



Full wwPDB EM Validation Report ⓘ

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PDB ID : 23CP / pdb_000023cp
EMDB ID : EMD-68865
Title : Cryo-EM structure of RSC complex from Chaetomium thermophilum
Authors : Ma, S.S.; Liu, M.D.; Shen, Q.T.; Chen, Y.
Deposited on : 2026-02-01
Resolution : 3.12 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:

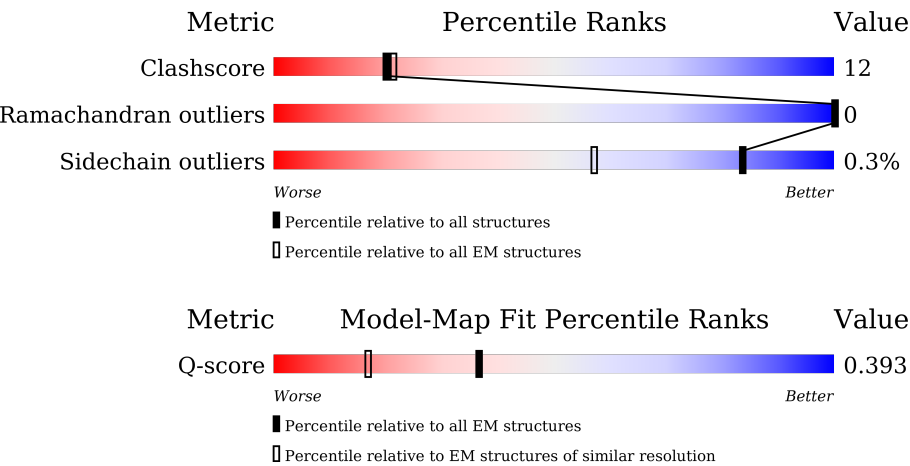
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.12 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	14478 (2.62 - 3.62)

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	K	1595	7% 90%
2	N	694	55% 14% 31%
2	O	694	37% 14% 49%
3	P	547	48% 20% 31%

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Mol	Chain	Length	Quality of chain
4	Q	769	29%14%56%
5	R	763	44%10%46%
6	S	607	5%58%8%34%
7	T	534	29%7%65%
8	V	990	29%12%59%
9	U	991	9%6%85%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25978 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 WD40 repeat-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	161	Total	C	N	O	S	0	0
			1321	824	262	226	9		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-58	GLY	-	expression tag	UNP G0SHD8
K	-57	SER	-	expression tag	UNP G0SHD8
K	-56	PRO	-	expression tag	UNP G0SHD8
K	-55	GLN	-	expression tag	UNP G0SHD8
K	-54	GLN	-	expression tag	UNP G0SHD8
K	-53	ASN	-	expression tag	UNP G0SHD8
K	-52	LYS	-	expression tag	UNP G0SHD8
K	-51	THR	-	expression tag	UNP G0SHD8
K	-50	ALA	-	expression tag	UNP G0SHD8
K	-49	ALA	-	expression tag	UNP G0SHD8
K	-48	LEU	-	expression tag	UNP G0SHD8
K	-47	ALA	-	expression tag	UNP G0SHD8
K	-46	GLN	-	expression tag	UNP G0SHD8
K	-45	HIS	-	expression tag	UNP G0SHD8
K	-44	ASP	-	expression tag	UNP G0SHD8
K	-43	GLU	-	expression tag	UNP G0SHD8
K	-42	ALA	-	expression tag	UNP G0SHD8
K	-41	ASP	-	expression tag	UNP G0SHD8
K	-40	TYR	-	expression tag	UNP G0SHD8
K	-39	LYS	-	expression tag	UNP G0SHD8
K	-38	ASP	-	expression tag	UNP G0SHD8
K	-37	HIS	-	expression tag	UNP G0SHD8
K	-36	ASP	-	expression tag	UNP G0SHD8
K	-35	GLY	-	expression tag	UNP G0SHD8
K	-34	ASP	-	expression tag	UNP G0SHD8
K	-33	TYR	-	expression tag	UNP G0SHD8
K	-32	LYS	-	expression tag	UNP G0SHD8
K	-31	ASP	-	expression tag	UNP G0SHD8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-30	HIS	-	expression tag	UNP G0SHD8
K	-29	ASP	-	expression tag	UNP G0SHD8
K	-28	ILE	-	expression tag	UNP G0SHD8
K	-27	ASP	-	expression tag	UNP G0SHD8
K	-26	TYR	-	expression tag	UNP G0SHD8
K	-25	LYS	-	expression tag	UNP G0SHD8
K	-24	ASP	-	expression tag	UNP G0SHD8
K	-23	ASP	-	expression tag	UNP G0SHD8
K	-22	ASP	-	expression tag	UNP G0SHD8
K	-21	ASP	-	expression tag	UNP G0SHD8
K	-20	LYS	-	expression tag	UNP G0SHD8
K	-19	GLY	-	expression tag	UNP G0SHD8
K	-18	GLY	-	expression tag	UNP G0SHD8
K	-17	SER	-	expression tag	UNP G0SHD8
K	-16	GLY	-	expression tag	UNP G0SHD8
K	-15	GLY	-	expression tag	UNP G0SHD8
K	-14	SER	-	expression tag	UNP G0SHD8
K	-13	LEU	-	expression tag	UNP G0SHD8
K	-12	GLU	-	expression tag	UNP G0SHD8
K	-11	VAL	-	expression tag	UNP G0SHD8
K	-10	LEU	-	expression tag	UNP G0SHD8
K	-9	PHE	-	expression tag	UNP G0SHD8
K	-8	GLN	-	expression tag	UNP G0SHD8
K	-7	GLY	-	expression tag	UNP G0SHD8
K	-6	PRO	-	expression tag	UNP G0SHD8
K	-5	GLY	-	expression tag	UNP G0SHD8
K	-4	GLY	-	expression tag	UNP G0SHD8
K	-3	SER	-	expression tag	UNP G0SHD8
K	-2	GLY	-	expression tag	UNP G0SHD8
K	-1	GLY	-	expression tag	UNP G0SHD8
K	0	SER	-	expression tag	UNP G0SHD8
K	1	GLY	-	expression tag	UNP G0SHD8
K	2	THR	-	expression tag	UNP G0SHD8
K	114	VAL	ILE	conflict	UNP G0SHD8
K	282	ILE	VAL	conflict	UNP G0SHD8
K	1513	THR	ALA	conflict	UNP G0SHD8

- Molecule 2 is a protein called Ssr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	478	Total	C	N	O	S	0	0
			3758	2347	667	723	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	354	Total	C	N	O	S	0	0
			2890	1815	514	543	18		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	687	ASP	-	expression tag	UNP G0S647
N	688	TYR	-	expression tag	UNP G0S647
N	689	LYS	-	expression tag	UNP G0S647
N	690	ASP	-	expression tag	UNP G0S647
N	691	ASP	-	expression tag	UNP G0S647
N	692	ASP	-	expression tag	UNP G0S647
N	693	ASP	-	expression tag	UNP G0S647
N	694	LYS	-	expression tag	UNP G0S647
O	687	ASP	-	expression tag	UNP G0S647
O	688	TYR	-	expression tag	UNP G0S647
O	689	LYS	-	expression tag	UNP G0S647
O	690	ASP	-	expression tag	UNP G0S647
O	691	ASP	-	expression tag	UNP G0S647
O	692	ASP	-	expression tag	UNP G0S647
O	693	ASP	-	expression tag	UNP G0S647
O	694	LYS	-	expression tag	UNP G0S647

- Molecule 3 is a protein called DM2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	376	Total	C	N	O	S	0	0
			3064	1937	547	571	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	191	ASP	ASN	conflict	UNP G0RYN3
P	540	ASP	-	expression tag	UNP G0RYN3
P	541	TYR	-	expression tag	UNP G0RYN3
P	542	LYS	-	expression tag	UNP G0RYN3
P	543	ASP	-	expression tag	UNP G0RYN3
P	544	ASP	-	expression tag	UNP G0RYN3
P	545	ASP	-	expression tag	UNP G0RYN3
P	546	ASP	-	expression tag	UNP G0RYN3
P	547	LYS	-	expression tag	UNP G0RYN3

- Molecule 4 is a protein called DUF1750-domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	338	Total	C	N	O	S	0	0
			2750	1759	495	486	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	763	ASP	-	expression tag	UNP G0SEZ9
Q	764	TYR	-	expression tag	UNP G0SEZ9
Q	765	LYS	-	expression tag	UNP G0SEZ9
Q	766	ASP	-	expression tag	UNP G0SEZ9
Q	767	ASP	-	expression tag	UNP G0SEZ9
Q	768	ASP	-	expression tag	UNP G0SEZ9
Q	769	ASP	-	expression tag	UNP G0SEZ9
Q	770	LYS	-	expression tag	UNP G0SEZ9

- Molecule 5 is a protein called Putative chromatin structure-remodeling complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	413	Total	C	N	O	S	0	0
			3289	2091	565	618	15		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	269	MET	-	initiating methionine	UNP G0S909
R	444	ILE	ASN	conflict	UNP G0S909
R	601	GLU	ASP	conflict	UNP G0S909
R	741	THR	SER	conflict	UNP G0S909
R	1026	HIS	-	expression tag	UNP G0S909
R	1027	HIS	-	expression tag	UNP G0S909
R	1028	HIS	-	expression tag	UNP G0S909
R	1029	HIS	-	expression tag	UNP G0S909
R	1030	HIS	-	expression tag	UNP G0S909
R	1031	HIS	-	expression tag	UNP G0S909

- Molecule 6 is a protein called Putative chromatin structure-remodeling complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	399	Total	C	N	O	S	0	0
			3184	2014	565	593	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	6	ASP	ASN	conflict	UNP G0S475
S	272	ILE	THR	conflict	UNP G0S475
S	600	ASP	-	expression tag	UNP G0S475
S	601	TYR	-	expression tag	UNP G0S475
S	602	LYS	-	expression tag	UNP G0S475
S	603	ASP	-	expression tag	UNP G0S475
S	604	ASP	-	expression tag	UNP G0S475
S	605	ASP	-	expression tag	UNP G0S475
S	606	ASP	-	expression tag	UNP G0S475
S	607	LYS	-	expression tag	UNP G0S475

- Molecule 7 is a protein called Rsc7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	189	Total	C	N	O	S	0	0
			1514	954	269	285	6		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	527	ASP	-	expression tag	UNP G0S6N5
T	528	TYR	-	expression tag	UNP G0S6N5
T	529	LYS	-	expression tag	UNP G0S6N5
T	530	ASP	-	expression tag	UNP G0S6N5
T	531	ASP	-	expression tag	UNP G0S6N5
T	532	ASP	-	expression tag	UNP G0S6N5
T	533	ASP	-	expression tag	UNP G0S6N5
T	534	LYS	-	expression tag	UNP G0S6N5

- Molecule 8 is a protein called Rsc58.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	407	Total	C	N	O	S	0	0
			3070	1916	530	614	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	300	GLU	ASP	conflict	UNP G0S281
V	612	HIS	PRO	conflict	UNP G0S281
V	985	HIS	-	expression tag	UNP G0S281

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Chain	Residue	Modelled	Actual	Comment	Reference
V	986	HIS	-	expression tag	UNP G0S281
V	987	HIS	-	expression tag	UNP G0S281
V	988	HIS	-	expression tag	UNP G0S281
V	989	HIS	-	expression tag	UNP G0S281
V	990	HIS	-	expression tag	UNP G0S281

- Molecule 9 is a protein called Rsc1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	150	Total	C	N	O	S	0	0
			1135	696	220	218	1		

There are 11 discrepancies between the modelled and reference sequences:

