



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 01:06 AM UTC

PDB ID : 7M7G / pdb_00007m7g
EMDB ID : EMD-23712
Title : 6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: State 2
Authors : Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.
Deposited on : 2021-03-28
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

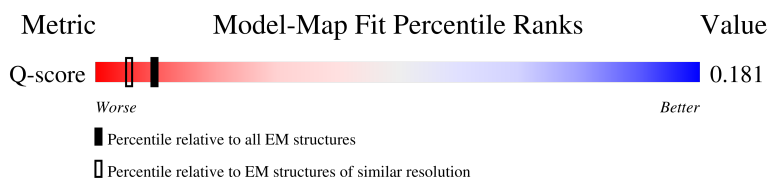
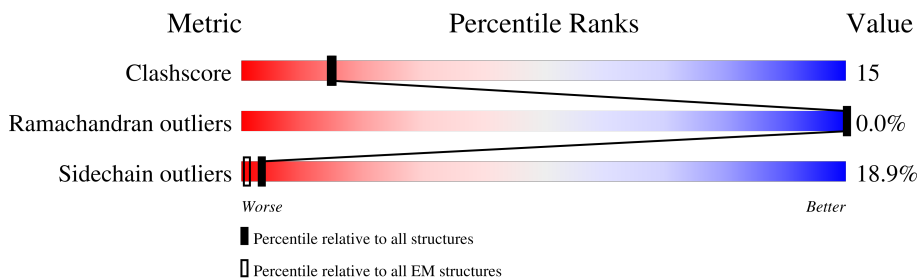
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	1784	23% 45% 26% • 24%
1	B	1784	20% 46% 25% 5% • 23%
2	C	249	44% 29% 8% • 18%
2	E	249	43% 32% 7% • 18%

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Mol	Chain	Length	Quality of chain
3	D	236	43% 39% • 13%
3	F	236	43% 40% • • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26480 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 EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1356	Total	C	N	O	S	0	0
			10046	6244	1845	1922	35		
1	B	1379	Total	C	N	O	S	0	0
			10220	6356	1875	1954	35		

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	1486	THR	-	linker	UNP Q5UNP6
A	1487	SER	-	linker	UNP Q5UNP6
A	1488	GLU	-	linker	UNP Q5UNP6
A	1489	LEU	-	linker	UNP Q5UNP6
A	1490	GLY	-	linker	UNP Q5UNP6
A	1768	SER	-	expression tag	UNP Q03133
A	1769	SER	-	expression tag	UNP Q03133
A	1770	VAL	-	expression tag	UNP Q03133
A	1771	ASP	-	expression tag	UNP Q03133
A	1772	LYS	-	expression tag	UNP Q03133
A	1773	LEU	-	expression tag	UNP Q03133
A	1774	ALA	-	expression tag	UNP Q03133
A	1775	ALA	-	expression tag	UNP Q03133
A	1776	ALA	-	expression tag	UNP Q03133
A	1777	LEU	-	expression tag	UNP Q03133
A	1778	GLU	-	expression tag	UNP Q03133
A	1779	HIS	-	expression tag	UNP Q03133
A	1780	HIS	-	expression tag	UNP Q03133
A	1781	HIS	-	expression tag	UNP Q03133
A	1782	HIS	-	expression tag	UNP Q03133
A	1783	HIS	-	expression tag	UNP Q03133
A	1784	HIS	-	expression tag	UNP Q03133
B	1	MET	-	expression tag	UNP Q5UNP6
B	2	ALA	-	expression tag	UNP Q5UNP6
B	3	SER	-	expression tag	UNP Q5UNP6
B	4	THR	-	expression tag	UNP Q5UNP6
B	5	ASP	-	expression tag	UNP Q5UNP6
B	6	SER	-	expression tag	UNP Q5UNP6
B	7	GLU	-	expression tag	UNP Q5UNP6
B	8	LYS	-	expression tag	UNP Q5UNP6
B	9	VAL	-	expression tag	UNP Q5UNP6
B	10	ALA	-	expression tag	UNP Q5UNP6
B	11	GLU	-	expression tag	UNP Q5UNP6
B	12	TYR	-	expression tag	UNP Q5UNP6
B	13	LEU	-	expression tag	UNP Q5UNP6
B	14	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ARG	-	expression tag	UNP Q5UNP6
B	16	ALA	-	expression tag	UNP Q5UNP6
B	17	THR	-	expression tag	UNP Q5UNP6
B	18	LEU	-	expression tag	UNP Q5UNP6
B	19	ASP	-	expression tag	UNP Q5UNP6
B	20	LEU	-	expression tag	UNP Q5UNP6
B	21	ARG	-	expression tag	UNP Q5UNP6
B	22	ALA	-	expression tag	UNP Q5UNP6
B	23	ALA	-	expression tag	UNP Q5UNP6
B	24	ARG	-	expression tag	UNP Q5UNP6
B	25	GLN	-	expression tag	UNP Q5UNP6
B	26	ARG	-	expression tag	UNP Q5UNP6
B	27	ILE	-	expression tag	UNP Q5UNP6
B	28	ARG	-	expression tag	UNP Q5UNP6
B	29	GLU	-	expression tag	UNP Q5UNP6
B	30	LEU	-	expression tag	UNP Q5UNP6
B	31	GLU	-	expression tag	UNP Q5UNP6
B	1486	THR	-	linker	UNP Q5UNP6
B	1487	SER	-	linker	UNP Q5UNP6
B	1488	GLU	-	linker	UNP Q5UNP6
B	1489	LEU	-	linker	UNP Q5UNP6
B	1490	GLY	-	linker	UNP Q5UNP6
B	1768	SER	-	expression tag	UNP Q03133
B	1769	SER	-	expression tag	UNP Q03133
B	1770	VAL	-	expression tag	UNP Q03133
B	1771	ASP	-	expression tag	UNP Q03133
B	1772	LYS	-	expression tag	UNP Q03133
B	1773	LEU	-	expression tag	UNP Q03133
B	1774	ALA	-	expression tag	UNP Q03133
B	1775	ALA	-	expression tag	UNP Q03133
B	1776	ALA	-	expression tag	UNP Q03133
B	1777	LEU	-	expression tag	UNP Q03133
B	1778	GLU	-	expression tag	UNP Q03133
B	1779	HIS	-	expression tag	UNP Q03133
B	1780	HIS	-	expression tag	UNP Q03133
B	1781	HIS	-	expression tag	UNP Q03133
B	1782	HIS	-	expression tag	UNP Q03133
B	1783	HIS	-	expression tag	UNP Q03133
B	1784	HIS	-	expression tag	UNP Q03133

- Molecule 2 is a protein called 1B2 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

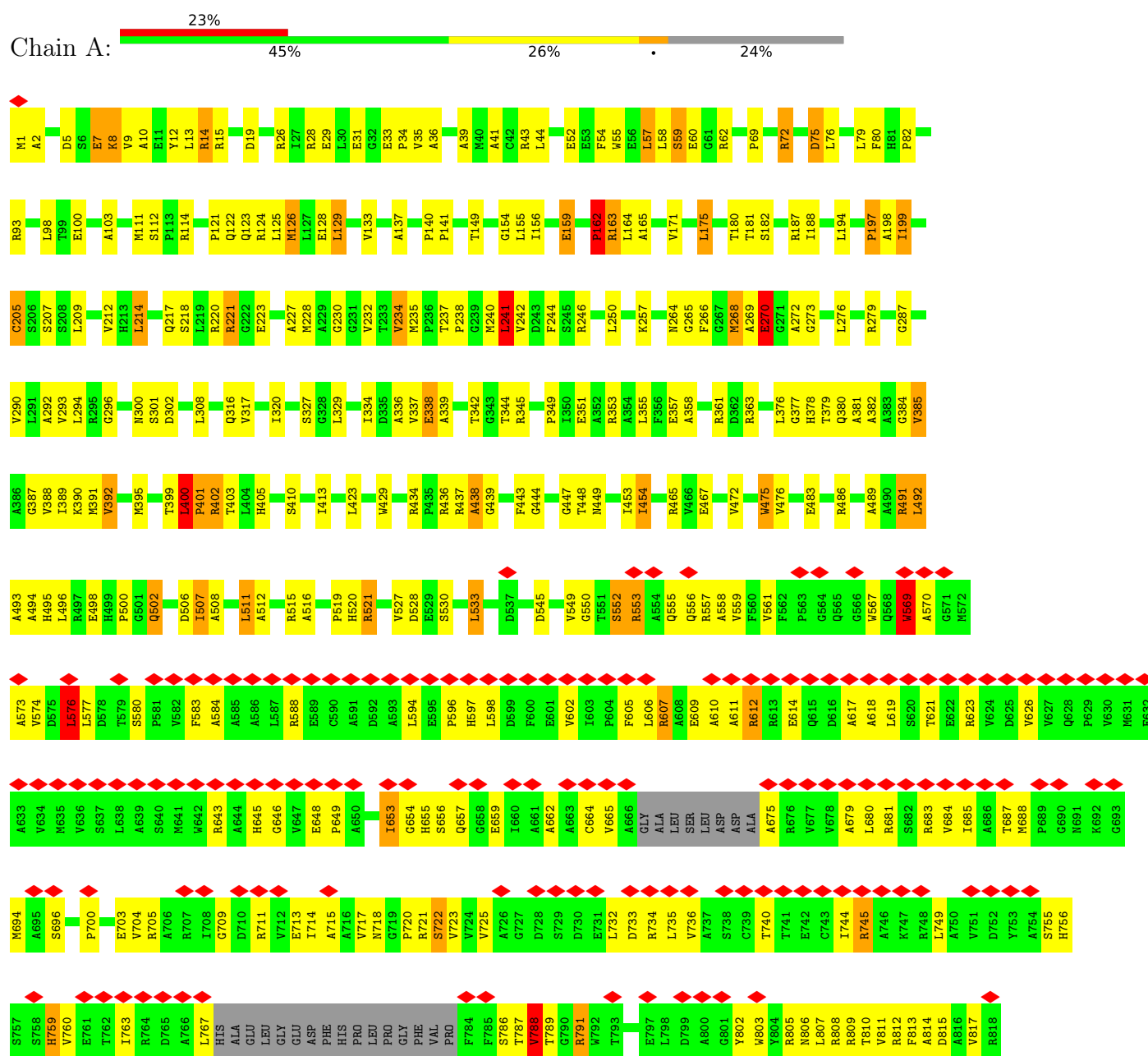
- Molecule 3 is a protein called 1B2 (light chain).

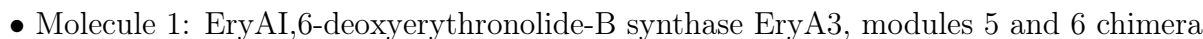
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

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.

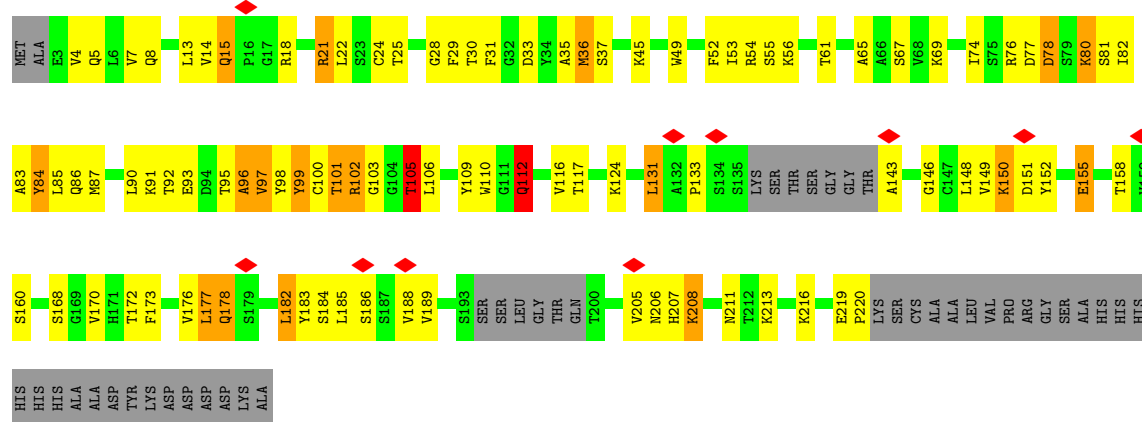
- Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera



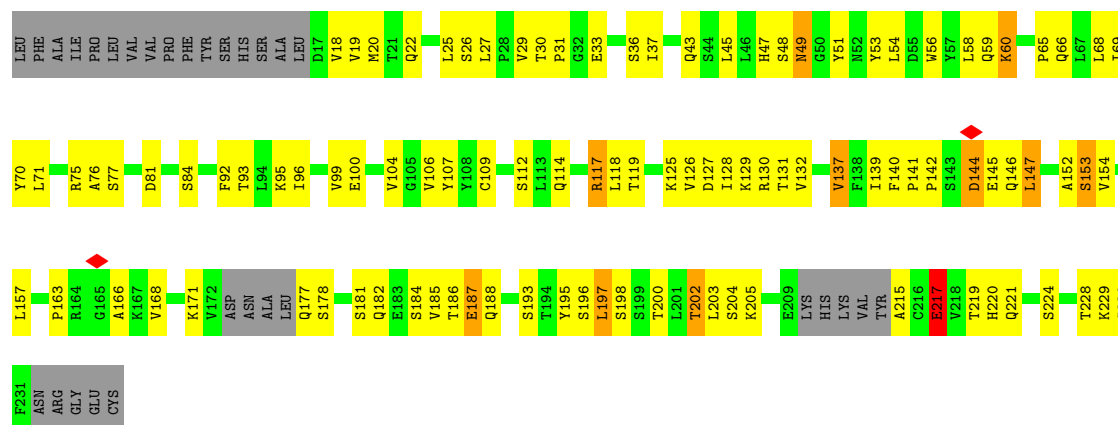




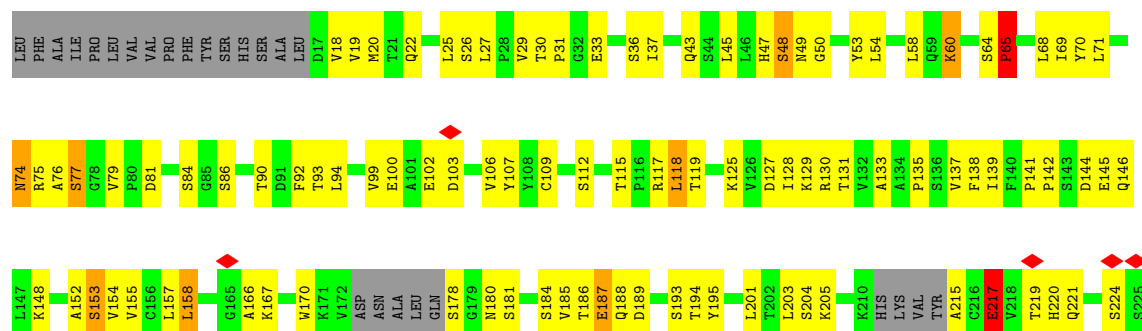
Chain E: 43% 32% 7% • 18%



Chain D: 43% 39% 1% 13%



Chain F: 43% 40% 2% 1% 13%



P226	T228	ASN	ARG	GLY	GLU	CYS
V227	K229	F231	ARG	GLY	GLU	CYS
S230						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56378	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.610	Depositor
Minimum map value	-1.457	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.325	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	0.90	50/10238 (0.5%)	1.14	87/13933 (0.6%)
1	B	0.93	52/10421 (0.5%)	1.22	77/14187 (0.5%)
2	C	0.86	9/1575 (0.6%)	1.12	12/2141 (0.6%)
2	E	0.81	5/1575 (0.3%)	1.18	11/2141 (0.5%)
3	D	0.58	0/1601	0.98	7/2175 (0.3%)
3	F	0.73	5/1601 (0.3%)	1.11	12/2174 (0.6%)
All	All	0.88	121/27011 (0.4%)	1.16	206/36751 (0.6%)

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	B	0	2
2	C	0	2
2	E	0	3
3	F	0	1
All	All	0	9

