression tag	UNP P68106
D	-27	VAL	-	expression tag	UNP P68106
D	-26	VAL	-	expression tag	UNP P68106
D	-25	GLU	-	expression tag	UNP P68106
D	-24	GLY	-	expression tag	UNP P68106
D	-23	LEU	-	expression tag	UNP P68106
D	-22	ALA	-	expression tag	UNP P68106
D	-21	GLY	-	expression tag	UNP P68106
D	-20	GLU	-	expression tag	UNP P68106
D	-19	LEU	-	expression tag	UNP P68106
D	-18	GLU	-	expression tag	UNP P68106
D	-17	GLN	-	expression tag	UNP P68106
D	-16	LEU	-	expression tag	UNP P68106
D	-15	ARG	-	expression tag	UNP P68106
D	-14	ALA	-	expression tag	UNP P68106
D	-13	ARG	-	expression tag	UNP P68106
D	-12	LEU	-	expression tag	UNP P68106
D	-11	GLU	-	expression tag	UNP P68106
D	-10	HIS	-	expression tag	UNP P68106
D	-9	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	PRO	-	expression tag	UNP P68106
D	-7	GLN	-	expression tag	UNP P68106
D	-6	GLY	-	expression tag	UNP P68106
D	-5	GLN	-	expression tag	UNP P68106
D	-4	ARG	-	expression tag	UNP P68106
D	-3	GLU	-	expression tag	UNP P68106
D	-2	PRO	-	expression tag	UNP P68106
D	-1	GLU	-	expression tag	UNP P68106
D	0	LEU	-	expression tag	UNP P68106
F	-50	MET	-	expression tag	UNP P68106
F	-49	ASN	-	expression tag	UNP P68106
F	-48	HIS	-	expression tag	UNP P68106
F	-47	LYS	-	expression tag	UNP P68106
F	-46	VAL	-	expression tag	UNP P68106
F	-45	HIS	-	expression tag	UNP P68106
F	-44	HIS	-	expression tag	UNP P68106
F	-43	HIS	-	expression tag	UNP P68106
F	-42	HIS	-	expression tag	UNP P68106
F	-41	HIS	-	expression tag	UNP P68106
F	-40	HIS	-	expression tag	UNP P68106
F	-39	MET	-	expression tag	UNP P68106
F	-38	ASP	-	expression tag	UNP P68106
F	-37	GLU	-	expression tag	UNP P68106
F	-36	LYS	-	expression tag	UNP P68106
F	-35	THR	-	expression tag	UNP P68106
F	-34	THR	-	expression tag	UNP P68106
F	-33	GLY	-	expression tag	UNP P68106
F	-32	TRP	-	expression tag	UNP P68106
F	-31	ARG	-	expression tag	UNP P68106
F	-30	GLY	-	expression tag	UNP P68106
F	-29	GLY	-	expression tag	UNP P68106
F	-28	HIS	-	expression tag	UNP P68106
F	-27	VAL	-	expression tag	UNP P68106
F	-26	VAL	-	expression tag	UNP P68106
F	-25	GLU	-	expression tag	UNP P68106
F	-24	GLY	-	expression tag	UNP P68106
F	-23	LEU	-	expression tag	UNP P68106
F	-22	ALA	-	expression tag	UNP P68106
F	-21	GLY	-	expression tag	UNP P68106
F	-20	GLU	-	expression tag	UNP P68106
F	-19	LEU	-	expression tag	UNP P68106
F	-18	GLU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-17	GLN	-	expression tag	UNP P68106
F	-16	LEU	-	expression tag	UNP P68106
F	-15	ARG	-	expression tag	UNP P68106
F	-14	ALA	-	expression tag	UNP P68106
F	-13	ARG	-	expression tag	UNP P68106
F	-12	LEU	-	expression tag	UNP P68106
F	-11	GLU	-	expression tag	UNP P68106
F	-10	HIS	-	expression tag	UNP P68106
F	-9	HIS	-	expression tag	UNP P68106
F	-8	PRO	-	expression tag	UNP P68106
F	-7	GLN	-	expression tag	UNP P68106
F	-6	GLY	-	expression tag	UNP P68106
F	-5	GLN	-	expression tag	UNP P68106
F	-4	ARG	-	expression tag	UNP P68106
F	-3	GLU	-	expression tag	UNP P68106
F	-2	PRO	-	expression tag	UNP P68106
F	-1	GLU	-	expression tag	UNP P68106
F	0	LEU	-	expression tag	UNP P68106
H	-50	MET	-	expression tag	UNP P68106
H	-49	ASN	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	LYS	-	expression tag	UNP P68106
H	-46	VAL	-	expression tag	UNP P68106
H	-45	HIS	-	expression tag	UNP P68106
H	-44	HIS	-	expression tag	UNP P68106
H	-43	HIS	-	expression tag	UNP P68106
H	-42	HIS	-	expression tag	UNP P68106
H	-41	HIS	-	expression tag	UNP P68106
H	-40	HIS	-	expression tag	UNP P68106
H	-39	MET	-	expression tag	UNP P68106
H	-38	ASP	-	expression tag	UNP P68106
H	-37	GLU	-	expression tag	UNP P68106
H	-36	LYS	-	expression tag	UNP P68106
H	-35	THR	-	expression tag	UNP P68106
H	-34	THR	-	expression tag	UNP P68106
H	-33	GLY	-	expression tag	UNP P68106
H	-32	TRP	-	expression tag	UNP P68106
H	-31	ARG	-	expression tag	UNP P68106
H	-30	GLY	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	HIS	-	expression tag	UNP P68106
H	-27	VAL	-	expression tag	UNP P68106

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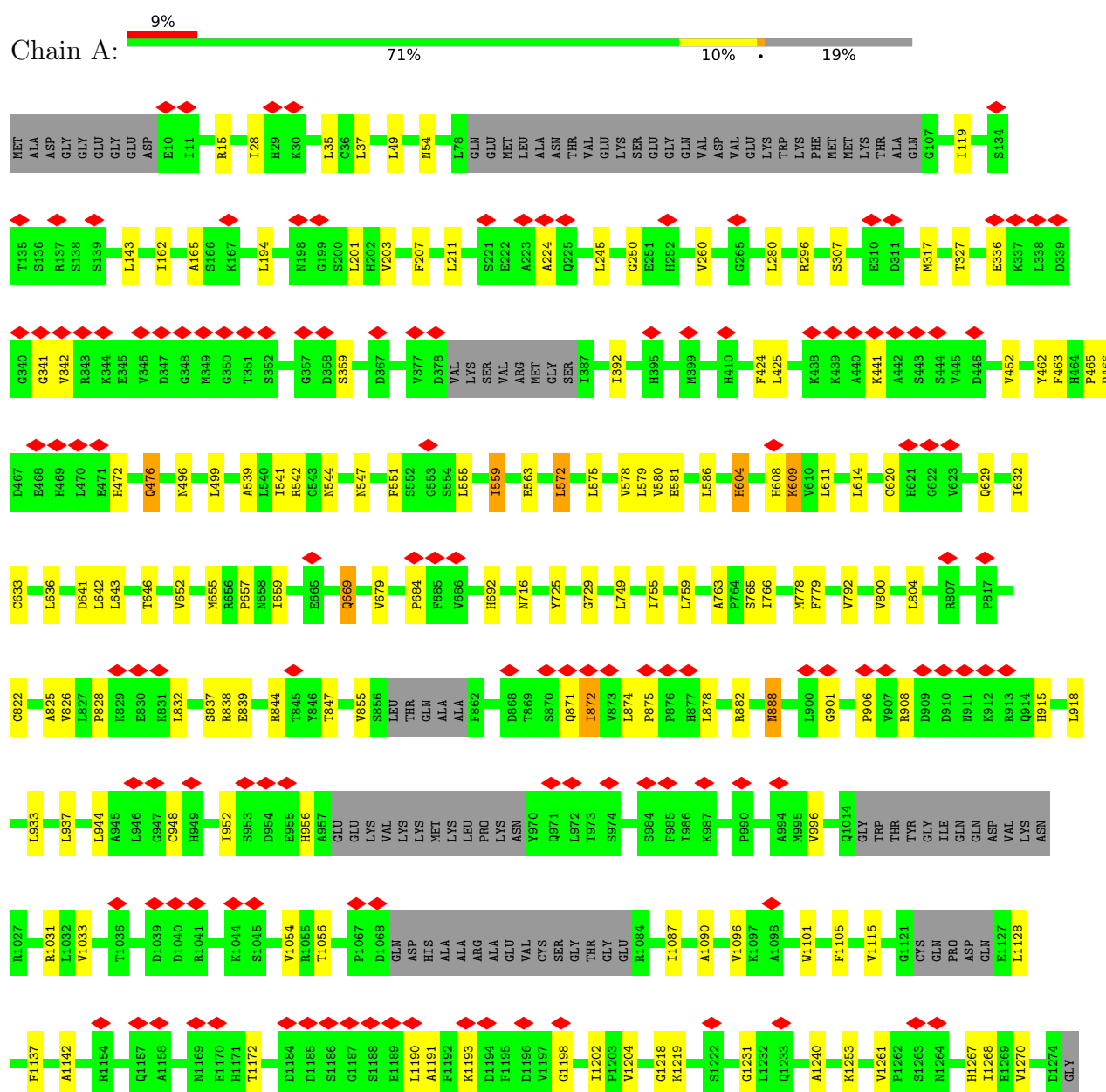
Chain	Residue	Modelled	Actual	Comment	Reference
H	-26	VAL	-	expression tag	UNP P68106
H	-25	GLU	-	expression tag	UNP P68106
H	-24	GLY	-	expression tag	UNP P68106
H	-23	LEU	-	expression tag	UNP P68106
H	-22	ALA	-	expression tag	UNP P68106
H	-21	GLY	-	expression tag	UNP P68106
H	-20	GLU	-	expression tag	UNP P68106
H	-19	LEU	-	expression tag	UNP P68106
H	-18	GLU	-	expression tag	UNP P68106
H	-17	GLN	-	expression tag	UNP P68106
H	-16	LEU	-	expression tag	UNP P68106
H	-15	ARG	-	expression tag	UNP P68106
H	-14	ALA	-	expression tag	UNP P68106
H	-13	ARG	-	expression tag	UNP P68106
H	-12	LEU	-	expression tag	UNP P68106
H	-11	GLU	-	expression tag	UNP P68106
H	-10	HIS	-	expression tag	UNP P68106
H	-9	HIS	-	expression tag	UNP P68106
H	-8	PRO	-	expression tag	UNP P68106
H	-7	GLN	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	GLN	-	expression tag	UNP P68106
H	-4	ARG	-	expression tag	UNP P68106
H	-3	GLU	-	expression tag	UNP P68106
H	-2	PRO	-	expression tag	UNP P68106
H	-1	GLU	-	expression tag	UNP P68106
H	0	LEU	-	expression tag	UNP P68106



### 3 Residue-property plots [i](#)

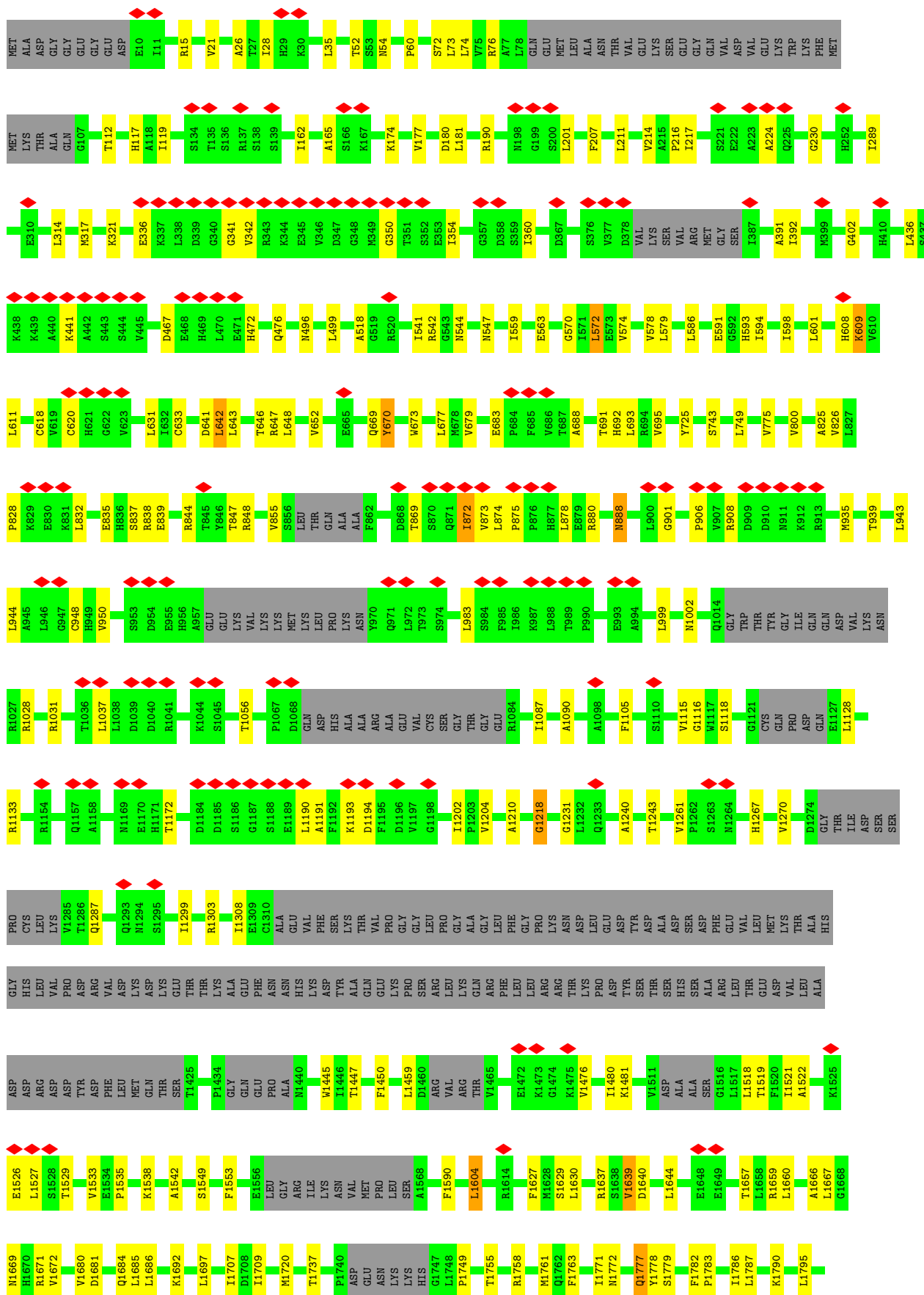
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