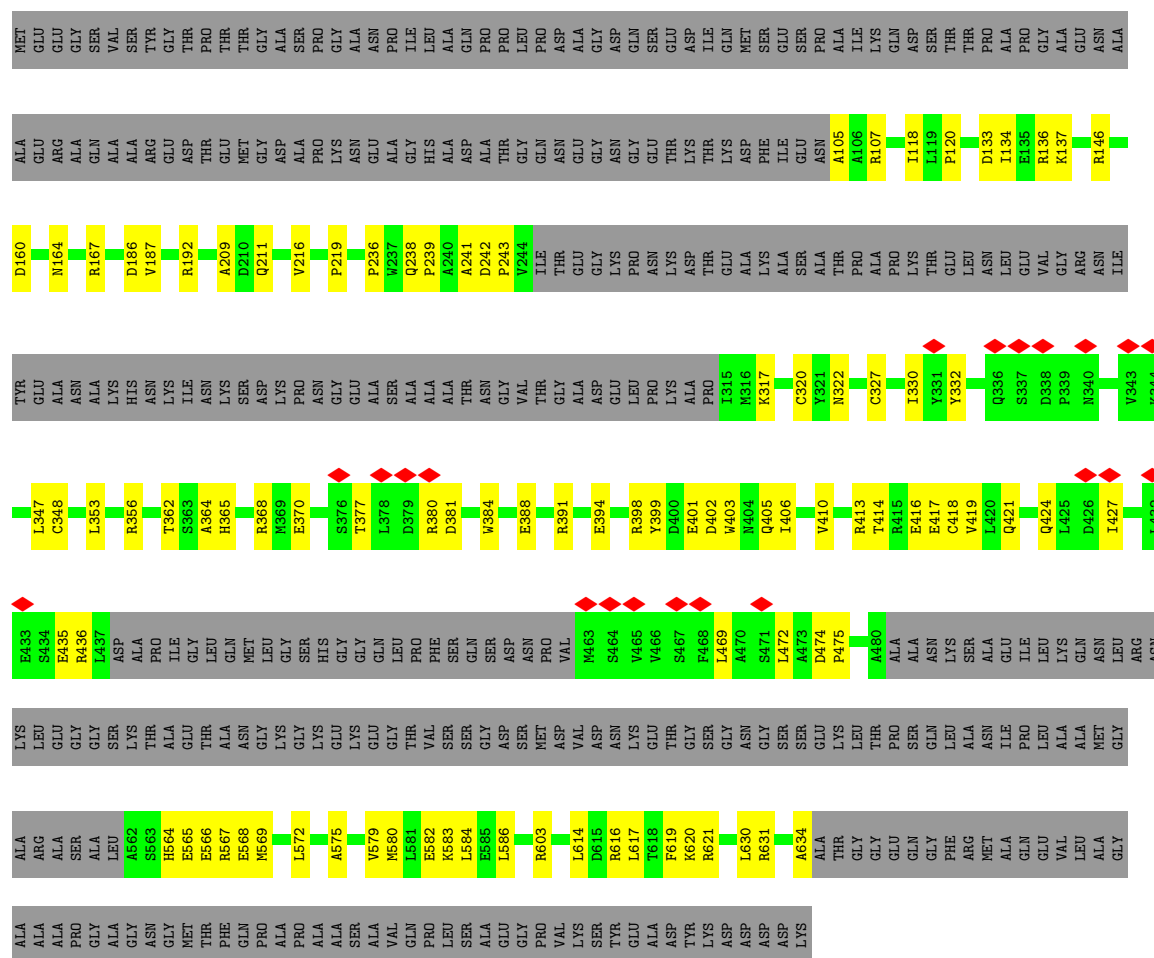
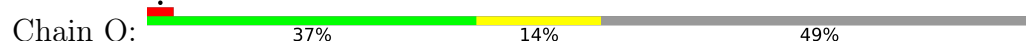
Chain	Residue	Modelled	Actual	Comment	Reference
U	294	GLY	ASP	conflict	UNP G0SB54
U	300	ASP	ASN	conflict	UNP G0SB54
U	363	HIS	TYR	conflict	UNP G0SB54
U	984	ASP	-	expression tag	UNP G0SB54
U	985	TYR	-	expression tag	UNP G0SB54
U	986	LYS	-	expression tag	UNP G0SB54
U	987	ASP	-	expression tag	UNP G0SB54
U	988	ASP	-	expression tag	UNP G0SB54
U	989	ASP	-	expression tag	UNP G0SB54
U	990	ASP	-	expression tag	UNP G0SB54
U	991	LYS	-	expression tag	UNP G0SB54

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

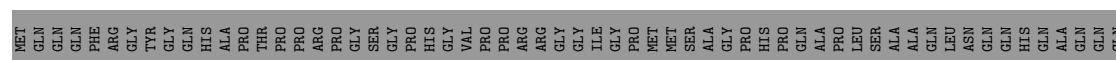
Mol	Chain	Residues	Atoms		AltConf
10	N	1	Total	Zn	0
			1	1	
10	O	1	Total	Zn	0
			1	1	
10	S	1	Total	Zn	0
			1	1	



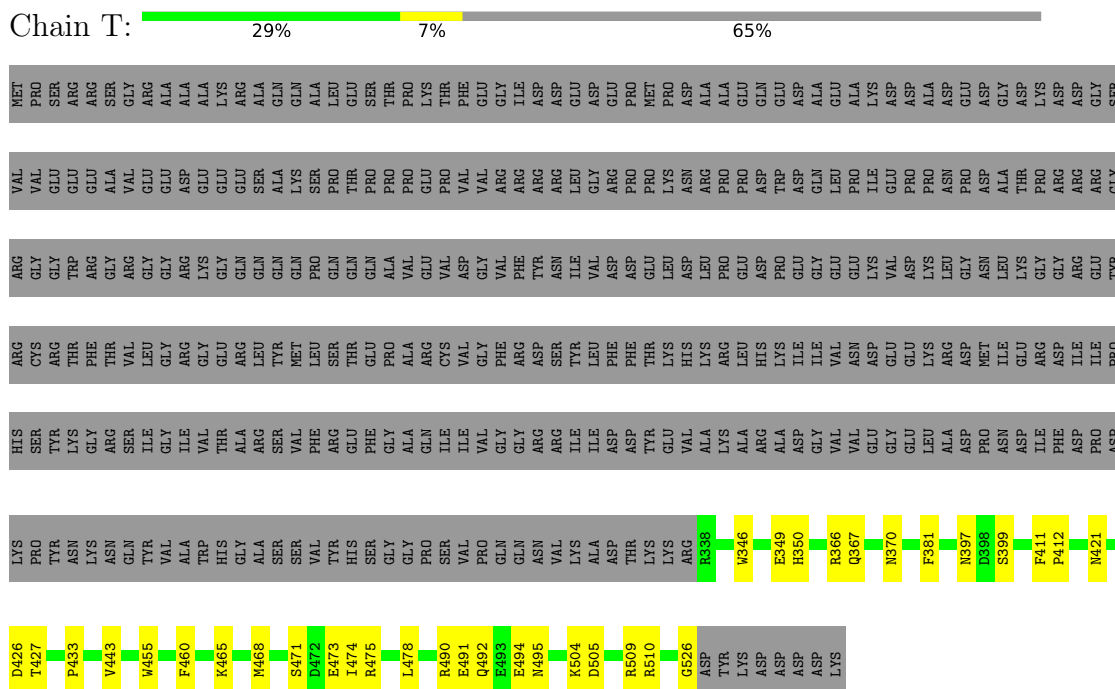
- Molecule 2: Ssr1



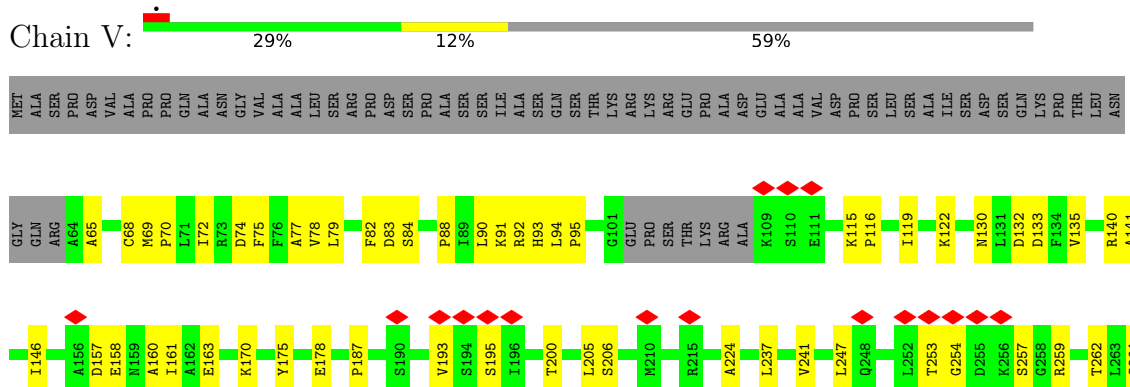
- Molecule 3: DM2 domain-containing protein



- Molecule 7: Rsc7



- Molecule 8: Rsc58





E844	E951	GLN	ASN	THR	VAL	THR	VAL	THR	VAL	TYR	PHE	LYS
V845	Q952	PRO	VAL	ASP	PRO	ASP	CTS	ARG	CTY	ARG	ARG	ASN
N851	K953	PRO	PRO	LEU	GLY	LEU	GLU	PRO	GLY	GLY	GLY	HIS
I852	K954	MET	GLY	LEU	VAL	LEU	SER	GLY	SER	ASP	ASP	LYS
D853	A955	MET	THR	LYS	THR	LYS	TYR	THR	GLN	THR	GLY	ARG
A854	E956	HIS	GLY	PRO	GLY	PRO	ASN	VAL	VAL	VAL	LYS	LYS
A855	A957	VAL	PRO	THR	PRO	THR	GLU	HIS	HIS	HIS	TYR	TYR
I856	R958	PRO	PRO	TRP	TRP	TRP	GLU	ARG	ARG	PRO	LEU	GLN
P857	E959	GLN	GLN	ARG	THR	THR	THR	PHE	PHE	ASN	LEU	ASN
K858	L960	PRO	PRO	SER	SER	SER	PHE	ALA	ALA	VAL	VAL	VAL
E862	L961	HIS	GLY	PRO	SER	PRO	LYS	LYS	LYS	SER	SER	ASP
Q863	E962	ALA	MET	ASN	TYR	ASN	PHE	ILE	ILE	GLY	GLY	GLY
C866	K963	MET	HIS	ALA	HIS	ALA	ASN	GLY	GLY	VAL	VAL	VAL
I872	V964	PRO	HIS	PRO	HIS	PRO	LYS	TYR	TYR	HIS	HIS	LEU
F876	R966	PRO	ALA	LEU	ALA	LEU	ILE	GLY	GLY	GLY	GLY	GLN
R882	D967	PRO	THR	ALA	THR	ILE	THR	VAL	VAL	ILE	ILE	ASP
N885	W968	GLN	GLN	ALA	THR	ALA	SER	VAL	VAL	TRP	TRP	ARG
V887	E871	GLN	MET	VAL	PRO	VAL	GLY	LYS	LYS	TRP	TRP	LYS
A888	I972	PRO	PRO	ARG	PRO	ARG	CTY	PHE	PHE	VAL	VAL	ASN
E889	D973	PRO	ALA	PRO	ALA	ALA	ASN	GLY	GLY	GLY	GLY	ASN
A890	R974	PRO	ALA	PRO	ALA	ARG	PRO	ASP	ASP	ASP	ASP	ASN
Y891	Q877	PRO	SER	PRO	SER	ARG	GLY	TRP	TRP	TRP	TRP	ALA
H896	L878	HIS	PRO	ARG	PRO	ARG	GLY	ARG	ARG	VAL	VAL	LYS
S897	L879	ALA	PHE	GLY	PRO	GLY	VAL	GLN	HIS	HIS	HIS	GLN
V898	R879	TYR	ILE	ASN	PRO	ASN	ARG	ASN	ILE	ILE	ILE	HIS
R899	L880	PRO	PRO	GLY	HIS	ASN	GLY	ARG	ARG	ARG	ARG	HIS
H900	R881	ALA	ALA	TYR	ALA	TYR	GLY	ILE	ILE	ASN	ASN	ASP
L901	E882	PRO	GLN	PRO	GLN	GLN	ASP	PRO	PRO	GLY	GLY	ASN
I904	D982	PRO	TYR	ARG	PRO	ARG	TYR	ASN	ASP	ASP	ASP	ASP
K905	L983	PRO	GLY	PRO	GLN	ARG	GLY	ASN	GLY	ASP	VAL	ALA
Q906	ASP	HIS	ALA	ASN	ALA	ASN	PRO	ILE	ILE	ASP	ALA	VAL
L907	TYR	ALA	GLN	ILE	ALA	ALA	PRO	GLN	GLN	LEU	GLU	VAL
R908	LYS	SER	PRO	THR	PRO	PRO	PRO	GLU	ASP	SER	GLN	GLU
E909	ASP	PRO	PRO	THR	PRO	PRO	PRO	LYS	ASP	LYS	TYR	TYR
E910	ASP	HIS	PRO	THR	PRO	PRO	PRO	ARG	PRO	PRO	PRO	GLY
R911	ASP	VAL	ALA	PRO	ALA	ALA	VAL	PHE	VAL	ILE	VAL	VAL
A912	ASP	PRO	GLN	ARG	PRO	GLN	ASP	CYS	PRO	ILE	ASP	ASP
R913	ASP	PRO	VAL	PRO	VAL	VAL	PHE	ARG	PRO	VAL	VAL	ALA
K914	ASP	PRO	PRO	PRO	VAL	VAL	ILE	THR	THR	ARG	ARG	LYS
E918	ASP	PRO	ASN	PRO	GLY	GLY	LYS	THR	THR	GLY	GLY	GLN
D919	ASP	ALA	TYR	ALA	PRO	PRO	PRO	ARG	ARG	GLY	ILE	ILE
R919	ASP	PRO	TYR	PRO	PRO	PRO	HIS	PRO	PRO	GLY	LYS	LYS
E920	ASP	ALA	GLN	GLN	GLN	GLN	LEU	TRP	TRP	LYS	TRP	TRP
A921	ASP	PRO	PRO	ALA	PRO	PRO	LEU	VAL	VAL	VAL	VAL	ALA
L922	ASP	ALA	PRO	ALA	ALA	ALA	ILE	ASN	ASN	ASN	ASN	ARG
E925	ASP	ASN	PRO	PHE	HIS	PRO	ASP	LYS	LYS	ALA	ALA	PRO
R926	ASP	HIS	GLN	GLN	ILE	ILE	LYS	CTR	CTR	CTR	CTR	ASP
A939	ASP	ALA	PRO	PRO	PRO	PRO	GLU	TRP	TRP	TRP	TRP	ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	250420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.887	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	K	0.32	0/1336	0.57	0/1774
2	N	0.23	0/3834	0.44	4/5197 (0.1%)
2	O	0.20	0/2952	0.42	0/3999
3	P	0.28	4/3125 (0.1%)	0.46	2/4220 (0.0%)
4	Q	0.41	6/2820 (0.2%)	0.58	4/3821 (0.1%)
5	R	0.18	1/3350 (0.0%)	0.36	0/4548
6	S	0.20	2/3271 (0.1%)	0.36	2/4452 (0.0%)
7	T	0.13	0/1556	0.31	0/2122
8	V	0.28	2/3122 (0.1%)	0.52	2/4243 (0.0%)
9	U	0.36	2/1150 (0.2%)	0.53	1/1552 (0.1%)
All	All	0.26	17/26516 (0.1%)	0.45	15/35928 (0.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	109	PHE	C-N	8.40	1.45	1.33
3	P	451	ALA	C-N	-7.46	1.24	1.33
4	Q	108	TYR	C-N	7.46	1.44	1.33
4	Q	321	PRO	C-N	7.06	1.42	1.33
3	P	339	PHE	C-N	-6.94	1.24	1.33
4	Q	315	GLU	C-N	-6.87	1.24	1.33
4	Q	322	TYR	C-N	-6.32	1.25	1.33
9	U	978	LEU	C-N	-6.16	1.25	1.33
9	U	882	ARG	C-N	-6.12	1.28	1.33
6	S	421	TYR	C-N	-6.08	1.24	1.33
3	P	340	ARG	C-N	-5.89	1.25	1.33
5	R	451	ARG	C-N	5.67	1.41	1.33
8	V	529	LEU	C-N	-5.39	1.26	1.33
4	Q	316	GLU	C-N	5.33	1.40	1.33
8	V	535	PRO	CA-C	5.33	1.57	1.52
3	P	452	PHE	C-N	5.18	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	420	ARG	C-N	-5.01	1.25	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	452	PHE	N-CA-C	11.09	123.11	111.14
4	Q	109	PHE	CA-C-N	-7.23	111.88	122.65
4	Q	109	PHE	C-N-CA	-7.23	111.88	122.65
8	V	535	PRO	N-CA-C	6.63	118.78	110.70
2	N	567	ARG	N-CA-C	-6.07	106.85	114.56
2	N	542	THR	CA-C-N	-5.97	113.03	119.24
2	N	542	THR	C-N-CA	-5.97	113.03	119.24
8	V	517	MET	N-CA-C	-5.85	104.90	111.28
2	N	542	THR	N-CA-C	5.63	122.25	109.81
3	P	339	PHE	O-C-N	-5.39	117.28	123.42
4	Q	322	TYR	CA-C-N	5.24	128.31	120.87
4	Q	322	TYR	C-N-CA	5.24	128.31	120.87
6	S	421	TYR	CA-C-N	5.08	129.41	123.16
6	S	421	TYR	C-N-CA	5.08	129.41	123.16
9	U	914	LYS	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1321	0	1360	44	0
2	N	3758	0	3653	116	0
2	O	2890	0	2804	121	0
3	P	3064	0	3018	100	0
4	Q	2750	0	2734	104	0
5	R	3289	0	3298	61	0
6	S	3184	0	3082	31	0
7	T	1514	0	1454	34	0
8	V	3070	0	3004	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	U	1135	0	1058	54	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	S	1	0	0	0	0
All	All	25978	0	25465	631	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 12.