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	442	SER	CA-CB	-14.40	1.30	1.53
1	B	207	SER	CA-CB	-14.17	1.28	1.53
1	A	197	PRO	C-O	-13.29	1.06	1.24
1	B	442	SER	C-O	-12.62	1.09	1.24
1	B	440	VAL	C-O	-12.46	1.10	1.24
1	A	399	THR	C-O	-12.09	1.08	1.23
1	A	43	ARG	C-O	-11.12	1.11	1.23
1	A	54	PHE	C-O	-10.88	1.10	1.24
1	A	388	VAL	C-O	-10.35	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	VAL	C-O	-9.88	1.12	1.24
1	B	234	VAL	C-O	-9.84	1.13	1.24
1	A	384	GLY	C-N	-9.75	1.22	1.33
1	A	230	GLY	C-O	-9.45	1.09	1.23
1	B	243	ASP	C-O	-9.21	1.12	1.24
1	A	475	TRP	C-O	-8.99	1.12	1.23
1	B	270	GLU	C-O	-8.96	1.12	1.23
1	B	233	THR	C-O	-8.93	1.13	1.24
1	B	441	SER	CA-CB	-8.90	1.36	1.53
1	A	454	ILE	C-O	-8.89	1.13	1.24
1	B	162	PRO	C-O	-8.89	1.12	1.23
1	B	116	ALA	C-O	-8.84	1.12	1.24
1	A	507	ILE	C-O	-8.74	1.14	1.24
1	B	94	GLY	C-O	-8.69	1.17	1.24
1	A	385	VAL	C-O	-8.69	1.14	1.24
1	A	439	GLY	C-O	-8.51	1.12	1.23
1	A	57	LEU	C-O	-8.36	1.11	1.23
1	A	59	SER	CA-CB	-8.36	1.40	1.53
1	B	236	PRO	C-O	-8.31	1.12	1.24
1	B	117	LEU	C-O	-8.31	1.13	1.24
1	B	155	LEU	C-O	-8.29	1.14	1.23
3	F	74	ASN	C-O	-8.20	1.13	1.23
2	E	97	VAL	C-O	-8.16	1.14	1.24
1	B	232	VAL	C-O	-8.16	1.15	1.24
2	C	101	THR	C-O	-8.10	1.13	1.23
1	B	441	SER	C-O	-8.07	1.14	1.24
1	B	156	ILE	C-O	-8.00	1.14	1.24
1	B	172	GLU	C-O	-8.00	1.13	1.24
2	C	99	TYR	C-O	-7.97	1.13	1.23
1	A	492	LEU	C-O	-7.91	1.14	1.24
1	A	266	PHE	C-O	-7.88	1.13	1.24
1	B	207	SER	C-O	-7.86	1.13	1.24
1	B	64	ALA	CA-CB	-7.80	1.42	1.53
1	A	162	PRO	C-O	-7.79	1.15	1.23
1	B	163	ARG	C-O	-7.74	1.14	1.23
1	A	8	LYS	C-O	-7.65	1.14	1.24
1	B	183	VAL	C-O	-7.58	1.11	1.23
1	B	62	ARG	C-O	-7.55	1.14	1.24
1	A	493	ALA	CA-CB	-7.51	1.41	1.53
2	E	101	THR	C-O	-7.49	1.14	1.23
1	A	198	ALA	CA-CB	-7.48	1.42	1.52
1	A	338	GLU	C-O	-7.46	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	HIS	C-O	-7.40	1.14	1.24
3	F	76	ALA	CA-CB	-7.29	1.43	1.53
2	C	98	TYR	C-O	-7.23	1.15	1.24
2	C	102	ARG	C-O	-7.22	1.14	1.24
1	B	443	PHE	C-O	-7.21	1.14	1.24
1	B	162	PRO	N-CA	-7.08	1.38	1.47
3	F	76	ALA	C-O	-7.07	1.15	1.24
1	B	116	ALA	CA-CB	-7.05	1.41	1.53
3	F	75	ARG	C-O	-6.99	1.15	1.23
1	B	175	LEU	C-O	-6.94	1.14	1.24
1	B	157	PRO	N-CA	-6.91	1.38	1.47
2	E	103	GLY	C-O	-6.82	1.14	1.23
2	C	39	VAL	C-O	-6.78	1.16	1.24
1	B	202	ASP	C-O	-6.76	1.15	1.23
1	A	162	PRO	N-CA	-6.74	1.39	1.46
1	B	243	ASP	CA-C	-6.71	1.46	1.52
2	E	102	ARG	C-O	-6.67	1.14	1.23
1	A	392	VAL	C-O	-6.66	1.15	1.24
1	B	159	GLU	C-O	-6.56	1.16	1.24
1	A	902	PRO	C-O	-6.54	1.15	1.24
1	B	266	PHE	C-O	-6.54	1.15	1.23
1	A	438	ALA	C-N	-6.51	1.24	1.33
1	A	197	PRO	N-CA	-6.43	1.39	1.47
1	A	494	ALA	C-O	-6.33	1.16	1.24
1	A	401	PRO	N-CA	-6.31	1.39	1.47
1	A	402	ARG	C-O	-6.28	1.15	1.23
1	A	491	ARG	C-O	-6.27	1.16	1.24
1	B	236	PRO	N-CA	-6.26	1.39	1.47
2	C	6	LEU	C-O	-6.23	1.15	1.23
1	A	401	PRO	C-O	-6.20	1.13	1.23
2	E	102	ARG	CA-C	-6.18	1.46	1.53
1	A	390	LYS	C-O	-6.12	1.16	1.24
1	B	177	THR	C-O	-6.11	1.15	1.24
1	B	65	VAL	C-O	-6.11	1.15	1.23
1	A	43	ARG	CA-C	-6.10	1.45	1.53
1	B	234	VAL	CA-C	-6.09	1.45	1.52
1	B	440	VAL	CA-C	-6.04	1.45	1.52
1	A	493	ALA	C-O	-5.89	1.17	1.24
1	B	244	PHE	C-O	-5.89	1.16	1.24
1	A	58	LEU	C-O	-5.87	1.16	1.24
1	B	92	GLN	C-O	-5.82	1.17	1.24
1	A	266	PHE	C-N	-5.81	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	HIS	C-O	-5.80	1.16	1.24
1	B	422	LEU	C-O	-5.79	1.17	1.23
1	A	234	VAL	CA-CB	-5.74	1.47	1.54
1	A	235	MET	C-O	-5.72	1.17	1.24
1	B	62	ARG	CA-C	-5.67	1.46	1.52
1	A	400	LEU	C-O	-5.67	1.17	1.24
1	A	511	LEU	C-O	-5.63	1.16	1.24
1	A	234	VAL	CA-C	-5.56	1.46	1.52
1	B	207	SER	CA-C	-5.43	1.45	1.52
2	C	101	THR	CA-C	-5.43	1.46	1.52
1	B	176	MET	C-O	-5.39	1.15	1.23
1	A	502	GLN	C-O	-5.33	1.17	1.24
1	B	63	ASP	C-O	-5.33	1.17	1.23
1	B	183	VAL	CA-C	-5.31	1.47	1.53
2	C	38	TRP	C-O	-5.26	1.18	1.24
1	A	57	LEU	CA-C	-5.25	1.45	1.52
1	B	174	TYR	C-O	-5.18	1.17	1.24
1	B	24	ARG	C-O	-5.17	1.17	1.24
1	A	338	GLU	C-N	-5.16	1.26	1.33
1	A	266	PHE	N-CA	5.16	1.52	1.46
1	B	1307	LEU	C-O	-5.14	1.21	1.25
1	B	157	PRO	C-O	-5.14	1.17	1.24
3	F	48	SER	CA-CB	-5.11	1.44	1.53
1	A	230	GLY	CA-C	-5.10	1.45	1.51
1	B	242	VAL	C-O	-5.10	1.16	1.24
1	A	403	THR	C-O	-5.10	1.18	1.24
2	C	37	SER	CA-CB	-5.09	1.43	1.54
1	A	475	TRP	CA-CB	-5.00	1.46	1.52

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	PRO	N-CA-CB	-23.63	83.47	103.32
1	B	159	GLU	CB-CA-C	-19.78	78.14	110.19
1	A	266	PHE	CA-CB-CG	17.76	131.56	113.80
1	A	902	PRO	CB-CA-C	-15.14	86.58	111.56
2	E	102	ARG	CB-CA-C	-14.80	89.92	112.12
1	B	233	THR	CA-CB-OG1	-14.72	87.52	109.60
1	B	157	PRO	N-CA-CB	-14.13	88.42	103.25
1	B	233	THR	CB-CA-C	-13.78	90.50	110.62
1	B	162	PRO	CB-CA-C	-13.64	93.93	111.39
1	A	493	ALA	N-CA-C	-12.40	97.75	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ILE	N-CA-C	-12.27	101.97	111.90
1	A	385	VAL	N-CA-C	-12.13	101.64	113.53
1	B	175	LEU	N-CA-C	-11.19	99.18	113.72
1	A	197	PRO	CB-CA-C	-11.06	93.30	111.56
1	B	234	VAL	N-CA-C	-10.91	92.84	108.11
1	B	270	GLU	CB-CG-CD	-10.77	94.29	112.60
1	A	54	PHE	CA-CB-CG	10.74	124.55	113.80
1	B	266	PHE	CA-CB-CG	10.70	124.50	113.80
1	B	243	ASP	CB-CA-C	-10.55	93.75	111.26
1	B	236	PRO	N-CA-CB	-10.49	92.01	103.23
2	C	102	ARG	CB-CA-C	-10.32	89.89	110.42
1	B	155	LEU	CA-C-N	-10.09	115.74	122.60
1	B	155	LEU	C-N-CA	-10.09	115.74	122.60
2	C	101	THR	N-CA-CB	-10.01	95.44	110.85
1	A	57	LEU	N-CA-C	-9.73	101.98	114.04
1	B	403	THR	N-CA-C	-9.70	90.83	107.99
1	B	174	TYR	CB-CA-C	-9.69	96.04	111.06
1	B	63	ASP	CB-CA-C	-9.62	93.25	109.50
1	A	72	ARG	CB-CG-CD	-9.59	89.24	111.30
2	E	99	TYR	CA-C-O	-9.49	110.01	121.11
1	A	401	PRO	N-CD-CG	-9.34	89.19	103.20
1	B	156	ILE	N-CA-C	-9.17	99.22	107.56
1	A	550	GLY	O-C-N	9.16	130.65	123.23
1	A	401	PRO	N-CA-CB	-8.89	91.93	102.86
1	B	92	GLN	CB-CG-CD	-8.69	97.83	112.60
1	B	1056	PHE	N-CA-C	-8.55	102.23	114.12
1	A	234	VAL	CA-C-O	-8.49	111.48	120.57
1	B	234	VAL	CA-C-O	-8.28	111.69	120.39
1	A	234	VAL	N-CA-C	-8.20	96.63	108.36
2	E	100	CYS	CB-CA-C	-8.20	97.54	110.74
2	C	100	CYS	CB-CA-C	-8.15	98.71	110.62
1	A	230	GLY	CA-C-O	-8.15	112.20	122.39
1	B	440	VAL	CA-C-O	-8.01	111.99	120.48
1	A	825	TYR	N-CA-C	-7.99	100.98	110.41
2	E	101	THR	N-CA-CB	-7.86	98.27	110.85
1	B	176	MET	N-CA-C	-7.79	103.62	113.43
3	F	180	ASN	CB-CA-C	-7.75	96.57	110.37
2	C	101	THR	CA-CB-OG1	-7.74	97.99	109.60
1	A	14	ARG	N-CA-C	-7.72	103.44	113.17
2	C	101	THR	CA-C-O	-7.63	112.33	121.56
1	A	511	LEU	N-CA-C	-7.62	102.63	112.23
1	B	233	THR	CA-C-O	-7.61	110.67	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	PHE	CB-CA-C	-7.58	95.79	110.11
1	A	266	PHE	CB-CA-C	-7.54	94.25	109.55
2	C	41	GLN	CB-CA-C	-7.52	99.59	111.17
1	A	266	PHE	N-CA-CB	7.47	122.09	110.44
1	A	198	ALA	CA-C-O	-7.43	113.07	121.39
3	F	50	GLY	N-CA-C	-7.42	104.34	115.32
1	B	1014	PRO	N-CA-C	-7.41	99.61	110.80
1	A	1014	PRO	N-CA-C	-7.39	99.64	110.80
1	A	26	ARG	N-CA-C	-7.35	104.45	113.41
1	A	230	GLY	CA-C-N	7.28	128.37	121.46
1	A	230	GLY	C-N-CA	7.28	128.37	121.46
1	B	731	GLU	N-CA-C	-7.27	106.33	114.62
1	B	156	ILE	CA-C-O	-7.26	115.05	119.12
2	E	86	GLN	CA-C-N	-7.23	113.02	123.00
2	E	86	GLN	C-N-CA	-7.23	113.02	123.00
1	B	183	VAL	CA-C-O	-7.16	112.98	120.14
1	B	162	PRO	CA-N-CD	-7.11	102.04	112.00
1	B	243	ASP	CA-CB-CG	-7.11	105.49	112.60
1	A	387	GLY	O-C-N	-7.09	114.55	122.28
1	B	53	GLU	N-CA-C	-7.01	104.20	112.89
1	A	54	PHE	N-CA-C	-6.96	102.78	112.45
1	A	7	GLU	N-CA-C	-6.92	102.89	112.30
1	A	491	ARG	CG-CD-NE	-6.89	96.85	112.00
1	A	399	THR	CA-C-O	-6.89	113.31	120.89
1	A	5	ASP	CB-CA-C	6.85	124.01	110.65
1	A	788	VAL	N-CA-C	-6.83	106.64	113.20
1	B	223	GLU	N-CA-C	-6.79	106.19	114.75
3	F	65	PRO	N-CA-CB	-6.79	97.01	103.39
1	A	72	ARG	N-CA-CB	-6.75	100.07	110.46
1	B	531	ALA	N-CA-C	-6.75	103.85	111.07
1	B	159	GLU	CA-C-O	-6.74	113.15	120.36
1	A	389	ILE	O-C-N	-6.72	114.21	121.80
1	A	198	ALA	N-CA-CB	-6.69	99.43	110.53
1	A	496	LEU	N-CA-C	-6.67	104.27	112.88
1	A	197	PRO	N-CA-CB	-6.66	96.26	103.25
1	B	158	GLN	CB-CG-CD	-6.66	101.29	112.60
1	A	241	LEU	N-CA-C	-6.64	104.66	112.89
1	A	399	THR	CB-CA-C	-6.62	98.05	110.16
3	F	60	LYS	CA-C-N	6.62	127.66	119.98
3	F	60	LYS	C-N-CA	6.62	127.66	119.98
1	A	576	LEU	N-CA-C	-6.61	104.26	112.72
1	B	243	ASP	N-CA-C	-6.58	103.31	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	ARG	CB-CA-C	-6.57	97.56	109.38
2	C	4	VAL	N-CA-C	-6.54	100.31	109.21
3	D	60	LYS	CB-CA-C	6.54	118.92	109.11
1	A	198	ALA	CB-CA-C	-6.52	100.79	111.68
1	B	236	PRO	N-CD-CG	-6.37	93.64	103.20
3	D	202	THR	CA-C-N	-6.33	111.19	122.45
3	D	202	THR	C-N-CA	-6.33	111.19	122.45
1	B	380	GLN	CB-CA-C	-6.31	109.28	116.54
1	B	441	SER	CA-C-O	-6.31	113.31	120.32
1	B	242	VAL	N-CA-C	-6.28	107.01	113.10
1	B	497	ARG	N-CA-C	-6.27	105.45	113.23
1	B	57	LEU	N-CA-C	-6.26	105.54	113.43
1	B	441	SER	CB-CA-C	-6.26	98.37	109.70
1	A	75	ASP	CB-CA-C	-6.23	101.10	110.88
1	B	760	VAL	N-CA-C	-6.22	107.43	113.53
2	C	101	THR	CB-CA-C	-6.18	98.58	109.71
1	A	337	VAL	O-C-N	-6.16	114.91	122.61
1	A	390	LYS	CB-CA-C	-6.12	97.89	110.38
1	B	443	PHE	CA-C-O	-6.08	114.14	120.70
1	B	162	PRO	CA-C-O	-6.06	114.64	121.43
1	A	265	GLY	CA-C-O	-5.99	117.48	122.33
1	A	498	GLU	N-CA-C	-5.98	105.80	114.12
1	A	489	ALA	N-CA-C	-5.95	106.16	113.41
2	C	99	TYR	CA-C-O	-5.94	114.67	121.68
3	D	217	GLU	CA-CB-CG	5.91	125.92	114.10
1	A	1380	ARG	CB-CA-C	5.90	121.33	110.11
1	A	439	GLY	CA-C-N	5.90	130.95	123.10
1	A	439	GLY	C-N-CA	5.90	130.95	123.10
1	A	387	GLY	CA-C-N	5.90	130.44	120.29
1	A	387	GLY	C-N-CA	5.90	130.44	120.29
3	F	217	GLU	CA-CB-CG	5.88	125.86	114.10
1	B	1380	ARG	CB-CA-C	5.87	121.27	110.11
1	A	403	THR	N-CA-C	-5.87	98.17	108.20
1	A	15	ARG	N-CA-C	-5.86	104.89	112.68
1	A	902	PRO	CA-N-CD	-5.85	103.81	112.00
1	B	838	THR	N-CA-C	-5.82	105.02	111.36
1	B	79	LEU	N-CA-C	-5.82	106.03	113.01
1	B	392	VAL	N-CA-C	-5.80	107.85	113.53
1	B	379	THR	N-CA-C	-5.77	106.47	112.93
1	B	117	LEU	N-CA-C	-5.74	105.11	111.71
1	A	495	HIS	N-CA-C	-5.71	106.27	113.18
1	A	494	ALA	CA-C-O	-5.70	114.47	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ALA	O-C-N	5.70	129.58	122.63
3	D	47	HIS	CA-CB-CG	5.68	119.48	113.80
1	A	912	PRO	CA-C-N	-5.66	116.55	122.89
1	A	912	PRO	C-N-CA	-5.66	116.55	122.89
1	A	390	LYS	N-CA-C	-5.65	105.11	112.23
1	B	176	MET	CB-CG-SD	-5.65	95.76	112.70
1	A	57	LEU	CB-CA-C	-5.64	99.11	109.15
1	B	93	ARG	N-CA-C	-5.62	105.62	112.88
2	E	98	TYR	CA-C-O	-5.62	114.96	121.15
1	B	158	GLN	CA-C-O	-5.62	114.77	121.11
1	B	1325	GLY	O-C-N	-5.60	116.17	121.77
1	B	117	LEU	O-C-N	5.59	128.77	122.22
1	A	162	PRO	CB-CA-C	5.58	118.98	110.21
3	F	75	ARG	CA-C-O	-5.58	114.85	121.16
3	D	49	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	1325	GLY	O-C-N	-5.53	116.24	121.77
1	A	400	LEU	N-CA-C	-5.52	101.02	109.64
1	A	511	LEU	CA-C-O	-5.52	113.27	119.79
1	B	340	HIS	N-CA-C	-5.51	104.96	110.97
2	C	38	TRP	CA-C-O	-5.51	114.37	120.33
1	B	174	TYR	CA-C-O	-5.50	113.05	120.15
1	A	401	PRO	CA-N-CD	5.50	119.70	112.00
1	B	914	PRO	N-CA-CB	5.49	106.09	102.25
1	A	43	ARG	N-CA-C	-5.48	96.24	107.70
1	B	492	LEU	N-CA-C	-5.47	104.96	111.69
1	B	377	GLY	CA-C-O	-5.47	115.75	122.15
1	B	511	LEU	N-CA-C	-5.47	107.16	113.88
1	B	266	PHE	CA-C-N	5.44	132.07	121.41
1	B	266	PHE	C-N-CA	5.44	132.07	121.41
1	A	218	SER	N-CA-C	-5.40	106.65	113.18
2	E	96	ALA	O-C-N	-5.38	117.45	123.04
1	A	43	ARG	CA-C-O	-5.38	113.05	120.52
1	A	270	GLU	CB-CA-C	5.36	119.89	109.33
1	A	902	PRO	N-CD-CG	-5.34	95.19	103.20
1	A	385	VAL	CA-C-O	-5.34	113.48	118.98
3	F	60	LYS	CA-C-O	-5.33	114.66	120.69
1	A	454	ILE	CA-C-O	-5.32	113.78	120.69
1	B	176	MET	CB-CA-C	-5.32	100.72	109.65
1	B	960	GLU	N-CA-C	-5.27	106.11	112.54
2	E	112	GLN	N-CA-CB	-5.27	101.81	110.40
1	A	960	GLU	N-CA-C	-5.27	106.11	112.54
2	E	105	THR	N-CA-C	-5.27	106.18	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ARG	N-CA-C	-5.26	106.91	113.38
1	A	475	TRP	CA-C-O	-5.21	115.50	120.92
1	B	376	LEU	CB-CA-C	-5.21	105.09	114.52
1	B	530	SER	N-CA-C	-5.21	105.21	112.45
3	D	147	LEU	N-CA-C	-5.21	105.78	111.82
1	A	500	PRO	N-CA-C	5.19	120.34	111.68
2	C	102	ARG	CB-CG-CD	-5.19	99.37	111.30
3	F	166	ALA	N-CA-CB	-5.16	102.47	110.57
1	A	552	SER	CA-C-O	-5.15	115.58	120.94
1	A	388	VAL	N-CA-C	-5.14	104.55	111.44
1	A	402	ARG	CB-CA-C	-5.14	99.52	109.76
3	F	76	ALA	CA-C-O	-5.12	114.75	120.54
1	B	1202	VAL	N-CA-C	-5.12	108.52	113.53
1	B	55	TRP	N-CA-C	-5.11	107.11	113.19
1	B	1377	ARG	CA-C-O	-5.11	115.27	120.63
1	B	233	THR	N-CA-C	-5.10	98.98	107.80
3	F	47	HIS	CA-C-O	-5.10	116.08	121.94
1	A	265	GLY	O-C-N	-5.09	119.10	123.43
1	A	657	GLN	N-CA-C	-5.08	106.86	113.16
1	A	1377	ARG	CA-C-O	-5.08	115.30	120.63
1	A	58	LEU	N-CA-C	-5.07	107.27	113.50
3	F	60	LYS	CB-CA-C	5.06	117.76	109.46
1	A	266	PHE	N-CA-C	5.02	119.46	113.23
1	A	1202	VAL	N-CA-C	-5.02	108.61	113.53
2	C	86	GLN	CA-CB-CG	5.01	124.13	114.10
2	E	97	VAL	CA-C-O	-5.01	114.51	120.78
1	B	1050	ALA	N-CA-C	-5.01	106.01	111.82
1	A	569	TRP	N-CA-C	-5.01	107.00	113.01