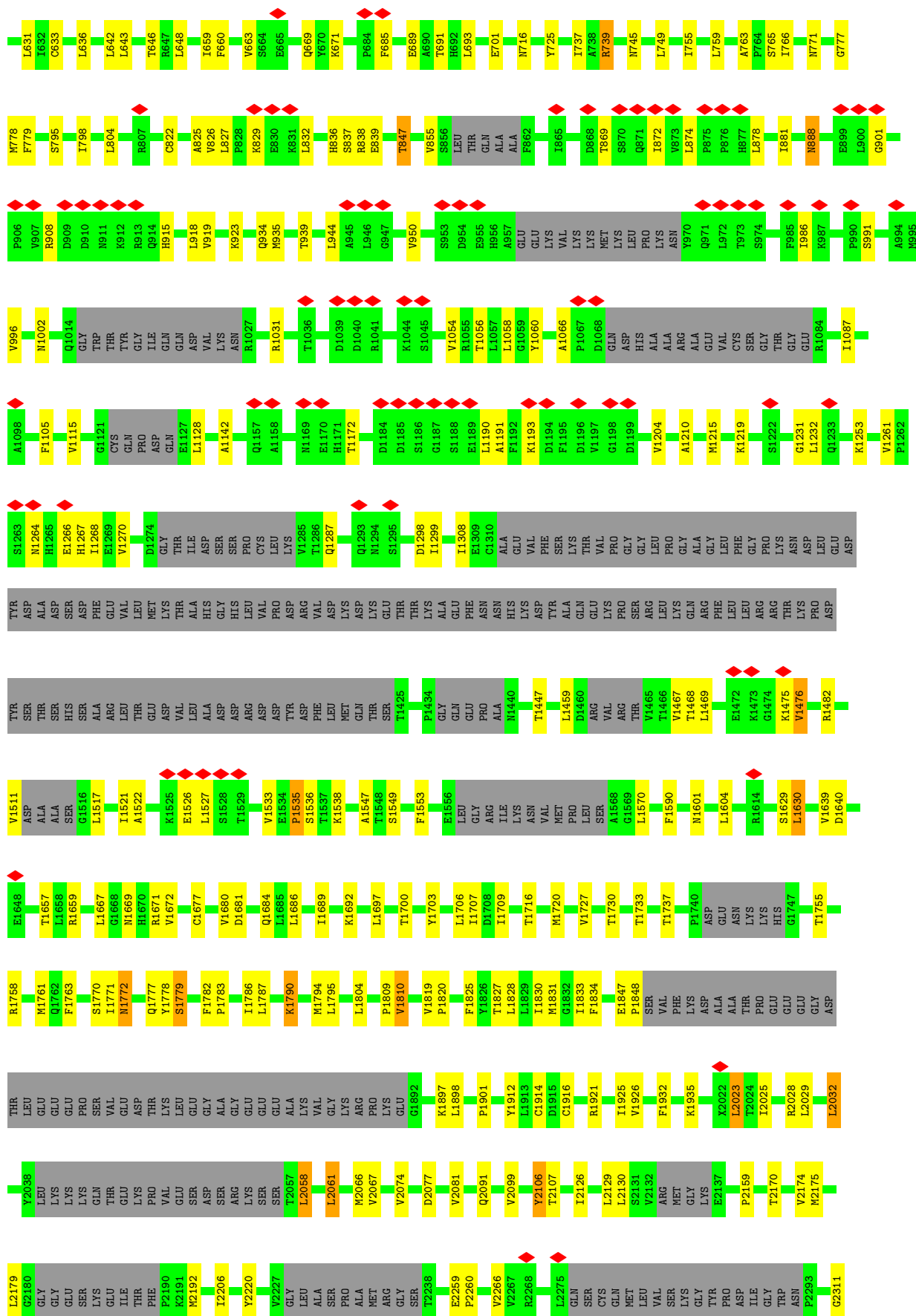










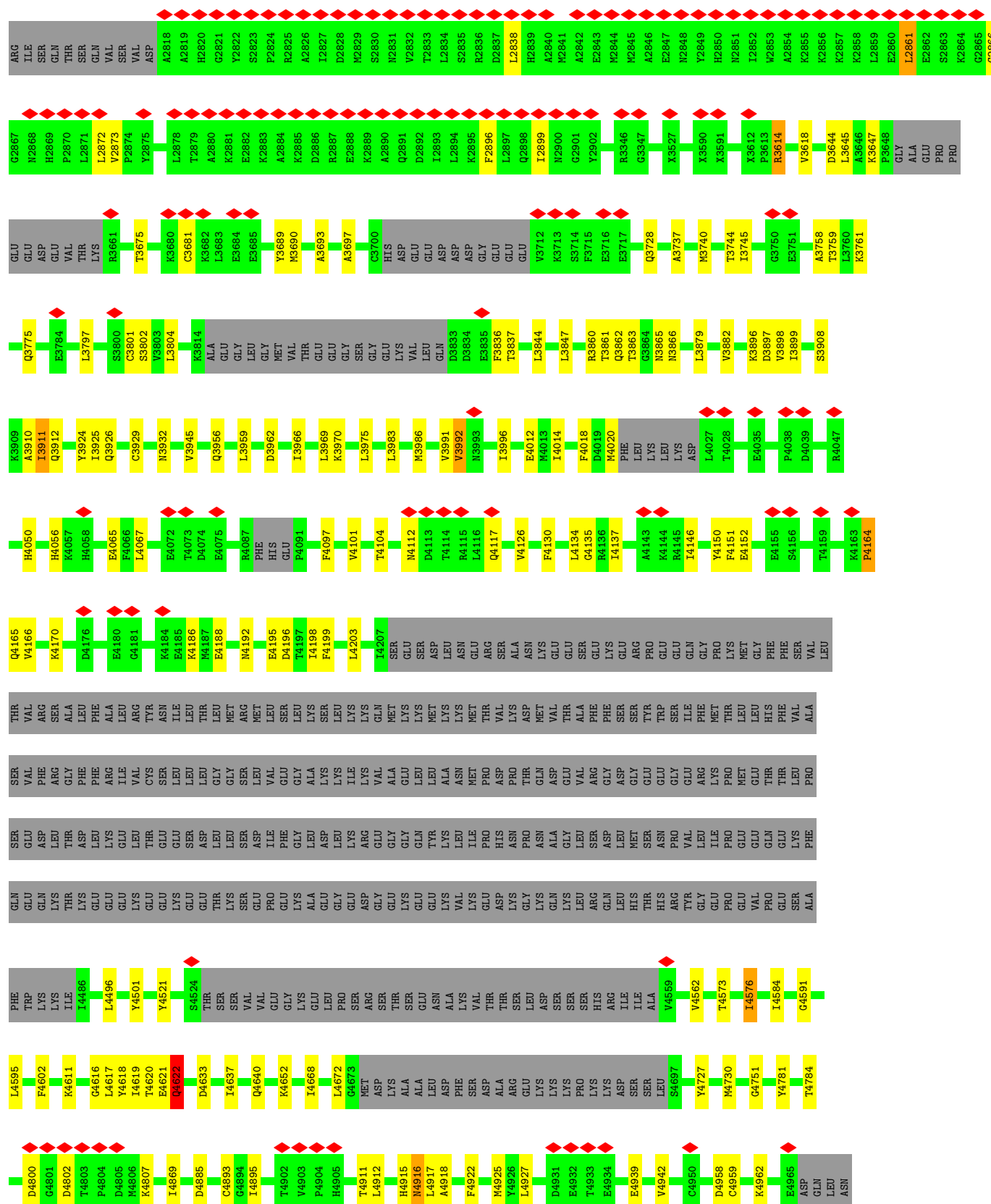


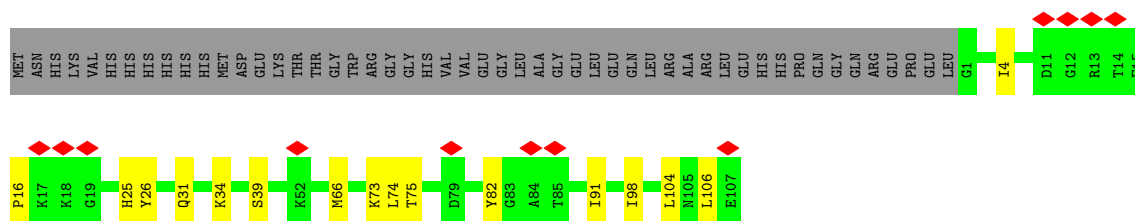




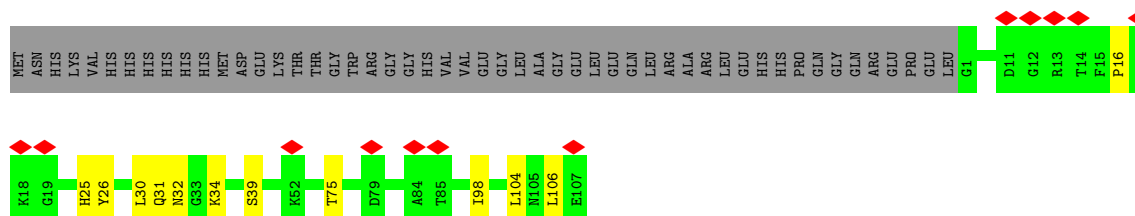




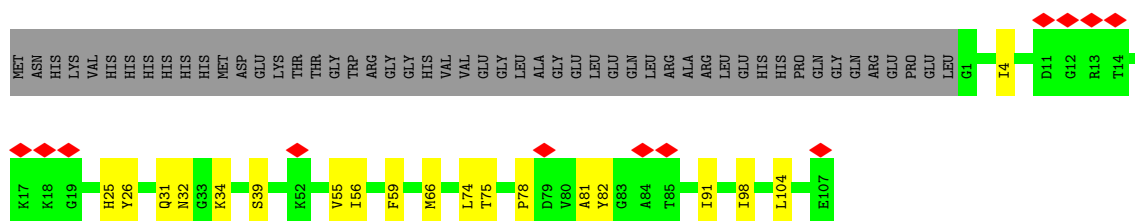




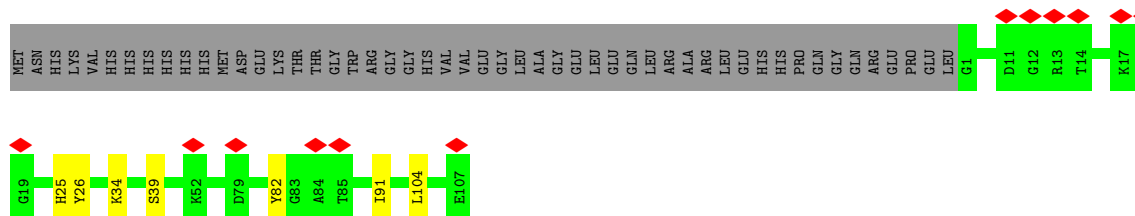
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	13158	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	62000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.046	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.035	Depositor
Map size ( $\text{\AA}$ )	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.34, 1.34, 1.34	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	0.78	0/25831	0.64	1/34865 (0.0%)
1	C	0.78	0/25831	0.64	1/34865 (0.0%)
1	E	0.78	0/25831	0.64	1/34865 (0.0%)
1	G	0.78	0/25831	0.64	0/34865
2	B	0.85	0/834	0.64	0/1123
2	D	0.85	0/834	0.63	0/1123
2	F	0.84	0/834	0.64	0/1123
2	H	0.86	0/834	0.65	0/1123
All	All	0.78	0/106660	0.64	3/143952 (0.0%)

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	1
1	C	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1630	LEU	CA-CB-CG	6.09	129.32	115.30
1	A	1630	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	1630	LEU	CA-CB-CG	5.38	127.68	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	604	HIS	Peptide
1	C	3614	ARG	Peptide
1	G	3614	ARG	Peptide

## 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	27416	0	25487	197	0
1	C	27416	0	25485	217	0
1	E	27416	0	25489	211	0
1	G	27416	0	25485	206	0
2	B	818	0	824	10	0
2	D	818	0	824	5	0
2	F	818	0	824	9	0
2	H	818	0	824	5	0
All	All	112936	0	105242	843	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 4.