All (631) 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)
2:N:642:PHE:CE2	2:O:634:ALA:HB3	1.72	1.22
2:N:642:PHE:CZ	2:O:634:ALA:HB3	1.76	1.19
2:O:603:ARG:HH12	5:R:981:ARG:HA	1.13	1.07
2:N:642:PHE:CE1	2:O:631:ARG:HA	1.95	1.00
2:N:642:PHE:CE2	2:O:634:ALA:CB	2.47	0.98
2:N:642:PHE:CE1	2:O:630:LEU:O	2.23	0.92
2:N:642:PHE:HE2	2:O:634:ALA:CB	1.83	0.91
2:N:642:PHE:HE2	2:O:634:ALA:HB3	1.35	0.90
2:N:642:PHE:HE1	2:O:630:LEU:C	1.80	0.88
5:R:998:ARG:O	5:R:998:ARG:NH1	2.07	0.88
3:P:448:ALA:HB1	3:P:452:PHE:CE2	2.11	0.85
2:O:402:ASP:HB2	2:O:405:GLN:HE22	1.41	0.84
2:O:384:TRP:HE1	2:O:413:ARG:HH11	1.22	0.84
2:N:642:PHE:CZ	2:O:630:LEU:O	2.31	0.83
2:N:642:PHE:HZ	2:O:634:ALA:HB3	1.45	0.80
1:K:323:ASN:HD21	8:V:482:ARG:HB3	1.45	0.80
2:O:469:LEU:HB2	9:U:966:ARG:HH21	1.48	0.79
2:O:243:PRO:HD2	7:T:510:ARG:HH12	1.50	0.77
3:P:452:PHE:CD2	5:R:428:GLN:HG2	2.19	0.76
2:O:320:CYS:SG	2:O:348:CYS:HB3	2.25	0.76
2:O:118:ILE:HG22	2:O:120:PRO:HD3	1.67	0.76
4:Q:46:LYS:HA	4:Q:49:ARG:HG2	1.68	0.75
6:S:437:LEU:HD21	6:S:445:ARG:HE	1.49	0.75
3:P:474:ASP:HA	3:P:477:ILE:HG22	1.67	0.75
2:N:642:PHE:CE1	2:O:630:LEU:C	2.64	0.74
2:O:565:GLU:OE1	2:O:565:GLU:N	2.21	0.74
8:V:90:LEU:HG	8:V:91:LYS:HD2	1.70	0.73
4:Q:41:LEU:HD13	4:Q:130:LEU:HB2	1.70	0.73
5:R:380:THR:HG21	5:R:388:MET:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:90:LEU:HB2	8:V:119:ILE:HD11	1.69	0.73
2:N:642:PHE:CZ	2:O:634:ALA:CB	2.66	0.73
9:U:858:LYS:NZ	9:U:866:CYS:SG	2.62	0.72
4:Q:106:GLU:HB2	4:Q:129:ARG:HG2	1.71	0.72
2:N:642:PHE:CE1	2:O:631:ARG:CA	2.72	0.72
3:P:285:ILE:HD11	3:P:374:LYS:HB3	1.70	0.71
3:P:164:ARG:HE	3:P:275:LYS:HB2	1.56	0.71
2:N:570:THR:OG1	2:O:569:MET:SD	2.48	0.71
3:P:448:ALA:HB1	3:P:452:PHE:CZ	2.25	0.70
2:N:180:ARG:NH2	2:N:191:MET:SD	2.60	0.70
2:O:603:ARG:NH1	5:R:981:ARG:HA	1.98	0.70
3:P:68:ARG:NH2	5:R:525:ARG:HD3	2.07	0.70
1:K:338:ASN:HD22	8:V:559:ARG:HB3	1.57	0.69
2:O:402:ASP:HA	8:V:534:LEU:HD13	1.74	0.69
2:O:384:TRP:HE1	2:O:413:ARG:NH1	1.91	0.69
8:V:88:PRO:HB2	8:V:91:LYS:HG2	1.74	0.69
4:Q:321:PRO:O	9:U:974:ARG:NH1	2.25	0.69
1:K:192:ASN:OD1	1:K:193:ALA:N	2.26	0.69
6:S:175:ARG:HH12	6:S:177:ARG:HH11	1.41	0.69
2:O:401:GLU:OE2	2:O:403:TRP:NE1	2.24	0.69
9:U:844:GLU:HG2	9:U:845:VAL:HG22	1.75	0.68
1:K:288:TYR:HA	4:Q:379:ARG:HH12	1.58	0.68
1:K:203:ILE:HB	8:V:465:LEU:HD11	1.75	0.68
5:R:928:ARG:HB3	5:R:1010:LEU:HD21	1.76	0.68
2:N:428:GLU:HB3	2:N:431:TYR:HE1	1.58	0.67
8:V:514:GLU:OE2	8:V:514:GLU:N	2.28	0.67
2:O:377:THR:HB	2:O:380:ARG:HH22	1.60	0.67
3:P:416:PHE:O	3:P:419:ASN:ND2	2.27	0.67
5:R:520:GLU:HG2	5:R:521:ARG:HG3	1.76	0.67
2:N:380:ARG:NH1	7:T:421:ASN:OD1	2.28	0.67
2:N:642:PHE:HE1	2:O:631:ARG:N	1.92	0.67
9:U:909:GLU:OE2	9:U:913:ARG:NH2	2.26	0.67
3:P:162:SER:HB2	3:P:275:LYS:HE2	1.77	0.66
2:N:614:LEU:HD11	2:N:661:MET:HB2	1.77	0.66
2:O:414:THR:N	2:O:417:GLU:OE1	2.24	0.66
5:R:414:ASP:OD1	5:R:415:ARG:N	2.28	0.66
1:K:294:ARG:HG3	4:Q:372:LEU:HD12	1.76	0.66
1:K:196:PRO:HA	2:N:433:GLU:HA	1.78	0.66
3:P:231:PHE:HA	3:P:284:VAL:HG23	1.77	0.65
3:P:480:GLY:O	3:P:484:ARG:N	2.29	0.65
9:U:962:GLU:O	9:U:966:ARG:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:452:PHE:CE2	5:R:428:GLN:HG2	2.32	0.65
4:Q:163:PRO:HG2	4:Q:166:ALA:HB2	1.79	0.65
2:N:557:ARG:HD2	9:U:971:GLU:HA	1.79	0.65
1:K:293:ARG:O	1:K:295:LYS:NZ	2.30	0.65
2:N:565:GLU:HB3	3:P:450:HIS:CD2	2.32	0.65
2:O:160:ASP:OD2	2:O:164:ASN:ND2	2.30	0.64
3:P:452:PHE:CD1	3:P:453:LEU:HD23	2.33	0.64
2:N:463:MET:HE1	4:Q:315:GLU:HG3	1.77	0.64
7:T:490:ARG:NH1	7:T:494:GLU:OE1	2.30	0.64
4:Q:110:GLN:NE2	4:Q:112:ALA:O	2.31	0.64
5:R:355:GLU:OE2	5:R:355:GLU:N	2.27	0.63
6:S:117:ARG:NH1	6:S:122:ASN:OD1	2.31	0.63
2:O:603:ARG:HH22	5:R:981:ARG:C	2.07	0.63
1:K:199:MET:O	1:K:203:ILE:HG12	1.98	0.63
3:P:452:PHE:HD1	3:P:453:LEU:HD23	1.63	0.63
5:R:370:GLU:O	5:R:374:GLU:HG2	1.99	0.63
2:N:557:ARG:NH1	9:U:971:GLU:O	2.32	0.62
2:O:568:GLU:HG3	2:O:569:MET:HE2	1.81	0.62
2:O:603:ARG:HE	5:R:985:PRO:HD3	1.63	0.62
2:N:642:PHE:HE1	2:O:631:ARG:CA	2.10	0.62
9:U:922:LEU:HA	9:U:925:GLU:HG2	1.81	0.62
4:Q:126:ARG:HB3	4:Q:128:PHE:CE2	2.34	0.62
4:Q:156:ALA:HB3	4:Q:161:ARG:HH12	1.64	0.62
7:T:504:LYS:NZ	7:T:505:ASP:OD1	2.32	0.62
4:Q:119:GLN:N	4:Q:119:GLN:OE1	2.32	0.62
1:K:313:LEU:HD12	1:K:313:LEU:H	1.64	0.62
8:V:65:ALA:O	8:V:68:CYS:N	2.33	0.62
2:N:577:VAL:HG11	2:O:572:LEU:HD21	1.82	0.62
3:P:226:ALA:HB3	3:P:289:TYR:HB2	1.81	0.62
4:Q:10:VAL:HG23	4:Q:205:ILE:HD11	1.81	0.62
1:K:384:MET:HE2	1:K:384:MET:HA	1.82	0.61
2:O:146:ARG:NH2	6:S:307:SER:O	2.31	0.61
2:O:413:ARG:NH2	2:O:417:GLU:OE2	2.33	0.61
7:T:397:ASN:ND2	7:T:399:SER:OG	2.33	0.61
5:R:976:ALA:HB3	5:R:979:ASN:HB2	1.81	0.61
2:N:386:ASP:N	2:N:386:ASP:OD1	2.32	0.61
1:K:336:PRO:HA	8:V:262:THR:HA	1.82	0.61
9:U:953:LYS:HE3	9:U:953:LYS:HA	1.82	0.61
2:N:119:LEU:HD11	2:N:202:LEU:HD23	1.83	0.61
5:R:901:ARG:NH1	5:R:908:ALA:O	2.34	0.61
6:S:204:LEU:O	6:S:207:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:968:TRP:O	9:U:972:ILE:HG12	2.00	0.61
3:P:510:ARG:O	3:P:510:ARG:NH1	2.34	0.60
3:P:448:ALA:HB1	3:P:452:PHE:HE2	1.64	0.60
8:V:380:PRO:HG2	8:V:383:GLN:HB2	1.83	0.60
2:O:603:ARG:NH2	5:R:980:GLU:O	2.33	0.60
2:O:368:ARG:HH12	2:O:370:GLU:HB2	1.67	0.60
4:Q:36:GLU:CD	4:Q:36:GLU:H	2.10	0.60
1:K:368:LEU:HG	2:N:422:PHE:HE1	1.66	0.59
2:O:394:GLU:HG2	9:U:896:HIS:CD2	2.37	0.59
4:Q:89:ALA:HA	4:Q:167:ILE:HG21	1.82	0.59
8:V:561:ASP:OD1	8:V:562:ASP:N	2.34	0.59
7:T:491:GLU:O	7:T:495:ASN:ND2	2.34	0.59
4:Q:33:GLU:OE2	4:Q:33:GLU:N	2.26	0.59
4:Q:191:ARG:HD3	4:Q:192:LYS:N	2.18	0.59
3:P:74:ASP:OD1	8:V:319:TRP:NE1	2.36	0.59
8:V:456:ASP:O	8:V:460:GLN:HG2	2.03	0.58
2:N:640:GLN:OE1	2:N:643:ARG:NH2	2.37	0.58
2:N:670:SER:OG	3:P:170:ARG:NH2	2.35	0.58
2:O:603:ARG:HH21	5:R:985:PRO:HD3	1.68	0.58
8:V:83:ASP:OD1	8:V:84:SER:N	2.36	0.58
1:K:177:ASN:HA	1:K:180:MET:HG3	1.83	0.58
2:N:168:LEU:HD11	2:O:219:PRO:HD2	1.84	0.58
8:V:257:SER:H	8:V:259:ARG:NH2	2.00	0.58
2:N:285:LYS:NZ	2:N:286:ILE:O	2.34	0.58
8:V:93:HIS:HB2	8:V:116:PRO:HB3	1.86	0.58
1:K:183:ILE:O	1:K:187:ARG:HG3	2.03	0.58
2:O:469:LEU:HD13	9:U:966:ARG:HE	1.69	0.58
2:O:566:GLU:OE1	3:P:88:HIS:NE2	2.36	0.58
7:T:367:GLN:O	7:T:367:GLN:NE2	2.35	0.58
4:Q:38:THR:O	4:Q:42:LEU:HG	2.04	0.57
6:S:590:MET:HE3	6:S:590:MET:HA	1.85	0.57
1:K:355:ALA:HA	1:K:358:LYS:HE2	1.85	0.57
2:N:354:GLU:OE1	2:N:354:GLU:N	2.38	0.57
2:N:348:CYS:SG	2:N:350:THR:OG1	2.57	0.57
5:R:444:ILE:HG12	5:R:488:LEU:HD13	1.85	0.57
4:Q:374:ASP:OD1	4:Q:375:GLU:N	2.38	0.57
8:V:314:LEU:HD12	8:V:378:ILE:HG21	1.85	0.57
3:P:426:LEU:HB3	8:V:360:LEU:HD22	1.86	0.57
7:T:346:TRP:O	7:T:350:HIS:ND1	2.37	0.57
8:V:526:GLN:O	8:V:530:ILE:HG12	2.04	0.57
5:R:451:ARG:HD2	5:R:494:GLU:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:580:MET:HA	2:O:584:LEU:HD12	1.85	0.57
5:R:350:VAL:HG21	5:R:445:GLU:CD	2.30	0.57
8:V:224:ALA:HA	9:U:863:GLN:HG3	1.87	0.57
2:N:404:ASN:OD1	2:N:415:ARG:NH1	2.38	0.56
8:V:69:MET:SD	8:V:70:PRO:HD3	2.45	0.56
8:V:562:ASP:N	8:V:562:ASP:OD1	2.37	0.56
2:N:238:GLN:NE2	7:T:433:PRO:O	2.38	0.56
2:O:401:GLU:HG3	8:V:534:LEU:HB3	1.87	0.56
7:T:504:LYS:HA	7:T:509:ARG:HD2	1.87	0.56
7:T:475:ARG:HA	7:T:478:LEU:HD13	1.86	0.56
4:Q:198:ASP:O	4:Q:202:TRP:NE1	2.38	0.56
4:Q:37:VAL:O	4:Q:41:LEU:HG	2.06	0.56
4:Q:205:ILE:HG13	4:Q:205:ILE:O	2.06	0.56
5:R:394:PHE:HB2	5:R:398:CYS:SG	2.46	0.56
2:N:652:ALA:O	2:O:620:LYS:NZ	2.33	0.56
2:N:320:CYS:SG	2:N:348:CYS:N	2.79	0.56
4:Q:126:ARG:HB3	4:Q:128:PHE:HE2	1.70	0.56
8:V:567:MET:HE3	8:V:567:MET:HA	1.87	0.56
2:N:546:LEU:HD13	9:U:960:LEU:HG	1.88	0.55
2:N:639:GLU:O	2:N:643:ARG:NH1	2.39	0.55
3:P:143:TRP:CZ3	3:P:144:GLN:HG3	2.42	0.55
2:N:463:MET:O	2:N:463:MET:HG2	2.05	0.55
1:K:179:LEU:O	1:K:183:ILE:HG13	2.07	0.55
2:N:599:GLN:NE2	4:Q:401:MET:SD	2.80	0.55
2:O:564:HIS:HA	2:O:567:ARG:HE	1.72	0.55
2:N:627:GLN:HE22	4:Q:432:LEU:HA	1.71	0.55
4:Q:111:ARG:HA	4:Q:111:ARG:HH11	1.71	0.55
5:R:377:LEU:O	5:R:380:THR:HG22	2.07	0.55
9:U:885:ASN:OD1	9:U:887:VAL:N	2.40	0.55
2:N:627:GLN:HE22	4:Q:433:GLU:H	1.53	0.55
1:K:176:LEU:O	1:K:180:MET:HG3	2.07	0.55
2:N:583:LYS:NZ	3:P:433:ASP:OD1	2.39	0.55
2:O:384:TRP:HB3	2:O:388:GLU:HB2	1.88	0.54
3:P:229:VAL:HB	3:P:248:ILE:HD11	1.88	0.54
2:O:399:TYR:HD2	2:O:406:ILE:HG12	1.72	0.54
2:N:272:VAL:HB	7:T:427:THR:HB	1.88	0.54
8:V:521:GLN:HA	8:V:524:LYS:NZ	2.23	0.54
2:N:609:ARG:HH21	4:Q:413:GLN:HA	1.71	0.54
4:Q:453:ASP:OD1	4:Q:454:GLU:N	2.39	0.54
8:V:557:GLU:N	8:V:557:GLU:OE2	2.41	0.54
2:N:614:LEU:HD11	2:N:661:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:466:TYR:HD2	5:R:469:VAL:HG23	1.71	0.54
1:K:293:ARG:HG3	4:Q:372:LEU:HD13	1.90	0.54
2:N:363:SER:OG	8:V:563:TYR:N	2.41	0.54
2:N:428:GLU:HB3	2:N:431:TYR:CE1	2.41	0.54
3:P:219:ARG:HE	3:P:270:ASP:HB2	1.72	0.54
4:Q:369:ASP:OD1	4:Q:369:ASP:N	2.38	0.54
5:R:592:ASP:OD1	5:R:593:LEU:N	2.41	0.54
8:V:75:PHE:HA	8:V:78:VAL:HG22	1.89	0.54
4:Q:19:HIS:CE1	4:Q:82:ALA:HB3	2.43	0.54
8:V:132:ASP:HA	8:V:135:VAL:HG12	1.89	0.54
2:N:557:ARG:NH1	9:U:971:GLU:OE2	2.42	0.53
6:S:177:ARG:HH12	6:S:449:ARG:HG3	1.73	0.53
9:U:974:ARG:HA	9:U:977:GLN:NE2	2.23	0.53
9:U:922:LEU:O	9:U:926:ARG:HG2	2.08	0.53
2:N:567:ARG:NH2	2:O:565:GLU:OE2	2.41	0.53
3:P:536:LEU:HA	7:T:526:GLY:HA3	1.91	0.53
1:K:379:ILE:O	1:K:383:MET:HG2	2.07	0.53
2:N:642:PHE:HZ	2:O:630:LEU:O	1.91	0.53
3:P:351:ARG:NH1	3:P:353:SER:O	2.41	0.53
2:N:666:ALA:H	3:P:131:ARG:NH2	2.07	0.53
1:K:184:LYS:O	1:K:188:MET:HG2	2.07	0.53
2:O:603:ARG:NE	5:R:984:ARG:HB3	2.24	0.53
3:P:481:GLU:HA	3:P:484:ARG:HB3	1.90	0.53
2:N:330:ILE:HD13	2:N:370:GLU:HB2	1.90	0.53
2:O:391:ARG:HD3	2:O:410:VAL:HA	1.91	0.53
2:N:322:ASN:HD22	2:N:356:ARG:HE	1.57	0.53
6:S:559:ALA:HB3	6:S:572:ASN:HB3	1.90	0.53
8:V:68:CYS:SG	8:V:69:MET:N	2.82	0.53
2:N:627:GLN:NE2	4:Q:433:GLU:H	2.07	0.52
