



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:40 AM UTC

PDB ID : 6D7T / pdb_00006d7t
EMDB ID : EMD-7825
Title : Cryo-EM structure of human TRPV6-Y467A in complex with 2-Aminoethoxy
ydiphenyl borate (2-APB)
Authors : Singh, A.K.; Saotome, K.; McGoldrick, L.L.; Sobolevsky, A.I.
Deposited on : 2018-04-25
Resolution : 4.44 Å(reported)

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

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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
Mogul : 2022.3.0, CSD as543be (2022)
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

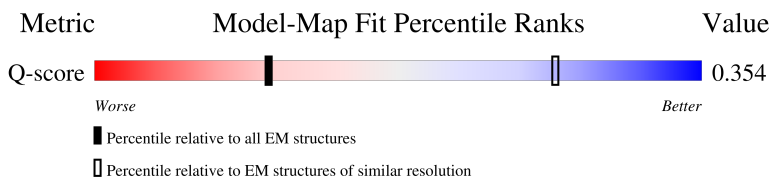
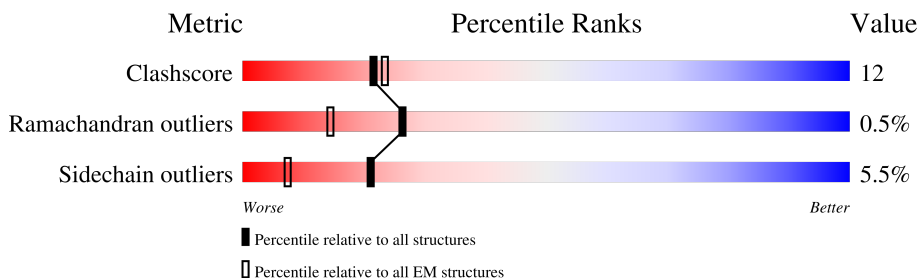
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.44 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	3025 (3.95 - 4.94)

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	742	
1	B	742	
1	C	742	
1	D	742	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19654 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 Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	611	Total	C	N	O	S	0	0
			4896	3162	830	864	40		
1	B	611	Total	C	N	O	S	0	0
			4896	3162	830	864	40		
1	C	611	Total	C	N	O	S	0	0
			4896	3162	830	864	40		
1	D	611	Total	C	N	O	S	0	0
			4896	3162	830	864	40		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	ALA	TYR	engineered mutation	UNP Q9H1D0
A	726	LEU	-	expression tag	UNP Q9H1D0
A	727	VAL	-	expression tag	UNP Q9H1D0
A	728	PRO	-	expression tag	UNP Q9H1D0
A	729	ARG	-	expression tag	UNP Q9H1D0
A	730	GLY	-	expression tag	UNP Q9H1D0
A	731	SER	-	expression tag	UNP Q9H1D0
A	732	ALA	-	expression tag	UNP Q9H1D0
A	733	ALA	-	expression tag	UNP Q9H1D0
A	734	ALA	-	expression tag	UNP Q9H1D0
A	735	TRP	-	expression tag	UNP Q9H1D0
A	736	SER	-	expression tag	UNP Q9H1D0
A	737	HIS	-	expression tag	UNP Q9H1D0
A	738	PRO	-	expression tag	UNP Q9H1D0
A	739	GLN	-	expression tag	UNP Q9H1D0
A	740	PHE	-	expression tag	UNP Q9H1D0
A	741	GLU	-	expression tag	UNP Q9H1D0
A	742	LYS	-	expression tag	UNP Q9H1D0
B	467	ALA	TYR	engineered mutation	UNP Q9H1D0
B	726	LEU	-	expression tag	UNP Q9H1D0
B	727	VAL	-	expression tag	UNP Q9H1D0