All (843) 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:E:3945:VAL:HG11	1:E:3983:LEU:HD21	1.47	0.94
1:A:874:LEU:HD23	1:A:878:LEU:HD13	1.50	0.94
1:E:1172:THR:HG21	1:E:1190:LEU:HD13	1.58	0.86
1:G:874:LEU:HD23	1:G:878:LEU:HD13	1.60	0.82
1:E:1261:VAL:HG11	1:E:1270:VAL:HG11	1.63	0.78
1:G:3945:VAL:HG11	1:G:3983:LEU:HD21	1.66	0.78
1:C:1172:THR:HG21	1:C:1190:LEU:HD13	1.66	0.77
1:G:1933:VAL:HG21	1:G:3618:VAL:HG22	1.66	0.76
1:A:1172:THR:HG21	1:A:1190:LEU:HD13	1.68	0.75
1:G:4617:LEU:O	1:G:4622:GLN:N	2.19	0.75
1:E:4617:LEU:O	1:E:4622:GLN:N	2.20	0.74
1:C:4617:LEU:O	1:C:4622:GLN:N	2.19	0.74
1:E:594:ILE:HD12	1:E:631:LEU:HD22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1105:PHE:HB2	1:G:1115:VAL:HG21	1.72	0.71
1:A:2075:ILE:HG12	1:A:2080:LEU:HD23	1.74	0.69
1:C:314:LEU:HD12	1:C:391:ALA:HB1	1.73	0.69
1:G:1543:VAL:HG11	1:G:1553:PHE:CZ	2.27	0.69
1:A:4617:LEU:O	1:A:4622:GLN:N	2.20	0.69
1:C:633:CYS:HB3	1:C:1672:VAL:HG11	1.73	0.69
1:C:874:LEU:HD23	1:C:878:LEU:HD13	1.75	0.68
1:A:3945:VAL:HG11	1:A:3983:LEU:HD21	1.74	0.68
1:C:1105:PHE:HB2	1:C:1115:VAL:HG21	1.76	0.67
2:D:26:TYR:N	2:D:39:SER:OG	2.27	0.67
1:E:874:LEU:HD23	1:E:878:LEU:HD13	1.78	0.66
1:E:1680:VAL:HG11	1:E:1709:ILE:HD13	1.78	0.66
1:C:26:ALA:HB3	1:C:35:LEU:HD13	1.77	0.65
1:E:314:LEU:HD12	1:E:391:ALA:HB1	1.77	0.65
1:G:633:CYS:HB3	1:G:1672:VAL:HG11	1.79	0.65
2:H:26:TYR:N	2:H:39:SER:OG	2.28	0.65
1:A:4192:ASN:HD22	1:A:4606:LYS:HE2	1.62	0.64
1:G:2266:VAL:HG12	1:G:2303:LEU:HD11	1.79	0.64
1:A:143:LEU:HD11	1:A:207:PHE:CD2	2.32	0.64
1:A:1219:LYS:HA	1:A:1240:ALA:HB3	1.80	0.64
1:E:4517:ILE:HG21	1:E:4574:LEU:HD23	1.80	0.64
2:B:26:TYR:N	2:B:39:SER:OG	2.29	0.64
1:A:1261:VAL:HG11	1:A:1270:VAL:HG11	1.80	0.64
1:A:2123:LEU:HD12	1:A:2127:ARG:NH1	2.12	0.64
1:A:4097:PHE:CZ	1:A:4152:GLU:HB2	2.32	0.64
1:A:1680:VAL:HG11	1:A:1709:ILE:HD13	1.80	0.63
1:E:4146:ILE:HD11	1:E:4958:ASP:HB3	1.80	0.63
1:G:1799:VAL:HG22	1:G:1893:LEU:HD22	1.80	0.63
1:A:4493:LEU:HD11	1:A:4590:ILE:HG21	1.81	0.63
1:C:1480:ILE:HG23	1:C:1481:LYS:HD2	1.81	0.63
1:E:633:CYS:HB3	1:E:1672:VAL:HG11	1.79	0.63
1:E:591:GLU:HA	1:E:631:LEU:HD21	1.81	0.63
1:A:3862:GLN:HE21	1:A:3865:ASN:HD22	1.48	0.62
1:C:4652:LYS:HG3	1:C:4672:LEU:HD23	1.82	0.62
1:G:3862:GLN:HE21	1:G:3865:ASN:HD22	1.48	0.62
1:A:888:ASN:ND2	1:A:1056:THR:HG21	2.15	0.61
1:E:2266:VAL:HG21	1:E:2324:LEU:HB3	1.82	0.61
1:A:37:LEU:HD13	1:A:203:VAL:HG11	1.81	0.61
1:E:1522:ALA:HB3	1:E:1527:LEU:HD11	1.81	0.61
1:A:1087:ILE:HD12	1:A:1128:LEU:HD23	1.82	0.61
1:A:4012:GLU:HG3	1:A:4122:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1522:ALA:HB3	1:G:1527:LEU:HD11	1.81	0.61
1:A:1522:ALA:HB3	1:A:1527:LEU:HD11	1.83	0.61
1:A:4146:ILE:HD11	1:A:4958:ASP:HB3	1.82	0.61
1:G:1261:VAL:HG11	1:G:1270:VAL:HG11	1.82	0.61
1:C:693:LEU:HG	1:C:749:LEU:HD12	1.83	0.60
1:E:2130:LEU:HA	1:E:2174:VAL:HG22	1.83	0.60
1:C:2130:LEU:HA	1:C:2174:VAL:HG22	1.82	0.60
1:C:28:ILE:HD11	1:C:201:LEU:HD11	1.83	0.60
2:H:26:TYR:H	2:H:39:SER:HG	1.50	0.60
1:C:4101:VAL:HG13	1:C:4150:TYR:HB2	1.84	0.60
1:G:1480:ILE:HG23	1:G:1481:LYS:HD2	1.82	0.60
1:G:766:ILE:HB	1:G:779:PHE:HB2	1.84	0.60
1:A:4916:ASN:O	1:A:4918:ALA:N	2.35	0.60
1:E:1727:VAL:HG11	1:E:1926:VAL:HG11	1.84	0.60
1:E:2067:VAL:HG21	1:E:3645:LEU:HD13	1.83	0.60
1:G:2130:LEU:HA	1:G:2174:VAL:HG22	1.84	0.59
2:H:26:TYR:N	2:H:39:SER:HG	2.00	0.59
1:A:4137:ILE:HG23	1:A:4151:PHE:CE2	2.37	0.59
1:C:3806:LEU:HD13	1:C:3889:PHE:HA	1.85	0.59
1:E:4101:VAL:HG13	1:E:4150:TYR:HB2	1.84	0.59
1:G:667:SER:HB2	1:G:1012:ILE:HD13	1.85	0.59
1:G:1707:ILE:HG23	1:G:1827:THR:HG21	1.84	0.59
1:E:4097:PHE:CZ	1:E:4152:GLU:HB2	2.37	0.59
1:G:1219:LYS:HA	1:G:1240:ALA:HB3	1.85	0.59
1:A:1480:ILE:HG23	1:A:1481:LYS:HD2	1.83	0.59
1:A:1090:ALA:HB3	1:A:1202:ILE:CG2	2.33	0.58
1:C:1090:ALA:HB3	1:C:1202:ILE:CG2	2.33	0.58
1:G:1700:THR:HG22	1:G:1820:PRO:HG3	1.85	0.58
1:G:4203:LEU:HD13	1:G:4595:LEU:HD12	1.85	0.58
1:C:826:VAL:HG21	1:C:832:LEU:HD22	1.85	0.58
1:A:1922:ILE:HD13	1:A:2105:THR:HG21	1.84	0.58
1:C:4916:ASN:O	1:C:4918:ALA:N	2.36	0.58
1:C:869:THR:HG21	1:C:1002:ASN:HD21	1.68	0.58
1:E:4014:ILE:HG22	1:E:4018:PHE:CE2	2.39	0.58
2:F:26:TYR:N	2:F:39:SER:OG	2.29	0.58
1:G:4195:GLU:HA	1:G:4198:ILE:HD12	1.85	0.58
1:A:4869:ILE:HG23	1:G:4869:ILE:HG21	1.85	0.58
1:C:1830:ILE:HG22	1:C:1912:TYR:CD1	2.39	0.58
1:G:4916:ASN:O	1:G:4918:ALA:N	2.37	0.58
1:E:4076:ASN:HB3	1:E:4078:THR:HG22	1.86	0.58
1:C:3778:MET:CE	1:C:3847:LEU:HD22	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3945:VAL:HG11	1:C:3983:LEU:HD21	1.86	0.57
1:C:4012:GLU:HG3	1:C:4122:LEU:HD21	1.84	0.57
1:E:4916:ASN:O	1:E:4918:ALA:N	2.37	0.57
1:A:4101:VAL:HG13	1:A:4150:TYR:HB2	1.87	0.57
1:C:4869:ILE:HG21	1:E:4869:ILE:HG23	1.86	0.57
1:A:2498:ARG:HB3	1:A:2517:LEU:HD11	1.86	0.57
1:C:611:LEU:HD22	1:C:1659:ARG:HD2	1.87	0.57
1:C:2159:PRO:HB3	1:C:2206:ILE:HD12	1.86	0.57
1:E:1087:ILE:HD12	1:E:1128:LEU:HD23	1.85	0.57
1:C:3879:LEU:HD11	1:C:3921:LEU:HD12	1.85	0.57
1:G:4014:ILE:HG22	1:G:4018:PHE:CE2	2.40	0.56
1:C:1519:THR:HG22	1:C:1529:THR:HG22	1.87	0.56
1:C:1680:VAL:HG11	1:C:1709:ILE:HD13	1.88	0.56
1:C:4618:TYR:OH	1:C:4633:ASP:HB2	2.05	0.56
1:A:2130:LEU:HA	1:A:2174:VAL:HG22	1.88	0.56
1:E:4618:TYR:OH	1:E:4633:ASP:HB2	2.06	0.56
2:D:25:HIS:CD2	2:D:104:LEU:HD11	2.41	0.56
1:A:1534:GLU:HG2	1:A:1539:LEU:HD11	1.87	0.56
1:A:3959:LEU:HD22	1:A:3965:GLN:HB3	1.87	0.56
1:C:673:TRP:CH2	1:C:825:ALA:HB2	2.40	0.56
1:G:4652:LYS:HG3	1:G:4672:LEU:HD23	1.88	0.56
1:G:3911:ILE:HD11	1:G:3975:LEU:HB2	1.88	0.55
1:A:4137:ILE:HG23	1:A:4151:PHE:HE2	1.71	0.55
1:E:2159:PRO:HB3	1:E:2206:ILE:HD12	1.89	0.55
1:A:1105:PHE:HB2	1:A:1115:VAL:HG21	1.87	0.55
2:B:25:HIS:CD2	2:B:104:LEU:HD11	2.41	0.55
1:C:4097:PHE:CZ	1:C:4152:GLU:HB2	2.41	0.55
1:G:4146:ILE:HD11	1:G:4958:ASP:HB3	1.87	0.55
1:A:749:LEU:HD22	1:A:755:ILE:HD11	1.88	0.55
1:A:1521:ILE:HG22	1:A:1526:GLU:HA	1.88	0.55
1:A:2861:LEU:HD22	1:A:2872:LEU:HD11	1.88	0.55
1:A:4191:VAL:HG21	1:A:4951:TRP:CH2	2.42	0.55
1:C:2067:VAL:HG11	1:C:3645:LEU:HD22	1.88	0.55
1:C:2067:VAL:HG21	1:C:3645:LEU:HD13	1.89	0.55
1:C:4146:ILE:HD11	1:C:4958:ASP:HB3	1.88	0.55
1:E:4137:ILE:HG23	1:E:4151:PHE:HE2	1.72	0.55
1:C:1261:VAL:HG11	1:C:1270:VAL:HG11	1.87	0.55
1:E:207:PHE:CE2	1:G:2326:ILE:HD12	2.42	0.55
1:C:4014:ILE:HG22	1:C:4018:PHE:CE2	2.42	0.55
1:C:1911:GLN:HB2	1:C:2087:LEU:HD11	1.88	0.55
1:C:3911:ILE:HD11	1:C:3975:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3614:ARG:O	1:E:3618:VAL:HG23	2.06	0.55
1:G:2861:LEU:HD22	1:G:2872:LEU:HD11	1.87	0.55
1:C:436:LEU:HD22	1:C:518:ALA:HA	1.89	0.55
1:C:872:ILE:HD13	1:C:873:VAL:N	2.21	0.55
1:E:2497:LEU:HD11	1:E:2873:VAL:HG12	1.90	0.55
1:G:3924:TYR:HB2	1:G:3925:ILE:HD12	1.89	0.55
1:C:1522:ALA:HB3	1:C:1527:LEU:HD11	1.87	0.54
1:C:4191:VAL:HG11	1:C:4951:TRP:CH2	2.43	0.54
2:F:25:HIS:CD2	2:F:104:LEU:HD11	2.42	0.54
1:G:3614:ARG:O	1:G:3618:VAL:HG23	2.07	0.54
1:A:1511:VAL:HA	1:A:1517:LEU:HD13	1.89	0.54
1:A:544:ASN:HB2	1:A:547:ASN:HD22	1.73	0.54
1:A:4199:PHE:CZ	1:A:4602:PHE:CD1	2.96	0.54
2:B:82:TYR:CD2	2:B:91:ILE:HG21	2.42	0.54
1:G:1736:ILE:HG13	1:G:1753:LEU:HD23	1.89	0.54
1:A:1268:ILE:HD11	1:A:1302:TYR:CE1	2.43	0.54
1:C:3614:ARG:O	1:C:3618:VAL:HG23	2.07	0.54
1:A:3614:ARG:O	1:A:3618:VAL:HG23	2.06	0.54
1:A:4014:ILE:HG22	1:A:4018:PHE:CE2	2.42	0.54
1:A:2067:VAL:HG21	1:A:3645:LEU:HD13	1.90	0.54
1:C:74:LEU:HD11	1:C:117:HIS:CE1	2.43	0.54
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.89	0.54
1:C:360:ILE:HD11	1:C:402:GLY:HA3	1.89	0.54
1:C:2266:VAL:HG21	1:C:2324:LEU:HD13	1.89	0.54
1:E:4619:ILE:HD12	1:E:4668:ILE:HD12	1.90	0.54
1:G:1096:VAL:HG11	1:G:1101:TRP:CD1	2.43	0.54
1:G:1218:GLY:HA2	1:G:1224:LEU:HD11	1.90	0.54
1:G:2470:VAL:HG21	1:G:2523:THR:CG2	2.38	0.53
1:E:1521:ILE:HG22	1:E:1526:GLU:HA	1.90	0.53
1:G:3693:ALA:HB1	1:G:3758:ALA:O	2.08	0.53
1:A:828:PRO:HG3	1:A:1033:VAL:HG11	1.91	0.53
1:C:3862:GLN:HE21	1:C:3865:ASN:HD22	1.55	0.53
1:G:601:LEU:HD23	1:G:642:LEU:HD21	1.89	0.53
1:G:4618:TYR:OH	1:G:4633:ASP:HB2	2.08	0.53
1:A:1460:ASP:HA	1:A:1496:UNK:H2	1.74	0.53
1:A:4570:MET:HA	1:A:4573:THR:HG22	1.91	0.53
1:G:618:CYS:SG	1:G:619:VAL:HG23	2.49	0.53
1:G:749:LEU:HD22	1:G:755:ILE:HD11	1.90	0.53
1:G:4020:MET:CE	1:G:4067:LEU:HD21	2.39	0.53
1:C:591:GLU:HA	1:C:631:LEU:HD21	1.90	0.53
1:A:4191:VAL:HG21	1:A:4951:TRP:CZ3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:HD22	1:A:1659:ARG:HD2	1.91	0.53
1:A:4076:ASN:HB3	1:A:4078:THR:HG22	1.91	0.53
1:E:360:ILE:HD11	1:E:402:GLY:HA3	1.91	0.53
1:G:828:PRO:HG3	1:G:1033:VAL:HG11	1.90	0.52
1:G:1680:VAL:HG11	1:G:1709:ILE:HD13	1.90	0.52
1:E:4195:GLU:HA	1:E:4198:ILE:HD12	1.90	0.52
1:G:4101:VAL:HG13	1:G:4150:TYR:HB2	1.91	0.52
1:C:688:ALA:HB1	1:C:691:THR:CB	2.39	0.52
1:G:4199:PHE:CZ	1:G:4602:PHE:CD1	2.97	0.52
2:B:26:TYR:N	2:B:39:SER:HG	2.07	0.52
1:C:688:ALA:HB1	1:C:691:THR:HB	1.91	0.52
1:E:2790:ILE:HG12	1:E:2904:VAL:HG12	1.92	0.52
1:G:3911:ILE:O	1:G:3911:ILE:HD13	2.09	0.52
1:A:35:LEU:HD22	1:A:49:LEU:HD13	1.91	0.52
1:E:4199:PHE:CZ	1:E:4602:PHE:CD1	2.97	0.52
1:E:4617:LEU:HA	1:E:4621:GLU:HB3	1.92	0.52
1:C:1894:LEU:HD12	1:C:2069:TRP:CZ2	2.44	0.52
1:G:1725:PHE:HB3	1:G:2105:THR:HG22	1.92	0.52
2:H:25:HIS:CD2	2:H:104:LEU:HD11	2.44	0.52
1:C:119:ILE:HG21	1:C:162:ILE:HD11	1.92	0.52
1:E:2718:LEU:HD22	1:E:2780:LEU:HD22	1.92	0.52
1:G:21:VAL:HG13	1:G:217:ILE:HD11	1.92	0.52
1:A:872:ILE:HD11	1:A:944:LEU:HD13	1.92	0.52
1:E:778:MET:O	1:E:1468:THR:OG1	2.28	0.52
1:E:1105:PHE:HB2	1:E:1115:VAL:HG21	1.91	0.52
1:G:1689:ILE:HD11	1:G:1790:LYS:HD3	1.91	0.52
1:E:633:CYS:SG	1:E:1669:ASN:ND2	2.83	0.52
1:G:935:MET:O	1:G:939:THR:HG23	2.10	0.52
1:G:2159:PRO:HB3	1:G:2206:ILE:HD12	1.92	0.52
1:C:572:LEU:HD13	1:C:609:LYS:HB2	1.90	0.51
1:E:611:LEU:HD22	1:E:1659:ARG:CD	2.40	0.51
1:A:307:SER:HB3	1:A:327:THR:HG22	1.93	0.51
1:A:2159:PRO:HB3	1:A:2206:ILE:HD12	1.92	0.51
1:C:3693:ALA:HB1	1:C:3758:ALA:O	2.10	0.51
1:E:804:LEU:HD22	1:E:822:CYS:HB3	1.92	0.51
1:A:3891:TRP:CZ2	1:G:76:ARG:HB2	2.45	0.51
1:C:4137:ILE:HG23	1:C:4151:PHE:CE2	2.45	0.51
1:E:4130:PHE:O	1:E:4134:LEU:N	2.43	0.51
1:A:633:CYS:SG	1:A:1669:ASN:ND2	2.83	0.51
1:E:991:SER:HB3	1:E:1066:ALA:HB2	1.93	0.51
1:G:436:LEU:HD11	1:G:447:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:541:ILE:HD12	1:E:578:VAL:HG22	1.93	0.51
1:E:659:ILE:HG23	1:E:825:ALA:HB1	1.92	0.51
1:E:745:ASN:HB2	1:E:771:ASN:HD21	1.75	0.51
1:G:1726:ILE:HG21	1:G:2120:LEU:HD21	1.92	0.51
1:C:436:LEU:HD13	1:C:518:ALA:HB2	1.91	0.51
1:C:4619:ILE:HD12	1:C:4668:ILE:HD12	1.93	0.51
1:E:888:ASN:ND2	1:E:1056:THR:HG21	2.25	0.51
1:E:1105:PHE:CB	1:E:1115:VAL:HG21	2.41	0.51
1:A:4958:ASP:O	1:A:4962:LYS:HB2	2.11	0.51
1:E:693:LEU:HD22	1:E:798:ILE:HD13	1.92	0.51
1:E:4191:VAL:HG21	1:E:4951:TRP:CZ3	2.46	0.51
1:E:143:LEU:HD21	1:E:207:PHE:CE2	2.47	0.50
1:E:2170:THR:O	1:E:2174:VAL:HG23	2.11	0.50
1:G:888:ASN:ND2	1:G:1056:THR:HG21	2.26	0.50
1:A:1830:ILE:HG22	1:A:1912:TYR:CD1	2.46	0.50
1:E:436:LEU:HD22	1:E:518:ALA:HA	1.94	0.50
1:G:660:PHE:CD2	1:G:827:LEU:HD11	2.45	0.50
1:G:3689:TYR:OH	1:G:3744:THR:HG21	2.11	0.50
2:F:82:TYR:CD2	2:F:91:ILE:HG21	2.47	0.50
1:C:677:LEU:HD22	1:C:695:VAL:HG21	1.93	0.50
1:E:633:CYS:CB	1:E:1672:VAL:HG11	2.40	0.50
1:E:4103:LEU:HD12	1:E:4127:LEU:HD11	1.94	0.50
1:E:4192:ASN:C	1:E:4192:ASN:HD22	2.14	0.50
1:G:2067:VAL:HG21	1:G:3645:LEU:HD13	1.93	0.50
1:G:3745:ILE:HG13	1:G:3759:THR:HG21	1.93	0.50
1:C:2470:VAL:HG21	1:C:2523:THR:CG2	2.42	0.50
1:E:915:HIS:HB3	1:E:918:LEU:HD13	1.93	0.50
1:G:688:ALA:HB3	1:G:795:SER:OG	2.12	0.50
1:C:633:CYS:CB	1:C:1672:VAL:HG11	2.41	0.50
1:C:1831:MET:HE1	1:C:1833:ILE:HD13	1.94	0.50
1:G:872:ILE:HD11	1:G:944:LEU:HD13	1.92	0.50
1:C:1116:GLY:O	1:C:1204:VAL:HG12	2.11	0.50
1:C:4927:LEU:HD11	1:C:4942:VAL:HG13	1.94	0.50
1:G:4097:PHE:CZ	1:G:4152:GLU:HB2	2.46	0.50
1:A:759:LEU:HD13	1:A:766:ILE:CG1	2.41	0.49
1:A:4617:LEU:HD13	1:A:4621:GLU:HB3	1.94	0.49
1:C:177:VAL:HG13	1:C:216:PRO:HD3	1.94	0.49
1:A:915:HIS:HB3	1:A:918:LEU:HD13	1.93	0.49
1:A:1507:ILE:HB	1:A:1521:ILE:HG13	1.94	0.49
1:A:2718:LEU:HD22	1:A:2780:LEU:HD22	1.94	0.49
1:C:4912:LEU:HA	1:C:4916:ASN:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4912:LEU:HA	1:E:4916:ASN:HB3	1.94	0.49
1:G:2423:ILE:HD13	1:G:2423:ILE:O	2.10	0.49
1:E:648:LEU:HD23	1:E:1684:GLN:HA	1.95	0.49
1:E:826:VAL:HG21	1:E:832:LEU:HD22	1.95	0.49
1:G:177:VAL:HG13	1:G:216:PRO:HD3	1.94	0.49
1:G:2159:PRO:CB	1:G:2206:ILE:HD12	2.43	0.49
1:G:2497:LEU:CD1	1:G:2873:VAL:HG12	2.43	0.49
1:A:4912:LEU:HA	1:A:4916:ASN:HB3	1.94	0.49
1:C:181:LEU:HD12	1:C:214:VAL:HG21	1.94	0.49
1:E:3899:ILE:HD12	1:E:3959:LEU:HD23	1.93	0.49
1:E:4191:VAL:HG11	1:E:4951:TRP:CH2	2.46	0.49
1:A:165:ALA:HB1	1:A:211:LEU:HD11	1.94	0.49
1:A:2473:LEU:HD21	1:A:2484:PHE:CE2	2.47	0.49
1:C:4046:LYS:HG2	1:C:4079:LEU:HD21	1.93	0.49
1:E:1782:PHE:CE2	1:E:1787:LEU:HD22	2.47	0.49
1:G:1689:ILE:HD11	1:G:1790:LYS:CD	2.43	0.49
1:C:3911:ILE:HD13	1:C:3911:ILE:O	2.12	0.49
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.93	0.49
1:G:826:VAL:HG21	1:G:832:LEU:HD22	1.94	0.49
1:G:4912:LEU:HA	1:G:4916:ASN:HB3	1.94	0.49
1:G:4958:ASP:O	1:G:4962:LYS:HB2	2.11	0.49
1:A:2304:ARG:HB2	1:A:2399:LEU:HD21	1.94	0.49
1:C:1445:TRP:CD1	1:C:1518:LEU:HD22	2.47	0.49
1:C:1826:TYR:CZ	1:C:1908:LEU:HD22	2.47	0.49
1:E:4617:LEU:HD13	1:E:4621:GLU:HB3	1.93	0.49
1:A:2470:VAL:HG11	1:A:2523:THR:HG22	1.94	0.49
1:C:28:ILE:CG1	1:C:201:LEU:HD11	2.42	0.49
1:C:1105:PHE:CB	1:C:1115:VAL:HG21	2.42	0.49
1:C:4958:ASP:O	1:C:4962:LYS:HB2	2.13	0.49
1:E:766:ILE:HB	1:E:779:PHE:HB2	1.95	0.49
1:G:660:PHE:CE2	1:G:827:LEU:HD11	2.48	0.49
1:G:3802:SER:HB2	1:G:3837:THR:HG21	1.95	0.49
1:A:3861:THR:HG23	1:A:3863:THR:HG23	1.94	0.48
1:G:659:ILE:N	1:G:659:ILE:HD12	2.28	0.48
1:G:1782:PHE:CE2	1:G:1787:LEU:HD22	2.47	0.48
1:E:601:LEU:HD23	1:E:642:LEU:HD21	1.95	0.48
1:E:881:ILE:HD11	1:E:1060:TYR:CD2	2.47	0.48
1:E:1831:MET:CE	1:E:1833:ILE:HD13	2.43	0.48
1:G:759:LEU:HD13	1:G:766:ILE:HG12	1.95	0.48
1:E:1087:ILE:HD12	1:E:1128:LEU:CD2	2.43	0.48
1:E:4099:VAL:O	1:E:4103:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1830:ILE:HG22	1:G:1912:TYR:CD1	2.48	0.48
1:E:2861:LEU:HD22	1:E:2872:LEU:HD11	1.94	0.48
1:E:3806:LEU:HD13	1:E:3889:PHE:HA	1.96	0.48
1:G:1475:LYS:O	1:G:1476:VAL:HG22	2.12	0.48
1:G:1483:SER:HB2	1:G:1533:VAL:HG23	1.94	0.48
1:G:4922:PHE:HA	1:G:4925:MET:HG2	1.93	0.48
1:A:2473:LEU:HD21	1:A:2484:PHE:HE2	1.78	0.48
1:C:579:LEU:HD22	1:C:586:LEU:HD23	1.95	0.48
1:C:3683:LEU:HD21	1:C:3747:ALA:HB1	1.95	0.48
1:E:3926:GLN:HA	1:E:3926:GLN:HE21	1.77	0.48
2:F:4:ILE:CD1	2:F:74:LEU:HD22	2.43	0.48
1:G:579:LEU:HD22	1:G:586:LEU:HD23	1.94	0.48
1:G:4496:LEU:HD22	1:G:4591:GLY:HA3	1.95	0.48
1:A:496:ASN:HA	1:A:499:LEU:HD12	1.95	0.48
2:B:4:ILE:CD1	2:B:74:LEU:HD22	2.44	0.48
1:C:541:ILE:HD12	1:C:578:VAL:HG22	1.95	0.48
1:E:4192:ASN:HD22	1:E:4193:PHE:N	2.11	0.48
2:F:56:ILE:HD13	2:F:82:TYR:CZ	2.48	0.48
1:G:869:THR:HG21	1:G:1002:ASN:HD21	1.77	0.48
1:A:1726:ILE:HG21	1:A:2120:LEU:HD21	1.95	0.48
1:E:986:ILE:HD13	1:E:1058:LEU:HB3	1.96	0.48
1:C:2123:LEU:HD12	1:C:2127:ARG:NE	2.29	0.48
1:C:3737:ALA:HA	1:C:3740:MET:HG2	1.96	0.48
1:E:4922:PHE:HA	1:E:4925:MET:HG2	1.94	0.48
1:G:759:LEU:HD13	1:G:766:ILE:CG1	2.44	0.48
1:G:1105:PHE:CB	1:G:1115:VAL:HG21	2.42	0.48
1:C:3775:GLN:NE2	1:C:3847:LEU:O	2.47	0.48
1:C:76:ARG:CB	1:E:3891:TRP:CZ2	2.97	0.48
1:C:4137:ILE:HG23	1:C:4151:PHE:HE2	1.78	0.48
1:C:4570:MET:HA	1:C:4573:THR:HG22	1.96	0.48
1:E:1686:LEU:HD22	1:E:1790:LYS:HE3	1.95	0.48
1:G:4521:TYR:CZ	1:G:4562:VAL:HG22	2.49	0.48
1:C:230:GLY:HA3	1:C:289:ILE:HD11	1.95	0.47
1:C:4617:LEU:HD13	1:C:4621:GLU:HB3	1.96	0.47
1:E:4652:LYS:HG3	1:E:4672:LEU:HD23	1.95	0.47
1:G:237:LEU:HD23	1:G:244:CYS:SG	2.53	0.47
1:G:436:LEU:HD13	1:G:518:ALA:HB2	1.95	0.47
1:C:559:ILE:HG21	1:C:593:HIS:HA	1.96	0.47
1:C:3802:SER:HB2	1:C:3837:THR:HG21	1.96	0.47
1:E:2497:LEU:CD1	1:E:2873:VAL:HG12	2.45	0.47
1:E:2861:LEU:HD22	1:E:2872:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4869:ILE:HG21	1:G:4869:ILE:HG23	1.95	0.47
1:E:4923:PHE:HZ	1:E:4942:VAL:HG11	1.79	0.47
1:G:4619:ILE:HD12	1:G:4668:ILE:HD12	1.96	0.47
1:A:3745:ILE:HG13	1:A:3759:THR:HG21	1.96	0.47
1:C:652:VAL:HG11	1:C:692:HIS:CD2	2.49	0.47
1:C:2498:ARG:CB	1:C:2517:LEU:HD11	2.45	0.47
1:E:1707:ILE:HG23	1:E:1827:THR:HG21	1.97	0.47
1:G:4104:THR:HG21	1:G:4134:LEU:HD11	1.97	0.47
1:A:4515:ASN:HD22	1:A:4745:LEU:HD21	1.80	0.47
1:C:935:MET:O	1:C:939:THR:HG23	2.14	0.47
1:C:52:THR:HG22	1:C:60:PRO:CB	2.45	0.47
1:C:1521:ILE:HG22	1:C:1526:GLU:HA	1.96	0.47
1:A:614:LEU:HD13	1:A:636:LEU:HD11	1.95	0.47
1:A:1686:LEU:HD22	1:A:1790:LYS:HE3	1.97	0.47
1:A:4619:ILE:HD12	1:A:4668:ILE:HD12	1.97	0.47
1:C:943:LEU:HD23	1:C:999:LEU:HD11	1.95	0.47
1:C:1303:ARG:HG2	1:C:1542:ALA:HB2	1.97	0.47
1:E:4923:PHE:CZ	1:E:4942:VAL:HG11	2.50	0.47
1:G:430:ILE:HD11	1:G:501:CYS:SG	2.55	0.47
1:G:1658:LEU:HD23	1:G:1701:GLY:HA3	1.96	0.47
1:C:2779:SER:OG	1:C:2849:TYR:OH	2.31	0.47
1:C:3778:MET:HE3	1:C:3847:LEU:HD13	1.96	0.47
1:E:3752:THR:HG23	1:E:3836:PHE:CE2	2.50	0.47
1:G:826:VAL:HG13	1:G:832:LEU:HD13	1.97	0.47
1:G:1521:ILE:HG22	1:G:1526:GLU:HA	1.97	0.47
1:G:3911:ILE:HG12	1:G:3975:LEU:HD22	1.97	0.47
1:A:559:ILE:HG12	1:A:575:LEU:HD11	1.97	0.47
1:A:3866:ASN:OD1	1:A:3867:THR:HG23	2.14	0.47
1:A:4652:LYS:HG3	1:A:4672:LEU:HD23	1.97	0.47
1:C:2259:GLU:N	1:C:2260:PRO:HD2	2.30	0.47
1:C:3911:ILE:HG12	1:C:3975:LEU:HD22	1.97	0.47
1:E:660:PHE:CD2	1:E:827:LEU:HD11	2.50	0.47
1:E:749:LEU:HD22	1:E:755:ILE:HD11	1.97	0.47
1:G:1090:ALA:HB3	1:G:1202:ILE:CG2	2.45	0.47
1:G:3804:LEU:HD13	1:G:3910:ALA:HB2	1.97	0.47
1:A:4160:GLN:HG2	1:A:4201:MET:HA	1.97	0.47
1:C:1910:LEU:HG	1:C:2062:ILE:HD12	1.97	0.47
1:E:919:VAL:HG21	1:E:923:LYS:HD3	1.96	0.47
1:G:436:LEU:HD22	1:G:518:ALA:HA	1.96	0.47
1:C:1087:ILE:HD12	1:C:1128:LEU:CD2	2.45	0.46
1:C:1118:SER:CB	1:C:1204:VAL:HG11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:737:ILE:HG21	1:G:1481:LYS:HG2	1.98	0.46
1:G:4137:ILE:HG23	1:G:4151:PHE:HE2	1.78	0.46
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.98	0.46
2:D:16:PRO:HG3	2:D:106:LEU:HD21	1.97	0.46
1:E:580:VAL:HG23	1:E:581:GLU:HG2	1.97	0.46
1:E:4607:GLU:O	1:E:4611:LYS:HG2	2.15	0.46
1:C:618:CYS:SG	1:C:1666:ALA:HA	2.55	0.46
1:C:1218:GLY:O	1:C:1240:ALA:HB3	2.15	0.46
1:C:2023:LEU:N	1:C:2023:LEU:HD23	2.31	0.46
1:G:2493:PHE:O	1:G:2497:LEU:HG	2.15	0.46
1:G:2498:ARG:HB3	1:G:2517:LEU:HD11	1.98	0.46
1:A:496:ASN:HD22	1:A:499:LEU:HD12	1.79	0.46
1:A:4611:LYS:O	1:A:4616:GLY:N	2.49	0.46
1:C:2075:ILE:HD11	1:C:2080:LEU:HD23	1.97	0.46
1:C:3756:VAL:HG13	1:C:3836:PHE:CE1	2.51	0.46
1:E:2491:VAL:O	1:E:2495:PRO:HD2	2.16	0.46
1:E:3737:ALA:HA	1:E:3740:MET:HG2	1.96	0.46
1:G:804:LEU:HD22	1:G:822:CYS:HB3	1.96	0.46
1:G:3737:ALA:HA	1:G:3740:MET:HG2	1.98	0.46
1:G:3899:ILE:HD12	1:G:3959:LEU:HD23	1.97	0.46
1:A:572:LEU:HD13	1:A:609:LYS:HB2	1.98	0.46
1:A:4939:GLU:HA	1:A:4942:VAL:HG12	1.98	0.46
1:C:4611:LYS:O	1:C:4616:GLY:N	2.49	0.46
1:E:1475:LYS:O	1:E:1476:VAL:HG22	2.16	0.46
1:E:4927:LEU:HD11	1:E:4942:VAL:HG13	1.98	0.46
1:A:778:MET:O	1:A:1468:THR:OG1	2.33	0.46
1:A:3737:ALA:HA	1:A:3740:MET:HG2	1.98	0.46
1:C:944:LEU:HD21	1:C:950:VAL:HG22	1.97	0.46
1:E:579:LEU:HD22	1:E:586:LEU:HD23	1.98	0.46
1:E:996:VAL:HG12	1:E:1054:VAL:HG11	1.97	0.46
1:E:3693:ALA:HB1	1:E:3758:ALA:O	2.15	0.46
1:G:4020:MET:HE3	1:G:4067:LEU:HD21	1.97	0.46
1:G:4617:LEU:HD13	1:G:4621:GLU:HB3	1.98	0.46
1:A:541:ILE:HG22	1:A:547:ASN:HB3	1.97	0.46
1:C:601:LEU:HD23	1:C:642:LEU:HD21	1.96	0.46
1:E:739:ARG:CZ	1:E:1467:VAL:HG13	2.45	0.46
1:E:4501:TYR:OH	1:E:4595:LEU:HD21	2.15	0.46
1:G:633:CYS:CB	1:G:1672:VAL:HG11	2.46	0.46
1:G:1253:LYS:NZ	1:G:1601:ASN:HD22	2.14	0.46
1:C:2485:LEU:HD11	1:C:2527:PRO:HB3	1.98	0.46
1:G:1738:LEU:HD12	1:G:1921:ARG:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HD11	1:A:201:LEU:HD13	1.98	0.46
1:C:4198:ILE:HG23	1:C:4925:MET:CE	2.46	0.46