8:V:95:PRO:HB2	8:V:140:ARG:HH21	1.74	0.52
2:N:242:ASP:N	2:N:242:ASP:OD1	2.35	0.52
1:K:332:LEU:HD23	1:K:362:GLU:HB2	1.91	0.52
2:O:362:THR:HG22	2:O:365:HIS:CE1	2.44	0.52
3:P:345:LEU:HD23	3:P:348:ILE:HD11	1.90	0.52
4:Q:169:LEU:O	4:Q:174:HIS:NE2	2.43	0.52
9:U:918:ARG:NH2	9:U:919:ASP:OD1	2.43	0.52
2:N:320:CYS:HB2	2:N:323:CYS:HB2	1.91	0.52
5:R:909:PRO:O	5:R:911:GLN:NE2	2.42	0.52
3:P:131:ARG:HD3	4:Q:475:ARG:HH22	1.75	0.52
2:N:322:ASN:ND2	2:N:356:ARG:HE	2.07	0.52
5:R:403:ALA:O	5:R:416:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:150:LEU:HD12	6:S:151:PRO:HD2	1.92	0.52
1:K:180:MET:HA	1:K:183:ILE:HD12	1.91	0.52
1:K:199:MET:SD	1:K:199:MET:N	2.82	0.52
4:Q:130:LEU:HD12	4:Q:131:LEU:H	1.74	0.52
8:V:193:VAL:HG12	8:V:195:SER:H	1.74	0.52
9:U:851:ASN:ND2	9:U:853:ASP:OD1	2.43	0.52
2:O:584:LEU:HB3	3:P:101:PHE:CZ	2.45	0.51
2:N:560:ALA:HB1	9:U:978:LEU:HD12	1.92	0.51
3:P:225:LYS:H	3:P:290:ARG:HA	1.75	0.51
7:T:443:VAL:HG13	7:T:455:TRP:CZ3	2.45	0.51
1:K:192:ASN:ND2	1:K:327:GLN:OE1	2.43	0.51
2:N:274:ARG:HB2	7:T:411:PHE:HE1	1.75	0.51
3:P:161:ALA:O	3:P:278:GLY:N	2.36	0.51
5:R:624:LEU:HA	5:R:888:THR:HB	1.90	0.51
8:V:559:ARG:HB2	9:U:885:ASN:HD22	1.75	0.51
2:O:436:ARG:NE	2:O:436:ARG:HA	2.26	0.51
4:Q:57:THR:OG1	4:Q:58:TYR:N	2.44	0.51
4:Q:179:PHE:O	4:Q:183:LEU:HG	2.11	0.51
1:K:197:ILE:HG22	1:K:201:LYS:HZ2	1.76	0.51
2:N:274:ARG:HB2	7:T:411:PHE:CE1	2.45	0.51
9:U:907:LEU:O	9:U:911:ARG:HG2	2.10	0.51
3:P:281:ASN:HA	3:P:379:ILE:O	2.11	0.51
4:Q:173:ILE:HA	4:Q:176:LEU:HG	1.93	0.51
7:T:455:TRP:HH2	7:T:465:LYS:HD2	1.75	0.51
2:O:398:ARG:HG3	2:O:399:TYR:CD1	2.46	0.51
2:O:564:HIS:O	2:O:567:ARG:HG2	2.10	0.51
8:V:535:PRO:HD2	8:V:536:PRO:HD3	1.92	0.51
2:N:464:SER:HA	2:N:468:PHE:HB3	1.92	0.50
3:P:536:LEU:HD12	7:T:526:GLY:HA3	1.93	0.50
4:Q:457:ALA:HA	4:Q:460:GLU:HG3	1.92	0.50
3:P:309:MET:HE1	3:P:316:GLU:HG2	1.94	0.50
7:T:491:GLU:OE2	7:T:492:GLN:NE2	2.43	0.50
8:V:157:ASP:OD1	8:V:157:ASP:N	2.44	0.50
4:Q:81:PHE:HD1	4:Q:82:ALA:N	2.09	0.50
4:Q:97:GLN:HE22	4:Q:99:MET:HB3	1.77	0.50
6:S:207:LYS:HE3	6:S:207:LYS:HA	1.94	0.50
7:T:471:SER:HB3	7:T:474:ILE:HG13	1.92	0.50
2:O:322:ASN:ND2	2:O:356:ARG:O	2.42	0.50
3:P:319:MET:O	3:P:323:GLU:HG2	2.12	0.50
4:Q:25:ARG:HH11	4:Q:25:ARG:HG2	1.76	0.50
2:N:551:LEU:HB3	3:P:460:PRO:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:464:ILE:O	8:V:468:ILE:HG12	2.10	0.50
2:O:403:TRP:HA	2:O:406:ILE:HD12	1.93	0.50
3:P:134:ILE:HG13	3:P:167:ILE:HG12	1.93	0.50
8:V:74:ASP:HA	9:U:898:VAL:HG11	1.93	0.50
1:K:329:TYR:HB2	1:K:365:LYS:HG2	1.93	0.50
2:N:431:TYR:O	2:N:435:GLU:HG2	2.12	0.50
4:Q:201:ASN:OD1	4:Q:201:ASN:N	2.44	0.50
4:Q:323:GLN:NE2	4:Q:324:ILE:O	2.45	0.50
2:O:362:THR:HG22	2:O:365:HIS:HE1	1.77	0.49
4:Q:58:TYR:CE1	4:Q:189:ILE:HG22	2.47	0.49
2:O:388:GLU:OE1	2:O:388:GLU:N	2.42	0.49
3:P:68:ARG:HH21	5:R:525:ARG:HD3	1.74	0.49
8:V:319:TRP:HZ2	8:V:385:SER:HB2	1.78	0.49
2:O:565:GLU:O	2:O:569:MET:HG2	2.13	0.49
5:R:428:GLN:HG3	5:R:430:SER:H	1.78	0.49
8:V:458:GLU:HA	8:V:461:VAL:HG22	1.94	0.49
4:Q:125:ARG:HH21	4:Q:127:ARG:HD2	1.77	0.49
4:Q:191:ARG:HD2	4:Q:193:GLU:CD	2.38	0.49
1:K:188:MET:HE1	1:K:196:PRO:HD3	1.95	0.49
2:O:403:TRP:CD1	8:V:534:LEU:HD22	2.48	0.49
4:Q:172:PRO:O	4:Q:175:GLN:HG3	2.13	0.49
6:S:447:GLY:O	6:S:450:GLU:HG3	2.13	0.49
9:U:980:ARG:HH12	9:U:983:LEU:HD22	1.76	0.49
9:U:980:ARG:O	9:U:980:ARG:HD3	2.13	0.48
9:U:887:VAL:HG23	9:U:887:VAL:O	2.14	0.48
4:Q:458:ARG:HA	4:Q:461:GLU:OE2	2.14	0.48
1:K:354:THR:O	1:K:358:LYS:HG3	2.14	0.48
2:N:642:PHE:HE2	2:O:634:ALA:HB1	1.74	0.48
2:O:187:VAL:HG11	6:S:345:PHE:CE1	2.49	0.48
5:R:890:ILE:HD12	5:R:892:ILE:HD11	1.95	0.48
9:U:837:TYR:CZ	9:U:840:PRO:HG2	2.48	0.48
2:O:362:THR:HG23	2:O:364:ALA:H	1.79	0.48
3:P:297:PHE:HD1	3:P:367:LEU:HB3	1.79	0.48
5:R:608:VAL:O	5:R:611:LEU:HB2	2.14	0.48
2:O:416:GLU:O	2:O:419:VAL:HG12	2.14	0.47
8:V:541:ARG:HD2	8:V:547:LEU:HD23	1.96	0.47
9:U:974:ARG:HA	9:U:977:GLN:HE21	1.79	0.47
1:K:294:ARG:HE	4:Q:372:LEU:HB2	1.80	0.47
2:N:580:MET:HG2	3:P:436:LEU:HD11	1.96	0.47
2:O:216:VAL:HG12	7:T:381:PHE:HB3	1.95	0.47
4:Q:14:LEU:HD11	4:Q:207:PHE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:353:LEU:HD22	2:O:353:LEU:H	1.80	0.47
3:P:452:PHE:HE1	4:Q:313:TRP:CZ3	2.32	0.47
9:U:958:ARG:O	9:U:962:GLU:HG2	2.14	0.47
2:N:620:LYS:O	2:N:623:VAL:HG12	2.14	0.47
8:V:187:PRO:HG3	9:U:889:GLU:HB3	1.96	0.47
2:O:242:ASP:HA	7:T:510:ARG:NH1	2.30	0.47
4:Q:198:ASP:OD1	4:Q:199:ARG:N	2.47	0.47
8:V:77:ALA:HB3	9:U:898:VAL:HG12	1.96	0.47
8:V:459:LYS:HA	8:V:462:ASP:OD2	2.14	0.47
2:N:609:ARG:NH2	4:Q:416:GLN:HB2	2.29	0.47
2:O:241:ALA:O	7:T:510:ARG:NH1	2.48	0.47
2:O:427:ILE:HG12	8:V:552:VAL:HG11	1.97	0.47
3:P:164:ARG:HH21	3:P:275:LYS:HD2	1.80	0.47
5:R:544:THR:OG1	5:R:545:GLU:OE1	2.32	0.47
5:R:994:PHE:HB2	5:R:1004:VAL:HG11	1.96	0.47
1:K:173:GLN:O	1:K:176:LEU:HB3	2.15	0.47
2:N:590:TYR:O	2:N:594:MET:HG2	2.15	0.47
2:O:384:TRP:CE2	2:O:421:GLN:HG3	2.50	0.47
3:P:485:ALA:HB1	8:V:304:TYR:HA	1.97	0.47
4:Q:17:HIS:HD2	4:Q:183:LEU:HD11	1.80	0.47
7:T:443:VAL:HG13	7:T:455:TRP:HZ3	1.77	0.47
8:V:461:VAL:O	8:V:464:ILE:HG13	2.14	0.47
9:U:882:ARG:HH12	9:U:891:TYR:HH	1.57	0.47
3:P:161:ALA:HB3	3:P:279:ASP:HA	1.96	0.47
9:U:979:LEU:HA	9:U:982:ASP:OD2	2.15	0.47
2:N:535:ASN:HB3	2:N:538:SER:HB3	1.96	0.47
2:N:591:PHE:HD1	3:P:109:MET:HE1	1.80	0.47
2:O:583:LYS:HZ3	4:Q:390:GLU:HG2	1.80	0.47
3:P:342:ASP:OD1	3:P:343:ASP:N	2.48	0.47
4:Q:313:TRP:CH2	4:Q:317:ILE:HG13	2.50	0.47
6:S:448:ASP:HA	6:S:451:ARG:HG2	1.96	0.47
2:N:609:ARG:HH12	4:Q:412:LYS:HE3	1.79	0.46
3:P:361:GLU:O	3:P:364:THR:OG1	2.32	0.46
4:Q:5:ASP:O	4:Q:8:GLN:HG2	2.14	0.46
4:Q:452:LEU:O	4:Q:456:VAL:HG12	2.15	0.46
6:S:117:ARG:HH12	6:S:122:ASN:HA	1.80	0.46
9:U:900:HIS:O	9:U:904:ILE:HG12	2.16	0.46
2:N:407:ALA:HB2	2:N:415:ARG:HB3	1.97	0.46
2:N:220:PHE:CD1	2:O:236:PRO:HG3	2.50	0.46
8:V:92:ARG:CZ	8:V:93:HIS:HB3	2.45	0.46
6:S:415:GLU:CD	6:S:415:GLU:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:205:LEU:HD12	8:V:206:SER:N	2.30	0.46
8:V:481:ASN:O	8:V:485:THR:HG23	2.15	0.46
9:U:853:ASP:HA	9:U:856:ILE:HG12	1.97	0.46
1:K:193:ALA:HA	1:K:324:ARG:HH21	1.81	0.46
2:O:362:THR:H	2:O:365:HIS:CE1	2.34	0.46
3:P:125:LYS:HB3	3:P:399:LEU:HD22	1.98	0.46
7:T:411:PHE:CZ	7:T:426:ASP:HB2	2.50	0.46
8:V:332:LYS:HD2	8:V:332:LYS:HA	1.72	0.46
1:K:192:ASN:CG	1:K:193:ALA:H	2.20	0.46
2:N:655:PRO:HG3	2:O:616:ARG:HH22	1.81	0.46
2:O:575:ALA:O	2:O:579:VAL:HG12	2.15	0.46
2:O:582:GLU:HB3	4:Q:391:ILE:HG21	1.98	0.46
6:S:13:SER:HB3	6:S:110:MET:HE1	1.97	0.46
3:P:64:LEU:HD21	5:R:571:ASP:HB2	1.98	0.46
4:Q:169:LEU:HB3	4:Q:174:HIS:NE2	2.30	0.46
1:K:380:GLY:HA2	1:K:383:MET:HG3	1.96	0.46
2:N:639:GLU:HA	2:N:642:PHE:CD2	2.50	0.46
4:Q:130:LEU:HD12	4:Q:131:LEU:N	2.31	0.46
8:V:535:PRO:CD	8:V:536:PRO:HD3	2.46	0.46
9:U:901:LEU:O	9:U:905:LYS:HG3	2.16	0.46
2:O:564:HIS:HA	2:O:567:ARG:NE	2.30	0.46
4:Q:109:PHE:HD1	4:Q:126:ARG:HG3	1.81	0.46
4:Q:111:ARG:HA	4:Q:111:ARG:NH1	2.31	0.46
2:N:623:VAL:HG23	2:O:619:PHE:CD1	2.51	0.45
8:V:175:TYR:HA	8:V:178:GLU:OE2	2.16	0.45
2:N:322:ASN:OD1	2:N:323:CYS:N	2.48	0.45
4:Q:126:ARG:HE	4:Q:152:HIS:CE1	2.34	0.45
8:V:119:ILE:HA	8:V:122:LYS:HB3	1.98	0.45
2:N:335:PRO:HD2	8:V:267:PHE:CE1	2.51	0.45
2:O:238:GLN:HB3	2:O:239:PRO:HD3	1.97	0.45
2:O:327:CYS:HB2	2:O:330:ILE:O	2.17	0.45
6:S:153:VAL:HG12	6:S:155:GLY:H	1.81	0.45
2:N:252:LYS:HD2	2:N:252:LYS:HA	1.79	0.45
2:O:621:ARG:HH11	2:O:621:ARG:HG2	1.82	0.45
3:P:113:ARG:HD3	3:P:113:ARG:C	2.41	0.45
3:P:377:TYR:CE2	3:P:379:ILE:HG12	2.52	0.45
4:Q:37:VAL:HA	4:Q:40:TRP:CE3	2.50	0.45
6:S:467:THR:HG22	6:S:530:TYR:H	1.81	0.45
3:P:452:PHE:CD1	3:P:453:LEU:N	2.84	0.45
9:U:978:LEU:HD23	9:U:978:LEU:HA	1.77	0.45
2:O:603:ARG:HH21	5:R:985:PRO:CD	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:603:ARG:CZ	5:R:984:ARG:HB3	2.46	0.45
2:O:614:LEU:HD11	5:R:973:ARG:NH2	2.32	0.45
3:P:228:THR:OG1	3:P:287:ASN:HB2	2.16	0.45
8:V:476:ALA:HA	8:V:479:GLN:OE1	2.17	0.45
8:V:521:GLN:HA	8:V:524:LYS:HZ3	1.81	0.45
9:U:953:LYS:O	9:U:956:GLU:HG3	2.16	0.45
5:R:370:GLU:HG3	5:R:466:TYR:OH	2.17	0.45
6:S:320:ILE:HG12	6:S:327:TYR:HB3	1.98	0.45
8:V:471:MET:O	8:V:475:LEU:HG	2.17	0.45
9:U:856:ILE:O	9:U:858:LYS:N	2.45	0.45
2:N:218:PRO:HD2	3:P:524:ARG:HH12	1.81	0.45
4:Q:170:PRO:HD2	4:Q:173:ILE:HD13	1.97	0.45
4:Q:306:ARG:H	4:Q:306:ARG:HG2	1.66	0.45
8:V:130:ASN:OD1	8:V:133:ASP:N	2.49	0.45
1:K:298:GLN:HG2	8:V:401:VAL:HG11	1.99	0.45
2:O:410:VAL:HG21	2:O:418:CYS:SG	2.56	0.45
3:P:306:ILE:HG23	3:P:307:VAL:HG23	1.98	0.45
7:T:370:ASN:OD1	7:T:370:ASN:C	2.60	0.45
8:V:262:THR:HG23	8:V:264:GLY:H	1.82	0.45
8:V:461:VAL:O	8:V:465:LEU:HD23	2.16	0.45
2:O:118:ILE:HD11	2:O:167:ARG:HG2	1.99	0.44
4:Q:115:ARG:N	4:Q:118:GLU:OE1	2.45	0.44
6:S:108:ASP:N	6:S:108:ASP:OD1	2.49	0.44
6:S:572:ASN:OD1	6:S:572:ASN:N	2.50	0.44
9:U:896:HIS:O	9:U:900:HIS:N	2.50	0.44
1:K:316:ASP:O	1:K:320:ILE:HG22	2.16	0.44
2:N:319:ASN:HB3	2:N:324:GLY:HA2	1.99	0.44
2:N:358:PRO:HB3	8:V:569:GLU:O	2.17	0.44
2:N:538:SER:O	2:N:542:THR:HG23	2.17	0.44
2:N:642:PHE:CD1	2:O:630:LEU:HD23	2.53	0.44
4:Q:43:GLN:O	4:Q:46:LYS:HG2	2.18	0.44
8:V:135:VAL:HG11	8:V:175:TYR:CE1	2.53	0.44
2:N:328:THR:O	2:N:371:ASN:ND2	2.51	0.44
5:R:974:ILE:HG13	5:R:1014:ASP:HB3	1.99	0.44
5:R:611:LEU:HD22	5:R:1000:LEU:HD13	1.99	0.44
2:O:474:ASP:OD1	2:O:475:PRO:HD3	2.18	0.44
2:O:134:ILE:HG13	7:T:474:ILE:HG23	1.98	0.44
3:P:531:LEU:HD12	3:P:531:LEU:HA	1.78	0.44
4:Q:19:HIS:HE1	4:Q:81:PHE:CE1	2.36	0.44
5:R:1014:ASP:N	5:R:1014:ASP:OD1	2.44	0.44
8:V:146:ILE:HD11	8:V:161:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:135:SER:HB3	3:P:391:PRO:HB3	1.99	0.44
2:O:192:ARG:HH21	7:T:460:PHE:HB2	1.82	0.44
8:V:200:THR:OG1	8:V:247:LEU:O	2.24	0.44
1:K:406:VAL:HG12	1:K:408:GLU:HG3	1.99	0.43
2:N:285:LYS:HD2	2:N:285:LYS:HA	1.85	0.43