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	ASP	Mainchain
1	B	171	VAL	Mainchain
1	B	799	ASP	Sidechain
2	C	155	GLU	Peptide
2	C	21	ARG	Sidechain
2	E	155	GLU	Peptide
2	E	21	ARG	Sidechain
2	E	96	ALA	Mainchain
3	F	115	THR	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	10046	0	9883	290	0
1	B	10220	0	10049	300	0
2	C	1539	0	1511	63	0
2	E	1539	0	1511	62	0
3	D	1568	0	1528	52	0
3	F	1568	0	1533	55	0
All	All	26480	0	26015	785	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 (785) 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:B:777:PRO:HG3	1:B:799:ASP:CG	1.62	1.23
2:C:86:GLN:HA	2:C:86:GLN:HE21	1.38	0.87
1:A:611:ALA:HB2	1:A:863:GLY:HA2	1.57	0.85
1:B:777:PRO:CG	1:B:799:ASP:CG	2.51	0.79
1:B:777:PRO:HG3	1:B:799:ASP:OD2	1.87	0.73
1:A:610:ALA:HB3	1:A:862:ASP:HB2	1.73	0.70
1:A:700:PRO:HA	1:A:720:PRO:HA	1.73	0.70
3:F:68:LEU:HA	3:F:79:VAL:HG21	1.74	0.69
3:F:58:LEU:HB2	3:F:68:LEU:HD11	1.75	0.68
1:B:1171:VAL:HG21	1:B:1211:LEU:HD13	1.74	0.67
1:B:1144:LEU:HD11	1:B:1211:LEU:HD11	1.77	0.67
1:A:662:ALA:HA	1:A:665:VAL:HG12	1.77	0.66
1:B:707:ARG:HH12	1:B:735:LEU:HD12	1.59	0.66
1:B:1052:ALA:HA	1:B:1116:ARG:HH21	1.61	0.66
1:A:561:VAL:HG11	1:A:837:LEU:HD13	1.78	0.66
1:B:1019:LEU:HD13	1:B:1244:ILE:HG22	1.79	0.65
1:B:981:VAL:HB	1:B:990:LEU:HD21	1.78	0.65
1:A:610:ALA:HB3	1:A:862:ASP:CB	2.26	0.65
2:C:86:GLN:HA	2:C:86:GLN:NE2	2.10	0.65
1:A:569:TRP:HB3	1:A:623:ARG:HH22	1.60	0.65
2:E:8:GLN:HE22	2:E:99:TYR:HA	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:ARG:HB2	1:B:1124:ARG:HG3	1.78	0.64
1:A:696:SER:HB2	1:A:745:ARG:HH11	1.61	0.64
1:A:553:ARG:HB2	1:A:853:SER:HA	1.78	0.64
1:A:14:ARG:HG2	3:D:51:TYR:HE2	1.62	0.64
1:A:683:ARG:HE	1:A:687:THR:HB	1.61	0.64
2:C:144:ALA:HB3	3:D:140:PHE:HZ	1.63	0.64
1:A:171:VAL:HG21	1:A:910:LEU:HD21	1.80	0.63
1:A:909:TRP:HD1	1:A:911:GLU:HG2	1.64	0.63
1:A:1000:VAL:HB	1:A:1039:LEU:HD21	1.81	0.63
1:B:817:VAL:HA	1:B:820:LEU:HD12	1.81	0.62
1:B:1000:VAL:HB	1:B:1039:LEU:HD21	1.81	0.62
2:E:87:MET:HB3	2:E:90:LEU:HD21	1.81	0.62
1:B:370:GLY:HA3	1:B:423:LEU:HD12	1.82	0.62
1:A:828:PHE:HB3	1:A:837:LEU:HD11	1.82	0.62
2:E:146:GLY:HA3	2:E:188:VAL:HG22	1.81	0.62
3:F:99:VAL:HG13	3:F:103:ASP:HB2	1.82	0.62
1:B:1231:LEU:HD13	1:B:1288:TYR:HB2	1.83	0.61
1:A:162:PRO:HB3	1:A:912:PRO:HG2	1.81	0.61
1:B:704:VAL:HG11	1:B:723:VAL:HG21	1.81	0.61
1:B:721:ARG:HB2	1:B:843:GLU:HB3	1.82	0.61
3:F:188:GLN:NE2	3:F:193:SER:HB2	2.16	0.61
1:A:76:LEU:H	1:A:79:LEU:HD13	1.65	0.61
1:A:1075:ALA:HB2	1:A:1082:TRP:HD1	1.66	0.61
1:B:13:LEU:HD21	3:F:71:LEU:HD11	1.81	0.61
1:B:1075:ALA:HB2	1:B:1082:TRP:HD1	1.66	0.61
3:D:188:GLN:NE2	3:D:193:SER:HB2	2.16	0.61
1:A:1231:LEU:HD13	1:A:1288:TYR:HB2	1.83	0.61
1:B:149:THR:HB	1:B:194:LEU:HD22	1.83	0.60
1:B:562:PHE:HB2	1:B:654:GLY:HA2	1.82	0.60
1:B:766:ALA:HA	1:B:770:GLU:HB3	1.83	0.60
3:D:203:LEU:HG	3:D:204:SER:H	1.66	0.60
1:B:155:LEU:HD11	1:B:184:ALA:HB3	1.83	0.60
1:B:642:TRP:HB3	1:B:647:VAL:HB	1.83	0.60
1:B:775:PHE:HB2	1:B:799:ASP:HB2	1.82	0.60
2:E:4:VAL:HA	2:E:28:GLY:HA3	1.83	0.60
1:B:117:LEU:HD12	1:B:908:VAL:HG12	1.83	0.60
1:A:205:CYS:HB2	1:A:444:GLY:HA2	1.84	0.60
3:F:203:LEU:HG	3:F:204:SER:H	1.66	0.60
1:A:558:ALA:HA	1:A:827:THR:HB	1.83	0.60
3:F:152:ALA:HB3	3:F:203:LEU:HB3	1.84	0.60
1:A:35:VAL:HA	1:A:279:ARG:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:GLU:HB2	1:B:838:THR:HG23	1.83	0.59
1:A:82:PRO:HB3	1:A:1306:GLY:HA2	1.83	0.59
1:A:680:LEU:O	1:A:684:VAL:HG23	2.02	0.59
1:B:531:ALA:HB1	1:B:534:ARG:HH21	1.66	0.59
1:B:629:PRO:HG3	1:B:679:ALA:HA	1.84	0.59
1:B:1070:VAL:O	1:B:1074:ILE:HG13	2.01	0.59
3:F:135:PRO:HB2	3:F:158:LEU:HD12	1.84	0.59
3:F:137:VAL:HG22	3:F:158:LEU:HD11	1.84	0.59
2:E:149:VAL:O	2:E:152:TYR:HD1	1.85	0.59
2:E:87:MET:HE1	2:E:116:VAL:HG11	1.84	0.59
1:B:493:ALA:HB2	1:B:536:LEU:HB3	1.83	0.59
3:D:29:VAL:O	3:D:129:LYS:N	2.36	0.59
1:A:1:MET:O	2:E:54:ARG:NH2	2.36	0.59
1:A:395:MET:O	1:A:436:ARG:NH2	2.35	0.59
1:A:822:GLU:OE2	1:A:848:SER:OG	2.21	0.59
1:A:13:LEU:HD21	3:D:71:LEU:HD11	1.84	0.59
1:B:1019:LEU:HG	1:B:1252:VAL:HG21	1.83	0.59
2:C:9:SER:HG	2:C:23:SER:HG	1.49	0.58
1:A:296:GLY:HA3	1:A:327:SER:HB3	1.84	0.58
1:B:610:ALA:HB2	1:B:613:ARG:HH21	1.68	0.58
1:A:162:PRO:HG2	1:A:175:LEU:HD11	1.86	0.58
3:D:152:ALA:HB3	3:D:203:LEU:HB3	1.84	0.58
1:A:1070:VAL:O	1:A:1074:ILE:HG13	2.01	0.58
1:B:1048:GLU:HG3	1:B:1090:ALA:HA	1.85	0.58
1:A:1222:SER:HA	1:A:1267:LEU:HA	1.86	0.58
2:E:4:VAL:HG23	2:E:29:PHE:HD1	1.68	0.58
1:B:720:PRO:HB2	1:B:721:ARG:HH11	1.69	0.58
1:B:945:LEU:N	1:B:972:ALA:O	2.37	0.58
2:E:65:ALA:HB1	3:F:118:LEU:HD11	1.85	0.57
3:F:29:VAL:O	3:F:129:LYS:N	2.36	0.57
1:A:966:ARG:HA	1:A:969:LEU:HB2	1.86	0.57
1:B:608:ALA:HB1	1:B:612:ARG:HG3	1.85	0.57
1:B:966:ARG:HA	1:B:969:LEU:HB2	1.86	0.57
1:B:1125:TRP:HH2	1:B:1362:ILE:HG13	1.70	0.57
1:A:1125:TRP:HH2	1:A:1362:ILE:HG13	1.70	0.57
1:B:331:PRO:O	1:B:363:ARG:NH1	2.38	0.57
1:B:316:GLN:HA	1:B:319:VAL:HG12	1.86	0.57
1:B:966:ARG:HB2	1:B:976:VAL:HG21	1.86	0.57
1:B:1222:SER:HA	1:B:1267:LEU:HA	1.86	0.57
1:A:29:GLU:HA	1:A:33:GLU:HB2	1.86	0.57
1:A:316:GLN:O	1:A:320:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:VAL:HG23	1:B:813:PHE:HZ	1.69	0.57
1:B:580:SER:HB3	1:B:865:LEU:HD22	1.87	0.57
3:D:188:GLN:HE21	3:D:193:SER:HB2	1.70	0.56
3:F:188:GLN:HE21	3:F:193:SER:HB2	1.70	0.56
1:A:705:ARG:HH21	1:A:814:ALA:HB3	1.69	0.56
1:A:966:ARG:HB2	1:A:976:VAL:HG21	1.86	0.56
1:A:1019:LEU:HG	1:A:1252:VAL:HG21	1.87	0.56
1:B:43:ARG:HD3	1:B:49:SER:HA	1.86	0.56
1:A:1060:ARG:HG3	1:A:1061:ASN:N	2.21	0.56
2:C:149:VAL:O	2:C:152:TYR:HD1	1.89	0.56
1:A:55:TRP:CH2	1:A:401:PRO:HG3	2.41	0.56
1:A:945:LEU:N	1:A:972:ALA:O	2.37	0.56
1:B:1031:VAL:HG13	1:B:1078:ASN:HD21	1.71	0.56
1:A:395:MET:HE1	1:A:454:ILE:O	2.06	0.56
1:B:334:ILE:HD13	1:B:359:TYR:HE1	1.70	0.56
2:C:6:LEU:O	2:C:111:GLY:HA2	2.04	0.56
2:E:155:GLU:HG2	2:E:183:TYR:CE2	2.41	0.56
1:B:302:ASP:OD1	1:B:449:ASN:ND2	2.35	0.56
2:E:95:THR:HG23	2:E:117:THR:HG23	1.86	0.56
1:A:817:VAL:HG21	1:A:840:ALA:HB1	1.88	0.56
1:A:1226:HIS:HD2	1:A:1258:LEU:HD12	1.71	0.56
1:A:618:ALA:HB3	1:A:623:ARG:HD3	1.88	0.55
1:A:476:VAL:HG11	1:A:884:TRP:CZ2	2.41	0.55
1:A:1031:VAL:HG13	1:A:1078:ASN:HD21	1.71	0.55
1:B:715:ALA:HB3	1:B:724:VAL:HG12	1.88	0.55
1:B:924:GLU:HA	1:B:1350:ASN:HD21	1.71	0.55
1:B:1058:ARG:HG3	1:B:1301:GLN:HB3	1.88	0.55
2:C:155:GLU:HG2	2:C:183:TYR:CE2	2.41	0.55
1:A:863:GLY:HA3	1:A:867:ASP:OD2	2.07	0.55
1:B:1048:GLU:HB3	1:B:1060:ARG:HE	1.71	0.55
2:E:110:TRP:CD2	3:F:65:PRO:HB2	2.41	0.55
1:A:577:LEU:H	1:A:577:LEU:HD12	1.71	0.55
1:A:1063:ALA:O	1:A:1066:ALA:HB3	2.07	0.55
1:B:565:GLN:OE1	1:B:657:GLN:NE2	2.40	0.55
2:E:15:GLN:HB2	2:E:18:ARG:HE	1.71	0.55
1:A:232:VAL:HG23	1:A:272:ALA:HB2	1.89	0.55
1:A:241:LEU:HA	1:A:250:LEU:HD11	1.88	0.55
1:A:1048:GLU:HG3	1:A:1090:ALA:HA	1.87	0.55
1:B:209:LEU:HD12	1:B:442:SER:OG	2.06	0.55
1:B:1063:ALA:O	1:B:1066:ALA:HB3	2.06	0.55
2:E:150:LYS:NZ	3:F:146:GLN:OE1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:LEU:HB2	3:D:68:LEU:HD11	1.89	0.55
3:F:54:LEU:HD11	3:F:109:CYS:SG	2.47	0.55
1:A:60:GLU:HG3	1:A:62:ARG:HG3	1.89	0.55
1:A:767:LEU:HD23	1:A:803:TRP:HB2	1.87	0.55
1:A:1222:SER:HB3	1:A:1268:THR:HG22	1.88	0.55
1:B:1222:SER:HB3	1:B:1268:THR:HG22	1.88	0.55
3:D:54:LEU:HD11	3:D:109:CYS:SG	2.47	0.54
1:B:8:LYS:HB2	2:C:105:THR:HG21	1.88	0.54
1:A:199:ILE:HG23	1:B:201:VAL:HG23	1.88	0.54
1:A:718:ASN:H	1:A:723:VAL:HG12	1.71	0.54
1:A:718:ASN:HD21	1:A:813:PHE:HB3	1.72	0.54
1:B:65:VAL:HG21	1:B:255:ARG:HG3	1.90	0.54
1:A:1148:GLY:HA3	1:A:1170:LEU:HB3	1.90	0.54
2:E:22:LEU:HB2	2:E:85:LEU:HB3	1.90	0.54
1:A:301:SER:HA	1:A:448:THR:HA	1.89	0.54
1:A:756:HIS:HB3	1:A:810:THR:HA	1.89	0.54
2:C:22:LEU:HB2	2:C:85:LEU:HB3	1.90	0.54
2:C:150:LYS:NZ	3:D:146:GLN:OE1	2.39	0.54
1:A:714:ILE:HG22	1:A:725:VAL:HG12	1.89	0.53
1:A:864:SER:H	1:A:867:ASP:HB3	1.72	0.53
3:D:171:LYS:HD3	3:D:177:GLN:HB3	1.90	0.53
2:E:77:ASP:O	2:E:81:SER:HA	2.08	0.53
3:F:130:ARG:NH1	3:F:133:ALA:HB2	2.23	0.53
1:A:945:LEU:HD21	1:A:1105:SER:HB3	1.90	0.53
1:A:1262:THR:HA	1:A:1265:LEU:HD13	1.88	0.53
1:B:156:ILE:O	1:B:157:PRO:C	2.51	0.53
2:E:149:VAL:HG13	2:E:205:VAL:HG11	1.89	0.53
3:F:30:THR:HB	3:F:129:LYS:HB3	1.91	0.53
1:A:598:LEU:HD21	1:A:679:ALA:HB2	1.90	0.53
1:B:162:PRO:HB2	1:B:175:LEU:HD21	1.89	0.53
1:B:1236:VAL:HA	1:B:1239:LEU:HB2	1.89	0.53
1:A:287:GLY:O	1:A:895:ARG:NH1	2.42	0.53
1:A:1143:VAL:HG11	1:A:1160:LEU:HD13	1.90	0.53
1:B:646:GLY:HA3	1:B:883:ASP:HB3	1.90	0.53
3:F:19:VAL:HG11	3:F:45:LEU:HD21	1.90	0.53
1:A:1272:LEU:HD23	1:A:1295:LEU:HD22	1.91	0.53
1:A:1302:ARG:HD3	1:A:1309:ALA:HB2	1.90	0.53
1:A:187:ARG:HA	1:B:308:LEU:HD11	1.89	0.53
1:A:521:ARG:HB2	1:A:877:ALA:HA	1.90	0.53
1:B:368:HIS:HB3	1:B:423:LEU:HD21	1.90	0.53
1:B:945:LEU:HD21	1:B:1105:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:ARG:HH22	2:C:68:VAL:HG11	1.73	0.53
2:C:173:PHE:CZ	3:D:196:SER:HB3	2.44	0.53
1:A:1072:ARG:HG2	1:A:1112:GLN:HE21	1.74	0.53
1:B:692:LYS:HG3	1:B:728:ASP:HA	1.90	0.53
1:B:950:LEU:HB2	1:B:1003:VAL:HG22	1.91	0.53
1:B:613:ARG:NH2	1:B:620:SER:OG	2.42	0.53
2:C:8:GLN:HE22	2:C:99:TYR:HA	1.74	0.53
3:F:142:PRO:HD3	3:F:154:VAL:HB	1.91	0.53
1:A:103:ALA:HB1	1:A:905:ARG:HB3	1.90	0.53
1:B:467:GLU:HG2	1:B:505:ARG:HH22	1.73	0.53
1:B:1272:LEU:HD23	1:B:1295:LEU:HD22	1.91	0.53
1:B:642:TRP:HZ3	1:B:831:VAL:HG13	1.73	0.52
1:B:1171:VAL:HG13	1:B:1200:CYS:HB3	1.90	0.52
3:D:19:VAL:HG11	3:D:45:LEU:HD21	1.90	0.52
3:D:142:PRO:HD3	3:D:154:VAL:HB	1.91	0.52
3:F:19:VAL:HG22	3:F:43:GLN:HB2	1.91	0.52
1:A:14:ARG:HG2	3:D:51:TYR:CE2	2.42	0.52
1:A:718:ASN:HB2	1:A:723:VAL:HA	1.91	0.52
1:A:1313:ALA:HB3	1:A:1360:ILE:HG23	1.91	0.52
3:D:56:TRP:HB2	3:D:69:ILE:HB	1.91	0.52
2:E:206:ASN:HB3	2:E:213:LYS:HG3	1.89	0.52
1:A:950:LEU:HB2	1:A:1003:VAL:HG22	1.91	0.52
3:D:19:VAL:HG22	3:D:43:GLN:HB2	1.91	0.52
1:A:339:ALA:HB1	1:A:351:GLU:OE2	2.10	0.52
1:A:1074:ILE:HG22	1:A:1082:TRP:HB2	1.91	0.52
2:C:77:ASP:O	2:C:81:SER:HA	2.08	0.52
3:D:27:LEU:HD13	3:D:37:ILE:HG13	1.92	0.52
1:B:1072:ARG:HG2	1:B:1112:GLN:HE21	1.74	0.52
1:B:153:VAL:HG12	1:B:155:LEU:HG	1.92	0.52
3:D:30:THR:HB	3:D:129:LYS:HB3	1.91	0.52
1:B:906:GLU:HG2	1:B:907:ARG:H	1.75	0.52
1:B:1074:ILE:HG22	1:B:1082:TRP:HB2	1.91	0.52
2:C:177:LEU:HD13	2:C:183:TYR:CE1	2.45	0.52
1:B:208:SER:HB2	1:B:385:VAL:HB	1.91	0.52
1:B:154:GLY:HA3	1:B:207:SER:HB3	1.91	0.52
1:B:776:HIS:HB2	2:C:213:LYS:NZ	2.26	0.51
3:D:130:ARG:HG3	3:D:131:THR:O	2.11	0.51
1:A:126:MET:HB3	1:A:188:ILE:HD11	1.92	0.51
1:A:133:VAL:HG22	1:A:276:LEU:HB2	1.91	0.51
1:A:519:PRO:O	1:A:520:HIS:ND1	2.44	0.51
1:B:82:PRO:HG2	1:B:1308:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:CYS:HB3	1:B:744:ILE:HG22	1.93	0.51
1:A:577:LEU:HD13	1:A:607:ARG:HD3	1.92	0.51
1:B:1313:ALA:HB3	1:B:1360:ILE:HG23	1.91	0.51
1:A:559:VAL:HG11	1:A:820:LEU:HD13	1.93	0.51
1:A:1068:TRP:HZ2	1:A:1087:ASP:HB2	1.76	0.51
1:B:777:PRO:HG3	1:B:799:ASP:OD1	2.05	0.51
3:F:27:LEU:HD13	3:F:37:ILE:HG13	1.92	0.51
1:B:38:VAL:N	1:B:276:LEU:O	2.40	0.51
1:B:155:LEU:HD23	1:B:232:VAL:HG13	1.92	0.51
1:B:571:GLY:O	1:B:574:VAL:HG13	2.11	0.51
2:E:101:THR:HG22	2:E:110:TRP:CD2	2.46	0.51
3:F:130:ARG:HG3	3:F:131:THR:O	2.11	0.51
1:A:1171:VAL:HG22	1:A:1198:ALA:HB3	1.92	0.51
1:A:1278:SER:OG	1:A:1289:ALA:O	2.29	0.51
1:B:373:LYS:HD3	1:B:378:HIS:HA	1.93	0.51
1:B:511:LEU:HD13	1:B:898:LEU:HD13	1.93	0.51
1:A:8:LYS:HG2	2:E:105:THR:HG21	1.92	0.51
1:A:149:THR:HB	1:A:194:LEU:HD22	1.92	0.51
1:B:92:GLN:HE21	1:B:254:GLY:HA2	1.75	0.51
1:B:293:VAL:HG23	1:B:455:GLU:HB3	1.93	0.51
1:B:619:LEU:HB2	1:B:623:ARG:HG3	1.91	0.51
3:D:127:ASP:OD1	3:D:195:TYR:OH	2.28	0.51
1:A:704:VAL:HG11	1:A:723:VAL:HG11	1.93	0.51
1:B:42:CYS:HB2	1:B:44:LEU:HD22	1.91	0.51
1:B:692:LYS:HE3	1:B:754:ALA:HA	1.91	0.51
2:C:24:CYS:HB3	2:C:83:ALA:HB3	1.92	0.51
2:E:24:CYS:HB3	2:E:83:ALA:HB3	1.92	0.51
3:F:127:ASP:OD1	3:F:195:TYR:OH	2.28	0.51
1:A:1087:ASP:HB3	1:A:1114:ALA:HA	1.93	0.51
1:B:577:LEU:HB2	1:B:584:ALA:HB2	1.93	0.51
1:B:367:LEU:HB3	1:B:420:ILE:HG12	1.92	0.50
1:B:471:VAL:HG11	1:B:865:LEU:HD23	1.93	0.50