1:E:3797:LEU:HD21	1:E:3836:PHE:HE2	1.80	0.46
2:F:75:THR:HG23	2:F:98:ILE:CD1	2.46	0.46
1:G:2170:THR:O	1:G:2174:VAL:HG23	2.15	0.46
1:C:230:GLY:CA	1:C:289:ILE:HD11	2.46	0.46
1:C:743:SER:OG	1:C:775:VAL:HG22	2.16	0.46
1:C:4794:PHE:HB2	1:C:4833:ILE:HD11	1.98	0.46
1:A:1105:PHE:CB	1:A:1115:VAL:HG21	2.46	0.45
1:A:2170:THR:O	1:A:2174:VAL:HG23	2.16	0.45
1:A:2521:LEU:HD11	1:A:2601:UNK:CB	2.46	0.45
2:B:75:THR:HG23	2:B:98:ILE:CD1	2.46	0.45
1:E:611:LEU:HD22	1:E:1659:ARG:CG	2.45	0.45
1:E:4958:ASP:O	1:E:4962:LYS:HB2	2.16	0.45
1:G:541:ILE:HG22	1:G:547:ASN:HB3	1.97	0.45
1:G:3966:ILE:O	1:G:3969:LEU:N	2.49	0.45
1:A:2086:VAL:HG13	1:A:2087:LEU:HD12	1.98	0.45
1:C:670:TYR:O	1:C:673:TRP:NE1	2.49	0.45
1:C:1782:PHE:CE2	1:C:1787:LEU:HD22	2.51	0.45
1:C:3992:VAL:HG13	1:C:4964:TYR:CE2	2.51	0.45
1:E:476:GLN:HE21	1:E:476:GLN:HA	1.81	0.45
1:E:559:ILE:HD12	1:E:596:SER:HB2	1.98	0.45
1:E:3966:ILE:O	1:E:3969:LEU:N	2.48	0.45
1:G:3844:LEU:HD13	1:G:3847:LEU:HD12	1.97	0.45
1:A:875:PRO:HD2	1:A:878:LEU:HD12	1.98	0.45
2:B:73:LYS:HZ1	2:B:98:ILE:HD12	1.80	0.45
1:C:4617:LEU:HA	1:C:4621:GLU:HB3	1.98	0.45
1:G:4165:GLN:HG3	1:G:4501:TYR:CZ	2.52	0.45
1:C:112:THR:HG21	1:C:174:LYS:HD3	1.99	0.45
1:C:2423:ILE:HD13	1:C:2423:ILE:O	2.16	0.45
1:G:1094:TYR:OH	1:G:1808:ASP:OD1	2.33	0.45
1:E:1253:LYS:NZ	1:E:1601:ASN:HD22	2.14	0.45
1:E:1831:MET:HE1	1:E:1833:ILE:HD13	1.97	0.45
1:E:3952:PHE:HZ	1:E:3975:LEU:HD23	1.82	0.45
1:E:4152:GLU:HB3	1:E:4926:TYR:CD1	2.50	0.45
1:G:611:LEU:HD22	1:G:1659:ARG:HD2	1.98	0.45
1:A:996:VAL:HG12	1:A:1054:VAL:HG11	1.99	0.45
1:E:2023:LEU:N	1:E:2023:LEU:HD23	2.30	0.45
1:G:1299:ILE:HG23	1:G:1301:PHE:CE1	2.52	0.45
1:G:4130:PHE:O	1:G:4134:LEU:N	2.50	0.45
1:C:72:SER:C	1:C:73:LEU:HD22	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2513:MET:O	1:C:2517:LEU:HD13	2.17	0.45
1:G:689:GLU:O	1:G:691:THR:HG22	2.16	0.45
1:G:2896:PHE:HA	1:G:2899:ILE:HG12	1.98	0.45
1:E:459:LEU:HB3	1:E:536:LEU:HD13	1.99	0.45
1:E:1692:LYS:HG2	1:E:1810:VAL:HG13	1.97	0.45
1:E:1914:CYS:HB2	1:E:2091:GLN:HE22	1.82	0.45
1:E:2259:GLU:N	1:E:2260:PRO:HD2	2.32	0.45
1:G:598:ILE:HG23	1:G:642:LEU:HD22	1.99	0.45
1:G:2259:GLU:N	1:G:2260:PRO:HD2	2.31	0.45
1:A:1782:PHE:CE2	1:A:1787:LEU:HD22	2.52	0.45
1:C:2095:ILE:HD11	1:C:3630:ILE:HG22	1.99	0.45
1:C:2176:VAL:HG22	1:C:2224:ASN:HD21	1.81	0.45
1:A:804:LEU:HD22	1:A:822:CYS:HB3	1.98	0.45
1:C:4496:LEU:HD22	1:C:4591:GLY:HA3	1.99	0.45
1:E:739:ARG:NE	1:E:1467:VAL:HG13	2.32	0.45
1:E:935:MET:O	1:E:939:THR:HG23	2.17	0.45
1:E:4137:ILE:HG23	1:E:4151:PHE:CE2	2.50	0.45
1:E:4939:GLU:HA	1:E:4942:VAL:HG12	1.99	0.45
1:G:217:ILE:HG22	1:G:286:GLY:HA3	2.00	0.45
1:G:4611:LYS:O	1:G:4616:GLY:N	2.50	0.45
1:A:633:CYS:CB	1:A:1672:VAL:HG11	2.47	0.44
1:A:759:LEU:HD13	1:A:766:ILE:HG12	1.98	0.44
1:A:826:VAL:HG21	1:A:832:LEU:HD22	1.99	0.44
1:A:2473:LEU:HD13	1:A:2473:LEU:O	2.17	0.44
1:A:3911:ILE:HD11	1:A:3975:LEU:HD22	1.98	0.44
1:A:4195:GLU:HA	1:A:4198:ILE:HD12	2.00	0.44
1:C:2106:TYR:CG	1:C:2107:THR:N	2.85	0.44
1:E:2067:VAL:HG11	1:E:3645:LEU:HD22	1.99	0.44
1:G:2266:VAL:HG21	1:G:2324:LEU:HB3	1.99	0.44
1:A:4607:GLU:O	1:A:4611:LYS:HG2	2.17	0.44
1:C:1639:VAL:HG21	1:C:1644:LEU:HD23	1.99	0.44
1:E:1629:SER:HA	1:E:1640:ASP:HA	1.99	0.44
1:G:743:SER:OG	1:G:775:VAL:HG22	2.17	0.44
1:A:3956:GLN:HE21	1:A:4014:ILE:HG23	1.83	0.44
1:C:76:ARG:HB3	1:E:3891:TRP:CZ2	2.51	0.44
1:C:598:ILE:HG23	1:C:642:LEU:HD22	1.98	0.44
1:E:944:LEU:HD21	1:E:950:VAL:HG22	1.99	0.44
1:E:2473:LEU:HD21	1:E:2484:PHE:CE2	2.51	0.44
1:G:2718:LEU:HD22	1:G:2780:LEU:HD22	1.99	0.44
1:G:4164:PRO:HG2	1:G:4166:VAL:HG22	2.00	0.44
1:G:679:VAL:HA	1:G:800:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2023:LEU:N	1:A:2023:LEU:HD23	2.32	0.44
1:A:4617:LEU:HA	1:A:4621:GLU:HB3	1.98	0.44
1:E:1689:ILE:HD11	1:E:1790:LYS:CD	2.47	0.44
1:E:2838:LEU:HD23	1:E:2841:MET:SD	2.57	0.44
1:A:4612:LEU:HD11	1:A:4637:ILE:HG12	2.00	0.44
1:E:2130:LEU:CA	1:E:2174:VAL:HG22	2.46	0.44
1:A:1253:LYS:NZ	1:A:1601:ASN:HD22	2.15	0.44
1:A:2259:GLU:N	1:A:2260:PRO:HD2	2.31	0.44
1:A:3992:VAL:HG13	1:A:4964:TYR:CE2	2.53	0.44
1:C:28:ILE:CD1	1:C:201:LEU:HD11	2.46	0.44
1:C:4191:VAL:HG21	1:C:4951:TRP:CZ3	2.52	0.44
1:C:4817:PHE:O	1:C:4821:VAL:HG22	2.18	0.44
1:C:4823:VAL:HG23	1:C:4824:ARG:HG3	1.99	0.44
1:E:826:VAL:CG2	1:E:832:LEU:HD13	2.48	0.44
1:G:1116:GLY:O	1:G:1204:VAL:HG12	2.18	0.44
1:G:3966:ILE:HD12	1:G:3969:LEU:HD23	1.99	0.44
1:G:3986:MET:SD	1:G:3996:ILE:HD11	2.57	0.44
1:A:1703:TYR:HB2	1:A:1820:PRO:HB3	1.99	0.44
1:A:4617:LEU:HA	1:A:4621:GLU:CB	2.48	0.44
1:C:4164:PRO:HG2	1:C:4166:VAL:HG22	1.99	0.44
1:E:3778:MET:HE1	1:E:3847:LEU:HD22	2.00	0.44
1:E:4611:LYS:O	1:E:4616:GLY:N	2.51	0.44
1:G:3697:ALA:HB2	1:G:3761:LYS:HB3	2.00	0.44
1:A:280:LEU:HD13	1:A:296:ARG:NH1	2.33	0.44
1:A:3775:GLN:NE2	1:A:3847:LEU:O	2.51	0.44
1:C:1090:ALA:HB3	1:C:1202:ILE:HG22	2.00	0.44
1:C:4846:ILE:CD1	1:E:4816:MET:HG3	2.47	0.44
1:E:759:LEU:HD13	1:E:766:ILE:CG1	2.48	0.44
1:G:737:ILE:HD13	1:G:1535:PRO:HG3	2.00	0.44
1:G:3879:LEU:HA	1:G:3882:VAL:HG22	2.00	0.44
1:A:655:MET:SD	1:A:1619:VAL:HG21	2.58	0.43
1:C:633:CYS:SG	1:C:1669:ASN:ND2	2.91	0.43
1:C:4191:VAL:HG21	1:C:4951:TRP:CH2	2.53	0.43
1:C:4607:GLU:O	1:C:4611:LYS:HG2	2.18	0.43
1:G:580:VAL:HG23	1:G:581:GLU:HG2	2.00	0.43
1:A:952:ILE:HD12	1:A:956:HIS:CE1	2.53	0.43
1:A:1090:ALA:HB3	1:A:1202:ILE:HG22	1.99	0.43
1:A:2075:ILE:CG1	1:A:2080:LEU:HD23	2.46	0.43
1:A:3802:SER:HB2	1:A:3837:THR:HG21	2.00	0.43
1:A:3804:LEU:HB3	1:A:3885:SER:HB3	2.00	0.43
1:C:1808:ASP:HB3	1:C:1809:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:PHE:CD1	1:E:452:VAL:HG21	2.53	0.43
1:E:3916:GLN:O	1:E:3920:THR:HG23	2.19	0.43
1:G:3797:LEU:HD21	1:G:3836:PHE:CE2	2.53	0.43
1:A:463:PHE:HB3	1:A:539:ALA:HB1	2.00	0.43
1:A:611:LEU:HD22	1:A:1659:ARG:CD	2.48	0.43
1:A:4496:LEU:HD12	1:A:4587:PHE:CZ	2.53	0.43
1:C:73:LEU:C	1:C:74:LEU:HD12	2.39	0.43
1:E:739:ARG:HG3	1:E:1469:LEU:HD21	2.01	0.43
1:E:1830:ILE:HG22	1:E:1912:TYR:CD1	2.53	0.43
1:E:1847:GLU:HB2	1:E:1848:PRO:HD3	2.00	0.43
1:A:580:VAL:HG23	1:A:581:GLU:HG2	2.00	0.43
1:A:2497:LEU:HD13	1:A:2874:PRO:HD2	1.99	0.43
1:A:4152:GLU:HB3	1:A:4926:TYR:CE1	2.53	0.43
1:A:4508:LEU:HD21	1:A:4748:ILE:HD13	2.00	0.43
1:A:4858:VAL:CG1	1:C:4864:ILE:HG21	2.49	0.43
1:C:2498:ARG:HB3	1:C:2517:LEU:HD11	1.99	0.43
1:C:4668:ILE:HD13	1:C:4671:LEU:HD12	2.00	0.43
1:C:4899:TYR:CE2	1:C:4962:LYS:HG2	2.53	0.43
1:E:1268:ILE:HG23	1:E:1268:ILE:O	2.18	0.43
1:E:4005:VAL:HG21	1:E:4115:ARG:HD3	2.00	0.43
1:G:364:GLN:HE21	1:G:369:GLY:HA2	1.83	0.43
1:G:656:ARG:NH2	1:G:835:GLU:OE2	2.51	0.43
1:G:4939:GLU:HA	1:G:4942:VAL:HG12	2.00	0.43
1:C:4651:VAL:O	1:C:4655:VAL:HG23	2.18	0.43
1:E:663:VAL:HG13	1:E:671:LYS:HD3	2.00	0.43
1:E:847:THR:HG21	1:E:1215:MET:O	2.18	0.43
1:E:1783:PRO:HB2	1:E:1786:ILE:HG22	2.01	0.43
1:E:1925:ILE:HD13	1:E:2032:LEU:HD21	2.00	0.43
1:G:2110:GLY:O	1:G:2113:VAL:HG13	2.18	0.43
1:G:2497:LEU:HD12	1:G:2873:VAL:HG12	2.01	0.43
1:A:4082:GLU:HA	1:A:4085:VAL:HG22	2.00	0.43
1:C:983:LEU:HD21	1:C:1056:THR:HG23	2.01	0.43
1:C:1783:PRO:HB2	1:C:1786:ILE:HG22	2.01	0.43
1:C:1894:LEU:HD11	1:C:2065:THR:HG21	2.01	0.43
1:C:3843:PHE:O	1:C:3847:LEU:HG	2.19	0.43
1:E:869:THR:HG21	1:E:1002:ASN:HD21	1.84	0.43
1:G:21:VAL:CG1	1:G:217:ILE:HD11	2.48	0.43
1:G:1808:ASP:HB3	1:G:1809:PRO:HA	2.00	0.43
1:G:2713:ILE:HD13	1:G:2714:ILE:N	2.34	0.43
1:G:4781:TYR:HA	1:G:4784:THR:HG22	2.00	0.43
1:C:2779:SER:HG	1:C:2849:TYR:HH	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1511:VAL:HA	1:E:1517:LEU:HD13	2.01	0.43
1:E:2497:LEU:HD13	1:E:2874:PRO:HD3	2.00	0.43
1:G:2023:LEU:N	1:G:2023:LEU:HD23	2.34	0.43
1:A:1808:ASP:HB3	1:A:1809:PRO:HA	2.00	0.43
1:A:1826:TYR:CZ	1:A:1908:LEU:HD22	2.54	0.43
1:A:4597:VAL:HA	1:A:4600:VAL:HG22	2.00	0.43
1:C:544:ASN:HB2	1:C:547:ASN:HD22	1.84	0.43
1:E:2058:LEU:HA	1:E:2061:LEU:HD23	2.01	0.43
1:E:2266:VAL:HG21	1:E:2324:LEU:HD13	2.00	0.43
1:G:693:LEU:HD13	1:G:798:ILE:HD13	2.00	0.43
1:A:3697:ALA:HB2	1:A:3761:LYS:HB3	2.01	0.43
1:A:3973:MET:O	1:A:4095:ILE:HD11	2.19	0.43
1:E:2130:LEU:CB	1:E:2174:VAL:HG22	2.49	0.43
1:E:4103:LEU:HD12	1:E:4127:LEU:CD1	2.49	0.43
1:G:611:LEU:HD22	1:G:1659:ARG:CG	2.49	0.43
1:G:643:LEU:HD22	1:G:1661:TYR:CZ	2.53	0.43
1:G:2513:MET:O	1:G:2517:LEU:HD13	2.18	0.43
1:A:633:CYS:HB3	1:A:1672:VAL:HG11	2.01	0.42
1:C:2266:VAL:HG21	1:C:2324:LEU:HB3	2.01	0.42
1:C:4781:TYR:HA	1:C:4784:THR:HG22	2.01	0.42
1:E:763:ALA:HB3	1:E:765:SER:N	2.34	0.42
1:G:763:ALA:HB3	1:G:765:SER:N	2.33	0.42
1:G:1686:LEU:HD22	1:G:1790:LYS:HD2	2.01	0.42
1:G:1799:VAL:HG11	1:G:1845:LEU:HD11	2.01	0.42
1:A:2326:ILE:HG23	1:G:207:PHE:CD1	2.54	0.42
1:A:4046:LYS:HG2	1:A:4079:LEU:HD21	2.00	0.42
1:A:4493:LEU:HD21	1:A:4590:ILE:CG2	2.48	0.42
1:A:4846:ILE:CD1	1:C:4816:MET:HG3	2.48	0.42
1:C:207:PHE:CG	1:E:2326:ILE:HG23	2.54	0.42
1:C:1928:PHE:CG	1:C:2032:LEU:HD22	2.53	0.42
1:C:2896:PHE:HA	1:C:2899:ILE:HG12	2.01	0.42
1:E:611:LEU:HD22	1:E:1659:ARG:HG3	2.01	0.42
1:E:614:LEU:HD13	1:E:636:LEU:HD11	2.00	0.42
1:E:3911:ILE:CD1	1:E:3975:LEU:HD22	2.49	0.42
1:G:636:LEU:HD13	1:G:1664:VAL:HG21	2.01	0.42
1:G:1087:ILE:HD12	1:G:1128:LEU:HD23	2.01	0.42
1:G:2470:VAL:HG21	1:G:2523:THR:HG23	2.01	0.42
1:A:646:THR:HG23	1:A:1684:GLN:NE2	2.34	0.42
1:A:763:ALA:HB3	1:A:765:SER:N	2.34	0.42
1:A:1749:PRO:HB2	1:A:1843:LEU:HD21	2.01	0.42
1:A:4899:TYR:CE2	1:A:4962:LYS:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:PRO:HG3	2:B:106:LEU:HD21	2.01	0.42
1:C:289:ILE:HG22	1:C:354:ILE:HD12	2.01	0.42
1:C:591:GLU:CA	1:C:631:LEU:HD21	2.49	0.42
1:C:875:PRO:HD2	1:C:878:LEU:HD12	2.01	0.42
1:C:4939:GLU:HA	1:C:4942:VAL:HG12	2.01	0.42
1:E:4617:LEU:HA	1:E:4621:GLU:CB	2.49	0.42
1:G:652:VAL:HG11	1:G:692:HIS:CD2	2.54	0.42
1:G:3797:LEU:HD21	1:G:3836:PHE:HE2	1.84	0.42
1:G:3924:TYR:HB3	1:G:3932:ASN:HD21	1.85	0.42
1:C:1680:VAL:HG21	1:C:1685:LEU:HD13	2.01	0.42
1:C:4195:GLU:HA	1:C:4198:ILE:HD12	2.00	0.42
1:E:1932:PHE:CE2	1:E:2025:ILE:HG13	2.54	0.42
1:G:606:ARG:HG2	1:G:610:VAL:HG21	2.00	0.42
1:A:629:GLN:HA	1:A:632:ILE:HD12	2.00	0.42
1:A:1459:LEU:HD13	1:A:1459:LEU:N	2.35	0.42
1:A:1828:LEU:HD23	1:A:1834:PHE:CZ	2.54	0.42
1:A:3911:ILE:CD1	1:A:3975:LEU:HD22	2.49	0.42
1:C:2420:ILE:O	1:C:2424:LEU:HD13	2.20	0.42
1:C:4082:GLU:HA	1:C:4085:VAL:HG22	2.01	0.42
1:E:611:LEU:HD22	1:E:1659:ARG:HD2	2.00	0.42
1:E:3950:HIS:N	1:E:4010:ASN:HD21	2.18	0.42
1:E:4097:PHE:O	1:E:4101:VAL:HG23	2.19	0.42
1:E:4781:TYR:HA	1:E:4784:THR:HG22	2.00	0.42
2:F:66:MET:SD	2:F:74:LEU:HD21	2.59	0.42
1:G:682:THR:HG22	1:G:798:ILE:HG12	2.01	0.42
1:G:3644:ASP:HA	1:G:3647:LYS:HD2	2.02	0.42
1:G:3775:GLN:NE2	1:G:3847:LEU:O	2.53	0.42
1:G:3861:THR:HG23	1:G:3863:THR:HG23	2.00	0.42
1:A:245:LEU:HD11	1:A:260:VAL:CG1	2.49	0.42
1:A:652:VAL:HG11	1:A:692:HIS:CD2	2.55	0.42
1:A:996:VAL:CG1	1:A:1054:VAL:HG11	2.49	0.42
1:A:3668:LEU:HD21	1:A:3692:TYR:CD1	2.54	0.42
1:A:4923:PHE:CZ	1:A:4942:VAL:HG11	2.55	0.42
1:C:4043:ILE:HD12	1:C:4078:THR:HG21	2.01	0.42
1:C:4204:ALA:HA	1:C:4207:ILE:HG22	2.01	0.42
1:E:194:LEU:HD11	1:E:201:LEU:HD13	2.00	0.42
1:E:3775:GLN:NE2	1:E:3847:LEU:O	2.52	0.42
1:G:1932:PHE:CD2	1:G:2025:ILE:HD11	2.54	0.42
1:G:3740:MET:O	1:G:3744:THR:HG22	2.19	0.42
1:A:659:ILE:HG23	1:A:825:ALA:HB1	2.02	0.42
1:A:792:VAL:HG13	1:A:792:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4191:VAL:HG11	1:A:4951:TRP:CH2	2.55	0.42
1:E:544:ASN:HB2	1:E:547:ASN:HD22	1.84	0.42
1:E:689:GLU:O	1:E:691:THR:HG22	2.19	0.42
1:E:4639:THR:HG22	1:E:4641:SER:H	1.84	0.42
1:G:625:VAL:HG13	1:G:2132:VAL:HG23	2.01	0.42
1:G:875:PRO:HD2	1:G:878:LEU:HD12	2.00	0.42
1:A:629:GLN:CD	1:A:1666:ALA:HB1	2.40	0.42
1:A:2719:GLU:OE1	1:A:2719:GLU:O	2.38	0.42
1:A:3950:HIS:N	1:A:4010:ASN:HD21	2.17	0.42
1:E:559:ILE:HG12	1:E:575:LEU:HD11	2.02	0.42
1:E:2106:TYR:CG	1:E:2107:THR:N	2.88	0.42
1:E:2493:PHE:O	1:E:2497:LEU:HG	2.19	0.42
1:E:3883:GLN:HE22	1:E:3947:GLY:HA3	1.84	0.42
1:E:3956:GLN:NE2	1:E:4014:ILE:HG23	2.35	0.42
1:E:3992:VAL:HG13	1:E:4964:TYR:CE2	2.55	0.42
1:G:115:TYR:HE1	1:G:181:LEU:HD22	1.85	0.42
1:G:555:LEU:HD13	1:G:578:VAL:HG11	2.02	0.42
1:G:1910:LEU:HD12	1:G:2062:ILE:HD12	2.01	0.42
1:G:2250:ASN:HB2	1:G:2253:LEU:HB2	2.01	0.42
1:G:2420:ILE:O	1:G:2424:LEU:HD13	2.19	0.42
1:A:874:LEU:HD22	1:A:882:ARG:NH2	2.34	0.42
1:A:1819:VAL:HG21	1:A:1901:PRO:HB2	2.02	0.42
1:A:1911:GLN:HB2	1:A:2087:LEU:HD11	2.01	0.42
1:A:3862:GLN:HE21	1:A:3865:ASN:ND2	2.15	0.42
1:C:1847:GLU:HB2	1:C:1848:PRO:HD3	2.02	0.42
1:C:4576:ILE:HD13	1:C:4576:ILE:O	2.20	0.42
1:E:119:ILE:HD13	1:E:162:ILE:HD11	2.02	0.42
1:G:718:VAL:HG22	1:G:791:VAL:HG13	2.00	0.42
1:G:2123:LEU:HD12	1:G:2127:ARG:NH1	2.35	0.42
1:A:2513:MET:O	1:A:2517:LEU:HD13	2.20	0.42
1:A:3756:VAL:HG13	1:A:3836:PHE:CE1	2.54	0.42
1:E:2420:ILE:O	1:E:2424:LEU:HD13	2.20	0.42
1:G:1819:VAL:HG21	1:G:1901:PRO:HB2	2.01	0.42
1:G:2106:TYR:CG	1:G:2107:THR:N	2.88	0.42
1:A:766:ILE:HB	1:A:779:PHE:HB2	2.02	0.41
1:C:646:THR:HG23	1:C:1684:GLN:NE2	2.35	0.41
1:C:4147:GLU:OE1	1:C:4938:GLN:NE2	2.53	0.41
1:E:1795:LEU:HD11	1:E:1825:PHE:HB2	2.01	0.41
1:E:3907:PHE:HE2	1:E:3972:LEU:HD21	1.85	0.41
1:A:207:PHE:CE2	1:C:2326:ILE:HD12	2.54	0.41
1:A:659:ILE:HD12	1:A:659:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3742:LEU:HD11	1:E:3778:MET:HG2	2.02	0.41
1:E:3911:ILE:HD11	1:E:3975:LEU:HD22	2.02	0.41
1:A:119:ILE:HG21	1:A:162:ILE:HD11	2.00	0.41
1:A:1096:VAL:HG13	1:A:1101:TRP:CD1	2.55	0.41
1:A:3952:PHE:HZ	1:A:3975:LEU:HD23	1.84	0.41
1:C:1629:SER:HA	1:C:1640:ASP:HA	2.02	0.41
1:C:1707:ILE:HD11	1:C:1824:LEU:HA	2.02	0.41
1:C:1828:LEU:HD23	1:C:1834:PHE:HZ	1.84	0.41
1:E:4833:ILE:HD13	1:E:4845:ARG:NH1	2.35	0.41
1:G:1761:MET:HB2	1:G:1776:TYR:CD2	2.55	0.41
1:G:2354:ILE:HG23	1:G:2386:GLY:HA3	2.02	0.41
1:G:4097:PHE:O	1:G:4101:VAL:HG23	2.20	0.41
1:A:28:ILE:CG1	1:A:201:LEU:HD11	2.50	0.41
1:A:49:LEU:HD11	1:A:194:LEU:HD21	2.03	0.41
1:A:657:PRO:CB	1:A:804:LEU:HD11	2.50	0.41
1:A:3966:ILE:O	1:A:3969:LEU:N	2.54	0.41
1:C:679:VAL:HA	1:C:800:VAL:HG12	2.02	0.41
1:C:1604:LEU:HD21	1:C:1627:PHE:HE1	1.86	0.41
1:E:1703:TYR:HB2	1:E:1820:PRO:HB3	2.02	0.41
1:E:1819:VAL:HG21	1:E:1901:PRO:HB2	2.02	0.41
1:E:3862:GLN:HG2	1:E:3865:ASN:HD22	1.85	0.41
1:G:1847:GLU:HB2	1:G:1848:PRO:HD3	2.03	0.41
1:A:476:GLN:HA	1:A:476:GLN:HE21	1.84	0.41
1:A:4639:THR:HG22	1:A:4641:SER:H	1.85	0.41
1:C:594:ILE:HD12	1:C:631:LEU:HD22	2.02	0.41
1:E:306:LEU:HD11	1:E:314:LEU:HD22	2.03	0.41
1:E:4049:PHE:HE2	1:E:4067:LEU:HD13	1.85	0.41
1:G:1685:LEU:HD22	1:G:1709:ILE:HD11	2.01	0.41
1:G:3862:GLN:HE21	1:G:3865:ASN:ND2	2.14	0.41
1:A:425:LEU:HD13	1:A:452:VAL:HG22	2.03	0.41
1:A:579:LEU:HD22	1:A:586:LEU:HD23	2.02	0.41
1:A:1629:SER:HA	1:A:1640:ASP:HA	2.03	0.41
1:A:4869:ILE:HG21	1:C:4869:ILE:HG23	2.01	0.41
2:B:66:MET:SD	2:B:74:LEU:HD21	2.60	0.41
1:C:648:LEU:HD23	1:C:1684:GLN:HA	2.02	0.41
1:C:3693:ALA:HB3	1:C:3758:ALA:HB1	2.02	0.41
1:E:4012:GLU:HG3	1:E:4122:LEU:HD21	2.03	0.41
1:E:4823:VAL:HG23	1:E:4824:ARG:HG3	2.02	0.41
1:G:4135:GLY:HA3	1:G:4151:PHE:CZ	2.55	0.41
1:A:4097:PHE:O	1:A:4101:VAL:HG23	2.21	0.41
1:A:4135:GLY:HA3	1:A:4151:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:VAL:CG1	1:C:217:ILE:HD11	2.51	0.41
1:C:165:ALA:HB3	1:C:211:LEU:HD21	2.02	0.41
1:C:2081:VAL:HG23	1:C:3671:LEU:HD12	2.03	0.41
1:E:42:PHE:CG	1:E:418:VAL:HG22	2.56	0.41
1:E:996:VAL:CG1	1:E:1054:VAL:HG11	2.51	0.41
1:G:1795:LEU:HD11	1:G:1825:PHE:CD1	2.55	0.41
1:G:2861:LEU:HD22	1:G:2872:LEU:CD1	2.51	0.41
1:G:3908:SER:HA	1:G:3911:ILE:HG22	2.01	0.41
1:A:4781:TYR:HA	1:A:4784:THR:HG22	2.02	0.41
1:C:572:LEU:HD13	1:C:609:LYS:CB	2.51	0.41
1:E:1730:THR:O	1:E:1733:THR:OG1	2.37	0.41
1:E:1772:ASN:N	1:E:1772:ASN:HD22	2.19	0.41
1:A:555:LEU:HD13	1:A:578:VAL:HG11	2.03	0.41
1:A:679:VAL:HA	1:A:800:VAL:HG12	2.02	0.41
1:A:933:LEU:O	1:A:937:LEU:HB2	2.21	0.41
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	2.02	0.41
1:C:888:ASN:ND2	1:C:1056:THR:HG21	2.35	0.41
1:C:1749:PRO:HB3	1:C:2058:LEU:HD23	2.02	0.41
1:C:1795:LEU:HD11	1:C:1825:PHE:CG	2.55	0.41
1:C:3950:HIS:N	1:C:4010:ASN:HD21	2.19	0.41
1:E:598:ILE:HG23	1:E:642:LEU:HD22	2.02	0.41
1:E:3778:MET:CE	1:E:3847:LEU:HD22	2.51	0.41
1:E:4893:CYS:HG	1:E:4915:HIS:HE2	1.68	0.41
2:F:55:VAL:HG21	2:F:59:PHE:HD1	1.86	0.41
1:G:657:PRO:HG2	1:G:790:PRO:HG2	2.02	0.41
1:G:792:VAL:O	1:G:792:VAL:HG13	2.21	0.41
1:G:1751:ILE:HD13	1:G:1920:HIS:CE1	2.56	0.41
1:G:3956:GLN:HE21	1:G:4014:ILE:HG23	1.84	0.41
1:G:4893:CYS:HG	1:G:4915:HIS:HE2	1.68	0.41
1:G:4911:THR:O	1:G:4916:ASN:N	2.50	0.41
1:A:1910:LEU:HG	1:A:2062:ILE:HD12	2.02	0.41
1:C:207:PHE:CZ	1:E:2423:ILE:HD12	2.56	0.41
1:C:570:GLY:O	1:C:574:VAL:HG23	2.21	0.41
1:C:828:PRO:HG2	1:C:1037:LEU:HB3	2.03	0.41
1:C:4015:LEU:HD13	1:C:4123:ALA:HA	2.03	0.41
1:E:2029:LEU:HD21	1:E:3629:TRP:CE3	2.56	0.41
1:E:4120:LEU:HA	1:E:4123:ALA:HB3	2.03	0.41
1:E:4611:LYS:HB3	1:E:4617:LEU:HD23	2.03	0.41
1:E:4911:THR:O	1:E:4916:ASN:N	2.51	0.41
1:G:1831:MET:HE1	1:G:1833:ILE:HD13	2.02	0.41
1:G:3896:LYS:O	1:G:3898:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3992:VAL:HG13	1:A:4964:TYR:CZ	2.56	0.40
1:C:496:ASN:HA	1:C:499:LEU:HD12	2.02	0.40
1:C:1828:LEU:HD23	1:C:1834:PHE:CZ	2.56	0.40
1:C:2103:PRO:O	1:C:2164:ALA:HB1	2.20	0.40
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.86	0.40
1:C:4148:ARG:NH2	1:C:4914:GLU:OE2	2.54	0.40
1:C:4785:VAL:HG21	1:E:4742:ALA:CB	2.50	0.40
1:C:4923:PHE:HZ	1:C:4942:VAL:HG11	1.86	0.40
1:E:646:THR:HG23	1:E:1684:GLN:NE2	2.36	0.40
1:E:881:ILE:HD11	1:E:1060:TYR:CE2	2.56	0.40
1:E:2894:LEU:CD1	1:E:2897:LEU:HD12	2.52	0.40
1:G:463:PHE:HB3	1:G:539:ALA:HB1	2.03	0.40
1:G:465:PRO:HA	1:G:466:PRO:HD3	1.96	0.40
1:G:1686:LEU:HD22	1:G:1790:LYS:HE3	2.02	0.40
1:A:207:PHE:CD2	1:C:2326:ILE:HD12	2.56	0.40
1:C:1686:LEU:HD22	1:C:1790:LYS:HE3	2.04	0.40
1:C:2159:PRO:CB	1:C:2206:ILE:HD12	2.49	0.40
1:C:2221:LEU:HD21	1:C:2242:VAL:HB	2.03	0.40
1:C:3966:ILE:O	1:C:3969:LEU:N	2.54	0.40
2:D:75:THR:HG23	2:D:98:ILE:CD1	2.51	0.40
1:E:3841:PHE:HB3	1:E:3920:THR:HG21	2.04	0.40
1:G:447:LEU:HD21	1:G:522:ALA:HB2	2.03	0.40
1:G:572:LEU:HD13	1:G:609:LYS:CB	2.51	0.40
1:G:1629:SER:HA	1:G:1640:ASP:HA	2.03	0.40
1:G:1828:LEU:HD23	1:G:1834:PHE:HZ	1.86	0.40
1:C:572:LEU:HD22	1:C:609:LYS:HB3	2.04	0.40
1:E:1828:LEU:HD23	1:E:1834:PHE:HZ	1.87	0.40
1:A:465:PRO:HA	1:A:466:PRO:HD3	1.97	0.40
1:A:1268:ILE:O	1:A:1268:ILE:HG23	2.21	0.40
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	2.03	0.40
1:C:611:LEU:HB2	1:C:1659:ARG:HG3	2.02	0.40
1:C:1686:LEU:HD22	1:C:1790:LYS:HD2	2.02	0.40
1:C:2713:ILE:HD13	1:C:2714:ILE:N	2.36	0.40
1:C:2894:LEU:HD11	1:C:2904:VAL:HG21	2.04	0.40
1:C:3908:SER:HA	1:C:3911:ILE:HG22	2.02	0.40
1:C:4097:PHE:O	1:C:4101:VAL:HG23	2.22	0.40
1:C:4165:GLN:HG3	1:C:4501:TYR:CZ	2.57	0.40
1:C:4794:PHE:CB	1:C:4833:ILE:HD11	2.52	0.40
1:E:763:ALA:HB3	1:E:765:SER:H	1.86	0.40
2:H:82:TYR:CD2	2:H:91:ILE:HG21	2.56	0.40
1:A:1782:PHE:CZ	1:A:1787:LEU:HD22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2241:ASP:OD1	1:A:2242:VAL:N	2.55	0.40
1:A:2713:ILE:HD13	1:A:2714:ILE:N	2.36	0.40
2:B:4:ILE:HD12	2:B:74:LEU:HD22	2.03	0.40
1:C:4843:ILE:O	1:C:4846:ILE:HG22	2.22	0.40
2:D:30:LEU:O	2:D:32:ASN:N	2.55	0.40
1:E:217:ILE:HG22	1:E:286:GLY:HA3	2.03	0.40
1:E:737:ILE:HD13	1:E:1535:PRO:HG3	2.04	0.40
1:E:1706:LEU:O	1:E:1706:LEU:HD13	2.22	0.40
1:E:4651:VAL:O	1:E:4655:VAL:HG23	2.22	0.40
1:G:4573:THR:HA	1:G:4576:ILE:HG22	2.03	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	3065/4387 (70%)	2784 (91%)	217 (7%)	64 (2%)	7	36
1	C	3065/4387 (70%)	2773 (90%)	236 (8%)	56 (2%)	8	40
1	E	3065/4387 (70%)	2765 (90%)	238 (8%)	62 (2%)	7	38
1	G	3065/4387 (70%)	2789 (91%)	211 (7%)	65 (2%)	7	36
2	B	105/158 (66%)	97 (92%)	7 (7%)	1 (1%)	15	55
2	D	105/158 (66%)	96 (91%)	8 (8%)	1 (1%)	15	55
2	F	105/158 (66%)	97 (92%)	6 (6%)	2 (2%)	8	38
2	H	105/158 (66%)	97 (92%)	8 (8%)	0	100	100
All	All	12680/18180 (70%)	11498 (91%)	931 (7%)	251 (2%)	11	38