2:O:402:ASP:HB2	2:O:405:GLN:NE2	2.21	0.43
3:P:109:MET:HE2	3:P:109:MET:HB2	1.87	0.43
2:O:317:LYS:HE2	2:O:317:LYS:HB2	1.82	0.43
2:O:417:GLU:H	2:O:417:GLU:HG3	1.58	0.43
3:P:77:LEU:N	3:P:78:PRO:HD2	2.32	0.43
4:Q:43:GLN:O	4:Q:47:ILE:HG12	2.17	0.43
5:R:427:ILE:HG23	5:R:482:MET:HE1	2.00	0.43
5:R:935:LEU:HD12	5:R:935:LEU:HA	1.87	0.43
4:Q:20:LEU:HD13	4:Q:56:TRP:CD2	2.53	0.43
4:Q:391:ILE:HG13	4:Q:392:GLU:N	2.33	0.43
1:K:417:LYS:HA	1:K:417:LYS:HD3	1.84	0.43
2:N:288:LYS:HA	2:N:288:LYS:HD2	1.81	0.43
4:Q:81:PHE:HB2	4:Q:127:ARG:CZ	2.49	0.43
3:P:448:ALA:O	3:P:452:PHE:CE2	2.71	0.43
4:Q:199:ARG:HA	4:Q:202:TRP:CE2	2.53	0.43
5:R:412:ASP:OD1	5:R:412:ASP:N	2.49	0.43
5:R:484:MET:HG3	5:R:485:LEU:HG	2.01	0.43
9:U:951:GLU:HA	9:U:954:LYS:HE3	2.01	0.43
4:Q:19:HIS:CE1	4:Q:81:PHE:HE1	2.36	0.43
4:Q:175:GLN:HA	4:Q:178:ASN:OD1	2.19	0.43
6:S:199:VAL:HG22	6:S:207:LYS:NZ	2.34	0.43
8:V:94:LEU:HD11	8:V:141:ALA:HB2	1.99	0.43
8:V:567:MET:HE1	9:U:875:PHE:HB2	2.01	0.43
3:P:344:MET:HE2	3:P:344:MET:HB3	1.75	0.43
5:R:341:GLU:HA	5:R:341:GLU:OE1	2.18	0.43
5:R:496:ALA:O	5:R:500:THR:OG1	2.21	0.43
5:R:597:THR:HG22	5:R:598:ILE:HG23	2.00	0.43
9:U:872:ILE:HD12	9:U:872:ILE:HA	1.91	0.43
2:N:599:GLN:HA	2:N:599:GLN:OE1	2.19	0.43
2:O:137:LYS:HZ3	7:T:473:GLU:CD	2.26	0.43
3:P:266:MET:HE3	3:P:266:MET:HB2	1.95	0.43
6:S:181:LEU:HD12	6:S:181:LEU:HA	1.84	0.43
2:O:133:ASP:HA	2:O:136:ARG:HG2	2.00	0.43
3:P:164:ARG:HA	3:P:275:LYS:HA	2.01	0.43
3:P:364:THR:HA	3:P:367:LEU:HD12	2.00	0.43
4:Q:35:GLN:OE1	4:Q:35:GLN:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:862:GLU:OE1	9:U:862:GLU:N	2.45	0.43
9:U:921:ALA:O	9:U:925:GLU:HG2	2.19	0.43
2:N:148:ARG:HE	2:N:148:ARG:HB2	1.68	0.42
2:O:584:LEU:HB3	3:P:101:PHE:CE1	2.54	0.42
3:P:293:ASP:HB2	3:P:294:PRO:HD3	2.00	0.42
5:R:584:TYR:CZ	5:R:590:ASN:HB3	2.54	0.42
5:R:587:GLU:OE2	5:R:587:GLU:N	2.51	0.42
8:V:82:PHE:CD2	8:V:170:LYS:HD3	2.54	0.42
8:V:170:LYS:C	8:V:170:LYS:HZ2	2.27	0.42
1:K:171:PHE:HA	1:K:175:GLN:NE2	2.34	0.42
1:K:173:GLN:HE22	8:V:546:LYS:NZ	2.17	0.42
2:N:549:ILE:HD13	2:N:549:ILE:HA	1.87	0.42
6:S:199:VAL:HG23	6:S:204:LEU:HD12	2.00	0.42
8:V:463:ASP:OD1	8:V:464:ILE:N	2.52	0.42
9:U:853:ASP:OD1	9:U:853:ASP:N	2.51	0.42
2:O:568:GLU:HG3	2:O:569:MET:CE	2.48	0.42
3:P:168:GLU:HG3	3:P:271:GLU:HG2	2.02	0.42
8:V:90:LEU:H	8:V:90:LEU:HD23	1.84	0.42
8:V:466:GLU:O	8:V:469:SER:OG	2.25	0.42
2:N:463:MET:HE1	4:Q:315:GLU:CG	2.46	0.42
2:N:288:LYS:NZ	2:N:289:SER:O	2.52	0.42
2:O:394:GLU:HG2	9:U:896:HIS:HD2	1.81	0.42
3:P:143:TRP:CE3	3:P:144:GLN:HG3	2.54	0.42
4:Q:198:ASP:OD1	4:Q:200:VAL:N	2.52	0.42
4:Q:374:ASP:OD1	4:Q:374:ASP:C	2.63	0.42
4:Q:453:ASP:HA	4:Q:456:VAL:HG12	2.02	0.42
8:V:276:LEU:HD23	8:V:276:LEU:H	1.84	0.42
2:O:580:MET:SD	3:P:97:GLN:HB3	2.59	0.42
4:Q:123:HIS:HB3	4:Q:153:TYR:CE2	2.55	0.42
5:R:519:LEU:HD11	5:R:532:LEU:HG	2.01	0.42
9:U:844:GLU:OE1	9:U:844:GLU:N	2.42	0.42
2:N:249:LYS:H	2:N:249:LYS:HG2	1.68	0.42
3:P:161:ALA:HB3	3:P:278:GLY:O	2.20	0.42
3:P:296:ARG:C	3:P:297:PHE:HD2	2.28	0.42
3:P:479:LEU:HD12	3:P:479:LEU:HA	1.84	0.42
6:S:197:GLN:OE1	6:S:197:GLN:HA	2.20	0.42
7:T:411:PHE:N	7:T:412:PRO:HD3	2.35	0.42
2:N:320:CYS:SG	2:N:348:CYS:HB3	2.59	0.42
2:O:406:ILE:O	2:O:410:VAL:HG22	2.18	0.42
6:S:161:THR:OG1	6:S:163:PRO:HD2	2.20	0.42
8:V:539:VAL:HG21	8:V:547:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:323:ASN:HB2	8:V:483:ASN:ND2	2.35	0.42
2:O:401:GLU:HB2	8:V:537:TRP:C	2.45	0.42
3:P:514:LYS:C	3:P:514:LYS:HD2	2.45	0.42
6:S:322:LEU:HD12	6:S:359:TRP:CE2	2.54	0.42
1:K:172:THR:H	1:K:175:GLN:NE2	2.18	0.42
2:N:360:ASN:HB3	8:V:573:ALA:HB2	2.01	0.42
2:N:642:PHE:CD1	2:O:631:ARG:NH1	2.88	0.42
2:O:209:ALA:C	2:O:211:GLN:H	2.27	0.42
3:P:165:LEU:HD21	3:P:274:PHE:CE2	2.54	0.42
8:V:460:GLN:HA	8:V:463:ASP:OD2	2.20	0.42
2:N:136:ARG:HA	2:N:143:PHE:CE2	2.55	0.41
8:V:115:LYS:H	8:V:115:LYS:HG2	1.67	0.41
2:N:627:GLN:NE2	4:Q:432:LEU:HD12	2.35	0.41
2:O:330:ILE:HD13	2:O:330:ILE:HA	1.89	0.41
2:O:398:ARG:O	2:O:398:ARG:HD2	2.21	0.41
3:P:70:ARG:HD2	8:V:318:VAL:HG13	2.01	0.41
3:P:115:ASP:OD1	3:P:115:ASP:C	2.63	0.41
4:Q:317:ILE:HD13	4:Q:317:ILE:HA	1.90	0.41
5:R:493:LEU:HD23	5:R:493:LEU:HA	1.82	0.41
1:K:368:LEU:C	1:K:370:SER:N	2.76	0.41
2:N:396:LEU:HD23	2:N:396:LEU:HA	1.88	0.41
2:N:540:LYS:HA	2:N:540:LYS:HD3	1.92	0.41
2:N:550:PRO:O	2:N:554:MET:HG3	2.20	0.41
2:O:332:TYR:N	2:O:347:LEU:O	2.47	0.41
3:P:144:GLN:OE1	3:P:144:GLN:O	2.37	0.41
3:P:248:ILE:HD12	3:P:274:PHE:CE2	2.55	0.41
4:Q:108:TYR:HB2	4:Q:127:ARG:HB2	2.02	0.41
5:R:516:MET:HE3	5:R:555:HIS:NE2	2.35	0.41
8:V:72:ILE:H	8:V:72:ILE:HG13	1.62	0.41
8:V:79:LEU:O	8:V:83:ASP:N	2.53	0.41
2:N:414:THR:HG22	2:N:417:GLU:OE1	2.21	0.41
2:O:381:ASP:OD1	2:O:381:ASP:N	2.53	0.41
6:S:584:LEU:HD23	6:S:584:LEU:HA	1.90	0.41
8:V:456:ASP:OD1	8:V:456:ASP:C	2.64	0.41
8:V:470:ASP:HA	8:V:473:GLU:HG2	2.03	0.41
8:V:542:LEU:HA	9:U:911:ARG:HE	1.84	0.41
2:N:579:VAL:HG13	3:P:432:LEU:HD22	2.03	0.41
2:O:586:LEU:HD23	2:O:586:LEU:HA	1.84	0.41
8:V:146:ILE:HD12	8:V:146:ILE:HA	1.86	0.41
8:V:158:GLU:H	8:V:158:GLU:HG2	1.68	0.41
8:V:160:ALA:HA	8:V:163:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:262:THR:N	8:V:265:GLU:OE2	2.48	0.41
8:V:557:GLU:N	8:V:557:GLU:CD	2.79	0.41
2:O:105:ALA:HA	2:O:107:ARG:NH1	2.35	0.41
2:O:211:GLN:CD	7:T:366:ARG:HH21	2.28	0.41
2:O:242:ASP:HA	7:T:510:ARG:HH12	1.85	0.41
3:P:301:PRO:HA	3:P:304:ALA:HB3	2.02	0.41
3:P:514:LYS:HD2	3:P:514:LYS:O	2.19	0.41
4:Q:6:PRO:C	4:Q:8:GLN:H	2.29	0.41
4:Q:6:PRO:C	4:Q:8:GLN:N	2.78	0.41
4:Q:28:THR:N	8:V:473:GLU:OE2	2.38	0.41
2:N:280:ASN:HB2	2:N:282:LYS:NZ	2.36	0.41
2:N:359:GLY:HA2	8:V:565:GLY:HA3	2.01	0.41
4:Q:114:TYR:CE1	4:Q:167:ILE:HD13	2.55	0.41
2:N:110:LEU:HD23	2:N:110:LEU:HA	1.82	0.41
2:O:472:LEU:C	2:O:475:PRO:HD2	2.46	0.41
3:P:224:PHE:HZ	3:P:396:ILE:HG21	1.86	0.41
3:P:456:MET:SD	3:P:458:ARG:NH1	2.89	0.41
4:Q:454:GLU:O	4:Q:458:ARG:HG3	2.21	0.41
6:S:113:ASN:ND2	6:S:193:TYR:OH	2.40	0.41
6:S:153:VAL:HG11	6:S:157:SER:HB2	2.02	0.41
6:S:562:ASP:HB3	6:S:567:PRO:HA	2.03	0.41
4:Q:62:PRO:HD2	4:Q:86:TYR:OH	2.20	0.41
4:Q:198:ASP:OD1	4:Q:198:ASP:C	2.63	0.41
4:Q:207:PHE:HD1	4:Q:208:PRO:HD2	1.86	0.41
5:R:347:ASN:O	5:R:351:LYS:HG2	2.21	0.41
5:R:451:ARG:HD3	5:R:491:LEU:HD22	2.03	0.41
5:R:592:ASP:OD1	5:R:592:ASP:C	2.64	0.41
5:R:913:ALA:HA	5:R:917:LEU:HD22	2.01	0.41
8:V:65:ALA:C	8:V:68:CYS:H	2.28	0.41
8:V:253:THR:HG22	8:V:254:GLY:N	2.35	0.41
9:U:852:ILE:HD12	9:U:855:ALA:HB3	2.03	0.41
9:U:885:ASN:OD1	9:U:885:ASN:C	2.64	0.41
2:O:356:ARG:HH21	8:V:193:VAL:HA	1.86	0.41
2:O:617:LEU:HD23	2:O:617:LEU:HA	1.91	0.41
4:Q:399:GLU:O	4:Q:402:MET:HG3	2.21	0.41
2:N:545:GLN:O	2:N:549:ILE:HG12	2.21	0.40
2:N:627:GLN:HE22	4:Q:433:GLU:N	2.17	0.40
2:O:186:ASP:OD1	2:O:187:VAL:N	2.55	0.40
2:O:424:GLN:NE2	2:O:435:GLU:HG2	2.36	0.40
3:P:422:TYR:O	3:P:426:LEU:HG	2.21	0.40
8:V:237:LEU:HB2	8:V:241:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:556:ILE:HG22	8:V:557:GLU:H	1.86	0.40
1:K:368:LEU:O	1:K:369:TYR:C	2.65	0.40
2:N:347:LEU:HD11	2:N:357:PHE:HB3	2.04	0.40
3:P:142:TYR:HE1	3:P:382:ASP:HA	1.86	0.40
3:P:165:LEU:HD21	3:P:274:PHE:CZ	2.56	0.40
4:Q:18:ILE:HD12	4:Q:18:ILE:HA	1.92	0.40
4:Q:453:ASP:HA	4:Q:456:VAL:CG1	2.51	0.40
5:R:484:MET:H	5:R:484:MET:HG2	1.75	0.40
8:V:205:LEU:HD22	8:V:241:VAL:HG13	2.03	0.40
2:N:278:GLU:OE1	2:N:278:GLU:N	2.55	0.40
3:P:224:PHE:CD1	3:P:288:LEU:HB3	2.56	0.40
3:P:425:THR:O	3:P:429:ILE:HG12	2.21	0.40
3:P:467:TRP:CE2	4:Q:318:LEU:HD22	2.56	0.40
8:V:119:ILE:H	8:V:119:ILE:HG12	1.70	0.40
2:N:609:ARG:HH12	4:Q:412:LYS:CE	2.34	0.40
2:N:639:GLU:HA	2:N:642:PHE:CE2	2.56	0.40
3:P:114:LEU:HA	3:P:117:VAL:HG12	2.02	0.40
3:P:424:THR:O	3:P:427:LYS:N	2.54	0.40
3:P:452:PHE:CD2	5:R:428:GLN:CG	2.99	0.40
4:Q:179:PHE:CE2	4:Q:183:LEU:HD21	2.56	0.40
7:T:349:GLU:H	7:T:349:GLU:HG2	1.70	0.40
7:T:468:MET:CE	7:T:494:GLU:HG3	2.51	0.40
8:V:92:ARG:HA	8:V:92:ARG:HD2	1.96	0.40
9:U:964:VAL:HA	9:U:967:ASP:OD2	2.22	0.40
3:P:174:ASP:OD1	3:P:174:ASP:N	2.54	0.40
3:P:297:PHE:N	3:P:297:PHE:CD2	2.89	0.40
3:P:481:GLU:OE1	3:P:484:ARG:NH1	2.54	0.40
3:P:534:GLN:OE1	3:P:534:GLN:HA	2.21	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	K	153/1595 (10%)	140 (92%)	13 (8%)	0	100	100
2	N	470/694 (68%)	450 (96%)	20 (4%)	0	100	100
2	O	346/694 (50%)	333 (96%)	13 (4%)	0	100	100
3	P	362/547 (66%)	339 (94%)	23 (6%)	0	100	100
4	Q	330/769 (43%)	316 (96%)	14 (4%)	0	100	100
5	R	405/763 (53%)	395 (98%)	10 (2%)	0	100	100
6	S	389/607 (64%)	375 (96%)	14 (4%)	0	100	100
7	T	187/534 (35%)	178 (95%)	9 (5%)	0	100	100
8	V	395/990 (40%)	366 (93%)	29 (7%)	0	100	100
9	U	148/991 (15%)	136 (92%)	12 (8%)	0	100	100
All	All	3185/8184 (39%)	3028 (95%)	157 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	K	135/1356 (10%)	134 (99%)	1 (1%)	76	80
2	N	398/562 (71%)	396 (100%)	2 (0%)	81	83
2	O	312/562 (56%)	312 (100%)	0	100	100
3	P	330/462 (71%)	328 (99%)	2 (1%)	78	81
4	Q	290/598 (48%)	290 (100%)	0	100	100
5	R	358/655 (55%)	357 (100%)	1 (0%)	86	86
6	S	341/493 (69%)	340 (100%)	1 (0%)	86	86
7	T	165/457 (36%)	165 (100%)	0	100	100
8	V	331/836 (40%)	329 (99%)	2 (1%)	78	81
9	U	102/861 (12%)	102 (100%)	0	100	100
All	All	2762/6842 (40%)	2753 (100%)	9 (0%)	84	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	366	LEU
2	N	203	ILE
2	N	605	LEU
3	P	68	ARG
3	P	361	GLU
5	R	435	GLU
6	S	583	LYS
8	V	539	VAL
8	V	542	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	173	GLN
1	K	175	GLN
1	K	323	ASN
1	K	338	ASN
2	N	215	HIS
2	N	280	ASN
2	N	284	ASN
2	N	287	ASN
2	N	319	ASN
2	N	371	ASN
2	N	627	GLN
2	N	673	GLN
2	O	204	ASN
2	O	610	GLN
2	O	632	GLN
4	Q	9	ASN
4	Q	19	HIS
4	Q	147	ASN
4	Q	152	HIS
4	Q	323	GLN
5	R	364	GLN
5	R	392	HIS
5	R	424	ASN
5	R	907	ASN
6	S	348	GLN
6	S	365	HIS
6	S	466	ASN
7	T	495	ASN