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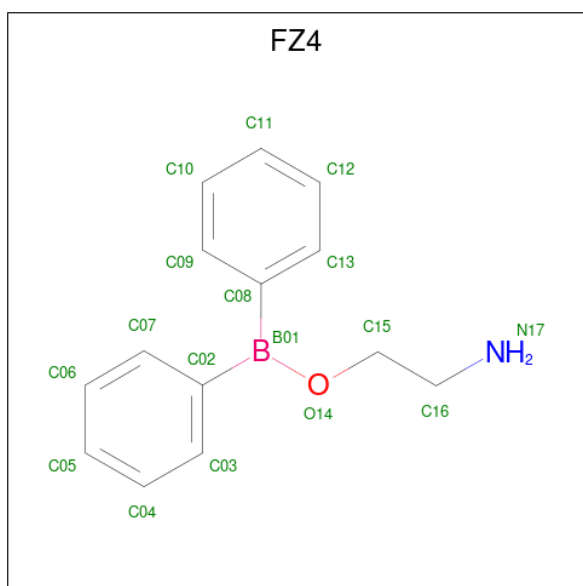
Chain	Residue	Modelled	Actual	Comment	Reference
B	728	PRO	-	expression tag	UNP Q9H1D0
B	729	ARG	-	expression tag	UNP Q9H1D0
B	730	GLY	-	expression tag	UNP Q9H1D0
B	731	SER	-	expression tag	UNP Q9H1D0
B	732	ALA	-	expression tag	UNP Q9H1D0
B	733	ALA	-	expression tag	UNP Q9H1D0
B	734	ALA	-	expression tag	UNP Q9H1D0
B	735	TRP	-	expression tag	UNP Q9H1D0
B	736	SER	-	expression tag	UNP Q9H1D0
B	737	HIS	-	expression tag	UNP Q9H1D0
B	738	PRO	-	expression tag	UNP Q9H1D0
B	739	GLN	-	expression tag	UNP Q9H1D0
B	740	PHE	-	expression tag	UNP Q9H1D0
B	741	GLU	-	expression tag	UNP Q9H1D0
B	742	LYS	-	expression tag	UNP Q9H1D0
C	467	ALA	TYR	engineered mutation	UNP Q9H1D0
C	726	LEU	-	expression tag	UNP Q9H1D0
C	727	VAL	-	expression tag	UNP Q9H1D0
C	728	PRO	-	expression tag	UNP Q9H1D0
C	729	ARG	-	expression tag	UNP Q9H1D0
C	730	GLY	-	expression tag	UNP Q9H1D0
C	731	SER	-	expression tag	UNP Q9H1D0
C	732	ALA	-	expression tag	UNP Q9H1D0
C	733	ALA	-	expression tag	UNP Q9H1D0
C	734	ALA	-	expression tag	UNP Q9H1D0
C	735	TRP	-	expression tag	UNP Q9H1D0
C	736	SER	-	expression tag	UNP Q9H1D0
C	737	HIS	-	expression tag	UNP Q9H1D0
C	738	PRO	-	expression tag	UNP Q9H1D0
C	739	GLN	-	expression tag	UNP Q9H1D0
C	740	PHE	-	expression tag	UNP Q9H1D0
C	741	GLU	-	expression tag	UNP Q9H1D0
C	742	LYS	-	expression tag	UNP Q9H1D0
D	467	ALA	TYR	engineered mutation	UNP Q9H1D0
D	726	LEU	-	expression tag	UNP Q9H1D0
D	727	VAL	-	expression tag	UNP Q9H1D0
D	728	PRO	-	expression tag	UNP Q9H1D0
D	729	ARG	-	expression tag	UNP Q9H1D0
D	730	GLY	-	expression tag	UNP Q9H1D0
D	731	SER	-	expression tag	UNP Q9H1D0
D	732	ALA	-	expression tag	UNP Q9H1D0
D	733	ALA	-	expression tag	UNP Q9H1D0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	734	ALA	-	expression tag	UNP Q9H1D0
D	735	TRP	-	expression tag	UNP Q9H1D0
D	736	SER	-	expression tag	UNP Q9H1D0
D	737	HIS	-	expression tag	UNP Q9H1D0
D	738	PRO	-	expression tag	UNP Q9H1D0
D	739	GLN	-	expression tag	UNP Q9H1D0
D	740	PHE	-	expression tag	UNP Q9H1D0
D	741	GLU	-	expression tag	UNP Q9H1D0
D	742	LYS	-	expression tag	UNP Q9H1D0

- Molecule 2 is 2-aminoethyl diphenylborinate (CCD ID: FZ4) (formula: C₁₄H₁₆BNO).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	B	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	C	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	D	1	Total	B	C	N	O	0
			17	1	14	1	1	

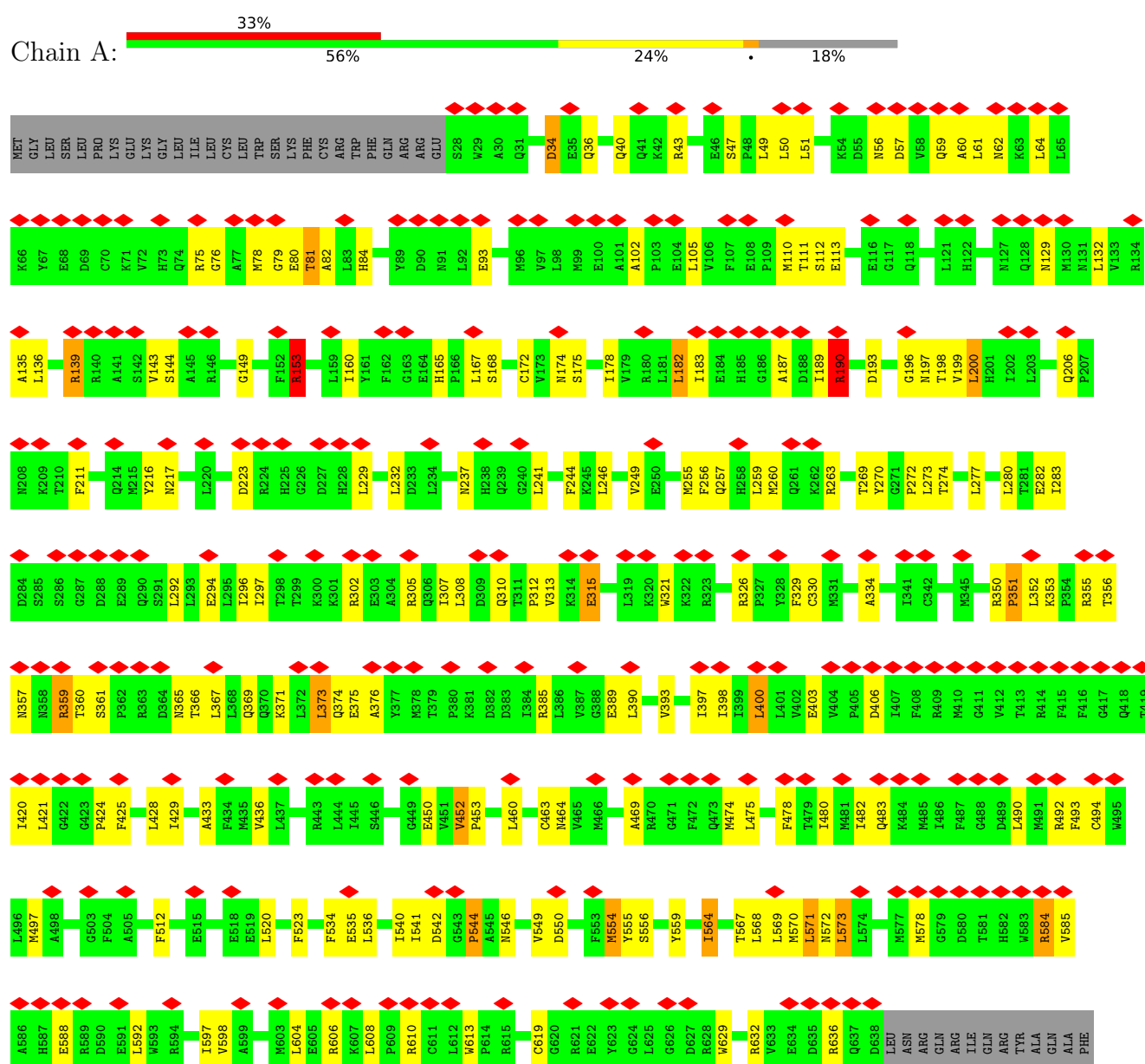
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