All (251) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	HIS
1	A	1476	VAL
1	A	1549	SER
1	A	1779	SER
1	A	3897	ASP
1	A	3992	VAL
1	A	4916	ASN
1	A	4917	LEU
1	C	472	HIS
1	C	1476	VAL
1	C	1549	SER
1	C	1779	SER
1	C	3897	ASP
1	C	4916	ASN
2	D	31	GLN
1	E	837	SER
1	E	855	VAL
1	E	1549	SER
1	E	1590	PHE
1	E	1779	SER
1	E	3897	ASP
1	E	3992	VAL
1	E	4916	ASN
1	E	4917	LEU
1	E	4959	CYS
1	G	472	HIS
1	G	837	SER
1	G	855	VAL
1	G	1549	SER
1	G	1639	VAL
1	G	1779	SER
1	G	3897	ASP
1	G	4916	ASN
1	G	4917	LEU
1	G	4959	CYS
1	A	250	GLY
1	A	838	ARG
1	A	855	VAL
1	A	901	GLY
1	A	1191	ALA
1	A	1535	PRO
1	A	1639	VAL
1	A	1737	THR

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Mol	Chain	Res	Type
1	A	4751	GLY
1	A	4959	CYS
1	C	855	VAL
1	C	901	GLY
1	C	906	PRO
1	C	1267	HIS
1	C	1535	PRO
1	C	1639	VAL
1	C	1681	ASP
1	C	1737	THR
1	C	1755	THR
1	C	2795	GLU
1	C	2797	ASP
1	C	3992	VAL
1	C	4917	LEU
1	C	4959	CYS
1	E	350	GLY
1	E	836	HIS
1	E	838	ARG
1	E	1191	ALA
1	E	1476	VAL
1	E	1667	LEU
1	E	1681	ASP
1	E	1737	THR
1	E	1755	THR
1	E	4038	PRO
1	G	188	SER
1	G	350	GLY
1	G	716	ASN
1	G	838	ARG
1	G	901	GLY
1	G	1191	ALA
1	G	1218	GLY
1	G	1456	GLY
1	G	1476	VAL
1	G	1535	PRO
1	G	1681	ASP
1	G	1755	THR
1	G	3992	VAL
1	A	359	SER
1	A	716	ASN
1	A	1667	LEU