1:B:558:ALA:HB2	1:B:880:VAL:HG13	1.92	0.50
1:A:41:ALA:HB1	1:A:129:LEU:HD12	1.93	0.50
1:A:1157:ALA:HA	1:A:1160:LEU:HD12	1.93	0.50
1:B:1278:SER:OG	1:B:1289:ALA:O	2.29	0.50
2:E:110:TRP:CE2	3:F:65:PRO:HB2	2.47	0.50
1:A:561:VAL:HG13	1:A:653:ILE:HD11	1.93	0.50
1:B:339:ALA:HB2	1:B:369:LEU:HD11	1.93	0.50
1:A:617:ALA:HB1	1:A:860:ARG:HE	1.75	0.50
1:B:158:GLN:NE2	1:B:240:MET:HE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1087:ASP:HB3	1:B:1114:ALA:HA	1.93	0.50
2:C:105:THR:HA	3:D:117:ARG:HH22	1.75	0.50
3:F:130:ARG:HD2	3:F:193:SER:OG	2.11	0.50
3:F:170:TRP:CD2	3:F:201:LEU:HD13	2.47	0.50
1:A:694:MET:HB2	1:A:749:LEU:HD12	1.93	0.50
1:B:1157:ALA:HA	1:B:1160:LEU:HD12	1.92	0.50
1:A:141:PRO:HD2	1:A:516:ALA:HB2	1.93	0.50
1:A:1337:ILE:HG22	1:A:1363:ASP:HB3	1.94	0.50
1:B:329:LEU:HD13	1:B:437:ARG:HD3	1.93	0.50
2:E:178:GLN:OE1	2:E:184:SER:OG	2.15	0.50
1:B:126:MET:HE2	1:B:232:VAL:HB	1.94	0.50
1:B:627:VAL:O	1:B:631:MET:HG2	2.11	0.50
2:C:91:LYS:HE3	2:C:93:GLU:HB3	1.94	0.50
1:A:597:HIS:HB2	1:A:675:ALA:HB1	1.94	0.50
1:A:709:GLY:H	1:A:713:GLU:HB2	1.77	0.50
1:A:292:ALA:HB3	1:A:392:VAL:HG22	1.94	0.50
1:B:1068:TRP:HZ2	1:B:1087:ASP:HB2	1.76	0.50
2:C:170:VAL:HG22	2:C:189:VAL:HG12	1.94	0.50
2:C:178:GLN:OE1	2:C:184:SER:OG	2.15	0.50
2:E:170:VAL:HG22	2:E:189:VAL:HG12	1.94	0.50
2:E:177:LEU:HB2	2:E:183:TYR:HE1	1.77	0.49
1:B:597:HIS:CE1	1:B:676:ARG:HB2	2.47	0.49
1:B:837:LEU:O	1:B:841:ILE:N	2.45	0.49
3:D:130:ARG:HD2	3:D:193:SER:OG	2.11	0.49
1:A:1171:VAL:HG11	1:A:1211:LEU:HD21	1.95	0.49
1:B:38:VAL:HG12	1:B:137:ALA:HB1	1.93	0.49
1:B:698:ALA:HA	1:B:722:SER:HA	1.94	0.49
1:B:1337:ILE:HG22	1:B:1363:ASP:HB3	1.94	0.49
2:C:133:PRO:HG2	2:C:220:PRO:HB3	1.94	0.49
1:A:93:ARG:NH2	1:A:1055:PRO:O	2.27	0.49
1:A:300:ASN:O	1:A:449:ASN:N	2.45	0.49
1:A:655:HIS:CE1	1:A:836:ILE:HG13	2.47	0.49
1:B:642:TRP:CD1	1:B:829:LEU:HD21	2.47	0.49
1:B:840:ALA:HA	1:B:843:GLU:OE1	2.13	0.49
1:B:921:GLU:HB2	1:B:1354:ARG:HA	1.94	0.49
1:B:1052:ALA:HA	1:B:1116:ARG:NH2	2.27	0.49
3:D:217:GLU:HB3	3:D:228:THR:HA	1.95	0.49
1:A:1068:TRP:CZ2	1:A:1087:ASP:HB2	2.48	0.49
1:B:103:ALA:HB1	1:B:905:ARG:HB3	1.95	0.49
1:B:841:ILE:O	1:B:844:ILE:HB	2.13	0.49
1:B:1383:ASP:OD1	1:B:1389:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1096:LEU:HA	1:B:1100:LEU:HG	1.94	0.49
2:E:177:LEU:HB2	2:E:183:TYR:CE1	2.47	0.49
1:A:162:PRO:HD2	1:A:175:LEU:HD21	1.94	0.49
1:B:305:SER:OG	1:B:307:GLY:O	2.29	0.49
3:D:25:LEU:O	3:D:125:LYS:N	2.41	0.49
1:B:1068:TRP:CZ2	1:B:1087:ASP:HB2	2.47	0.49
1:A:709:GLY:N	1:A:713:GLU:HB2	2.28	0.49
1:A:1383:ASP:OD1	1:A:1389:ARG:NH2	2.46	0.49
1:B:243:ASP:O	1:B:244:PHE:C	2.52	0.49
1:A:1270:PHE:O	1:A:1272:LEU:HD12	2.13	0.48
1:B:108:PHE:HZ	1:B:131:TRP:CE2	2.30	0.48
1:B:838:THR:HA	1:B:841:ILE:HB	1.95	0.48
2:C:160:SER:HB3	2:C:164:GLY:H	1.78	0.48
2:C:177:LEU:HD13	2:C:183:TYR:HE1	1.76	0.48
2:E:133:PRO:HG2	2:E:220:PRO:HB3	1.95	0.48
1:A:718:ASN:ND2	1:A:813:PHE:HB3	2.28	0.48
1:B:40:MET:HE1	1:B:393:LEU:HD21	1.95	0.48
1:B:704:VAL:HG22	1:B:714:ILE:HD11	1.95	0.48
1:B:1143:VAL:HG11	1:B:1160:LEU:HD13	1.94	0.48
1:B:1270:PHE:O	1:B:1272:LEU:HD12	2.13	0.48
1:A:559:VAL:HB	1:A:825:TYR:HB3	1.95	0.48
2:C:6:LEU:HD11	2:C:102:ARG:HG3	1.96	0.48
2:C:151:ASP:HA	2:C:182:LEU:HB3	1.95	0.48
1:A:98:LEU:HD12	1:A:234:VAL:HG22	1.96	0.48
1:B:54:PHE:C	1:B:56:GLU:H	2.21	0.48
1:B:156:ILE:HG13	1:B:381:ALA:HB2	1.95	0.48
1:A:810:THR:HG23	1:A:812:ARG:HG2	1.96	0.48
1:A:981:VAL:HB	1:A:990:LEU:HD21	1.94	0.48
1:A:1096:LEU:HA	1:A:1100:LEU:HG	1.94	0.48
1:B:1313:ALA:HB3	1:B:1360:ILE:HA	1.95	0.48
3:F:217:GLU:HB3	3:F:228:THR:HA	1.95	0.48
1:A:736:VAL:O	1:A:740:THR:HG23	2.14	0.48
2:C:149:VAL:CG1	2:C:205:VAL:HG11	2.43	0.48
3:D:187:GLU:OE1	3:D:187:GLU:N	2.47	0.48
3:F:187:GLU:N	3:F:187:GLU:OE1	2.47	0.48
1:A:257:LYS:HG3	1:A:405:HIS:HB3	1.96	0.48
1:A:475:TRP:CD1	1:A:508:ALA:HB2	2.48	0.48
1:A:491:ARG:HD3	1:A:902:PRO:HD3	1.96	0.48
1:B:15:ARG:HH21	3:D:76:ALA:HB1	1.79	0.48
1:A:302:ASP:N	1:A:447:GLY:O	2.46	0.48
1:B:1000:VAL:HG12	1:B:1002:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:THR:HG23	2:C:117:THR:HG23	1.95	0.48
3:D:58:LEU:HD13	3:D:107:TYR:CZ	2.49	0.48
1:A:391:MET:HE1	1:A:400:LEU:HD21	1.95	0.48
1:A:558:ALA:H	1:A:649:PRO:HA	1.78	0.48
2:C:131:LEU:HD11	2:C:148:LEU:HG	1.95	0.48
2:C:155:GLU:HG2	2:C:183:TYR:CD2	2.49	0.47
1:A:19:ASP:OD1	3:F:77:SER:HB3	2.13	0.47
1:A:241:LEU:HD23	1:A:268:MET:HE2	1.94	0.47
2:C:36:MET:HB3	2:C:36:MET:HE3	1.23	0.47
2:C:177:LEU:O	3:D:182:GLN:NE2	2.24	0.47
1:A:429:TRP:HH2	1:A:438:ALA:HB2	1.79	0.47
1:B:1158:ARG:HG3	1:B:1188:LEU:HD23	1.96	0.47
2:E:185:LEU:HD23	2:E:186:SER:N	2.29	0.47
1:A:273:GLY:HA3	1:A:385:VAL:HG13	1.97	0.47
1:A:602:VAL:HG22	1:A:606:LEU:HG	1.96	0.47
1:B:40:MET:HB3	1:B:389:ILE:HG12	1.96	0.47
1:B:197:PRO:HD2	1:B:224:SER:HB3	1.96	0.47
1:B:568:GLN:OE1	1:B:568:GLN:N	2.36	0.47
2:E:155:GLU:HG2	2:E:183:TYR:CD2	2.49	0.47
3:F:58:LEU:HD13	3:F:107:TYR:CZ	2.49	0.47
1:A:12:TYR:CD1	2:E:106:LEU:HD22	2.49	0.47
1:A:242:VAL:O	1:A:246:ARG:HG2	2.14	0.47
1:A:329:LEU:HD13	1:A:437:ARG:HD3	1.97	0.47
1:A:1313:ALA:HB3	1:A:1360:ILE:HA	1.95	0.47
1:B:1188:LEU:H	1:B:1188:LEU:HG	1.50	0.47
3:D:184:SER:HB3	3:D:198:SER:HB3	1.96	0.47
2:E:151:ASP:HA	2:E:182:LEU:HB3	1.96	0.47
1:A:555:GLN:HB3	1:A:646:GLY:O	2.15	0.47
1:B:688:MET:N	1:B:689:PRO:HD2	2.30	0.47
1:A:159:GLU:HG2	1:B:163:ARG:HE	1.79	0.47
1:A:308:LEU:HD21	1:B:183:VAL:HB	1.97	0.47
1:A:502:GLN:HB2	1:A:507:ILE:HD11	1.96	0.47
1:A:715:ALA:O	1:A:811:VAL:HG12	2.15	0.47
1:A:1239:LEU:HD22	1:A:1244:ILE:HG12	1.97	0.47
1:B:312:ASN:HD22	1:B:315:ALA:HB2	1.79	0.47
1:B:652:VAL:HG21	1:B:666:ALA:HB2	1.96	0.47
1:B:1028:LEU:HD11	1:B:1244:ILE:HD11	1.97	0.47
1:A:391:MET:O	1:A:395:MET:HG3	2.14	0.47
1:A:596:PRO:HG2	1:A:597:HIS:ND1	2.29	0.47
3:D:163:PRO:O	3:D:220:HIS:NE2	2.48	0.47
1:A:154:GLY:HA3	1:A:207:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HD12	1:B:278:GLU:HB2	1.96	0.47
1:B:555:GLN:O	1:B:557:ARG:HG2	2.15	0.47
2:E:36:MET:HE3	2:E:36:MET:HB3	1.58	0.47
1:A:28:ARG:HH21	3:D:75:ARG:HH21	1.63	0.47
1:A:472:VAL:HG21	1:A:866:ALA:HA	1.97	0.47
1:A:594:LEU:HD22	1:A:675:ALA:HA	1.97	0.47
1:A:1000:VAL:HG12	1:A:1002:GLY:H	1.78	0.47
1:A:1019:LEU:HD13	1:A:1244:ILE:HG22	1.97	0.47
1:B:478:SER:O	1:B:488:GLN:NE2	2.48	0.47
1:B:856:HIS:CE1	1:B:859:ARG:HG2	2.50	0.47
1:B:340:HIS:ND1	1:B:442:SER:HA	2.30	0.46
1:A:681:ARG:HH11	1:A:685:ILE:HD11	1.81	0.46
1:A:1236:VAL:HA	1:A:1239:LEU:HB2	1.98	0.46
1:B:495:HIS:NE2	1:B:897:PRO:O	2.47	0.46
1:B:1176:PRO:HD2	1:B:1199:ALA:HB2	1.97	0.46
2:E:7:VAL:HG23	2:E:25:THR:HB	1.98	0.46
1:A:163:ARG:NH1	1:B:914:PRO:HD2	2.29	0.46
1:A:828:PHE:H	1:A:853:SER:H	1.63	0.46
1:A:1079:PRO:HB3	1:A:1377:ARG:HG2	1.98	0.46
1:B:317:VAL:HG13	1:B:358:ALA:HB2	1.98	0.46
1:B:485:LEU:HD21	1:B:522:ALA:HB2	1.95	0.46
1:B:638:LEU:HB3	1:B:642:TRP:CZ3	2.51	0.46
1:B:660:ILE:HG22	1:B:674:ALA:HB1	1.96	0.46
1:A:69:PRO:CG	1:A:72:ARG:HD2	2.45	0.46
1:B:125:LEU:HD23	1:B:125:LEU:HA	1.77	0.46
1:B:1079:PRO:HB3	1:B:1377:ARG:HG2	1.98	0.46
2:C:87:MET:HE2	2:C:87:MET:HB3	1.78	0.46
3:D:166:ALA:HB2	3:D:220:HIS:HB2	1.97	0.46
2:E:131:LEU:HB2	2:E:146:GLY:C	2.40	0.46
2:E:152:TYR:HB2	2:E:207:HIS:CD2	2.50	0.46
2:E:208:LYS:HA	2:E:208:LYS:HD2	1.70	0.46
1:A:931:ARG:HE	1:A:931:ARG:HB2	1.57	0.46
1:B:45:PRO:HD2	1:B:376:LEU:HD22	1.98	0.46
1:B:118:ALA:HB2	1:B:171:VAL:HG12	1.97	0.46
1:A:400:LEU:HD22	1:A:423:LEU:HD11	1.98	0.46
1:A:1137:TRP:HE1	1:A:1268:THR:HG23	1.81	0.46
1:A:1176:PRO:HD2	1:A:1199:ALA:HB2	1.97	0.46
1:A:1272:LEU:HD23	1:A:1295:LEU:CD2	2.46	0.46
1:A:336:ALA:HB2	1:A:400:LEU:HD11	1.98	0.46
1:A:755:SER:HA	1:A:807:LEU:HA	1.96	0.46
1:B:349:PRO:HA	1:B:413:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:VAL:O	1:B:511:LEU:HG	2.16	0.46
2:E:13:LEU:HD13	2:E:117:THR:HB	1.98	0.46
1:A:129:LEU:HD12	1:A:129:LEU:HA	1.81	0.46
1:A:580:SER:HB3	1:A:583:PHE:HB3	1.98	0.46
1:B:86:ARG:HE	1:B:86:ARG:HB2	1.57	0.46
1:B:584:ALA:O	1:B:588:ARG:HG2	2.15	0.46
1:B:907:ARG:NH1	1:B:909:TRP:HB3	2.31	0.46
1:B:1068:TRP:O	1:B:1072:ARG:HG3	2.16	0.46
1:B:1272:LEU:HD23	1:B:1295:LEU:CD2	2.46	0.46
3:D:144:ASP:HA	3:D:147:LEU:HD12	1.98	0.46
2:E:31:PHE:CE2	2:E:76:ARG:HB2	2.51	0.46
2:E:31:PHE:HB3	2:E:78:ASP:OD1	2.16	0.46
2:E:188:VAL:HG21	3:F:157:LEU:HD12	1.98	0.46
1:A:339:ALA:HB2	1:A:355:LEU:HD11	1.99	0.45
1:B:241:LEU:HB3	1:B:268:MET:CE	2.47	0.45
1:B:692:LYS:NZ	1:B:726:ALA:HB1	2.31	0.45
1:B:1302:ARG:HD3	1:B:1309:ALA:HB2	1.97	0.45
1:A:207:SER:HB2	1:A:381:ALA:HB1	1.98	0.45
1:B:78:SER:C	1:B:80:PHE:N	2.72	0.45
1:B:510:SER:HB3	1:B:895:ARG:HB2	1.98	0.45
2:E:37:SER:HB2	2:E:101:THR:OG1	2.15	0.45
1:A:205:CYS:HB3	1:A:378:HIS:NE2	2.32	0.45
1:B:1137:TRP:HE1	1:B:1268:THR:HG23	1.81	0.45
2:E:143:ALA:HA	3:F:138:PHE:HE2	1.81	0.45
1:A:2:ALA:HA	2:E:54:ARG:HH21	1.81	0.45
1:A:443:PHE:CD1	1:A:449:ASN:HB3	2.50	0.45
1:A:802:TYR:O	1:A:805:ARG:HG2	2.15	0.45
2:C:31:PHE:HB3	2:C:78:ASP:OD1	2.16	0.45
1:A:351:GLU:HG3	1:A:443:PHE:HE2	1.81	0.45
1:A:1229:ALA:HB1	1:A:1288:TYR:HE1	1.82	0.45
1:B:194:LEU:HD11	1:B:228:MET:HE2	1.98	0.45
1:B:388:VAL:HG22	1:B:440:VAL:HG21	1.99	0.45
2:C:31:PHE:CE2	2:C:76:ARG:HB2	2.51	0.45
1:A:165:ALA:O	1:B:242:VAL:HG11	2.15	0.45
1:A:1377:ARG:HA	1:A:1377:ARG:HD2	1.77	0.45
1:B:17:THR:HG23	3:F:74:ASN:HD21	1.81	0.45
2:C:77:ASP:O	2:C:81:SER:CA	2.64	0.45
2:E:77:ASP:O	2:E:81:SER:CA	2.64	0.45
1:B:44:LEU:HG	1:B:376:LEU:CD1	2.47	0.45
3:F:137:VAL:HB	3:F:229:LYS:NZ	2.32	0.45
1:B:826:ARG:HG3	1:B:852:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:VAL:HG23	2:C:25:THR:HB	1.98	0.45
1:A:121:PRO:HB2	1:A:234:VAL:HG11	1.99	0.45
1:A:732:LEU:HD23	1:A:735:LEU:HD12	1.98	0.45
2:E:176:VAL:CG2	3:F:184:SER:HB2	2.47	0.45
1:B:103:ALA:HA	1:B:906:GLU:O	2.17	0.45
1:B:370:GLY:HA2	1:B:403:THR:OG1	2.17	0.45
3:D:58:LEU:HD13	3:D:107:TYR:CE2	2.52	0.45
3:F:70:TYR:O	3:F:71:LEU:C	2.60	0.45
1:A:1034:MET:SD	1:A:1081:VAL:HG13	2.57	0.44
1:B:176:MET:HB3	1:B:176:MET:HE3	1.00	0.44
1:B:465:ARG:HD2	1:B:465:ARG:HA	1.38	0.44
1:B:736:VAL:HG11	1:B:748:ARG:HD3	2.00	0.44
1:B:1156:ILE:HD13	1:B:1156:ILE:HA	1.82	0.44
3:F:137:VAL:HG22	3:F:158:LEU:CD1	2.46	0.44
1:B:539:LEU:HD22	1:B:539:LEU:HA	1.70	0.44
1:B:1110:GLU:HB2	1:B:1113:LEU:HD21	1.99	0.44
1:B:1163:ARG:HA	1:B:1163:ARG:HD3	1.39	0.44
1:B:1171:VAL:HG21	1:B:1211:LEU:CD1	2.46	0.44
1:B:1229:ALA:HB1	1:B:1288:TYR:HE1	1.82	0.44
1:B:1377:ARG:HD2	1:B:1377:ARG:HA	1.77	0.44
3:F:58:LEU:HD13	3:F:107:TYR:CE2	2.52	0.44
1:A:79:LEU:HD21	1:A:238:PRO:HB3	1.99	0.44
1:A:1139:PRO:HB2	1:A:1165:ALA:HA	1.99	0.44
1:A:1310:THR:HG22	1:A:1312:VAL:HG13	1.98	0.44
1:A:1362:ILE:HB	1:A:1364:VAL:HG12	2.00	0.44
1:B:531:ALA:O	1:B:534:ARG:HB3	2.17	0.44
1:B:926:SER:H	1:B:1346:ARG:HH12	1.65	0.44
1:B:1028:LEU:HD21	1:B:1070:VAL:HG21	1.99	0.44
1:B:1034:MET:SD	1:B:1081:VAL:HG13	2.57	0.44
1:B:1093:VAL:HB	1:B:1096:LEU:HD12	1.98	0.44
2:E:148:LEU:HD21	3:F:155:VAL:HG21	2.00	0.44
2:E:207:HIS:O	2:E:211:ASN:N	2.49	0.44
1:A:8:LYS:C	1:A:10:ALA:H	2.25	0.44
1:B:763:ILE:HB	1:B:767:LEU:HB2	1.99	0.44
1:B:1139:PRO:HB2	1:B:1165:ALA:HA	1.99	0.44
2:C:52:PHE:CE1	2:C:63:GLU:HB3	2.52	0.44
2:E:131:LEU:HD12	2:E:131:LEU:HA	1.81	0.44
1:A:1043:LEU:N	1:A:1081:VAL:O	2.48	0.44
1:A:1068:TRP:O	1:A:1072:ARG:HG3	2.16	0.44
1:B:54:PHE:C	1:B:56:GLU:N	2.74	0.44
1:B:329:LEU:HD12	1:B:453:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:SER:HB2	1:B:518:LEU:HD22	2.00	0.44
3:D:58:LEU:O	3:D:66:GLN:N	2.40	0.44
1:A:44:LEU:HD22	1:A:376:LEU:HD13	1.99	0.44
1:A:349:PRO:HA	1:A:413:ILE:HG12	1.99	0.44
1:B:302:ASP:HB3	1:B:312:ASN:HB2	2.00	0.44
1:B:720:PRO:HB2	1:B:721:ARG:HD2	1.99	0.44
1:A:234:VAL:HA	1:A:270:GLU:HG3	2.00	0.44
1:A:483:GLU:OE1	1:A:486:ARG:NH2	2.50	0.44
1:B:1209:ARG:HA	1:B:1261:LEU:HD21	1.99	0.44
2:E:35:ALA:CB	2:E:54:ARG:HA	2.48	0.44
3:F:25:LEU:O	3:F:125:LYS:N	2.41	0.44
1:A:1188:LEU:H	1:A:1188:LEU:HG	1.50	0.44
1:B:619:LEU:HD12	1:B:619:LEU:HA	1.71	0.44
1:B:1071:GLY:HA3	1:B:1085:LEU:HD11	2.00	0.44
1:A:317:VAL:HG13	1:A:358:ALA:HB2	1.99	0.44
1:A:512:ALA:HB1	1:A:884:TRP:HB3	2.00	0.44