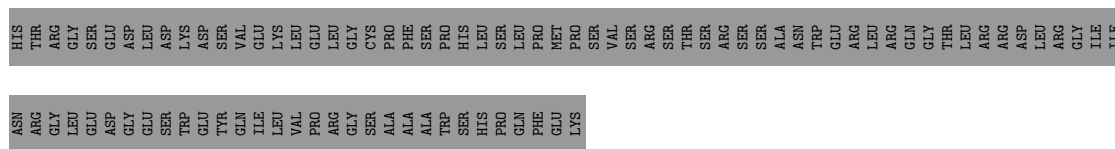
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	

3 Residue-property plots

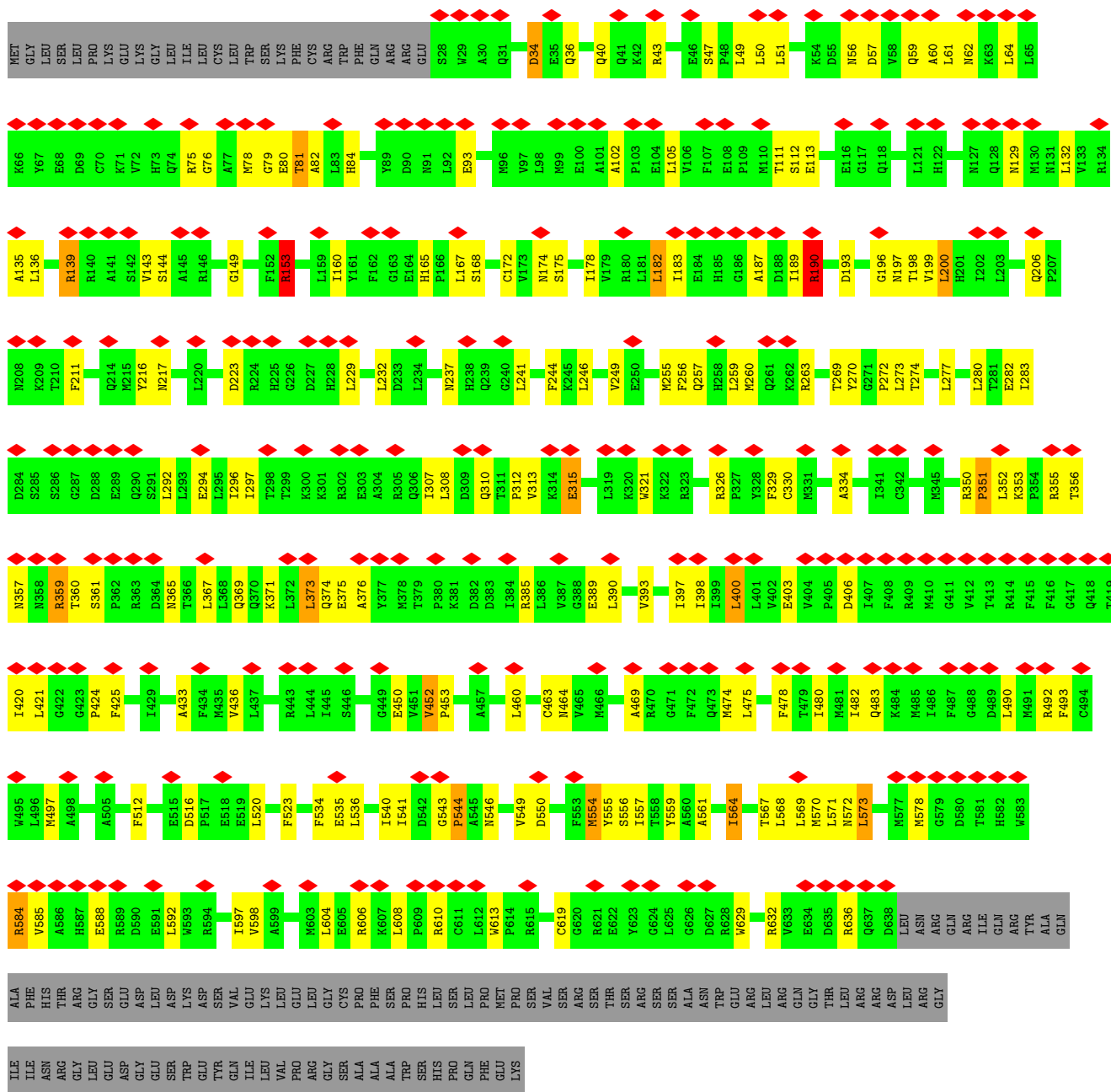
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transient receptor potential cation channel subfamily V member 6