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Mol	Chain	Res	Type
8	V	125	GLN
8	V	460	GLN
8	V	483	ASN
9	U	906	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

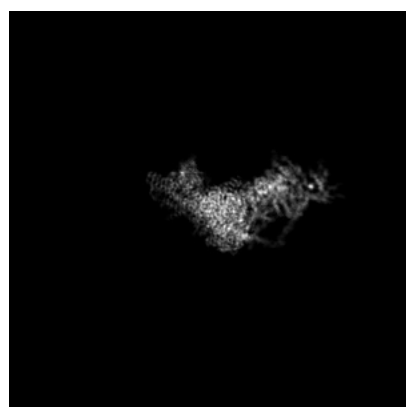
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68865. These allow visual inspection of the internal detail of the map and identification of artifacts.

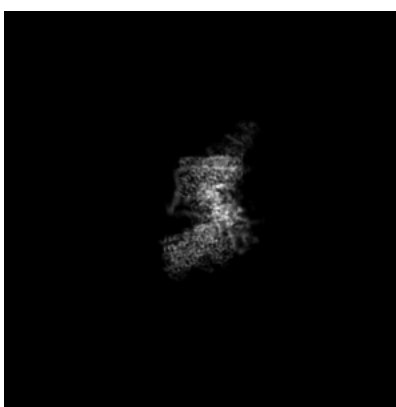
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