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Mol	Chain	Res	Type
1	A	1681	ASP
1	A	1755	THR
1	A	2106	TYR
1	A	2864	LYS
1	A	4038	PRO
1	A	4112	ASN
1	C	224	ALA
1	C	838	ARG
1	C	1191	ALA
1	C	1590	PHE
1	C	1667	LEU
1	C	2106	TYR
1	C	4112	ASN
1	C	4957	GLY
1	E	716	ASN
1	E	901	GLY
1	E	1639	VAL
1	E	4112	ASN
2	F	31	GLN
1	G	224	ALA
1	G	906	PRO
1	G	1219	LYS
1	G	1231	GLY
1	G	1590	PHE
1	G	1667	LEU
1	G	2106	TYR
1	G	2797	ASP
1	G	4112	ASN
1	A	224	ALA
1	A	641	ASP
1	A	642	LEU
1	A	669	GLN
1	A	837	SER
1	A	1218	GLY
1	A	1472	GLU
1	A	1725	PHE
1	A	1758	ARG
1	A	1834	PHE
1	A	2074	VAL
1	A	2077	ASP
1	A	4056	HIS
1	C	350	GLY

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Mol	Chain	Res	Type
1	C	620	CYS
1	C	847	THR
1	C	1231	GLY
1	C	1604	LEU
1	C	1758	ARG
1	C	2077	ASP
1	C	2710	SER
1	E	63	SER
1	E	224	ALA
1	E	472	HIS
1	E	1210	ALA
1	E	1535	PRO
1	E	1536	SER
1	E	1758	ARG
1	E	1770	SER
1	E	2074	VAL
1	E	2077	ASP
1	E	2106	TYR
1	E	2797	ASP
1	E	3686	ASP
2	F	32	ASN
1	G	467	ASP
1	G	642	LEU
1	G	836	HIS
1	G	847	THR
1	G	1725	PHE
1	G	1737	THR
1	G	2074	VAL
1	G	2077	ASP
1	G	2710	SER
1	G	3681	CYS
1	G	4056	HIS
1	G	4802	ASP
1	A	620	CYS
1	A	839	GLU
1	A	847	THR
1	A	871	GLN
1	A	1142	ALA
1	A	1267	HIS
1	A	2311	GLY
1	A	4164	PRO
1	A	4622	GLN

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Mol	Chain	Res	Type
1	C	641	ASP
1	C	642	LEU
1	C	837	SER
1	C	839	GLU
1	C	1210	ALA
1	C	1299	ILE
1	C	2074	VAL
1	C	3991	VAL
1	C	4622	GLN
1	E	685	PHE
1	E	829	LYS
1	E	839	GLU
1	E	1142	ALA
1	E	1231	GLY
1	E	1547	ALA
1	E	1604	LEU
1	E	3788	VAL
1	E	4056	HIS
1	E	4164	PRO
1	E	4181	GLY
1	E	4743	ALA
1	G	341	GLY
1	G	620	CYS
1	G	839	GLU
1	G	1299	ILE
1	G	1472	GLU
1	G	1758	ARG
1	G	1770	SER
1	G	1777	GLN
1	G	1834	PHE
1	G	4622	GLN
1	G	4751	GLY
1	G	4800	ASP
1	A	1299	ILE
1	A	4800	ASP
2	B	31	GLN
1	C	341	GLY
1	C	467	ASP
1	C	670	TYR
1	C	1194	ASP
1	C	1777	GLN
1	C	1810	VAL

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Mol	Chain	Res	Type
1	C	2311	GLY
1	E	777	GLY
1	E	847	THR
1	E	1267	HIS
1	E	1299	ILE
1	E	2311	GLY
1	E	3681	CYS
1	E	4622	GLN
1	G	1810	VAL
1	A	341	GLY
1	A	1231	GLY
1	A	1810	VAL
1	E	341	GLY
1	E	3991	VAL
1	G	2866	GLY
1	A	906	PRO
1	A	3991	VAL
1	A	4623	PRO
1	E	1810	VAL
1	G	3991	VAL
1	A	729	GLY
1	A	1198	GLY
1	A	4957	GLY
1	C	1218	GLY
1	C	4623	PRO
1	E	4623	PRO
1	G	4164	PRO
1	A	684	PRO
1	C	3788	VAL
1	E	4830	GLY
1	G	834	VAL
1	G	1533	VAL
1	G	4895	ILE
1	A	2865	GLY
1	A	3788	VAL
1	G	2311	GLY
1	G	1809	PRO
1	C	1809	PRO
1	A	1809	PRO
1	E	1809	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2774/3480 (80%)	2648 (96%)	126 (4%)	27	52
1	C	2774/3480 (80%)	2639 (95%)	135 (5%)	25	50
1	E	2774/3480 (80%)	2624 (95%)	150 (5%)	22	47
1	G	2774/3480 (80%)	2642 (95%)	132 (5%)	25	51
2	B	88/131 (67%)	87 (99%)	1 (1%)	73	84
2	D	88/131 (67%)	87 (99%)	1 (1%)	73	84
2	F	88/131 (67%)	87 (99%)	1 (1%)	73	84
2	H	88/131 (67%)	87 (99%)	1 (1%)	73	84
All	All	11448/14444 (79%)	10901 (95%)	547 (5%)	29	51

All (547) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	54	ASN
1	A	317	MET
1	A	336	GLU
1	A	342	VAL
1	A	392	ILE
1	A	424	PHE
1	A	441	LYS
1	A	462	TYR
1	A	476	GLN
1	A	542	ARG
1	A	551	PHE
1	A	559	ILE
1	A	563	GLU
1	A	572	LEU
1	A	604	HIS
1	A	608	HIS
1	A	609	LYS
1	A	643	LEU

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Mol	Chain	Res	Type
1	A	669	GLN
1	A	725	TYR
1	A	844	ARG
1	A	872	ILE
1	A	888	ASN
1	A	908	ARG
1	A	948	CYS
1	A	1031	ARG
1	A	1137	PHE
1	A	1193	LYS
1	A	1204	VAL
1	A	1287	GLN
1	A	1298	ASP
1	A	1302	TYR
1	A	1308	ILE
1	A	1447	THR
1	A	1450	PHE
1	A	1459	LEU
1	A	1533	VAL
1	A	1538	LYS
1	A	1553	PHE
1	A	1554	GLN
1	A	1595	LEU
1	A	1630	LEU
1	A	1657	THR
1	A	1671	ARG
1	A	1689	ILE
1	A	1697	LEU
1	A	1700	THR
1	A	1716	THR
1	A	1720	MET
1	A	1721	MET
1	A	1763	PHE
1	A	1771	ILE
1	A	1776	TYR
1	A	1777	GLN
1	A	1778	TYR
1	A	1779	SER
1	A	1794	MET
1	A	1804	LEU
1	A	1833	ILE
1	A	1897	LYS

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Mol	Chain	Res	Type
1	A	1898	LEU
1	A	1900	GLU
1	A	1910	LEU
1	A	1935	LYS
1	A	2023	LEU
1	A	2028	ARG
1	A	2066	MET
1	A	2126	ILE
1	A	2129	LEU
1	A	2179	LEU
1	A	2192	MET
1	A	2220	TYR
1	A	2354	ILE
1	A	2423	ILE
1	A	2466	LYS
1	A	2473	LEU
1	A	2474	ASP
1	A	2517	LEU
1	A	2713	ILE
1	A	2717	LYS
1	A	2723	ASN
1	A	2746	GLU
1	A	2747	ILE
1	A	2750	ASP
1	A	2762	LYS
1	A	2770	GLU
1	A	2843	GLU
1	A	2858	LYS
1	A	3675	THR
1	A	3690	MET
1	A	3728	GLN
1	A	3797	LEU
1	A	3844	LEU
1	A	3860	ARG
1	A	3911	ILE
1	A	3912	GLN
1	A	3929	CYS
1	A	3956	GLN
1	A	3962	ASP
1	A	3969	LEU
1	A	3970	LYS
1	A	3992	VAL

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Mol	Chain	Res	Type
1	A	4065	GLU
1	A	4078	THR
1	A	4154	SER
1	A	4170	LYS
1	A	4172	GLN
1	A	4186	LYS
1	A	4188	GLU
1	A	4192	ASN
1	A	4491	LYS
1	A	4573	THR
1	A	4576	ILE
1	A	4584	ILE
1	A	4622	GLN
1	A	4637	ILE
1	A	4670	GLU
1	A	4730	MET
1	A	4752	PHE
1	A	4807	LYS
1	A	4855	PHE
1	A	4860	LEU
1	A	4885	ASP
1	A	4925	MET
1	A	4927	LEU
2	B	34	LYS
1	C	15	ARG
1	C	54	ASN
1	C	180	ASP
1	C	190	ARG
1	C	317	MET
1	C	321	LYS
1	C	336	GLU
1	C	342	VAL
1	C	392	ILE
1	C	441	LYS
1	C	476	GLN
1	C	542	ARG
1	C	563	GLU
1	C	572	LEU
1	C	608	HIS
1	C	609	LYS
1	C	643	LEU
1	C	647	ARG

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Mol	Chain	Res	Type
1	C	669	GLN
1	C	683	GLU
1	C	725	TYR
1	C	835	GLU
1	C	844	ARG
1	C	848	ARG
1	C	872	ILE
1	C	880	ARG
1	C	888	ASN
1	C	908	ARG
1	C	948	CYS
1	C	1028	ARG
1	C	1031	ARG
1	C	1133	ARG
1	C	1193	LYS
1	C	1243	THR
1	C	1287	GLN
1	C	1308	ILE
1	C	1447	THR
1	C	1450	PHE
1	C	1459	LEU
1	C	1533	VAL
1	C	1538	LYS
1	C	1553	PHE
1	C	1637	ARG
1	C	1657	THR
1	C	1660	LEU
1	C	1671	ARG
1	C	1692	LYS
1	C	1697	LEU
1	C	1720	MET
1	C	1761	MET
1	C	1763	PHE
1	C	1771	ILE
1	C	1772	ASN
1	C	1777	GLN
1	C	1778	TYR
1	C	1804	LEU
1	C	1897	LYS
1	C	1908	LEU
1	C	1910	LEU
1	C	1919	ARG

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Mol	Chain	Res	Type
1	C	1925	ILE
1	C	1935	LYS
1	C	2023	LEU
1	C	2028	ARG
1	C	2032	LEU
1	C	2036	VAL
1	C	2077	ASP
1	C	2099	VAL
1	C	2126	ILE
1	C	2129	LEU
1	C	2139	GLU
1	C	2192	MET
1	C	2220	TYR
1	C	2298	ARG
1	C	2354	ILE
1	C	2399	LEU
1	C	2423	ILE
1	C	2517	LEU
1	C	2713	ILE
1	C	2717	LYS
1	C	2723	ASN
1	C	2747	ILE
1	C	2750	ASP
1	C	2762	LYS
1	C	2770	GLU
1	C	2795	GLU
1	C	2858	LYS
1	C	2861	LEU
1	C	3616	ARG
1	C	3662	VAL
1	C	3675	THR
1	C	3690	MET
1	C	3728	GLN
1	C	3797	LEU
1	C	3801	CYS
1	C	3860	ARG
1	C	3866	ASN
1	C	3876	VAL
1	C	3887	SER
1	C	3911	ILE
1	C	3912	GLN
1	C	3926	GLN

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Mol	Chain	Res	Type
1	C	3929	CYS
1	C	3951	VAL
1	C	3962	ASP
1	C	3969	LEU
1	C	3970	LYS
1	C	3979	MET
1	C	3992	VAL
1	C	4032	THR
1	C	4065	GLU
1	C	4117	GLN
1	C	4120	LEU
1	C	4152	GLU
1	C	4167	LYS
1	C	4170	LYS
1	C	4178	VAL
1	C	4186	LYS
1	C	4188	GLU
1	C	4192	ASN
1	C	4200	GLU
1	C	4494	ASN
1	C	4576	ILE
1	C	4584	ILE
1	C	4622	GLN
1	C	4637	ILE
1	C	4730	MET
1	C	4752	PHE
1	C	4807	LYS
1	C	4840	GLU
1	C	4860	LEU
1	C	4865	GLN
1	C	4875	LEU
1	C	4882	VAL
1	C	4885	ASP
2	D	34	LYS
1	E	15	ARG
1	E	18	ASP
1	E	54	ASN
1	E	143	LEU
1	E	179	ASP
1	E	180	ASP
1	E	198	ASN
1	E	313	ASN

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Mol	Chain	Res	Type
1	E	317	MET
1	E	336	GLU
1	E	342	VAL
1	E	374	TYR
1	E	392	ILE
1	E	424	PHE
1	E	441	LYS
1	E	462	TYR
1	E	476	GLN
1	E	542	ARG
1	E	551	PHE
1	E	559	ILE
1	E	562	LEU
1	E	563	GLU
1	E	572	LEU
1	E	589	ILE
1	E	608	HIS
1	E	609	LYS
1	E	643	LEU
1	E	669	GLN
1	E	701	GLU
1	E	725	TYR
1	E	739	ARG
1	E	795	SER
1	E	872	ILE
1	E	888	ASN
1	E	908	ARG
1	E	934	GLN
1	E	1031	ARG
1	E	1193	LYS
1	E	1204	VAL
1	E	1219	LYS
1	E	1232	LEU
1	E	1264	ASN
1	E	1266	GLU
1	E	1287	GLN
1	E	1298	ASP
1	E	1308	ILE
1	E	1447	THR
1	E	1459	LEU
1	E	1482	ARG
1	E	1533	VAL

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Mol	Chain	Res	Type
1	E	1538	LYS
1	E	1553	PHE
1	E	1570	LEU
1	E	1630	LEU
1	E	1657	THR
1	E	1671	ARG
1	E	1677	CYS
1	E	1697	LEU
1	E	1700	THR
1	E	1716	THR
1	E	1720	MET
1	E	1761	MET
1	E	1763	PHE
1	E	1771	ILE
1	E	1772	ASN
1	E	1777	GLN
1	E	1778	TYR
1	E	1779	SER
1	E	1790	LYS
1	E	1794	MET
1	E	1804	LEU
1	E	1897	LYS
1	E	1898	LEU
1	E	1916	CYS
1	E	1921	ARG
1	E	1935	LYS
1	E	2023	LEU
1	E	2028	ARG
1	E	2032	LEU
1	E	2058	LEU
1	E	2061	LEU
1	E	2066	MET
1	E	2081	VAL
1	E	2099	VAL
1	E	2126	ILE
1	E	2129	LEU
1	E	2175	MET
1	E	2179	LEU
1	E	2192	MET
1	E	2220	TYR
1	E	2326	ILE
1	E	2354	ILE

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Mol	Chain	Res	Type
1	E	2399	LEU
1	E	2423	ILE
1	E	2462	CYS
1	E	2511	THR
1	E	2517	LEU
1	E	2713	ILE
1	E	2717	LYS
1	E	2723	ASN
1	E	2746	GLU
1	E	2747	ILE
1	E	2750	ASP
1	E	2762	LYS
1	E	2770	GLU
1	E	2795	GLU
1	E	2858	LYS
1	E	2861	LEU
1	E	2864	LYS
1	E	3671	LEU
1	E	3675	THR
1	E	3690	MET
1	E	3728	GLN
1	E	3801	CYS
1	E	3860	ARG
1	E	3911	ILE
1	E	3912	GLN
1	E	3926	GLN
1	E	3929	CYS
1	E	3951	VAL
1	E	3959	LEU
1	E	3962	ASP
1	E	3969	LEU
1	E	3970	LYS
1	E	3979	MET
1	E	3992	VAL
1	E	4033	PHE
1	E	4065	GLU
1	E	4117	GLN
1	E	4120	LEU
1	E	4170	LYS
1	E	4186	LYS
1	E	4192	ASN
1	E	4491	LYS

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Mol	Chain	Res	Type
1	E	4573	THR
1	E	4576	ILE
1	E	4584	ILE
1	E	4596	LYS
1	E	4620	THR
1	E	4622	GLN
1	E	4637	ILE
1	E	4722	LEU
1	E	4730	MET
1	E	4752	PHE
1	E	4807	LYS
1	E	4840	GLU
1	E	4865	GLN
1	E	4876	ARG
1	E	4885	ASP
1	E	4927	LEU
2	F	34	LYS
1	G	15	ARG
1	G	18	ASP
1	G	54	ASN
1	G	180	ASP
1	G	238	HIS
1	G	317	MET
1	G	342	VAL
1	G	373	THR
1	G	392	ILE
1	G	417	ARG
1	G	424	PHE
1	G	441	LYS
1	G	462	TYR
1	G	476	GLN
1	G	542	ARG
1	G	551	PHE
1	G	558	LEU
1	G	563	GLU
1	G	572	LEU
1	G	575	LEU
1	G	604	HIS
1	G	609	LYS
1	G	643	LEU
1	G	680	ASP
1	G	725	TYR