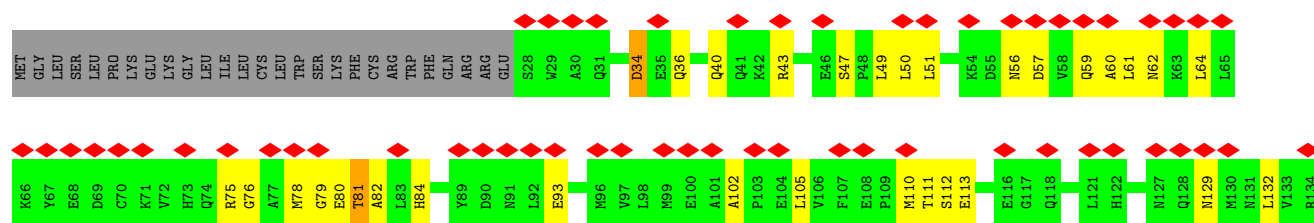


- Molecule 1: Transient receptor potential cation channel subfamily V member 6



- Molecule 1: Transient receptor potential cation channel subfamily V member 6





SER	GLU	ASP	GLY	LEU	ASP	ASP	ASP	ASP	SER	SER	VAL	GLN	ILE	LEU	VAL	PRO	GLU	LEU	LEU	GLY	CYS	PRO	PHE	ALA	ALA	ALA	TRP	HIS	SER	HIS	PRO	PRO	GLN	PHE	GLU	LYS																						
D590	E591	L592	W593	R594	I597	V598	A599	M603	L604	E605	R606	R607	L608	P609	R610	C611	L612	W613	P614	R615	C619	G620	R621	E622	W623	G624	L625	G626	D627	R628	W629	R632	V633	E634	D635	G636	Q637	D638	LEU	ASN	ARG	GLN	ARG	GLY	ILE	ILE	ASN	ARG	ARG	GLY	ALA	GLN	ALA	PHE	HIS	THR	ARG	GLY
G503	F512	E515	E518	E519	G520	G521	L522	W523	F534	E535	L536	I540	I541	D542	G543	P544	A545	N546	V549	D550	F553	W554	W555	S556	Y559	I564	W567	L568	L569	M570	N571	N572	L573	L574	L575	A576	W577	M578	G579	D580	W581	H582	W583	R584	V585	A586	H587	E588	W589									
P424	F425	L428	I429	A433	F434	M435	V436	L437	R443	L444	I445	S446	G449	E450	V451	V452	P453	L460	C463	N464	V465	M466	A469	R470	G471	F472	Q473	M474	L475	F478	T479	I480	M481	I482	Q483	K484	M485	I486	F487	G488	D489	L490	M491	R492	F493	C494	V495	M497	A498									
R359	T360	S361	P362	R363	D364	N365	T366	L367	Q368	Q369	K371	L372	L373	Q374	E375	A376	Y377	M378	D382	D383	I384	R385	L386	V387	G388	E389	L390	V393	I397	I398	I399	L400	L401	V402	E403	V404	P405	D406	I407	F408	R409	M410	G411	V412	T413	R414	F415	F416	G417	Q418	T419	I420	L421	G422	G423			
N208	K209	T210	F211	Q214	M215	Y216	N217	D223	R224	H225	G226	D227	H228	L229	L232	D233	Y234	L234	N237	H238	Q239	G240	L241	F244	K245	L246	V249	E250	M255	F256	Q257	H258	L259	M260	Q261	K262	R263	T269	Y270	G271	P272	L273	T274	L277	L280	T281	E282	I283	D284	S285								
A135	L136	R139	R140	A141	S142	V143	S144	A145	R146	G149	F152	R153	L159	I160	Y161	F162	G163	E164	H165	P166	L167	S168	C172	V173	M174	S175	I178	V179	R180	L181	L182	I183	E184	H185	G186	A187	D188	I189	R190	D193	G196	N197	T198	V199	L200	H201	I202	L203	Q206	P207								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0669	Depositor
Map size ($\text{\AA}$)	248.88, 248.88, 248.88	wwPDB
Map dimensions	204, 204, 204	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.22, 1.22, 1.22	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FZ4, CA

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	0.47	2/5008 (0.0%)	0.86	13/6795 (0.2%)
1	B	0.47	2/5008 (0.0%)	0.86	13/6795 (0.2%)
1	C	0.49	2/5008 (0.0%)	0.85	11/6795 (0.2%)
1	D	0.68	3/5008 (0.1%)	0.89	17/6795 (0.3%)
All	All	0.54	9/20032 (0.0%)	0.87	54/27180 (0.2%)

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	3
1	B	0	3
1	C	0	4
1	D	0	4
All	All	0	14