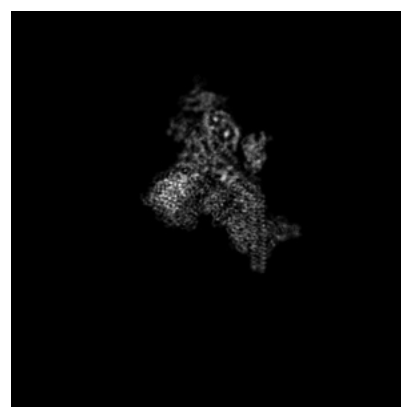
6.1.1 Primary map



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: 242



Y Index: 214

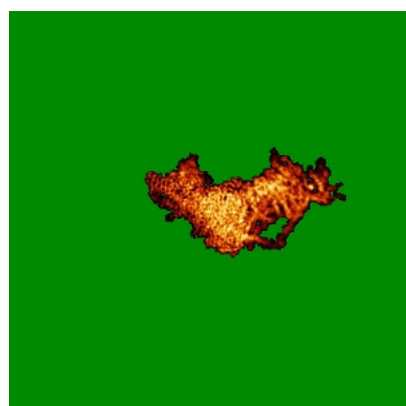


Z Index: 212

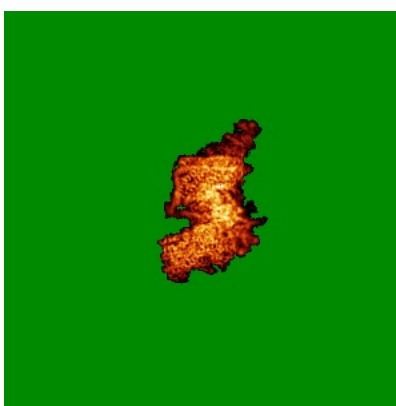
The images above show the largest variance slices of the map in three orthogonal directions.

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

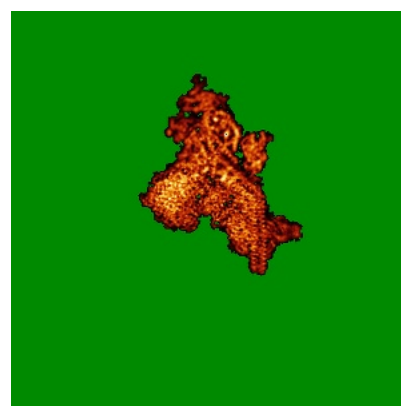
6.4.1 Primary map



X



Y

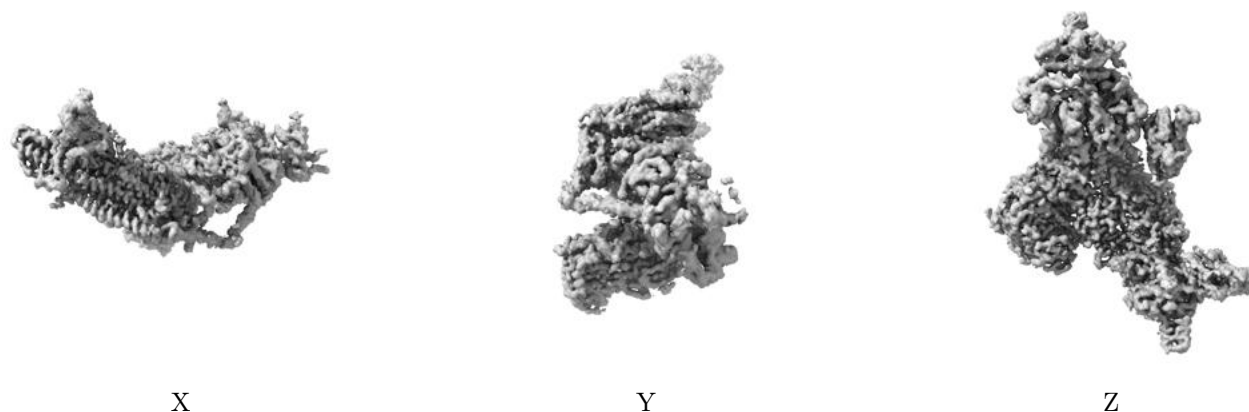


Z

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 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

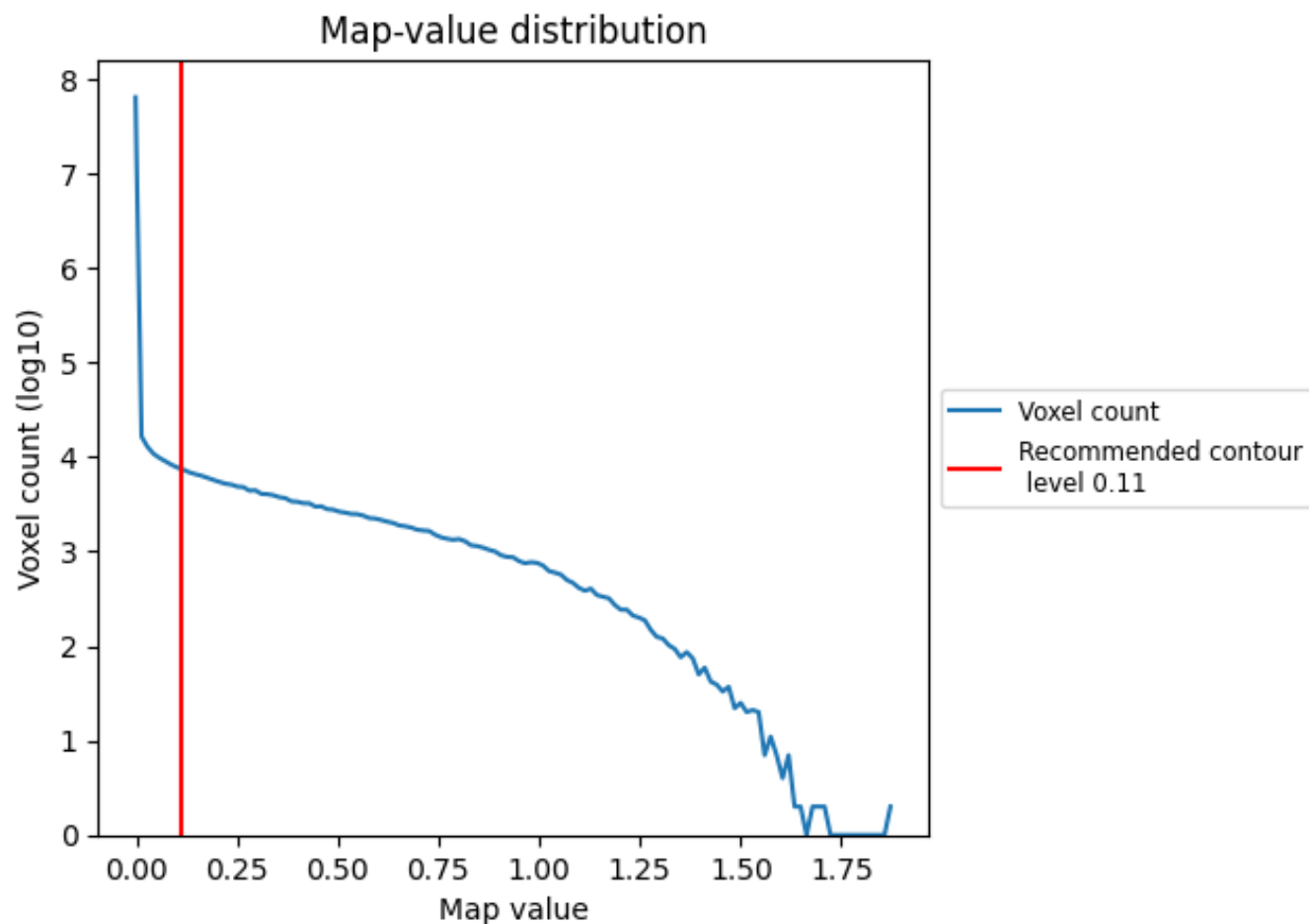
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