1:A:835:PRO:HB2	1:A:837:LEU:HD23	2.00	0.44
1:A:1093:VAL:HB	1:A:1096:LEU:HD12	1.98	0.44
1:A:1156:ILE:HD13	1:A:1156:ILE:HA	1.83	0.44
1:A:1224:VAL:HB	1:A:1270:PHE:HD1	1.83	0.44
1:B:568:GLN:HE21	1:B:621:THR:HG21	1.83	0.44
1:B:655:HIS:NE2	1:B:724:VAL:HG21	2.33	0.44
1:A:34:PRO:HB2	1:A:293:VAL:HG11	1.99	0.43
1:A:580:SER:HB3	1:A:583:PHE:CB	2.48	0.43
1:A:865:LEU:HD22	1:A:865:LEU:HA	1.74	0.43
1:B:682:SER:HA	1:B:685:ILE:HG22	2.00	0.43
1:B:1088:VAL:HG11	1:B:1096:LEU:HD23	2.00	0.43
1:B:1224:VAL:HB	1:B:1270:PHE:HD1	1.83	0.43
2:C:37:SER:O	2:C:101:THR:OG1	2.36	0.43
1:A:8:LYS:C	1:A:10:ALA:N	2.75	0.43
1:A:722:SER:HB2	1:A:744:ILE:HG13	2.00	0.43
1:A:755:SER:OG	1:A:806:ASN:O	2.31	0.43
1:A:805:ARG:HA	1:A:809:ARG:HG3	2.00	0.43
1:A:1096:LEU:HD22	1:A:1100:LEU:HD11	2.00	0.43
1:A:1110:GLU:HB2	1:A:1113:LEU:HD21	1.99	0.43
1:B:1096:LEU:HD22	1:B:1100:LEU:HD11	2.00	0.43
1:B:1371:LEU:H	1:B:1371:LEU:HG	1.45	0.43
3:F:22:GLN:N	3:F:22:GLN:OE1	2.51	0.43
1:A:379:THR:HB	1:A:382:ALA:HB3	1.99	0.43
1:A:567:TRP:CD1	1:A:832:SER:HB2	2.53	0.43
1:A:654:GLY:HA3	1:A:659:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:LEU:HD21	1:A:1070:VAL:HG21	1.99	0.43
1:B:778:LEU:HD22	1:B:778:LEU:HA	1.80	0.43
2:E:112:GLN:H	2:E:112:GLN:HG3	1.17	0.43
1:A:1071:GLY:HA3	1:A:1085:LEU:HD11	2.00	0.43
1:B:573:ALA:HB1	1:B:576:LEU:HB3	2.00	0.43
1:B:795:PRO:HD2	1:B:798:LEU:HB2	2.00	0.43
1:B:1033:ALA:O	1:B:1037:ALA:N	2.50	0.43
3:F:158:LEU:HD13	3:F:158:LEU:HA	1.82	0.43
1:A:338:GLU:O	1:A:338:GLU:HG3	2.18	0.43
1:A:492:LEU:HD21	1:A:511:LEU:HD11	2.01	0.43
1:B:641:MET:HG2	1:B:868:PHE:CZ	2.53	0.43
1:B:703:GLU:HG2	1:B:704:VAL:N	2.34	0.43
1:B:705:ARG:HG2	1:B:714:ILE:HG13	2.00	0.43
3:D:128:ILE:HB	3:D:188:GLN:NE2	2.34	0.43
3:F:31:PRO:HA	3:F:99:VAL:O	2.19	0.43
1:A:80:PHE:CE1	1:A:93:ARG:HD2	2.53	0.43
1:B:39:ALA:HB2	1:B:137:ALA:HB2	2.00	0.43
1:B:149:THR:HA	1:B:226:LEU:O	2.19	0.43
1:B:155:LEU:HD12	1:B:200:SER:OG	2.19	0.43
1:B:177:THR:O	1:B:183:VAL:HG21	2.19	0.43
1:B:367:LEU:O	1:B:421:SER:N	2.39	0.43
1:B:380:GLN:HB3	1:B:381:ALA:H	1.48	0.43
1:B:949:TRP:HZ3	1:B:1044:TRP:HD1	1.65	0.43
1:B:1167:HIS:CD2	1:B:1219:VAL:HG11	2.53	0.43
1:B:1339:MET:H	1:B:1339:MET:HG3	1.56	0.43
1:A:688:MET:HE1	1:A:759:HIS:O	2.18	0.43
1:A:756:HIS:HE1	1:A:788:VAL:HG13	1.84	0.43
1:B:734:ARG:HD3	1:B:734:ARG:HA	1.61	0.43
3:D:22:GLN:OE1	3:D:22:GLN:N	2.52	0.43
3:D:137:VAL:HB	3:D:229:LYS:NZ	2.34	0.43
2:E:80:LYS:O	2:E:82:ILE:HG12	2.18	0.43
1:A:680:LEU:HD22	1:A:803:TRP:CE2	2.54	0.43
1:A:760:VAL:HG23	1:A:763:ILE:HG13	2.01	0.43
1:A:865:LEU:HB3	1:A:866:ALA:H	1.66	0.43
1:A:949:TRP:HZ3	1:A:1044:TRP:HD1	1.66	0.43
1:A:1088:VAL:HG11	1:A:1096:LEU:HD23	2.00	0.43
1:B:610:ALA:HA	1:B:613:ARG:HE	1.83	0.43
1:B:1362:ILE:HB	1:B:1364:VAL:HG12	2.00	0.43
2:E:22:LEU:HD23	2:E:22:LEU:HA	1.88	0.43
3:F:29:VAL:HB	3:F:99:VAL:HG11	2.00	0.43
1:A:1209:ARG:HA	1:A:1261:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:ALA:HB1	1:B:672:ASP:HA	2.00	0.43
1:B:748:ARG:H	1:B:748:ARG:HG2	1.57	0.43
1:B:1212:LEU:HD13	1:B:1261:LEU:HD22	2.01	0.43
2:C:8:GLN:HE21	2:C:100:CYS:HB2	1.84	0.43
2:C:49:TRP:HZ2	2:C:52:PHE:HD1	1.66	0.43
3:D:31:PRO:HA	3:D:99:VAL:O	2.19	0.43
3:F:106:VAL:HG22	3:F:125:LYS:HD2	2.01	0.43
1:A:1033:ALA:O	1:A:1037:ALA:N	2.50	0.43
1:B:44:LEU:HG	1:B:376:LEU:HD11	2.00	0.43
1:B:72:ARG:H	1:B:72:ARG:HG2	1.61	0.43
1:B:235:MET:HA	1:B:236:PRO:HD2	1.83	0.43
1:B:512:ALA:HB1	1:B:884:TRP:CG	2.54	0.43
2:E:53:ILE:HB	2:E:74:ILE:HG22	2.01	0.43
2:E:205:VAL:O	2:E:213:LYS:HA	2.19	0.43
3:F:58:LEU:HD21	3:F:60:LYS:HG3	2.01	0.43
1:B:78:SER:C	1:B:80:PHE:H	2.26	0.42
1:B:406:ALA:HB1	1:B:422:LEU:HD13	2.01	0.42
1:B:921:GLU:CB	1:B:1354:ARG:HA	2.49	0.42
2:C:185:LEU:HD23	2:C:186:SER:N	2.34	0.42
1:A:576:LEU:HA	1:A:576:LEU:HD12	1.72	0.42
1:B:608:ALA:HA	1:B:612:ARG:HE	1.85	0.42
2:C:80:LYS:O	2:C:82:ILE:HG12	2.19	0.42
3:D:141:PRO:HA	3:D:154:VAL:HG23	2.01	0.42
1:A:36:ALA:HB1	1:A:290:VAL:HG13	2.02	0.42
1:A:681:ARG:NH1	1:A:685:ILE:HD11	2.34	0.42
1:B:29:GLU:HA	1:B:33:GLU:HB2	2.01	0.42
1:B:1043:LEU:N	1:B:1081:VAL:O	2.48	0.42
1:B:1331:PHE:HB3	1:B:1336:VAL:HG13	2.02	0.42
3:F:215:ALA:HA	3:F:230:SER:HA	2.01	0.42
1:A:126:MET:HE2	1:A:232:VAL:HB	2.01	0.42
1:A:269:ALA:HB2	1:A:377:GLY:HA3	2.01	0.42
1:A:841:ILE:HG23	1:A:852:LEU:HD13	2.01	0.42
1:B:337:VAL:HG23	1:B:367:LEU:HD11	2.02	0.42
1:B:495:HIS:CG	1:B:899:PRO:HD3	2.55	0.42
3:D:29:VAL:HB	3:D:99:VAL:HG11	2.00	0.42
1:A:228:MET:HG2	1:A:276:LEU:HD13	2.01	0.42
1:A:349:PRO:O	1:A:353:ARG:HG3	2.18	0.42
1:A:1163:ARG:HA	1:A:1163:ARG:HD3	1.42	0.42
1:A:1331:PHE:HB3	1:A:1336:VAL:HG13	2.02	0.42
1:B:338:GLU:N	1:B:439:GLY:O	2.46	0.42
1:A:35:VAL:HG23	1:A:294:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ILE:O	1:A:363:ARG:NH1	2.33	0.42
1:A:410:SER:HB3	1:A:413:ILE:HD12	2.02	0.42
1:A:944:ARG:HD3	1:A:944:ARG:HA	1.92	0.42
1:A:1339:MET:H	1:A:1339:MET:HG3	1.56	0.42
2:C:206:ASN:HD22	2:C:213:LYS:HG3	1.85	0.42
3:F:128:ILE:HB	3:F:188:GLN:NE2	2.34	0.42
1:A:556:GLN:NE2	1:B:304:ALA:HB1	2.34	0.42
1:A:1049:SER:N	1:A:1088:VAL:O	2.50	0.42
2:C:69:LYS:HA	2:C:69:LYS:HD3	1.85	0.42
1:A:683:ARG:O	1:A:687:THR:HG22	2.20	0.42
1:A:733:ASP:OD1	1:A:734:ARG:N	2.52	0.42
1:A:1222:SER:HB3	1:A:1268:THR:H	1.85	0.42
1:B:265:GLY:HA2	1:B:344:THR:HA	2.02	0.42
1:B:577:LEU:HD23	1:B:577:LEU:H	1.85	0.42
1:B:628:GLN:HB2	1:B:682:SER:HB2	2.02	0.42
2:C:38:TRP:O	2:C:50:VAL:HB	2.19	0.42
3:D:168:VAL:HG21	3:D:197:LEU:HD22	2.02	0.42
1:A:378:HIS:CD2	1:A:380:GLN:H	2.38	0.42
1:A:434:ARG:HE	1:A:434:ARG:HB3	1.61	0.42
1:A:612:ARG:H	1:A:612:ARG:HG3	1.45	0.42
1:A:1007:LEU:H	1:A:1007:LEU:HG	1.42	0.42
1:B:506:ASP:OD2	1:B:894:ARG:NH1	2.53	0.42
1:B:589:GLU:HG2	1:B:590:CYS:N	2.35	0.42
3:F:118:LEU:HD13	3:F:118:LEU:HA	1.83	0.42
1:A:760:VAL:CG1	1:A:808:ARG:HB2	2.49	0.42
1:B:121:PRO:HB2	1:B:234:VAL:HG11	2.02	0.42
1:B:556:GLN:HG3	1:B:881:ALA:HB2	2.02	0.42
1:B:1007:LEU:H	1:B:1007:LEU:HG	1.42	0.42
2:C:149:VAL:HG13	2:C:205:VAL:HG11	2.01	0.42
1:A:787:THR:O	1:A:811:VAL:HG23	2.20	0.41
1:A:837:LEU:O	1:A:841:ILE:N	2.49	0.41
1:B:1053:THR:HG22	1:B:1114:ALA:CB	2.49	0.41
1:B:1169:LEU:HD13	1:B:1169:LEU:HA	1.89	0.41
1:B:1222:SER:HB3	1:B:1268:THR:H	1.85	0.41
1:A:34:PRO:HB2	1:A:293:VAL:CG1	2.50	0.41
1:A:400:LEU:HA	1:A:401:PRO:HD3	1.88	0.41
1:A:711:ARG:HH21	1:A:759:HIS:HB2	1.85	0.41
1:B:12:TYR:CE1	3:D:70:TYR:HB2	2.55	0.41
1:B:253:ASP:OD2	1:B:255:ARG:HD3	2.20	0.41
1:B:311:PRO:HG2	1:B:350:ILE:HD12	2.01	0.41
2:C:18:ARG:HA	2:C:18:ARG:HD3	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:49:TRP:HZ2	2:E:52:PHE:HD1	1.66	0.41
1:A:244:PHE:HD2	1:A:268:MET:HE1	1.85	0.41
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.75	0.41
1:A:570:ALA:HB3	1:A:605:PHE:HE2	1.85	0.41
1:A:584:ALA:O	1:A:588:ARG:HD3	2.19	0.41
1:A:864:SER:HA	1:A:868:PHE:HB2	2.03	0.41
1:B:378:HIS:C	1:B:380:GLN:H	2.26	0.41
3:D:106:VAL:HG22	3:D:125:LYS:HD2	2.01	0.41
1:A:39:ALA:HB2	1:A:137:ALA:HB2	2.01	0.41
1:A:55:TRP:O	1:A:59:SER:HB3	2.20	0.41
1:A:122:GLN:HB3	1:A:155:LEU:HD23	2.03	0.41
1:A:227:ALA:O	1:A:276:LEU:HD12	2.20	0.41
1:B:811:VAL:HG12	1:B:813:PHE:HB2	2.01	0.41
1:B:921:GLU:HB3	1:B:922:VAL:H	1.63	0.41
3:D:215:ALA:HA	3:D:230:SER:HA	2.01	0.41
2:E:21:ARG:NH1	2:E:84:TYR:CD2	2.88	0.41
2:E:80:LYS:NZ	2:E:82:ILE:HG13	2.36	0.41
1:A:221:ARG:HD2	1:A:223:GLU:HB2	2.03	0.41
1:A:329:LEU:HD12	1:A:453:ILE:HG21	2.03	0.41
1:B:76:LEU:H	1:B:76:LEU:HG	1.36	0.41
1:B:139:ILE:HD12	1:B:139:ILE:H	1.85	0.41
1:B:604:PRO:HB3	1:B:607:ARG:HH21	1.86	0.41
1:B:773:GLU:H	1:B:773:GLU:HG3	1.47	0.41
1:B:1137:TRP:CD1	1:B:1268:THR:HG1	2.38	0.41
2:C:6:LEU:HD22	2:C:24:CYS:SG	2.61	0.41
1:A:1030:LEU:O	1:A:1034:MET:HG3	2.21	0.41
1:B:1100:LEU:O	1:B:1104:VAL:HG22	2.21	0.41
1:B:1171:VAL:HG22	1:B:1198:ALA:HB3	2.02	0.41
1:B:1366:TRP:HA	1:B:1369:PHE:HB3	2.02	0.41
3:D:59:GLN:OE1	3:D:65:PRO:HG3	2.20	0.41
3:D:146:GLN:OE1	3:D:153:SER:HB2	2.20	0.41
2:E:53:ILE:HG23	2:E:76:ARG:HH11	1.84	0.41
1:A:140:PRO:HA	1:A:141:PRO:HD3	1.96	0.41
1:A:717:VAL:HA	1:A:723:VAL:HB	2.03	0.41
1:B:562:PHE:HB3	1:B:635:MET:HE1	2.03	0.41
1:B:625:ASP:HB3	1:B:686:ALA:HB2	2.02	0.41
1:B:739:CYS:HA	1:B:742:GLU:HB2	2.03	0.41
1:B:1025:ALA:HA	1:B:1241:GLY:H	1.86	0.41
2:C:21:ARG:NH1	2:C:84:TYR:CD2	2.88	0.41
2:C:80:LYS:NZ	2:C:82:ILE:HG13	2.36	0.41
2:E:77:ASP:O	2:E:81:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:141:PRO:HA	3:F:154:VAL:HG23	2.01	0.41
1:A:512:ALA:HB1	1:A:884:TRP:CG	2.56	0.41
1:A:1054:GLY:HA3	1:A:1056:PHE:CE1	2.56	0.41
2:C:31:PHE:HE2	2:C:76:ARG:HB2	1.86	0.41
2:C:126:PRO:HB3	2:C:149:VAL:CG1	2.51	0.41
3:F:146:GLN:OE1	3:F:153:SER:HB2	2.20	0.41
1:A:465:ARG:HH12	1:A:467:GLU:CD	2.29	0.41
1:A:511:LEU:O	1:A:515:ARG:HB2	2.20	0.41
1:A:910:LEU:HD12	1:A:910:LEU:HA	1.81	0.41
1:B:92:GLN:HB2	1:B:250:LEU:HD23	2.01	0.41
1:B:104:PHE:HB3	1:B:908:VAL:CG2	2.51	0.41
1:B:141:PRO:HG2	1:B:516:ALA:HB2	2.03	0.41
1:B:1170:LEU:HB2	1:B:1197:VAL:HG23	2.03	0.41
2:C:161:TRP:HD1	2:C:170:VAL:HG13	1.85	0.41
3:D:54:LEU:HD13	3:D:92:PHE:CG	2.55	0.41
1:A:162:PRO:HD3	1:A:910:LEU:HG	2.03	0.41
1:A:357:GLU:HA	1:A:361:ARG:HG2	2.02	0.41
1:A:619:LEU:HG	1:A:621:THR:H	1.85	0.41
1:A:718:ASN:HD22	1:A:718:ASN:HA	1.72	0.41
1:A:1318:ALA:HB3	1:A:1341:PRO:HD3	2.03	0.41
1:A:1334:HIS:HA	1:A:1368:ARG:HB3	2.03	0.41
2:C:37:SER:HB3	2:C:52:PHE:HB3	2.03	0.41
2:C:77:ASP:O	2:C:81:SER:N	2.54	0.41
2:C:149:VAL:HG12	2:C:152:TYR:CD1	2.55	0.41
3:F:189:ASP:OD1	3:F:194:THR:N	2.49	0.41
1:A:1229:ALA:H	1:A:1322:MET:HE2	1.86	0.40
1:B:692:LYS:HE2	1:B:757:SER:OG	2.20	0.40
1:B:865:LEU:HD12	1:B:865:LEU:HA	1.86	0.40
2:E:173:PHE:O	2:E:185:LEU:HG	2.20	0.40
3:F:53:TYR:O	3:F:112:SER:N	2.54	0.40
3:F:130:ARG:HH12	3:F:133:ALA:HB2	1.85	0.40
1:A:588:ARG:HD3	1:A:588:ARG:N	2.37	0.40
1:A:788:VAL:HG11	1:A:805:ARG:HG3	2.04	0.40
1:A:1078:ASN:CG	1:A:1081:VAL:HB	2.46	0.40
1:B:1030:LEU:O	1:B:1034:MET:HG3	2.21	0.40
2:C:159:VAL:HG22	2:C:205:VAL:HG13	2.03	0.40
3:D:104:VAL:HG23	3:D:126:VAL:HG12	2.03	0.40
1:A:506:ASP:HB3	1:A:896:VAL:HG21	2.03	0.40
1:A:573:ALA:HA	1:A:862:ASP:OD2	2.21	0.40
1:A:791:ARG:HG2	1:A:815:ASP:HB3	2.02	0.40
1:A:829:LEU:HG	1:A:855:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ARG:HE	1:B:93:ARG:HB3	1.42	0.40
1:B:1067:LEU:O	1:B:1071:GLY:N	2.45	0.40
1:B:1285:LEU:O	1:B:1289:ALA:N	2.54	0.40
2:C:40:ARG:N	2:C:48:GLU:O	2.46	0.40
2:E:31:PHE:O	2:E:76:ARG:NH2	2.54	0.40
3:F:135:PRO:HG3	3:F:220:HIS:HB3	2.04	0.40
1:A:214:LEU:HD12	1:A:214:LEU:HA	1.83	0.40
1:A:217:GLN:HG3	1:B:221:ARG:NH1	2.37	0.40
1:A:718:ASN:ND2	1:A:840:ALA:HB2	2.37	0.40
1:A:931:ARG:H	1:A:931:ARG:HG3	1.47	0.40
1:A:1321:GLY:HA2	1:A:1324:GLU:HB3	2.04	0.40
1:B:51:PRO:HA	1:B:54:PHE:HB3	2.03	0.40
1:B:76:LEU:HA	1:B:79:LEU:HB2	2.03	0.40
1:B:443:PHE:HA	1:B:449:ASN:HA	2.04	0.40
1:B:467:GLU:HB2	1:B:468:ALA:H	1.81	0.40
1:B:682:SER:O	1:B:685:ILE:HG22	2.21	0.40
2:C:6:LEU:HD23	2:C:6:LEU:HA	1.93	0.40
2:C:13:LEU:HD13	2:C:117:THR:HB	2.04	0.40
1:A:163:ARG:HE	1:B:159:GLU:HG2	1.86	0.40
1:B:640:SER:HA	1:B:643:ARG:HD3	2.04	0.40
1:B:1000:VAL:H	1:B:1039:LEU:HD11	1.87	0.40
1:B:1147:GLY:HA2	1:B:1172:SER:HB3	2.03	0.40
2:C:31:PHE:O	2:C:76:ARG:NH2	2.54	0.40
2:C:86:GLN:HE21	2:C:86:GLN:CA	2.21	0.40
3:D:53:TYR:O	3:D:112:SER:N	2.54	0.40
2:E:5:GLN:HA	2:E:109:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1348/1784 (76%)	1233 (92%)	114 (8%)	1 (0%)	48	81
1	B	1375/1784 (77%)	1243 (90%)	132 (10%)	0	100	100
2	C	199/249 (80%)	177 (89%)	22 (11%)	0	100	100
2	E	199/249 (80%)	175 (88%)	24 (12%)	0	100	100
3	D	200/236 (85%)	185 (92%)	15 (8%)	0	100	100
3	F	200/236 (85%)	187 (94%)	13 (6%)	0	100	100
All	All	3521/4538 (78%)	3200 (91%)	320 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	656	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	999/1325 (75%)	833 (83%)	166 (17%)	2	12
1	B	1017/1325 (77%)	819 (80%)	198 (20%)	1	9
2	C	170/203 (84%)	134 (79%)	36 (21%)	1	6
2	E	170/203 (84%)	136 (80%)	34 (20%)	1	9
3	D	182/208 (88%)	143 (79%)	39 (21%)	1	6
3	F	182/208 (88%)	142 (78%)	40 (22%)	1	6
All	All	2720/3472 (78%)	2207 (81%)	513 (19%)	3	10