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Mol	Chain	Res	Type
1	G	739	ARG
1	G	851	LEU
1	G	872	ILE
1	G	888	ASN
1	G	908	ARG
1	G	948	CYS
1	G	1027	ARG
1	G	1031	ARG
1	G	1137	PHE
1	G	1189	GLU
1	G	1193	LYS
1	G	1232	LEU
1	G	1259	LEU
1	G	1287	GLN
1	G	1298	ASP
1	G	1308	ILE
1	G	1447	THR
1	G	1459	LEU
1	G	1465	VAL
1	G	1533	VAL
1	G	1538	LYS
1	G	1553	PHE
1	G	1554	GLN
1	G	1643	GLU
1	G	1657	THR
1	G	1671	ARG
1	G	1677	CYS
1	G	1697	LEU
1	G	1720	MET
1	G	1721	MET
1	G	1761	MET
1	G	1763	PHE
1	G	1771	ILE
1	G	1772	ASN
1	G	1778	TYR
1	G	1804	LEU
1	G	1897	LYS
1	G	1898	LEU
1	G	1910	LEU
1	G	1919	ARG
1	G	1925	ILE
1	G	2023	LEU

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Mol	Chain	Res	Type
1	G	2028	ARG
1	G	2036	VAL
1	G	2058	LEU
1	G	2066	MET
1	G	2077	ASP
1	G	2086	VAL
1	G	2117	ILE
1	G	2126	ILE
1	G	2129	LEU
1	G	2179	LEU
1	G	2192	MET
1	G	2220	TYR
1	G	2328	ARG
1	G	2354	ILE
1	G	2399	LEU
1	G	2423	ILE
1	G	2426	SER
1	G	2511	THR
1	G	2517	LEU
1	G	2522	CYS
1	G	2713	ILE
1	G	2717	LYS
1	G	2723	ASN
1	G	2746	GLU
1	G	2747	ILE
1	G	2750	ASP
1	G	2762	LYS
1	G	2770	GLU
1	G	2795	GLU
1	G	2838	LEU
1	G	2861	LEU
1	G	3675	THR
1	G	3690	MET
1	G	3728	GLN
1	G	3801	CYS
1	G	3860	ARG
1	G	3866	ASN
1	G	3911	ILE
1	G	3912	GLN
1	G	3926	GLN
1	G	3929	CYS
1	G	3962	ASP

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Mol	Chain	Res	Type
1	G	3970	LYS
1	G	3992	VAL
1	G	4012	GLU
1	G	4050	HIS
1	G	4065	GLU
1	G	4117	GLN
1	G	4126	VAL
1	G	4170	LYS
1	G	4186	LYS
1	G	4188	GLU
1	G	4192	ASN
1	G	4196	ASP
1	G	4576	ILE
1	G	4584	ILE
1	G	4620	THR
1	G	4622	GLN
1	G	4637	ILE
1	G	4640	GLN
1	G	4727	TYR
1	G	4730	MET
1	G	4807	LYS
1	G	4885	ASP
1	G	4927	LEU
2	H	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	375	GLN
1	A	476	GLN
1	A	486	GLN
1	A	487	ASN
1	A	496	ASN
1	A	547	ASN
1	A	669	GLN
1	A	692	HIS
1	A	746	GLN
1	A	888	ASN
1	A	956	HIS
1	A	1002	ASN
1	A	1046	ASN
1	A	1063	ASN

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Mol	Chain	Res	Type
1	A	1601	ASN
1	A	1684	GLN
1	A	1772	ASN
1	A	1773	ASN
1	A	1905	GLN
1	A	2152	ASN
1	A	2209	GLN
1	A	2891	GLN
1	A	3775	GLN
1	A	3865	ASN
1	A	3956	GLN
1	A	4010	ASN
1	A	4192	ASN
1	A	4515	ASN
1	A	4644	ASN
1	A	4738	ASN
1	A	4765	ASN
1	A	4818	HIS
1	A	4879	GLN
1	A	4919	ASN
2	B	25	HIS
2	B	65	GLN
1	C	54	ASN
1	C	364	GLN
1	C	476	GLN
1	C	487	ASN
1	C	496	ASN
1	C	547	ASN
1	C	669	GLN
1	C	692	HIS
1	C	771	ASN
1	C	888	ASN
1	C	956	HIS
1	C	1002	ASN
1	C	1772	ASN
1	C	1773	ASN
1	C	1905	GLN
1	C	2152	ASN
1	C	2224	ASN
1	C	2891	GLN
1	C	3775	GLN
1	C	3862	GLN

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Mol	Chain	Res	Type
1	C	3932	ASN
1	C	3956	GLN
1	C	3976	GLN
1	C	4010	ASN
1	C	4192	ASN
1	C	4644	ASN
1	C	4818	HIS
1	C	4879	GLN
1	C	4919	ASN
2	D	25	HIS
1	E	476	GLN
1	E	547	ASN
1	E	607	ASN
1	E	746	GLN
1	E	771	ASN
1	E	888	ASN
1	E	1002	ASN
1	E	1147	GLN
1	E	1601	ASN
1	E	1772	ASN
1	E	1773	ASN
1	E	1905	GLN
1	E	2091	GLN
1	E	2482	GLN
1	E	2848	ASN
1	E	3775	GLN
1	E	3865	ASN
1	E	3912	GLN
1	E	3926	GLN
1	E	3932	ASN
1	E	4192	ASN
1	E	4631	GLN
1	E	4644	ASN
1	E	4818	HIS
1	E	4919	ASN
2	F	25	HIS
1	G	33	GLN
1	G	54	ASN
1	G	476	GLN
1	G	487	ASN
1	G	544	ASN
1	G	547	ASN

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Mol	Chain	Res	Type
1	G	692	HIS
1	G	746	GLN
1	G	771	ASN
1	G	773	GLN
1	G	888	ASN
1	G	956	HIS
1	G	1002	ASN
1	G	1147	GLN
1	G	1601	ASN
1	G	1631	HIS
1	G	1691	ASN
1	G	1772	ASN
1	G	1773	ASN
1	G	2071	GLN
1	G	2091	GLN
1	G	2152	ASN
1	G	2848	ASN
1	G	2891	GLN
1	G	3775	GLN
1	G	3799	GLN
1	G	3865	ASN
1	G	3912	GLN
1	G	3916	GLN
1	G	3926	GLN
1	G	3932	ASN
1	G	3965	GLN
1	G	4010	ASN
1	G	4192	ASN
1	G	4768	GLN
1	G	4879	GLN
1	G	4919	ASN
2	H	25	HIS
2	H	65	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	27
1	G	27
1	E	27
1	A	27

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3612:UNK	C	3613:PRO	N	76.52
1	G	3612:UNK	C	3613:PRO	N	75.29
1	E	3612:UNK	C	3613:PRO	N	74.52
1	A	3612:UNK	C	3613:PRO	N	74.10
1	E	2701:UNK	C	2702:PHE	N	43.29
1	C	2701:UNK	C	2702:PHE	N	43.25
1	G	2701:UNK	C	2702:PHE	N	42.68
1	A	2701:UNK	C	2702:PHE	N	41.57
1	E	3589:UNK	C	3590:UNK	N	41.47
1	A	3589:UNK	C	3590:UNK	N	40.67
1	G	3589:UNK	C	3590:UNK	N	38.79
1	C	3589:UNK	C	3590:UNK	N	37.92
1	G	3436:UNK	C	3437:UNK	N	22.01
1	A	3347:GLY	C	3348:UNK	N	21.94
1	E	3347:GLY	C	3348:UNK	N	21.63
1	C	2529:LEU	C	2578:UNK	N	21.47
1	E	3436:UNK	C	3437:UNK	N	21.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3347:GLY	C	3348:UNK	N	21.29
1	E	2529:LEU	C	2578:UNK	N	20.68
1	G	3347:GLY	C	3348:UNK	N	20.37
1	C	3436:UNK	C	3437:UNK	N	20.35
1	A	2529:LEU	C	2578:UNK	N	20.28
1	A	3436:UNK	C	3437:UNK	N	20.21
1	A	2659:UNK	C	2660:UNK	N	19.56
1	G	2529:LEU	C	2578:UNK	N	19.18
1	G	2659:UNK	C	2660:UNK	N	18.25
1	E	1943:ARG	C	2008:UNK	N	18.00
1	G	1943:ARG	C	2008:UNK	N	17.56
1	C	3414:UNK	C	3415:UNK	N	17.36
1	G	3496:UNK	C	3497:UNK	N	17.23
1	E	3371:UNK	C	3372:UNK	N	17.18
1	A	1943:ARG	C	2008:UNK	N	17.12
1	E	2659:UNK	C	2660:UNK	N	16.94
1	G	3478:UNK	C	3479:UNK	N	16.94
1	G	1500:UNK	C	1501:ASN	N	16.90
1	E	3478:UNK	C	3479:UNK	N	16.86
1	C	3478:UNK	C	3479:UNK	N	16.82
1	A	3414:UNK	C	3415:UNK	N	16.74
1	C	1500:UNK	C	1501:ASN	N	16.69
1	E	2597:UNK	C	2598:UNK	N	16.38
1	C	2659:UNK	C	2660:UNK	N	16.36
1	C	1943:ARG	C	2008:UNK	N	16.33
1	E	3414:UNK	C	3415:UNK	N	16.18
1	C	3496:UNK	C	3497:UNK	N	16.05
1	E	1500:UNK	C	1501:ASN	N	16.00
1	A	3510:UNK	C	3511:UNK	N	15.98
1	A	1500:UNK	C	1501:ASN	N	15.96
1	C	2597:UNK	C	2598:UNK	N	15.85
1	G	3414:UNK	C	3415:UNK	N	15.79
1	C	2679:UNK	C	2680:UNK	N	15.57
1	A	3478:UNK	C	3479:UNK	N	15.52
1	G	3510:UNK	C	3511:UNK	N	15.50
1	E	2636:UNK	C	2637:UNK	N	15.08
1	G	3371:UNK	C	3372:UNK	N	15.08
1	G	2022:UNK	C	2023:LEU	N	14.88
1	A	3496:UNK	C	3497:UNK	N	14.87
1	E	3510:UNK	C	3511:UNK	N	14.76
1	A	2022:UNK	C	2023:LEU	N	14.71
1	A	2597:UNK	C	2598:UNK	N	14.71

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2022:UNK	C	2023:LEU	N	14.64
1	G	3548:UNK	C	3549:UNK	N	14.53
1	E	2022:UNK	C	2023:LEU	N	14.45
1	G	3571:UNK	C	3572:UNK	N	14.26
1	C	3510:UNK	C	3511:UNK	N	13.96
1	G	2679:UNK	C	2680:UNK	N	13.82
1	C	2636:UNK	C	2637:UNK	N	13.74
1	C	3571:UNK	C	3572:UNK	N	13.65
1	G	2636:UNK	C	2637:UNK	N	13.56
1	C	3371:UNK	C	3372:UNK	N	13.49
1	A	2679:UNK	C	2680:UNK	N	13.34
1	A	3548:UNK	C	3549:UNK	N	13.33
1	E	3496:UNK	C	3497:UNK	N	12.80
1	C	3528:UNK	C	3529:UNK	N	12.75
1	A	2636:UNK	C	2637:UNK	N	12.73
1	G	2597:UNK	C	2598:UNK	N	12.44
1	E	3528:UNK	C	3529:UNK	N	12.40
1	G	3391:UNK	C	3392:UNK	N	12.33
1	E	3571:UNK	C	3572:UNK	N	12.27
1	C	3548:UNK	C	3549:UNK	N	12.03
1	E	3457:UNK	C	3458:UNK	N	11.91
1	E	3391:UNK	C	3392:UNK	N	11.75
1	E	2679:UNK	C	2680:UNK	N	11.67
1	C	3457:UNK	C	3458:UNK	N	11.62
1	A	3528:UNK	C	3529:UNK	N	11.43
1	A	2460:UNK	C	2461:PHE	N	10.92
1	A	3571:UNK	C	3572:UNK	N	10.38
1	A	3371:UNK	C	3372:UNK	N	10.05
1	E	2460:UNK	C	2461:PHE	N	9.63
1	G	2460:UNK	C	2461:PHE	N	9.03
1	C	2460:UNK	C	2461:PHE	N	9.00
1	G	3528:UNK	C	3529:UNK	N	8.96
1	A	3457:UNK	C	3458:UNK	N	8.73
1	A	3391:UNK	C	3392:UNK	N	8.48
1	E	2616:UNK	C	2617:UNK	N	8.34
1	G	3457:UNK	C	3458:UNK	N	8.29
1	E	3548:UNK	C	3549:UNK	N	6.74
1	C	2616:UNK	C	2617:UNK	N	6.50
1	G	2616:UNK	C	2617:UNK	N	6.26
1	C	1484:ASN	C	1496:UNK	N	5.85
1	A	1484:ASN	C	1496:UNK	N	5.47
1	C	2427:LEU	C	2447:UNK	N	5.34

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2427:LEU	C	2447:UNK	N	5.15
1	G	1484:ASN	C	1496:UNK	N	4.71
1	A	2616:UNK	C	2617:UNK	N	4.70
1	C	3391:UNK	C	3392:UNK	N	4.48
1	A	2427:LEU	C	2447:UNK	N	4.21
1	E	1484:ASN	C	1496:UNK	N	4.12
1	G	2427:LEU	C	2447:UNK	N	3.84

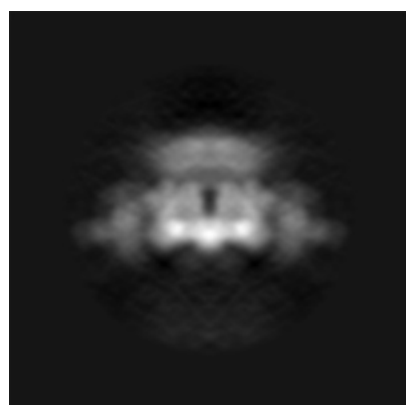
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8303. These allow visual inspection of the internal detail of the map and identification of artifacts.

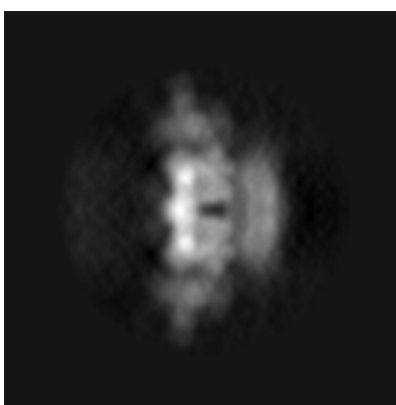
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

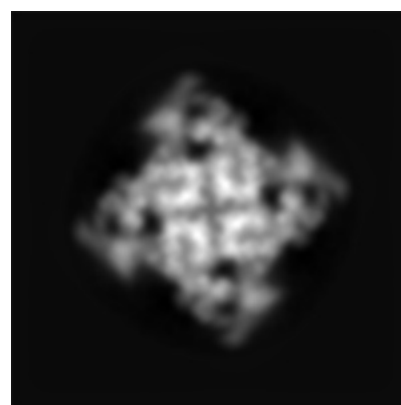
#### 6.1.1 Primary map



X



Y

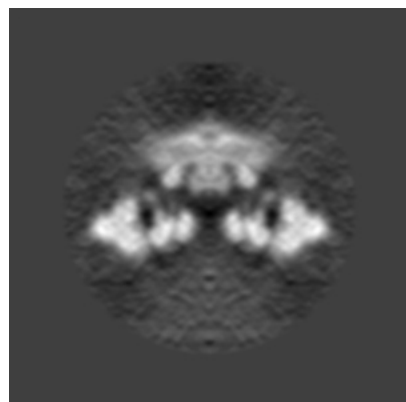


Z

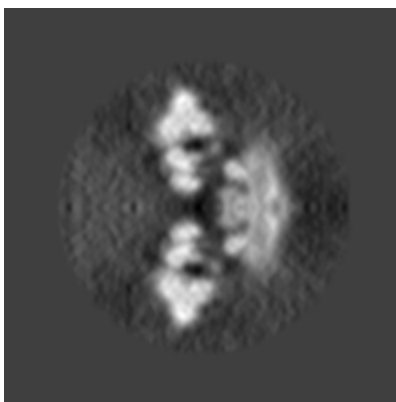
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

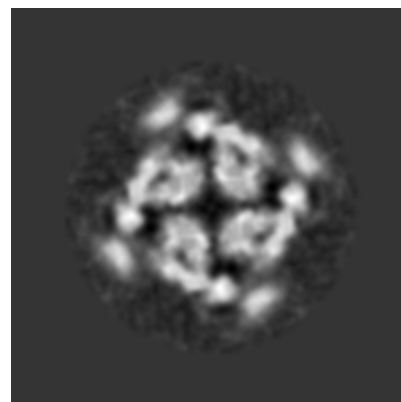
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



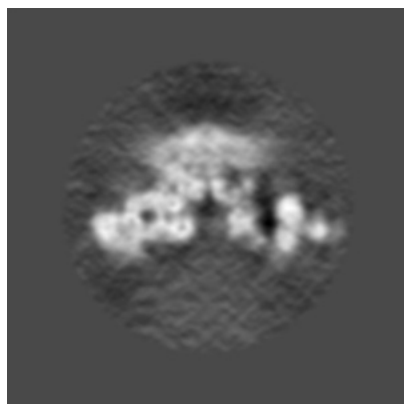
Z Index: 200



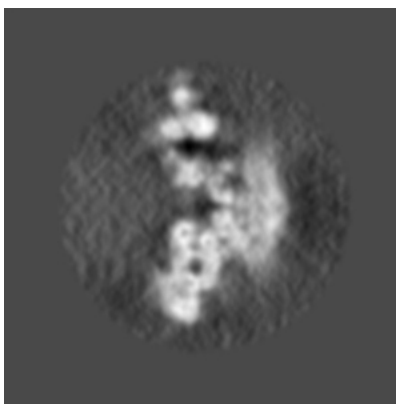
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

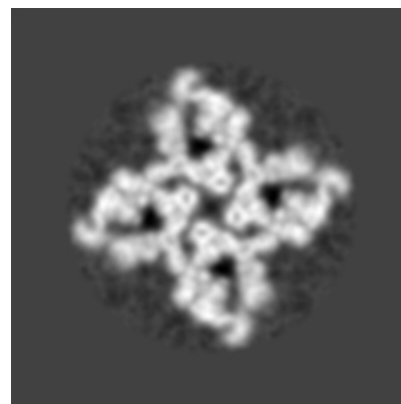
### 6.3.1 Primary map



X Index: 190



Y Index: 210

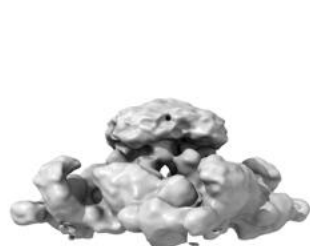


Z Index: 181

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

## 6.4 Orthogonal surface views [i](#)

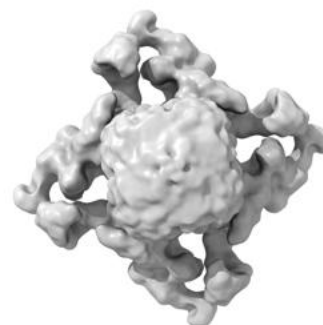
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