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	544	PRO	C-N	32.19	1.73	1.33
1	D	540	ILE	C-N	17.08	1.55	1.34
1	C	540	ILE	C-N	-13.26	1.10	1.33
1	A	540	ILE	C-N	10.28	1.51	1.33
1	B	540	ILE	C-N	10.28	1.51	1.33
1	A	361	SER	C-N	5.36	1.39	1.33
1	C	361	SER	C-N	5.30	1.39	1.33
1	B	361	SER	C-N	5.28	1.39	1.33
1	D	361	SER	C-N	5.23	1.39	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	544	PRO	O-C-N	-11.76	110.57	123.03
1	D	540	ILE	CA-C-N	-11.07	102.63	120.13
1	D	540	ILE	C-N-CA	-11.07	102.63	120.13
1	D	540	ILE	O-C-N	7.95	132.50	122.57
1	A	153	ARG	CG-CD-NE	6.98	127.36	112.00
1	B	153	ARG	CG-CD-NE	6.98	127.35	112.00
1	D	153	ARG	CG-CD-NE	6.97	127.34	112.00
1	C	153	ARG	CG-CD-NE	6.95	127.29	112.00
1	B	190	ARG	NE-CZ-NH2	6.94	125.44	119.20
1	D	190	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	A	190	ARG	NE-CZ-NH2	6.91	125.41	119.20
1	C	190	ARG	NE-CZ-NH2	6.91	125.41	119.20
1	B	588	GLU	N-CA-C	6.52	118.77	110.61
1	D	588	GLU	N-CA-C	6.52	118.77	110.61
1	C	588	GLU	N-CA-C	6.52	118.76	110.61
1	A	588	GLU	N-CA-C	6.49	118.73	110.61
1	B	544	PRO	O-C-N	5.97	129.79	123.10
1	B	544	PRO	CA-C-N	-5.97	110.14	121.54
1	B	544	PRO	C-N-CA	-5.97	110.14	121.54
1	A	544	PRO	CA-C-N	-5.96	110.16	121.54
1	A	544	PRO	C-N-CA	-5.96	110.16	121.54
1	A	544	PRO	O-C-N	5.94	129.75	123.10
1	B	112	SER	CA-C-N	5.87	132.76	121.54
1	B	112	SER	C-N-CA	5.87	132.76	121.54
1	D	112	SER	CA-C-N	5.86	132.74	121.54
1	D	112	SER	C-N-CA	5.86	132.74	121.54
1	C	112	SER	CA-C-N	5.86	132.73	121.54
1	C	112	SER	C-N-CA	5.86	132.73	121.54
1	A	112	SER	CA-C-N	5.84	132.69	121.54
1	A	112	SER	C-N-CA	5.84	132.69	121.54
1	C	190	ARG	CD-NE-CZ	5.76	132.46	124.40
1	A	190	ARG	CD-NE-CZ	5.74	132.44	124.40
1	B	190	ARG	CD-NE-CZ	5.72	132.40	124.40
1	D	190	ARG	CD-NE-CZ	5.72	132.40	124.40
1	D	190	ARG	CG-CD-NE	5.58	124.28	112.00
1	B	190	ARG	CG-CD-NE	5.58	124.28	112.00
1	A	190	ARG	CG-CD-NE	5.56	124.22	112.00
1	C	190	ARG	CG-CD-NE	5.55	124.20	112.00
1	A	584	ARG	CA-C-N	5.39	131.68	121.97
1	A	584	ARG	C-N-CA	5.39	131.68	121.97
1	D	584	ARG	CA-C-N	5.39	131.67	121.97
1	D	584	ARG	C-N-CA	5.39	131.67	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	584	ARG	CA-C-N	5.38	131.65	121.97
1	B	584	ARG	C-N-CA	5.38	131.65	121.97
1	C	584	ARG	CA-C-N	5.38	131.65	121.97
1	C	584	ARG	C-N-CA	5.38	131.65	121.97
1	B	315	GLU	CA-CB-CG	5.23	124.56	114.10
1	D	315	GLU	CA-CB-CG	5.23	124.56	114.10
1	A	315	GLU	CA-CB-CG	5.23	124.56	114.10
1	C	315	GLU	CA-CB-CG	5.22	124.53	114.10
1	D	544	PRO	CA-C-N	5.13	129.89	121.58
1	D	544	PRO	C-N-CA	5.13	129.89	121.58
1	D	372	LEU	CA-CB-CG	5.01	133.84	116.30
1	C	372	LEU	CA-CB-CG	5.00	133.80	116.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASN	Peptide
1	A	223	ASP	Peptide
1	A	351	PRO	Peptide
1	B	129	ASN	Peptide
1	B	223	ASP	Peptide
1	B	351	PRO	Peptide
1	C	129	ASN	Peptide
1	C	223	ASP	Peptide
1	C	351	PRO	Peptide
1	C	544	PRO	Mainchain
1	D	129	ASN	Peptide
1	D	223	ASP	Peptide
1	D	351	PRO	Peptide
1	D	540	ILE	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4896	0	4954	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4896	0	4954	119	0
1	C	4896	0	4953	129	0
1	D	4896	0	4953	134	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
2	C	17	0	0	0	0