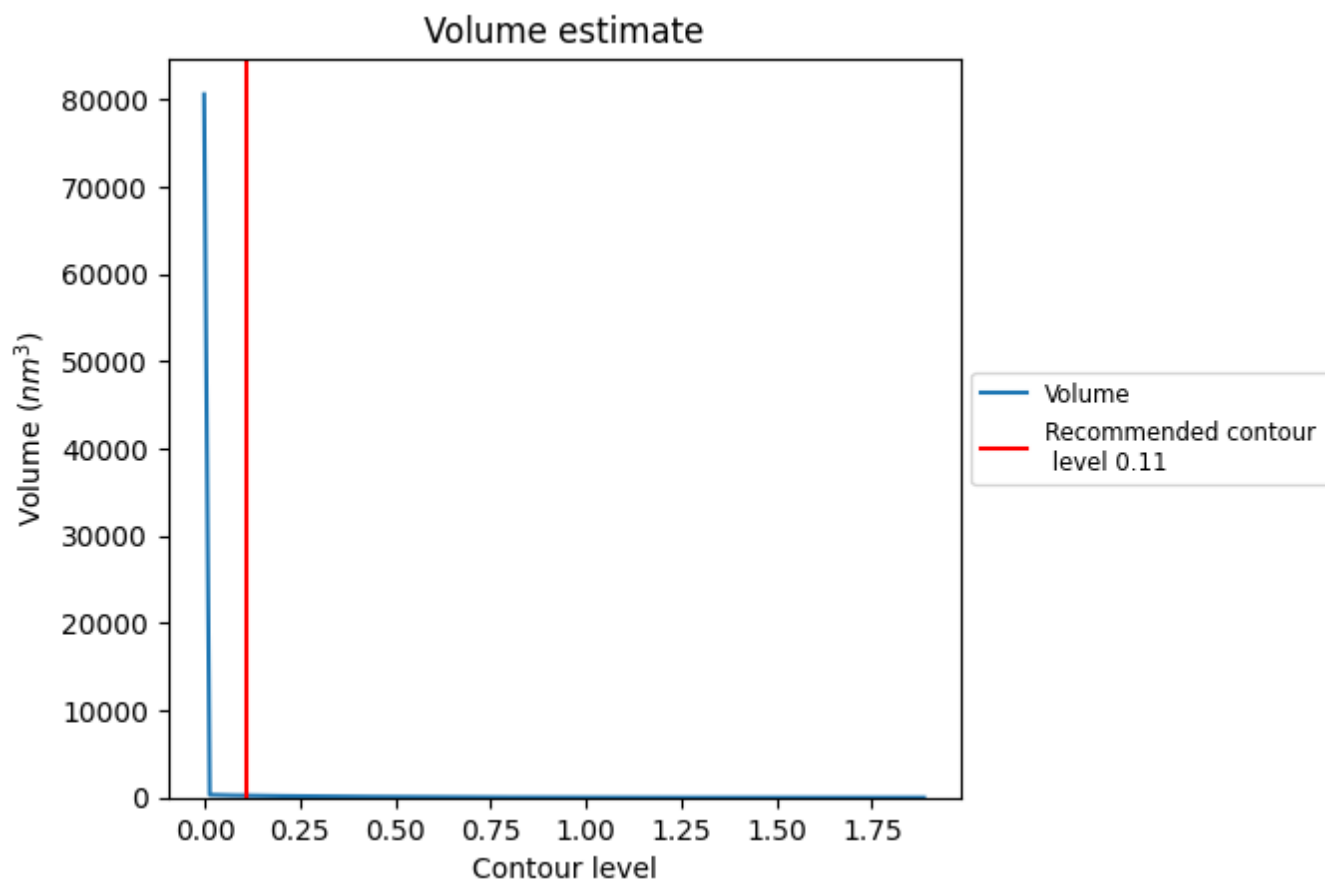
This section contains the results of statistical analysis of the map.

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.

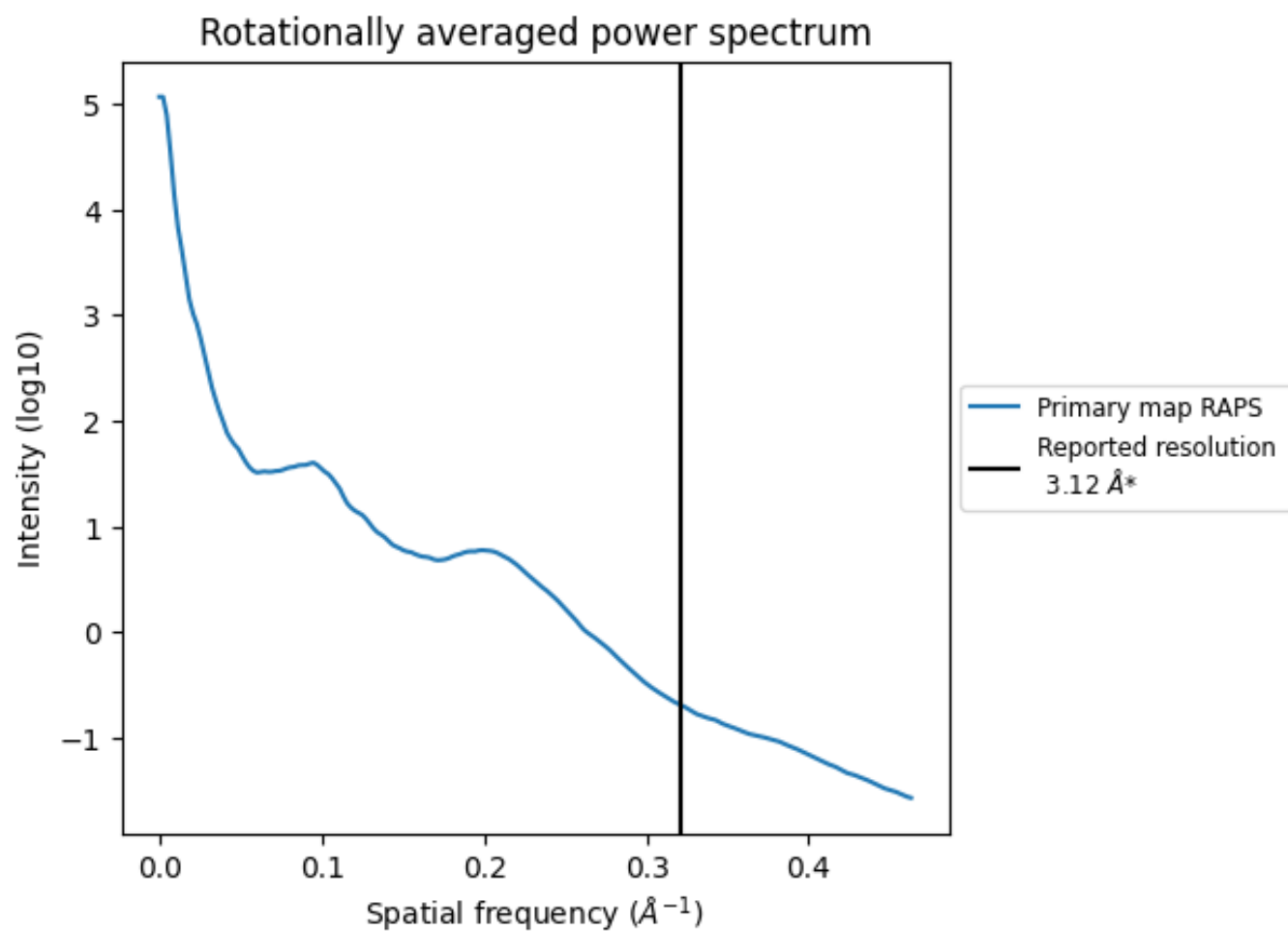
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm³; this corresponds to an approximate mass of 208 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 0.321 $\text{\AA}^{-1}$

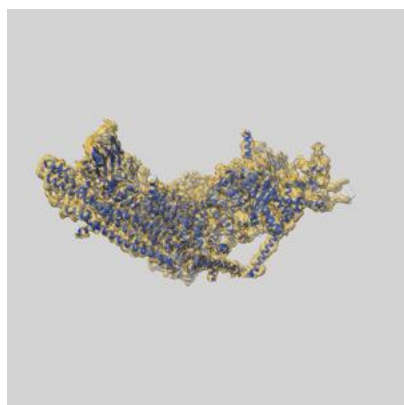
8 Fourier-Shell correlation ⓘ

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

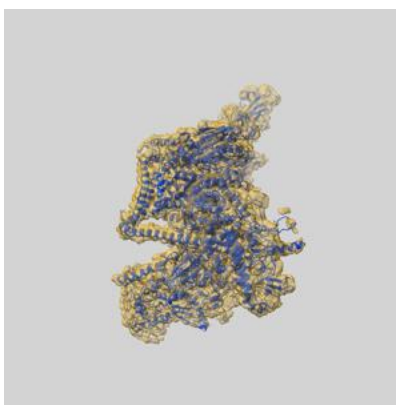
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68865 and PDB model 23CP. Per-residue inclusion information can be found in section [3](#) on page [10](#).

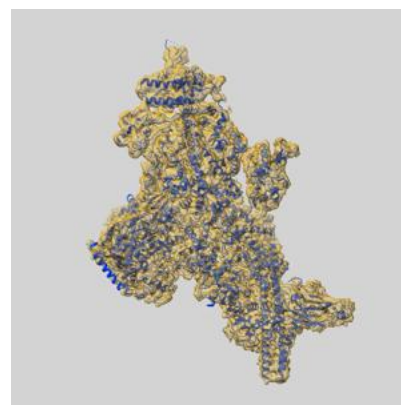
9.1 Map-model overlay [i](#)



X



Y



Z

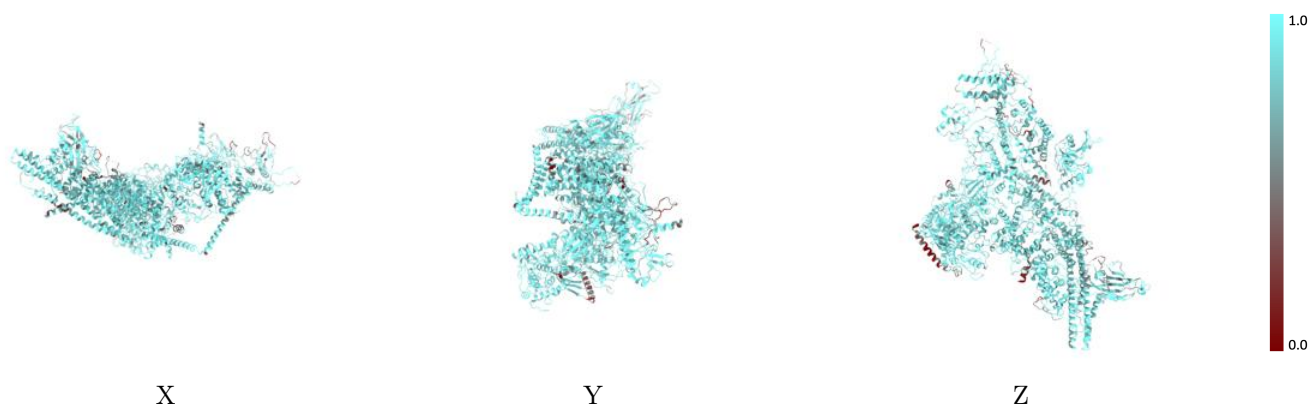
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



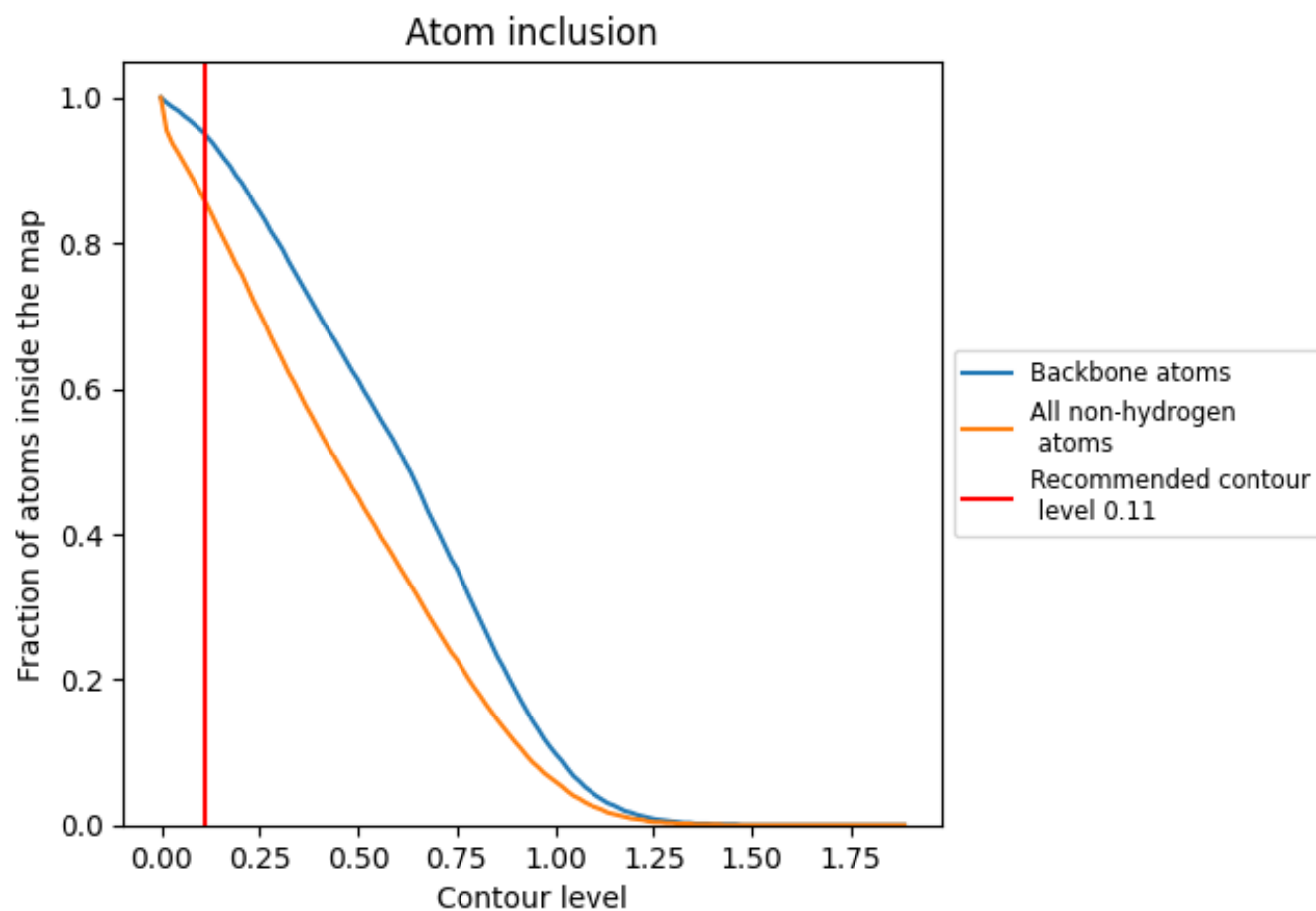
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.3930
K	0.7990	0.3260
N	0.8870	0.4190
O	0.8500	0.3820
P	0.8110	0.3750
Q	0.8620	0.3370
R	0.9190	0.4990
S	0.8560	0.4650
T	0.9360	0.4720
U	0.8500	0.2410
V	0.8100	0.2990

1.0

0.0

<0.0