All (513) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	9	VAL
1	A	31	GLU
1	A	52	GLU

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Mol	Chain	Res	Type
1	A	57	LEU
1	A	75	ASP
1	A	100	GLU
1	A	111	MET
1	A	112	SER
1	A	114	ARG
1	A	123	GLN
1	A	124	ARG
1	A	125	LEU
1	A	126	MET
1	A	128	GLU
1	A	129	LEU
1	A	156	ILE
1	A	159	GLU
1	A	162	PRO
1	A	163	ARG
1	A	164	LEU
1	A	175	LEU
1	A	180	THR
1	A	181	THR
1	A	182	SER
1	A	197	PRO
1	A	199	ILE
1	A	205	CYS
1	A	209	LEU
1	A	212	VAL
1	A	214	LEU
1	A	220	ARG
1	A	221	ARG
1	A	237	THR
1	A	240	MET
1	A	241	LEU
1	A	264	ASN
1	A	268	MET
1	A	270	GLU
1	A	342	THR
1	A	344	THR
1	A	345	ARG
1	A	400	LEU
1	A	402	ARG
1	A	521	ARG
1	A	527	VAL

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Mol	Chain	Res	Type
1	A	528	ASP
1	A	530	SER
1	A	533	LEU
1	A	549	VAL
1	A	552	SER
1	A	553	ARG
1	A	557	ARG
1	A	569	TRP
1	A	574	VAL
1	A	576	LEU
1	A	607	ARG
1	A	609	GLU
1	A	612	ARG
1	A	614	GLU
1	A	626	VAL
1	A	643	ARG
1	A	645	HIS
1	A	648	GLU
1	A	653	ILE
1	A	664	CYS
1	A	703	GLU
1	A	721	ARG
1	A	722	SER
1	A	745	ARG
1	A	759	HIS
1	A	786	SER
1	A	788	VAL
1	A	789	THR
1	A	791	ARG
1	A	826	ARG
1	A	852	LEU
1	A	853	SER
1	A	855	ILE
1	A	856	HIS
1	A	857	SER
1	A	858	LEU
1	A	859	ARG
1	A	862	ASP
1	A	865	LEU
1	A	868	PHE
1	A	873	SER
1	A	874	ARG

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Mol	Chain	Res	Type
1	A	908	VAL
1	A	910	LEU
1	A	911	GLU
1	A	915	VAL
1	A	920	THR
1	A	922	VAL
1	A	923	ASP
1	A	925	VAL
1	A	928	LEU
1	A	930	TYR
1	A	931	ARG
1	A	948	THR
1	A	950	LEU
1	A	961	THR
1	A	977	ARG
1	A	978	GLU
1	A	980	VAL
1	A	981	VAL
1	A	982	ASP
1	A	988	ASP
1	A	992	GLU
1	A	1004	LEU
1	A	1007	LEU
1	A	1010	ASP
1	A	1015	GLU
1	A	1125	TRP
1	A	1144	LEU
1	A	1145	VAL
1	A	1156	ILE
1	A	1163	ARG
1	A	1168	LEU
1	A	1169	LEU
1	A	1170	LEU
1	A	1172	SER
1	A	1173	ARG
1	A	1179	ASP
1	A	1184	LEU
1	A	1188	LEU
1	A	1194	ARG
1	A	1195	THR
1	A	1196	THR
1	A	1209	ARG

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Mol	Chain	Res	Type
1	A	1210	GLU
1	A	1211	LEU
1	A	1212	LEU
1	A	1235	THR
1	A	1237	ASP
1	A	1238	THR
1	A	1243	ARG
1	A	1244	ILE
1	A	1246	ARG
1	A	1249	ARG
1	A	1251	LYS
1	A	1253	LEU
1	A	1263	ARG
1	A	1296	ASP
1	A	1300	GLN
1	A	1303	ARG
1	A	1304	SER
1	A	1307	LEU
1	A	1327	VAL
1	A	1330	ARG
1	A	1333	ARG
1	A	1336	VAL
1	A	1339	MET
1	A	1342	GLU
1	A	1357	VAL
1	A	1360	ILE
1	A	1362	ILE
1	A	1363	ASP
1	A	1364	VAL
1	A	1367	ASP
1	A	1371	LEU
1	A	1376	GLN
1	A	1377	ARG
1	A	1379	THR
1	A	1380	ARG
1	A	1385	ILE
1	B	1	MET
1	B	3	SER
1	B	5	ASP
1	B	7	GLU
1	B	8	LYS
1	B	9	VAL

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Mol	Chain	Res	Type
1	B	40	MET
1	B	44	LEU
1	B	50	THR
1	B	56	GLU
1	B	57	LEU
1	B	62	ARG
1	B	65	VAL
1	B	70	THR
1	B	72	ARG
1	B	76	LEU
1	B	79	LEU
1	B	85	THR
1	B	86	ARG
1	B	92	GLN
1	B	93	ARG
1	B	98	LEU
1	B	117	LEU
1	B	120	ASP
1	B	124	ARG
1	B	126	MET
1	B	157	PRO
1	B	158	GLN
1	B	159	GLU
1	B	162	PRO
1	B	163	ARG
1	B	176	MET
1	B	179	THR
1	B	180	THR
1	B	203	THR
1	B	207	SER
1	B	220	ARG
1	B	232	VAL
1	B	233	THR
1	B	243	ASP
1	B	247	MET
1	B	250	LEU
1	B	266	PHE
1	B	342	THR
1	B	374	SER
1	B	379	THR
1	B	380	GLN
1	B	390	LYS