2	D	17	0	0	0	0
3	A	2	0	0	0	0
All	All	19654	0	19814	463	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 (463) 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:D:544:PRO:C	1:D:545:ALA:N	1.73	1.46
1:D:535:GLU:OE1	1:D:541:ILE:HB	1.54	1.06
1:D:535:GLU:CD	1:D:541:ILE:HB	1.93	0.93
1:B:535:GLU:HG3	1:C:559:TYR:HE2	1.58	0.68
1:A:535:GLU:HG3	1:B:559:TYR:HE2	1.58	0.68
1:D:535:GLU:OE2	1:D:541:ILE:N	2.27	0.68
1:A:374:GLN:HG3	1:A:375:GLU:HG2	1.76	0.68
1:C:40:GLN:NE2	1:C:78:MET:SD	2.66	0.68
1:A:40:GLN:NE2	1:A:78:MET:SD	2.66	0.68
1:D:40:GLN:NE2	1:D:78:MET:SD	2.66	0.68
1:D:263:ARG:NH2	1:D:282:GLU:OE2	2.28	0.67
1:A:263:ARG:NH2	1:A:282:GLU:OE2	2.28	0.67
1:B:578:MET:HG3	1:C:578:MET:HE1	1.76	0.67
1:D:374:GLN:HG3	1:D:375:GLU:HG2	1.76	0.67
1:A:559:TYR:HE2	1:D:535:GLU:HG3	1.59	0.67
1:B:40:GLN:NE2	1:B:78:MET:SD	2.66	0.67
1:D:57:ASP:HB3	1:D:60:ALA:HB3	1.77	0.67
1:B:263:ARG:NH2	1:B:282:GLU:OE2	2.27	0.66
1:C:263:ARG:NH2	1:C:282:GLU:OE2	2.28	0.66
1:A:57:ASP:HB3	1:A:60:ALA:HB3	1.77	0.66
1:A:578:MET:HG3	1:B:578:MET:HE1	1.78	0.66
1:C:57:ASP:HB3	1:C:60:ALA:HB3	1.77	0.66
1:B:56:ASN:ND2	1:B:93:GLU:OE2	2.29	0.66
1:B:374:GLN:HG3	1:B:375:GLU:HG2	1.76	0.65
1:C:535:GLU:HG3	1:D:559:TYR:HE2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:MET:HE1	1:D:578:MET:HG3	1.79	0.65
1:C:374:GLN:HG3	1:C:375:GLU:HG2	1.76	0.65
1:D:56:ASN:ND2	1:D:93:GLU:OE2	2.30	0.65
1:A:56:ASN:ND2	1:A:93:GLU:OE2	2.29	0.65
1:B:57:ASP:HB3	1:B:60:ALA:HB3	1.77	0.65
1:C:578:MET:HG3	1:D:578:MET:HE1	1.79	0.65
1:C:56:ASN:ND2	1:C:93:GLU:OE2	2.30	0.64
1:C:353:LYS:HB3	1:C:373:LEU:HG	1.80	0.64
1:C:360:THR:HG1	1:C:366:THR:HG1	1.46	0.63
1:B:353:LYS:HB3	1:B:373:LEU:HG	1.80	0.63
1:D:149:GLY:O	1:D:153:ARG:NH2	2.32	0.63
1:D:175:SER:HB3	1:D:178:ILE:HD13	1.80	0.63
1:B:175:SER:HB3	1:B:178:ILE:HD13	1.80	0.63
1:C:149:GLY:O	1:C:153:ARG:NH2	2.32	0.62
1:B:149:GLY:O	1:B:153:ARG:NH2	2.32	0.62
1:B:297:ILE:HD11	1:B:598:VAL:HG23	1.81	0.62
1:C:175:SER:HB3	1:C:178:ILE:HD13	1.80	0.62
1:A:149:GLY:O	1:A:153:ARG:NH2	2.32	0.62
1:A:297:ILE:HD11	1:A:598:VAL:HG23	1.82	0.62
1:A:353:LYS:HB3	1:A:373:LEU:HG	1.80	0.62
1:C:297:ILE:HD11	1:C:598:VAL:HG23	1.82	0.62
1:D:353:LYS:HB3	1:D:373:LEU:HG	1.80	0.62
1:D:297:ILE:HD11	1:D:598:VAL:HG23	1.81	0.62
1:B:490:LEU:HD13	1:C:568:LEU:HD12	1.82	0.62
1:C:353:LYS:NZ	1:C:356:THR:OG1	2.33	0.62
1:A:175:SER:HB3	1:A:178:ILE:HD13	1.80	0.61
1:B:353:LYS:NZ	1:B:356:THR:OG1	2.33	0.61
1:D:353:LYS:NZ	1:D:356:THR:OG1	2.33	0.61
1:C:554:MET:SD	1:C:554:MET:N	2.74	0.60
1:A:36:GLN:NE2	1:A:113:GLU:OE2	2.35	0.60
1:B:554:MET:SD	1:B:554:MET:N	2.74	0.60
1:C:277:LEU:HD23	1:C:632:ARG:HB3	1.84	0.60
1:B:36:GLN:NE2	1:B:113:GLU:OE2	2.35	0.60
1:D:277:LEU:HD23	1:D:632:ARG:HB3	1.84	0.60
1:A:554:MET:SD	1:A:554:MET:N	2.74	0.60
1:A:353:LYS:NZ	1:A:356:THR:OG1	2.33	0.59
1:B:478:PHE:O	1:B:482:ILE:N	2.35	0.59
1:C:190:ARG:HG3	1:C:232:LEU:HD12	1.85	0.59
1:D:478:PHE:O	1:D:482:ILE:N	2.35	0.59
1:D:522:HIS:ND1	1:D:544:PRO:HB3	2.16	0.59
1:C:452:VAL:HB	1:D:554:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ARG:HG3	1:D:232:LEU:HD12	1.85	0.59
1:C:36:GLN:NE2	1:C:113:GLU:OE2	2.35	0.59
1:D:36:GLN:NE2	1:D:113:GLU:OE2	2.35	0.59
1:D:554:MET:N	1:D:554:MET:SD	2.74	0.59