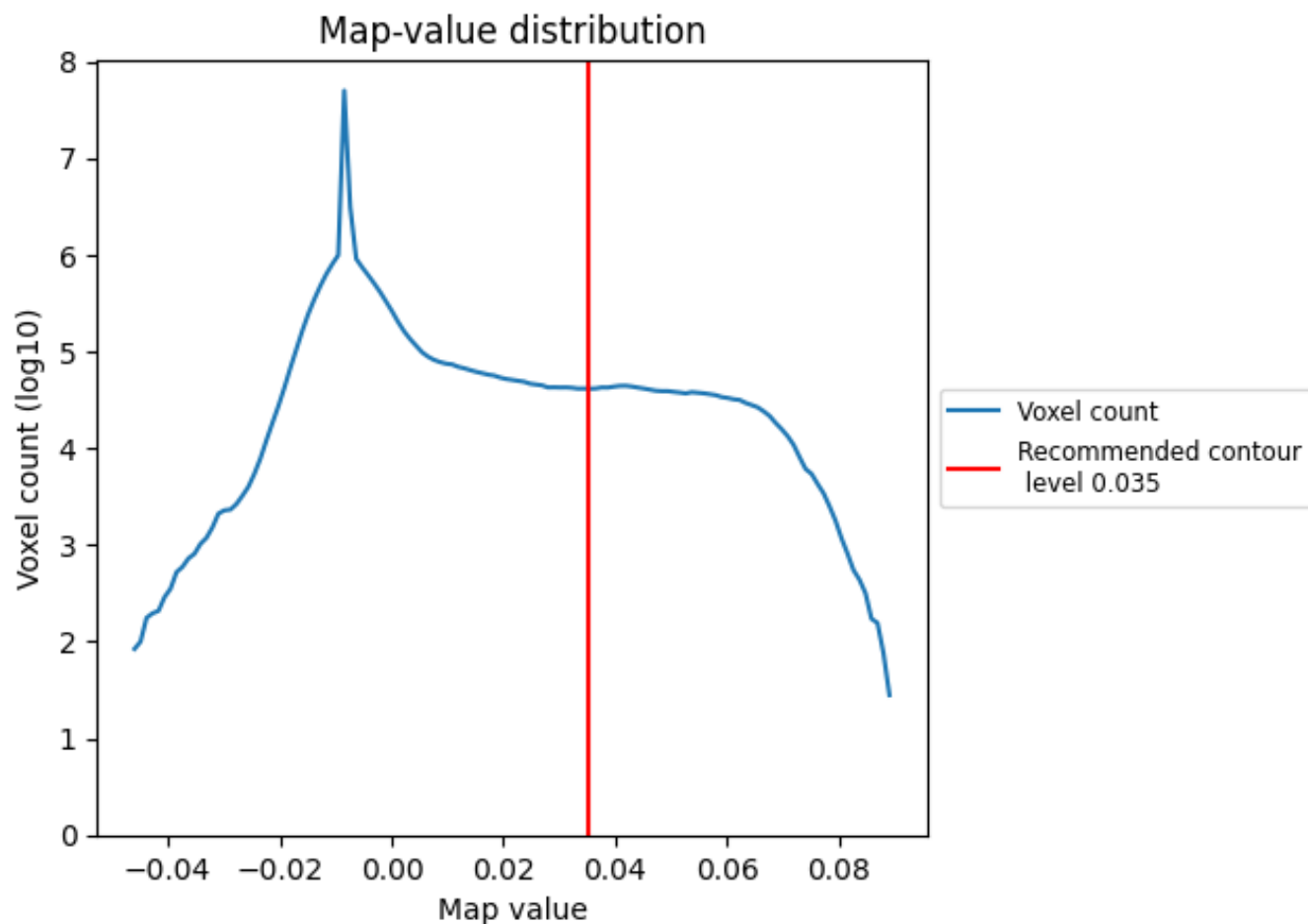
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

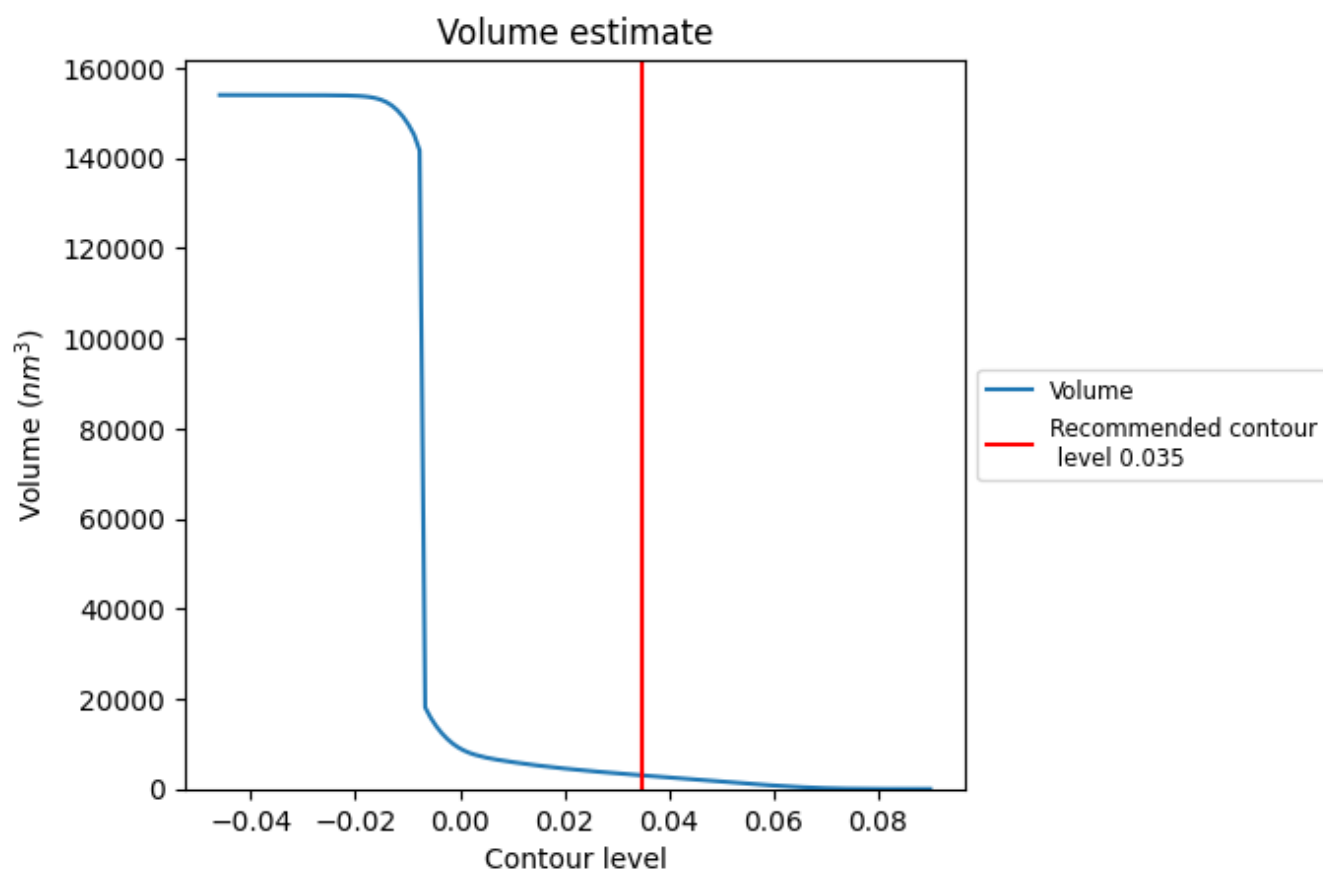
This section contains the results of statistical analysis of the map.

### 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.

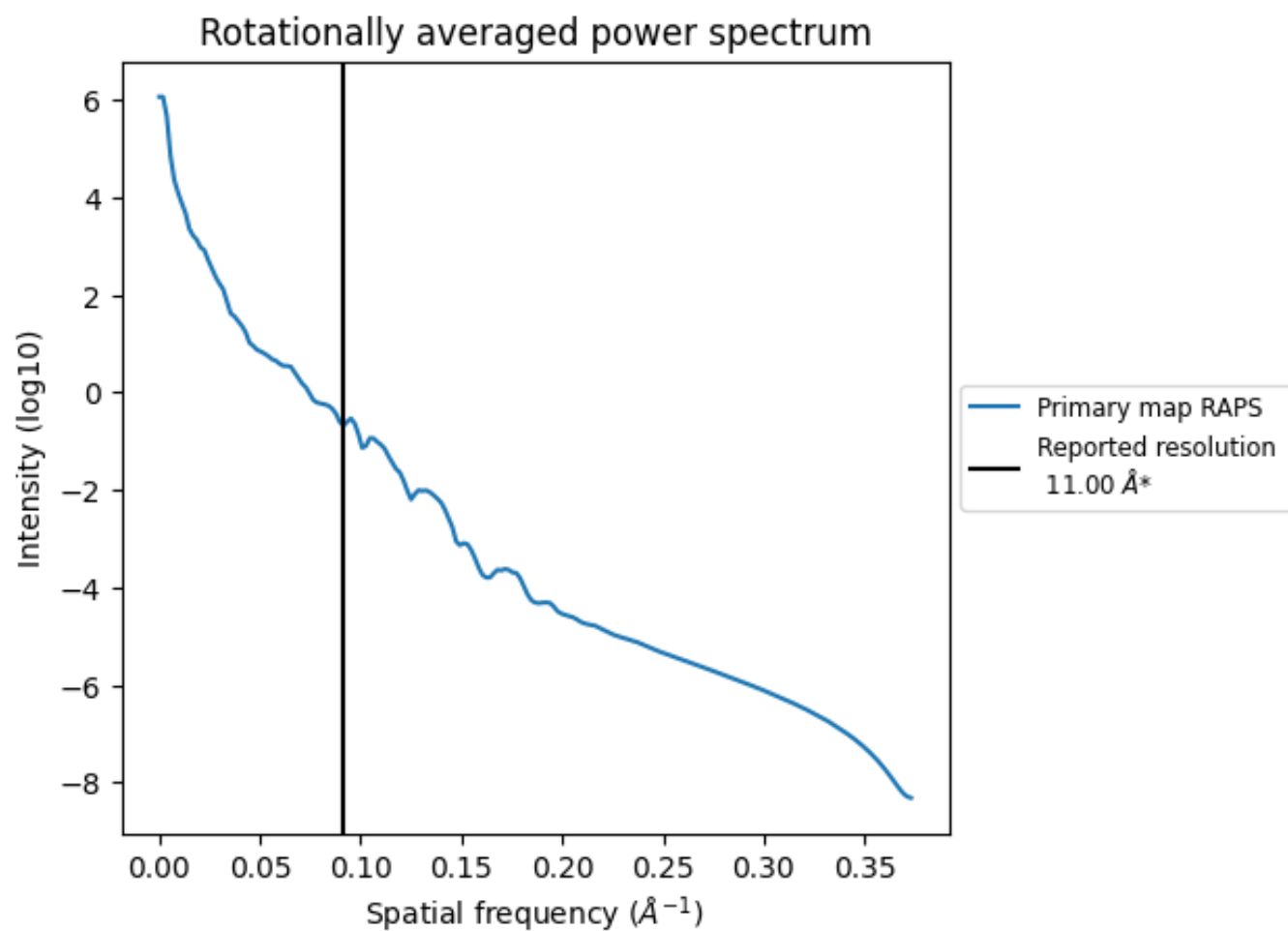
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3008 nm<sup>3</sup>; this corresponds to an approximate mass of 2718 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 0.091 Å<sup>-1</sup>

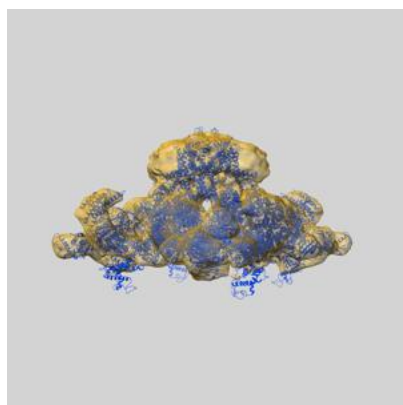
## 8 Fourier-Shell correlation ⓘ

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

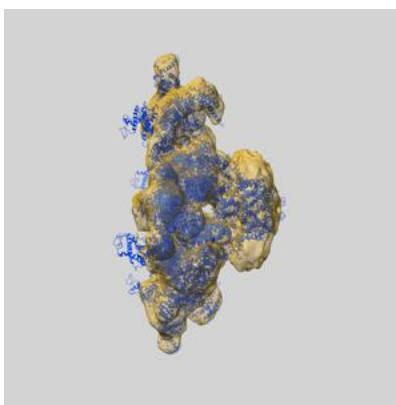
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8303 and PDB model 5L1D. Per-residue inclusion information can be found in section [3](#) on page [9](#).

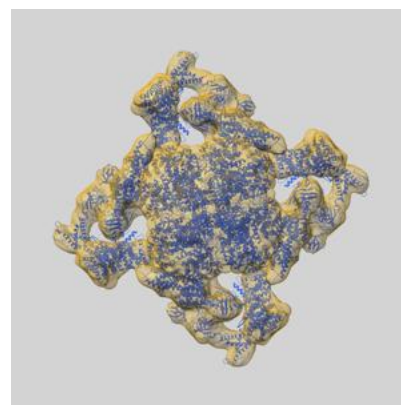
### 9.1 Map-model overlay [i](#)



X



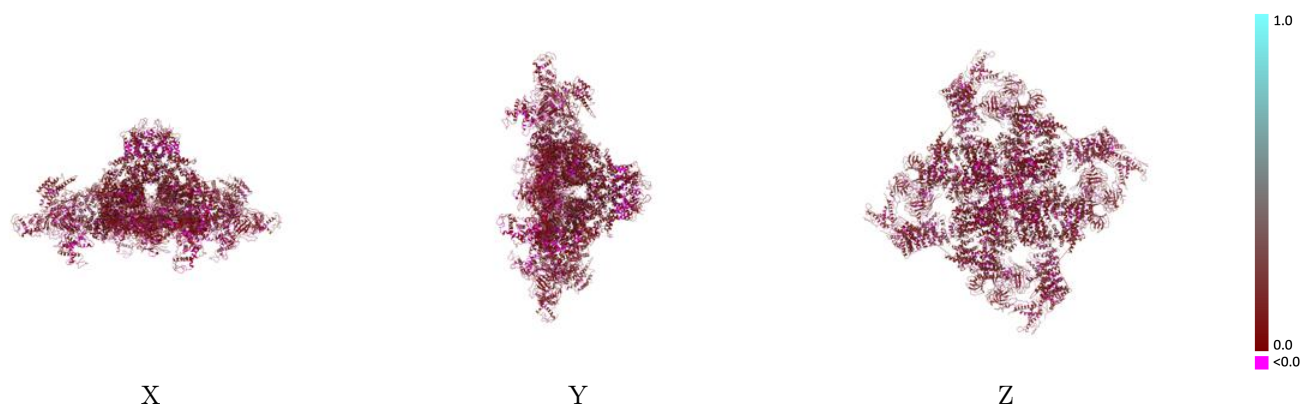
Y



Z

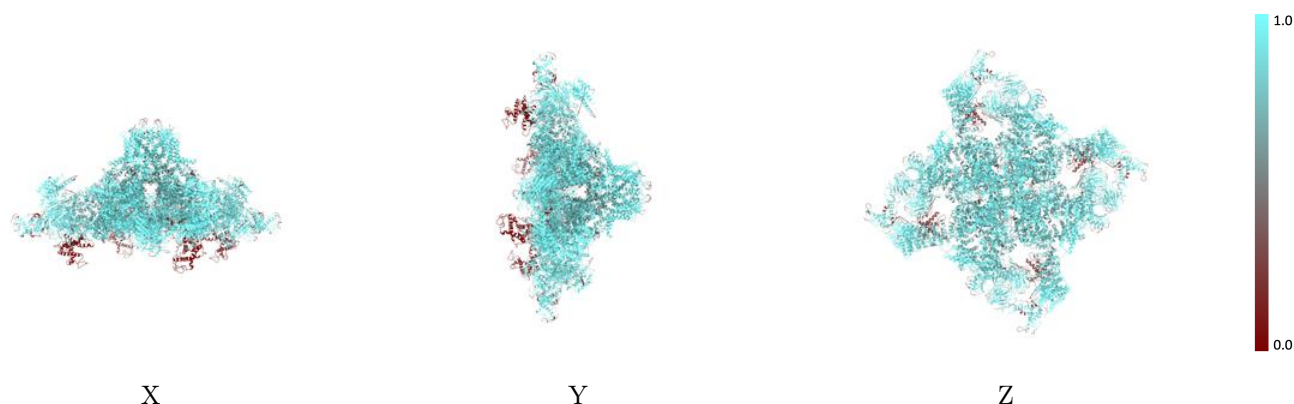
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

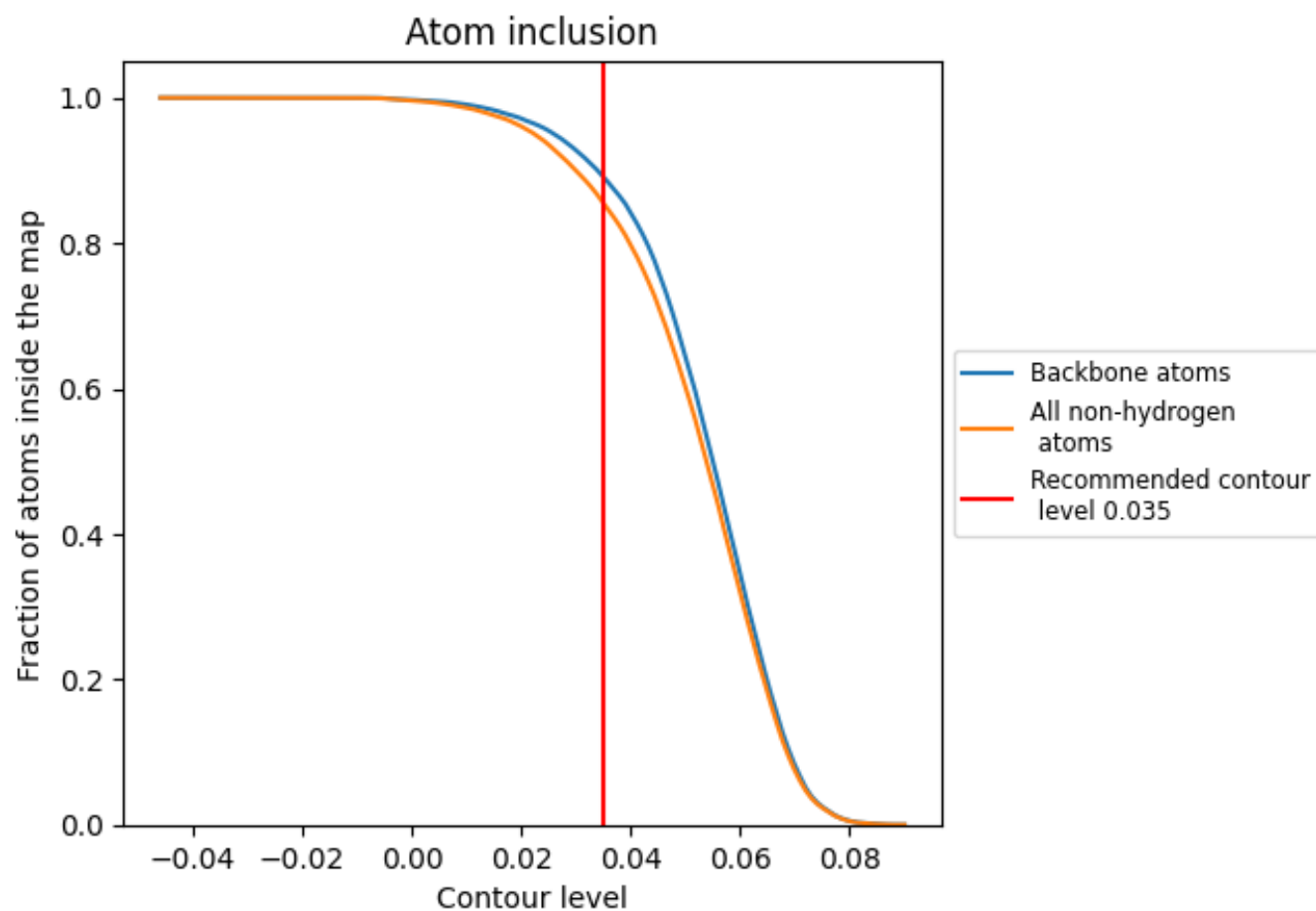
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.035).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8553</div>	<div><div></div>0.0820</div>
A	<div><div></div>0.8562</div>	<div><div></div>0.0820</div>
B	<div><div></div>0.8474</div>	<div><div></div>0.0660</div>
C	<div><div></div>0.8557</div>	<div><div></div>0.0820</div>
D	<div><div></div>0.8462</div>	<div><div></div>0.0720</div>
E	<div><div></div>0.8547</div>	<div><div></div>0.0820</div>
F	<div><div></div>0.8437</div>	<div><div></div>0.0750</div>
G	<div><div></div>0.8561</div>	<div><div></div>0.0830</div>
H	<div><div></div>0.8375</div>	<div><div></div>0.0700</div>

1.0

0.0

<0.0