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Mol	Chain	Res	Type
1	B	404	LEU
1	B	422	LEU
1	B	460	VAL
1	B	461	VAL
1	B	462	GLU
1	B	464	GLU
1	B	465	ARG
1	B	498	GLU
1	B	505	ARG
1	B	515	ARG
1	B	527	VAL
1	B	528	ASP
1	B	533	LEU
1	B	534	ARG
1	B	535	VAL
1	B	539	LEU
1	B	599	ASP
1	B	601	GLU
1	B	619	LEU
1	B	623	ARG
1	B	627	VAL
1	B	683	ARG
1	B	703	GLU
1	B	704	VAL
1	B	711	ARG
1	B	717	VAL
1	B	722	SER
1	B	723	VAL
1	B	731	GLU
1	B	732	LEU
1	B	733	ASP
1	B	734	ARG
1	B	735	LEU
1	B	740	THR
1	B	744	ILE
1	B	747	LYS
1	B	748	ARG
1	B	759	HIS
1	B	762	THR
1	B	763	ILE
1	B	765	ASP
1	B	767	LEU

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Mol	Chain	Res	Type
1	B	770	GLU
1	B	771	LEU
1	B	773	GLU
1	B	775	PHE
1	B	777	PRO
1	B	778	LEU
1	B	782	VAL
1	B	784	PHE
1	B	785	PHE
1	B	786	SER
1	B	793	THR
1	B	794	GLN
1	B	797	GLU
1	B	798	LEU
1	B	799	ASP
1	B	805	ARG
1	B	826	ARG
1	B	841	ILE
1	B	853	SER
1	B	855	ILE
1	B	859	ARG
1	B	867	ASP
1	B	870	GLU
1	B	908	VAL
1	B	915	VAL
1	B	919	SER
1	B	920	THR
1	B	926	SER
1	B	928	LEU
1	B	929	ARG
1	B	931	ARG
1	B	933	GLU
1	B	935	ARG
1	B	948	THR
1	B	950	LEU
1	B	961	THR
1	B	977	ARG
1	B	978	GLU
1	B	980	VAL
1	B	981	VAL
1	B	982	ASP
1	B	1004	LEU

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Mol	Chain	Res	Type
1	B	1007	LEU
1	B	1010	ASP
1	B	1015	GLU
1	B	1053	THR
1	B	1057	GLU
1	B	1058	ARG
1	B	1060	ARG
1	B	1125	TRP
1	B	1144	LEU
1	B	1145	VAL
1	B	1156	ILE
1	B	1163	ARG
1	B	1168	LEU
1	B	1169	LEU
1	B	1170	LEU
1	B	1172	SER
1	B	1173	ARG
1	B	1179	ASP
1	B	1184	LEU
1	B	1188	LEU
1	B	1194	ARG
1	B	1195	THR
1	B	1196	THR
1	B	1205	ARG
1	B	1206	GLU
1	B	1211	LEU
1	B	1212	LEU
1	B	1217	ASP
1	B	1235	THR
1	B	1237	ASP
1	B	1238	THR
1	B	1240	THR
1	B	1242	GLU
1	B	1244	ILE
1	B	1245	GLU
1	B	1246	ARG
1	B	1249	ARG
1	B	1251	LYS
1	B	1253	LEU
1	B	1261	LEU
1	B	1263	ARG
1	B	1264	GLU

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Mol	Chain	Res	Type
1	B	1265	LEU
1	B	1296	ASP
1	B	1300	GLN
1	B	1303	ARG
1	B	1307	LEU
1	B	1312	VAL
1	B	1327	VAL
1	B	1330	ARG
1	B	1333	ARG
1	B	1336	VAL
1	B	1339	MET
1	B	1342	GLU
1	B	1357	VAL
1	B	1360	ILE
1	B	1362	ILE
1	B	1363	ASP
1	B	1364	VAL
1	B	1367	ASP
1	B	1371	LEU
1	B	1376	GLN
1	B	1377	ARG
1	B	1379	THR
1	B	1380	ARG
1	B	1385	ILE
2	C	4	VAL
2	C	5	GLN
2	C	18	ARG
2	C	30	THR
2	C	36	MET
2	C	37	SER
2	C	45	LYS
2	C	56	LYS
2	C	61	THR
2	C	67	SER
2	C	69	LYS
2	C	78	ASP
2	C	80	LYS
2	C	84	TYR
2	C	86	GLN
2	C	87	MET
2	C	91	LYS
2	C	92	THR

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Mol	Chain	Res	Type
2	C	93	GLU
2	C	101	THR
2	C	106	LEU
2	C	108	ASP
2	C	112	GLN
2	C	114	THR
2	C	124	LYS
2	C	150	LYS
2	C	158	THR
2	C	168	SER
2	C	172	THR
2	C	178	GLN
2	C	182	LEU
2	C	202	ILE
2	C	204	ASN
2	C	206	ASN
2	C	216	LYS
2	C	219	GLU
3	D	18	VAL
3	D	20	MET
3	D	26	SER
3	D	33	GLU
3	D	36	SER
3	D	48	SER
3	D	49	ASN
3	D	60	LYS
3	D	77	SER
3	D	81	ASP
3	D	84	SER
3	D	93	THR
3	D	95	LYS
3	D	96	ILE
3	D	100	GLU
3	D	114	GLN
3	D	117	ARG
3	D	118	LEU
3	D	119	THR
3	D	132	VAL
3	D	137	VAL
3	D	139	ILE
3	D	144	ASP
3	D	145	GLU

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Mol	Chain	Res	Type
3	D	153	SER
3	D	157	LEU
3	D	178	SER
3	D	181	SER
3	D	185	VAL
3	D	186	THR
3	D	187	GLU
3	D	197	LEU
3	D	200	THR
3	D	202	THR
3	D	205	LYS
3	D	217	GLU
3	D	219	THR
3	D	221	GLN
3	D	224	SER
2	E	14	VAL
2	E	15	GLN
2	E	30	THR
2	E	33	ASP
2	E	36	MET
2	E	45	LYS
2	E	55	SER
2	E	56	LYS
2	E	61	THR
2	E	67	SER
2	E	69	LYS
2	E	78	ASP
2	E	80	LYS
2	E	84	TYR
2	E	91	LYS
2	E	92	THR
2	E	93	GLU
2	E	97	VAL
2	E	102	ARG
2	E	105	THR
2	E	112	GLN
2	E	124	LYS
2	E	131	LEU
2	E	150	LYS
2	E	158	THR
2	E	160	SER
2	E	168	SER

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Mol	Chain	Res	Type
2	E	172	THR
2	E	177	LEU
2	E	178	GLN
2	E	182	LEU
2	E	208	LYS
2	E	216	LYS
2	E	219	GLU
3	F	18	VAL
3	F	20	MET
3	F	26	SER
3	F	33	GLU
3	F	36	SER
3	F	48	SER
3	F	49	ASN
3	F	64	SER
3	F	65	PRO
3	F	69	ILE
3	F	77	SER
3	F	81	ASP
3	F	84	SER
3	F	86	SER
3	F	90	THR
3	F	92	PHE
3	F	93	THR
3	F	94	LEU
3	F	100	GLU
3	F	102	GLU
3	F	117	ARG
3	F	118	LEU
3	F	119	THR
3	F	139	ILE
3	F	144	ASP
3	F	145	GLU
3	F	148	LYS
3	F	153	SER
3	F	158	LEU
3	F	167	LYS
3	F	178	SER
3	F	181	SER
3	F	185	VAL
3	F	186	THR
3	F	187	GLU

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Mol	Chain	Res	Type
3	F	205	LYS
3	F	217	GLU
3	F	219	THR
3	F	221	GLN
3	F	224	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	213	HIS
1	A	217	GLN
1	A	449	ASN
1	A	655	HIS
1	A	718	ASN
1	A	904	GLN
1	A	1112	GLN
1	A	1167	HIS
1	A	1226	HIS
1	A	1292	ASN
1	A	1334	HIS
1	A	1349	GLN
1	A	1350	ASN
1	B	217	GLN
1	B	312	ASN
1	B	375	ASN
1	B	380	GLN
1	B	597	HIS
1	B	776	HIS
1	B	1112	GLN
1	B	1226	HIS
1	B	1292	ASN
1	B	1334	HIS
1	B	1349	GLN
1	B	1350	ASN
2	C	8	GLN
2	C	41	GLN
2	C	86	GLN
2	C	112	GLN
2	C	171	HIS
2	C	178	GLN
3	D	52	ASN

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Mol	Chain	Res	Type
3	D	111	GLN
3	D	180	ASN
3	D	188	GLN
2	E	178	GLN
2	E	207	HIS
3	F	52	ASN
3	F	111	GLN
3	F	169	GLN
3	F	188	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

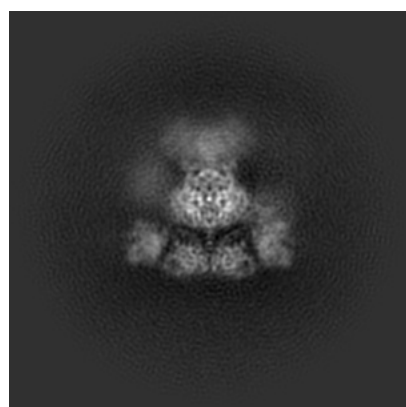
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23712. These allow visual inspection of the internal detail of the map and identification of artifacts.

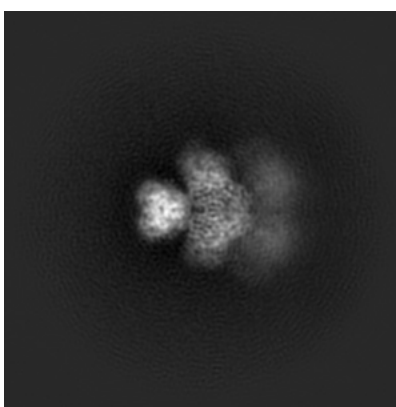
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

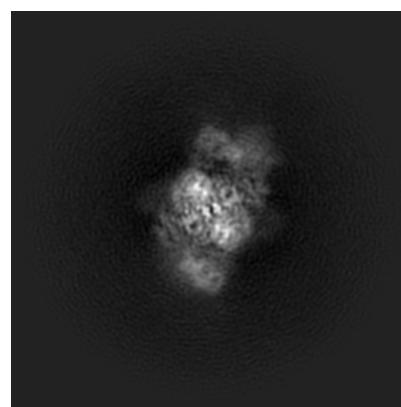
6.1.1 Primary map



X



Y

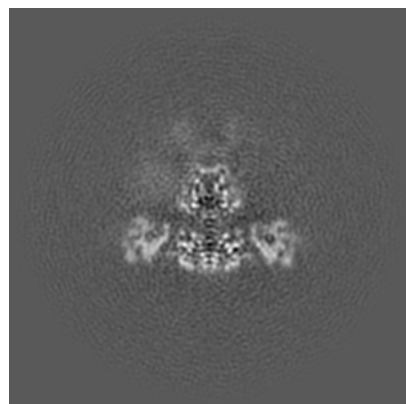


Z

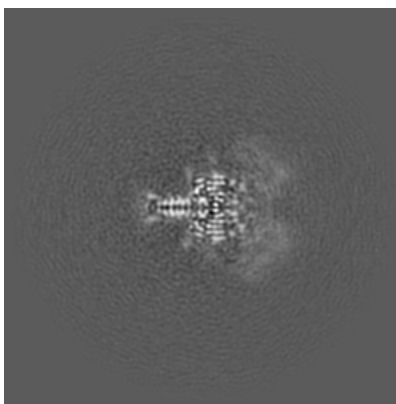
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

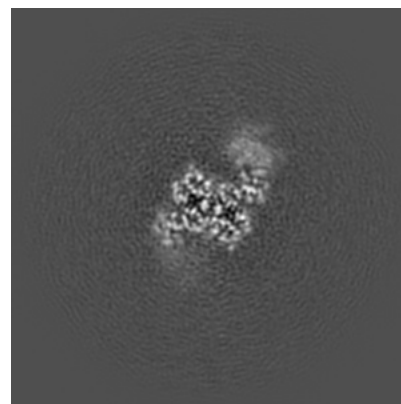
6.2.1 Primary map



X Index: 168



Y Index: 168

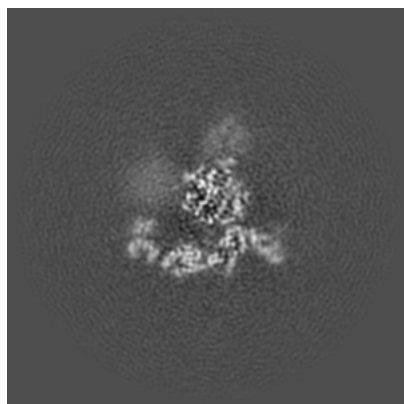


Z Index: 168

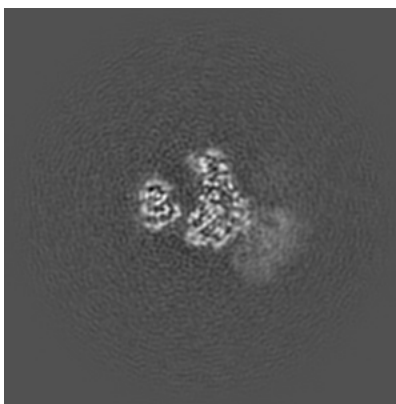
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

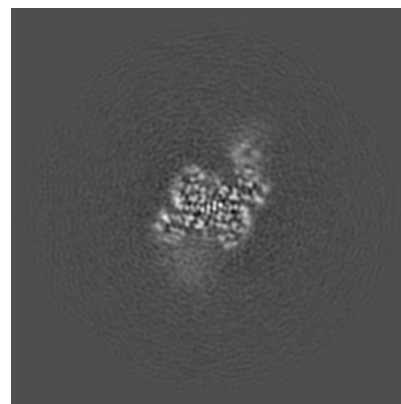
6.3.1 Primary map



X Index: 157



Y Index: 182

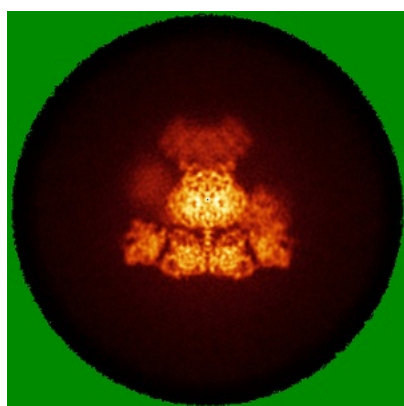


Z Index: 177

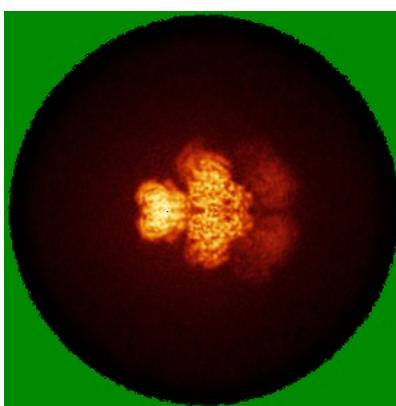
The images above show the largest variance slices of the map in three orthogonal directions.

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

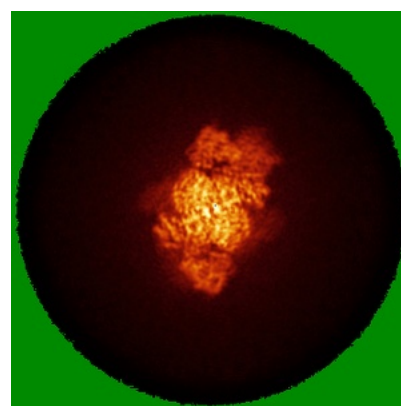
6.4.1 Primary map



X



Y

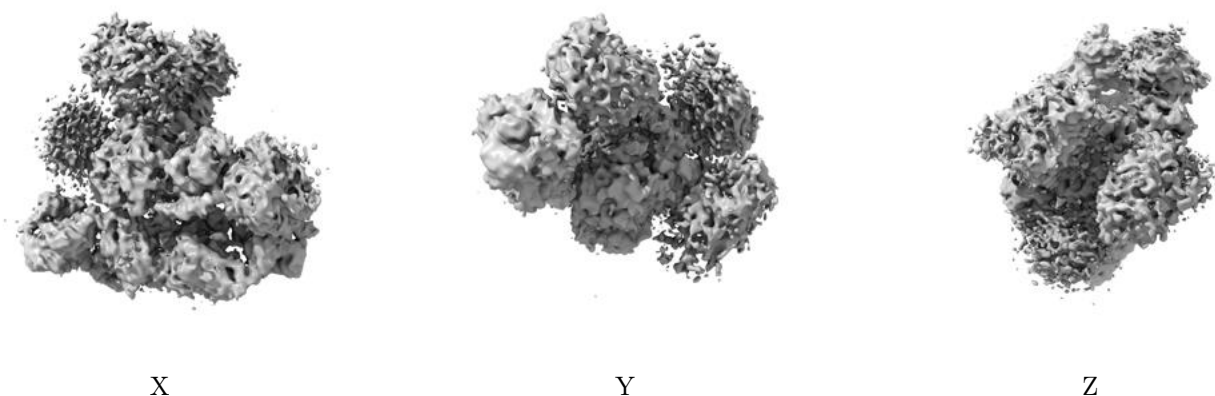


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

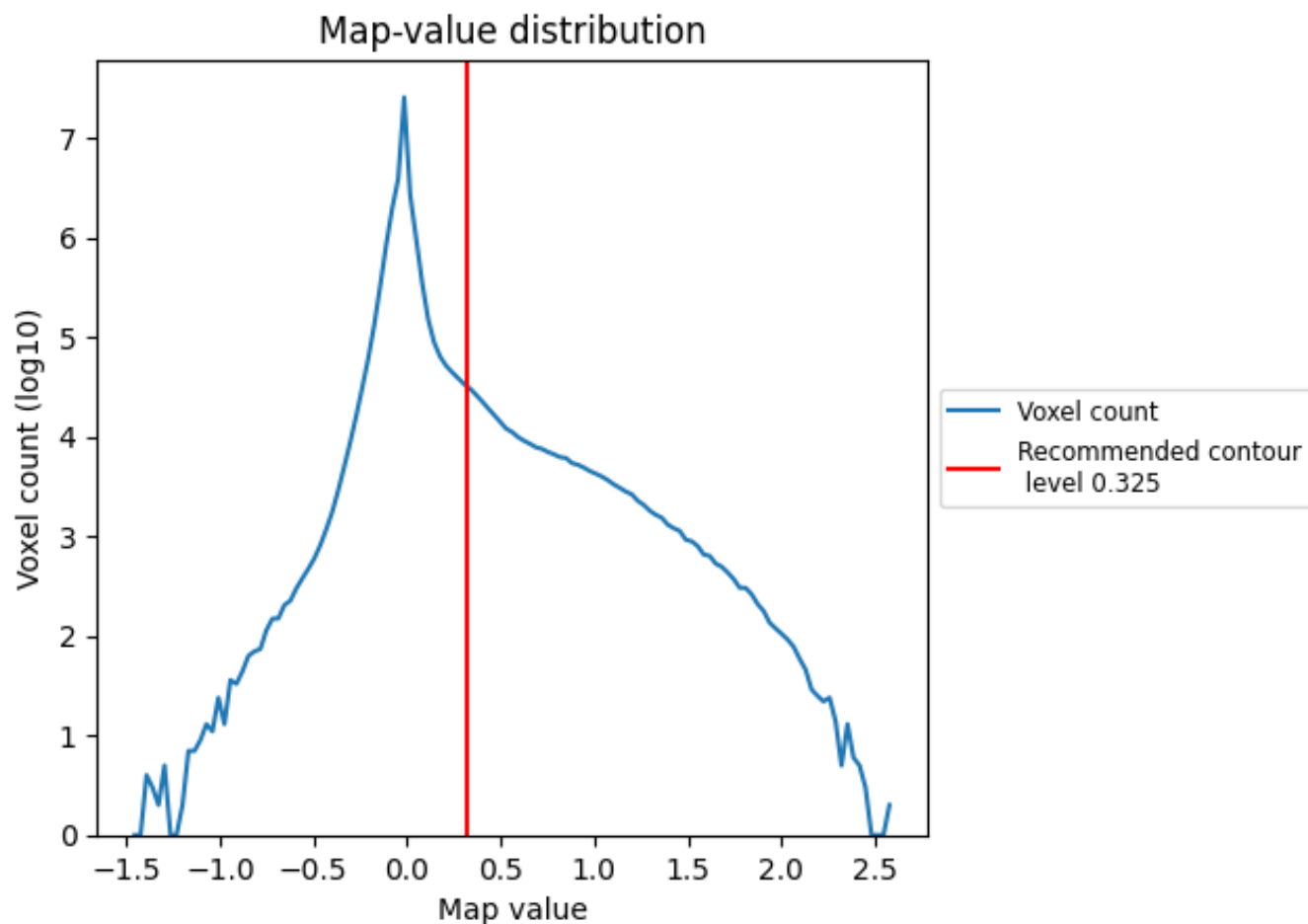
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