1:B:280:LEU:HD12	1:B:283:ILE:HB	1.85	0.59
1:A:280:LEU:HD12	1:A:283:ILE:HB	1.85	0.59
1:B:174:ASN:ND2	1:B:211:PHE:O	2.36	0.59
1:C:280:LEU:HD12	1:C:283:ILE:HB	1.85	0.59
1:D:174:ASN:ND2	1:D:211:PHE:O	2.36	0.59
1:B:76:GLY:H	1:B:80:GLU:H	1.51	0.58
1:C:452:VAL:HG13	1:C:453:PRO:HD3	1.85	0.58
1:A:277:LEU:HD23	1:A:632:ARG:HB3	1.84	0.58
1:B:190:ARG:HG3	1:B:232:LEU:HD12	1.84	0.58
1:C:174:ASN:ND2	1:C:211:PHE:O	2.36	0.58
1:A:174:ASN:ND2	1:A:211:PHE:O	2.36	0.58
1:A:216:TYR:HB2	1:A:255:MET:HE1	1.85	0.58
1:A:490:LEU:HD13	1:B:568:LEU:HD12	1.84	0.58
1:B:452:VAL:HG13	1:B:453:PRO:HD3	1.85	0.58
1:A:190:ARG:HG3	1:A:232:LEU:HD12	1.85	0.58
1:B:277:LEU:HD23	1:B:632:ARG:HB3	1.84	0.58
1:A:452:VAL:HG13	1:A:453:PRO:HD3	1.85	0.58
1:C:76:GLY:H	1:C:80:GLU:H	1.51	0.58
1:A:549:VAL:HG21	1:D:367:LEU:HD13	1.85	0.58
1:D:280:LEU:HD12	1:D:283:ILE:HB	1.85	0.58
1:D:452:VAL:HG13	1:D:453:PRO:HD3	1.85	0.58
1:D:351:PRO:HB3	1:D:373:LEU:HB2	1.86	0.57
1:A:568:LEU:HD12	1:D:490:LEU:HD13	1.85	0.57
1:A:76:GLY:H	1:A:80:GLU:H	1.51	0.57
1:C:172:CYS:SG	1:C:206:GLN:NE2	2.77	0.57
1:C:478:PHE:O	1:C:482:ILE:N	2.35	0.57
1:A:172:CYS:SG	1:A:206:GLN:NE2	2.77	0.57
1:B:172:CYS:SG	1:B:206:GLN:NE2	2.77	0.57
1:C:216:TYR:HB2	1:C:255:MET:HE1	1.85	0.57
1:D:360:THR:OG1	1:D:366:THR:OG1	2.23	0.57
1:A:478:PHE:O	1:A:482:ILE:N	2.35	0.57
1:C:490:LEU:HD13	1:D:568:LEU:HD12	1.87	0.57
1:D:172:CYS:SG	1:D:206:GLN:NE2	2.77	0.57
1:A:554:MET:HE3	1:D:452:VAL:HB	1.87	0.57
1:B:351:PRO:HB3	1:B:373:LEU:HB2	1.86	0.57
1:D:216:TYR:HB2	1:D:255:MET:HE1	1.85	0.57
1:B:216:TYR:HB2	1:B:255:MET:HE1	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:GLY:H	1:D:80:GLU:H	1.51	0.56
1:A:351:PRO:HB3	1:A:373:LEU:HB2	1.86	0.56
1:C:193:ASP:OD1	1:C:197:ASN:N	2.38	0.56
1:C:351:PRO:HB3	1:C:373:LEU:HB2	1.86	0.56
1:D:272:PRO:HB2	1:D:636:ARG:HG3	1.88	0.56
1:D:546:ASN:HD22	1:D:549:VAL:HG22	1.70	0.56
1:A:272:PRO:HB2	1:A:636:ARG:HG3	1.88	0.56
1:D:536:LEU:HD11	1:D:544:PRO:HD2	1.88	0.56
1:B:193:ASP:OD1	1:B:197:ASN:N	2.38	0.56
1:B:237:ASN:OD1	1:B:241:LEU:N	2.38	0.56
1:B:469:ALA:HB1	1:B:475:LEU:HG	1.88	0.56
1:A:360:THR:OG1	1:A:366:THR:OG1	2.23	0.56
1:D:544:PRO:O	1:D:555:TYR:OH	2.16	0.56
1:A:350:ARG:NH2	1:A:450:GLU:OE1	2.39	0.56
1:A:546:ASN:HD22	1:A:549:VAL:HG22	1.70	0.56
1:B:350:ARG:NH2	1:B:450:GLU:OE1	2.39	0.56
1:A:193:ASP:OD1	1:A:197:ASN:N	2.38	0.56
1:A:469:ALA:HB1	1:A:475:LEU:HG	1.88	0.56
1:B:367:LEU:HD13	1:C:549:VAL:HG21	1.87	0.56
1:D:350:ARG:NH2	1:D:450:GLU:OE1	2.39	0.56
1:A:367:LEU:HD13	1:B:549:VAL:HG21	1.87	0.55
1:B:482:ILE:HD13	1:C:572:ASN:HD22	1.72	0.55
1:C:350:ARG:NH2	1:C:450:GLU:OE1	2.39	0.55
1:D:193:ASP:OD1	1:D:197:ASN:N	2.38	0.55
1:C:81:THR:OG1	1:C:82:ALA:N	2.39	0.55
1:B:452:VAL:HB	1:C:554:MET:HE3	1.89	0.55
1:C:272:PRO:HB2	1:C:636:ARG:HG3	1.88	0.55
1:C:367:LEU:HD13	1:D:549:VAL:HG21	1.87	0.55
1:D:237:ASN:OD1	1:D:241:LEU:N	2.38	0.55
1:A:357:ASN:H	1:A:371:LYS:HZ3	1.55	0.55
1:C:469:ALA:HB1	1:C:475:LEU:HG	1.88	0.55
1:C:546:ASN:HD22	1:C:549:VAL:HG22	1.70	0.55
1:B:272:PRO:HB2	1:B:636:ARG:HG3	1.88	0.54
1:A:452:VAL:HB	1:B:554:MET:HE3	1.88	0.54
1:B:546:ASN:HD22	1:B:549:VAL:HG22	1.70	0.54
1:D:102:ALA:HB1	1:D:105:LEU:HD13	1.90	0.54
1:D:469:ALA:HB1	1:D:475:LEU:HG	1.88	0.54