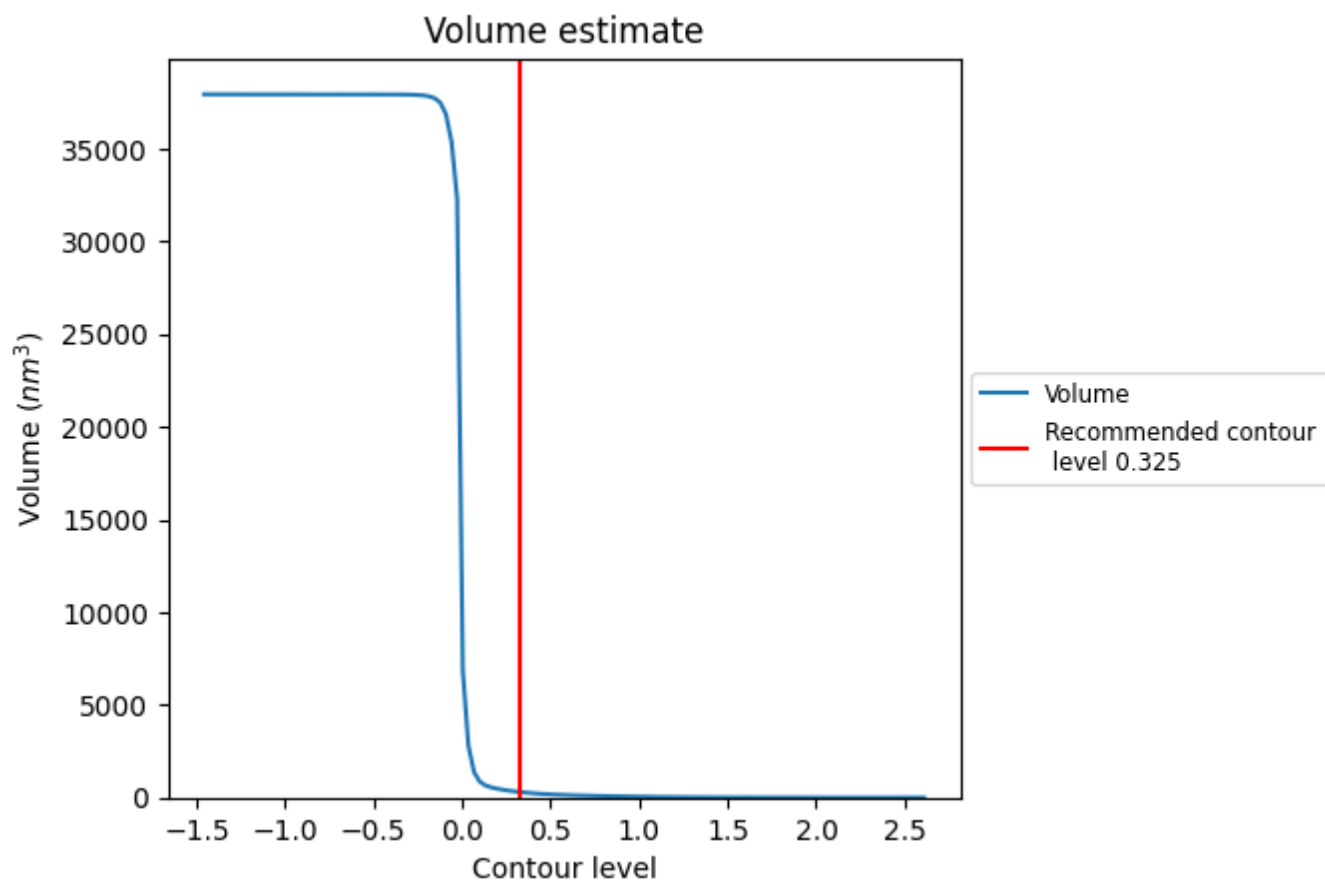
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

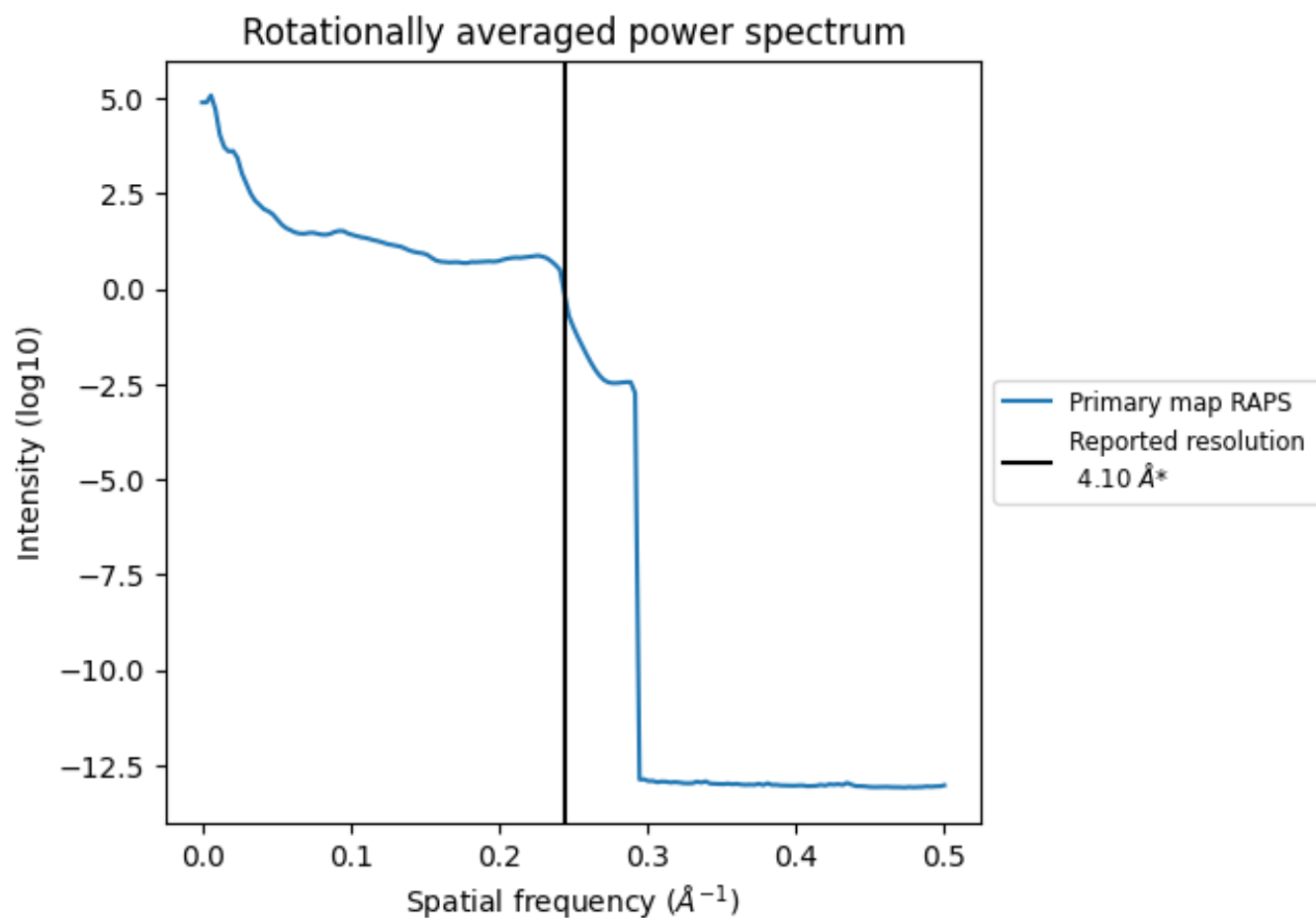
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm^3 ; this corresponds to an approximate mass of 270 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 0.244 Å⁻¹

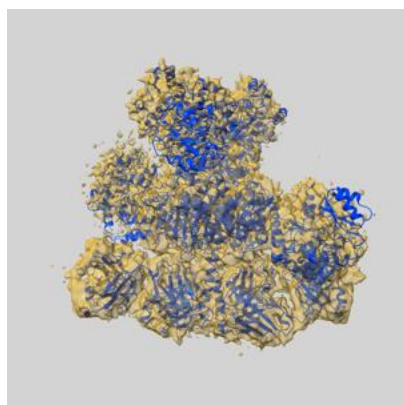
8 Fourier-Shell correlation ⓘ

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

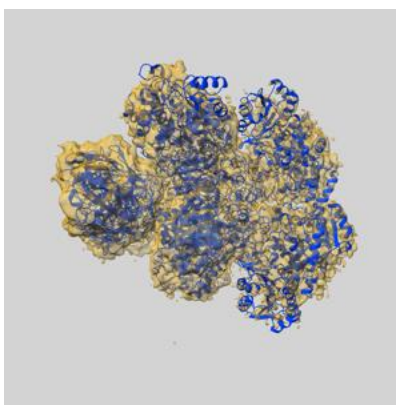
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23712 and PDB model 7M7G. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

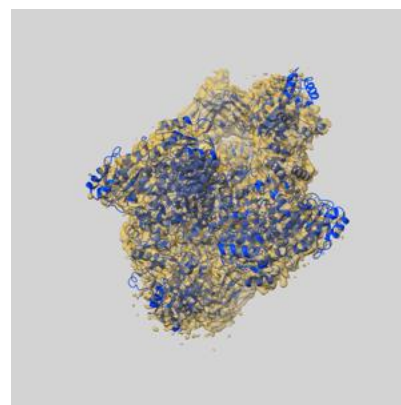
9.1 Map-model overlay [i](#)



X



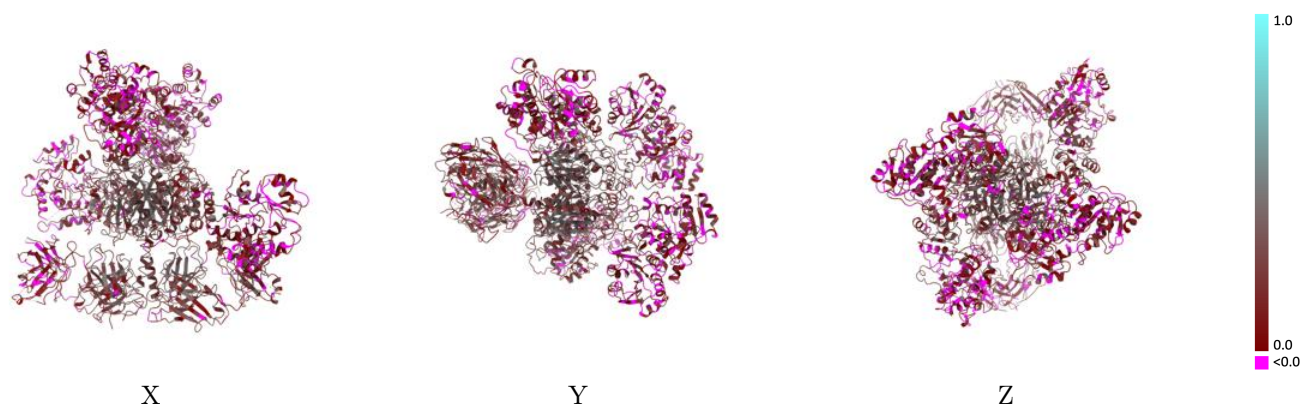
Y



Z

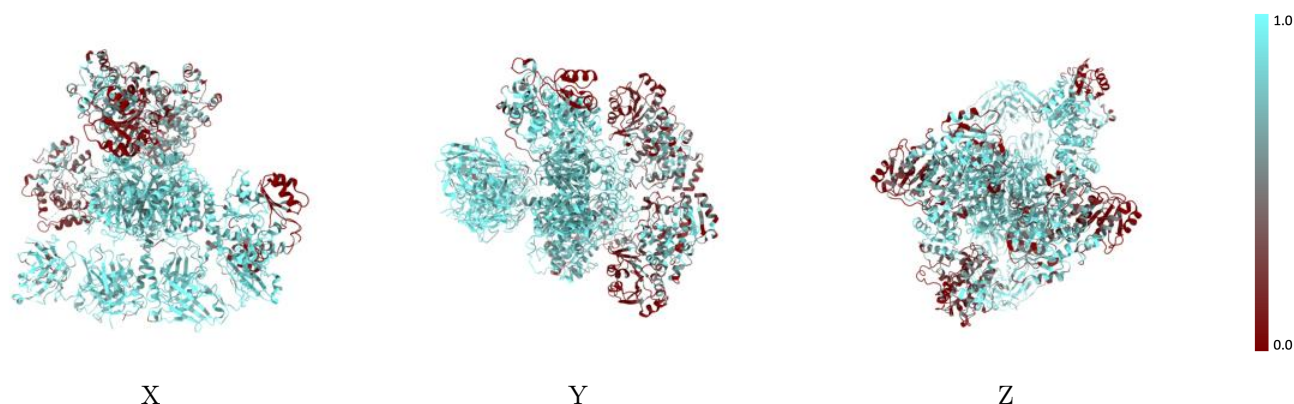
The images above show the 3D surface view of the map at the recommended contour level 0.325 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



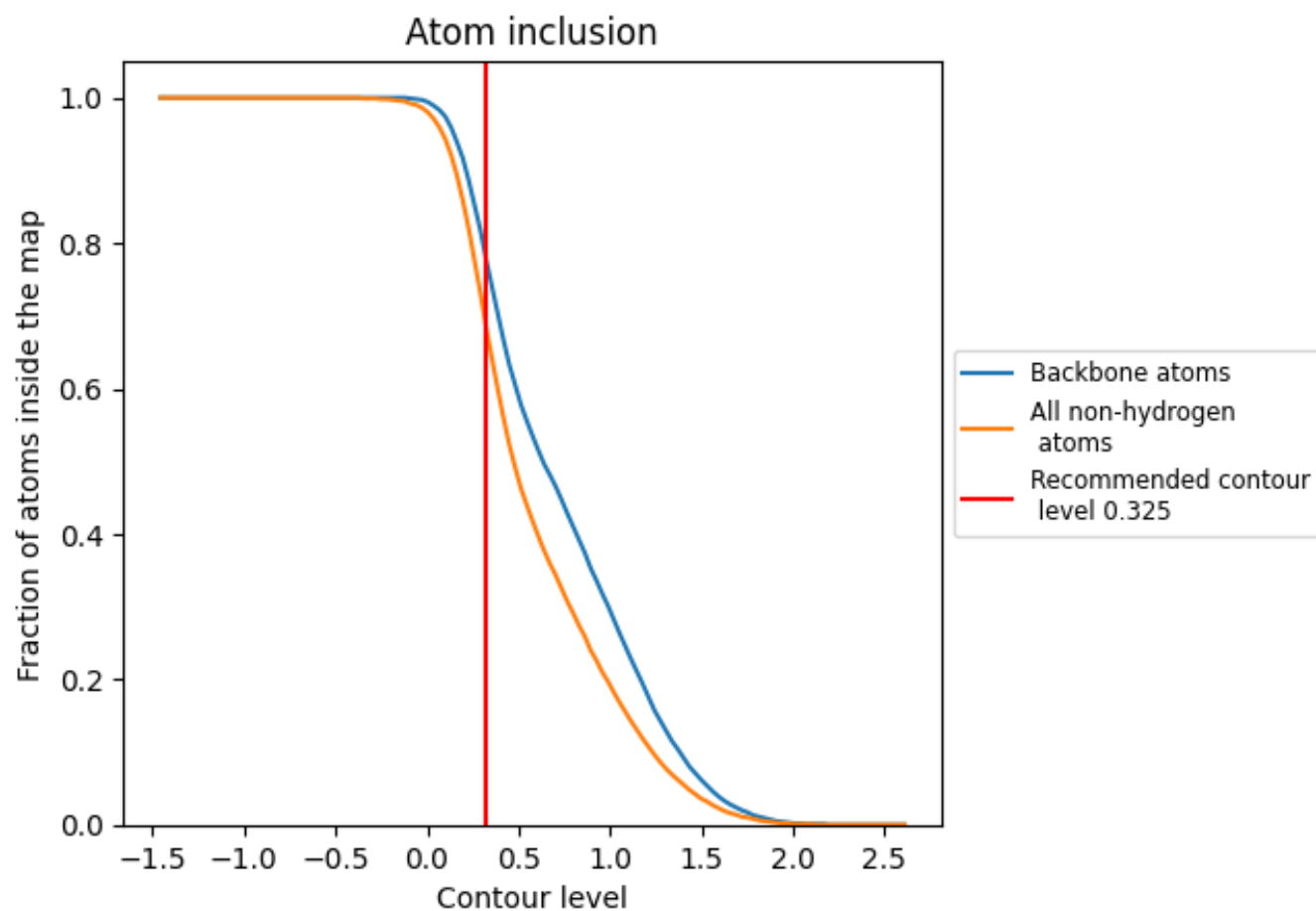
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.325).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 68% 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 (0.325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6810	0.1810
A	0.6040	0.1680
B	0.6460	0.1690
C	0.8680	0.2240
D	0.8710	0.2570
E	0.8580	0.1780
F	0.8480	0.2210

1.0

0.0

<0.0