1:A:81:THR:OG1	1:A:82:ALA:N	2.39	0.54
1:C:237:ASN:OD1	1:C:241:LEU:N	2.38	0.54
1:A:237:ASN:OD1	1:A:241:LEU:N	2.38	0.54
1:A:102:ALA:HB1	1:A:105:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ALA:HB1	1:B:105:LEU:HD13	1.90	0.54
1:A:482:ILE:HD13	1:B:572:ASN:HD22	1.73	0.54
1:C:102:ALA:HB1	1:C:105:LEU:HD13	1.90	0.54
1:C:482:ILE:HD13	1:D:572:ASN:HD22	1.72	0.54
1:A:355:ARG:HH22	1:A:360:THR:HB	1.73	0.53
1:B:355:ARG:HH22	1:B:360:THR:HB	1.73	0.53
1:D:244:PHE:HA	1:D:259:LEU:HD21	1.91	0.53
1:A:572:ASN:HD22	1:D:482:ILE:HD13	1.73	0.53
1:C:355:ARG:HH22	1:C:360:THR:HB	1.73	0.53
1:B:81:THR:OG1	1:B:82:ALA:N	2.39	0.53
1:B:198:THR:HG23	1:B:200:LEU:H	1.74	0.53
1:D:355:ARG:HH22	1:D:360:THR:HB	1.73	0.53
1:B:357:ASN:H	1:B:371:LYS:HZ3	1.55	0.53
1:C:198:THR:HG23	1:C:200:LEU:H	1.74	0.53
1:D:81:THR:OG1	1:D:82:ALA:N	2.39	0.53
1:B:365:ASN:HB2	1:C:550:ASP:H	1.73	0.53
1:C:357:ASN:H	1:C:371:LYS:HZ3	1.55	0.53
1:C:244:PHE:HA	1:C:259:LEU:HD21	1.91	0.52
1:D:198:THR:HG23	1:D:200:LEU:H	1.74	0.52
1:B:257:GLN:NE2	1:B:310:GLN:OE1	2.35	0.52
1:D:143:VAL:HG21	1:D:187:ALA:HA	1.91	0.52
1:A:244:PHE:HA	1:A:259:LEU:HD21	1.91	0.52
1:A:168:SER:HA	1:A:199:VAL:HG23	1.92	0.52
1:A:198:THR:HG23	1:A:200:LEU:H	1.74	0.52
1:A:143:VAL:HG21	1:A:187:ALA:HA	1.91	0.52
1:A:460:LEU:HA	1:A:463:CYS:HB3	1.92	0.52
1:B:143:VAL:HG21	1:B:187:ALA:HA	1.91	0.52
1:D:168:SER:HA	1:D:199:VAL:HG23	1.92	0.52
1:D:512:PHE:HD2	1:D:523:PHE:HD2	1.57	0.52
1:A:326:ARG:HA	1:A:329:PHE:HB3	1.93	0.51
1:B:244:PHE:HA	1:B:259:LEU:HD21	1.91	0.51
1:C:257:GLN:NE2	1:C:310:GLN:OE1	2.35	0.51
1:A:512:PHE:HD2	1:A:523:PHE:HD2	1.57	0.51
1:C:143:VAL:HG21	1:C:187:ALA:HA	1.91	0.51
1:B:460:LEU:HA	1:B:463:CYS:HB3	1.92	0.51
1:C:168:SER:HA	1:C:199:VAL:HG23	1.92	0.51
1:D:357:ASN:H	1:D:371:LYS:HZ3	1.58	0.51
1:A:294:GLU:OE1	1:A:606:ARG:NH2	2.43	0.51
1:A:365:ASN:HB2	1:B:550:ASP:H	1.76	0.51
1:B:326:ARG:HA	1:B:329:PHE:HB3	1.93	0.51
1:D:200:LEU:HD11	1:D:216:TYR:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD11	1:A:216:TYR:HE1	1.76	0.51
1:C:460:LEU:HA	1:C:463:CYS:HB3	1.92	0.51
1:D:294:GLU:OE1	1:D:606:ARG:NH2	2.43	0.51
1:B:294:GLU:OE1	1:B:606:ARG:NH2	2.43	0.51
1:B:168:SER:HA	1:B:199:VAL:HG23	1.92	0.51
1:C:326:ARG:HA	1:C:329:PHE:HB3	1.92	0.51
1:D:40:GLN:NE2	1:D:80:GLU:OE2	2.44	0.50
1:D:535:GLU:OE2	1:D:541:ILE:CA	2.59	0.50
1:B:200:LEU:HD11	1:B:216:TYR:HE1	1.76	0.50
1:B:351:PRO:HD3	1:B:385:ARG:HH12	1.77	0.50
1:B:512:PHE:HD2	1:B:523:PHE:HD2	1.57	0.50
1:C:512:PHE:HD2	1:C:523:PHE:HD2	1.57	0.50
1:D:351:PRO:HD3	1:D:385:ARG:HH12	1.77	0.50
1:A:40:GLN:NE2	1:A:80:GLU:OE2	2.44	0.50
1:B:40:GLN:NE2	1:B:80:GLU:OE2	2.44	0.50
1:C:200:LEU:HD11	1:C:216:TYR:HE1	1.76	0.50
1:D:460:LEU:HA	1:D:463:CYS:HB3	1.92	0.50
1:C:294:GLU:OE1	1:C:606:ARG:NH2	2.43	0.50
1:A:351:PRO:HD3	1:A:385:ARG:HH12	1.77	0.50
1:C:198:THR:OG1	1:C:199:VAL:N	2.45	0.50
1:B:198:THR:OG1	1:B:199:VAL:N	2.45	0.49
1:C:385:ARG:O	1:C:389:GLU:N	2.45	0.49
1:D:326:ARG:HA	1:D:329:PHE:HB3	1.92	0.49
1:C:40:GLN:NE2	1:C:80:GLU:OE2	2.44	0.49
1:C:351:PRO:HD3	1:C:385:ARG:HH12	1.77	0.49
1:A:260:MET:HE3	1:A:312:PRO:HG3	1.94	0.49
1:D:385:ARG:O	1:D:389:GLU:N	2.45	0.49
1:A:34:ASP:HB2	1:D:632:ARG:HD3	1.93	0.49
1:D:198:THR:OG1	1:D:199:VAL:N	2.45	0.49
1:D:257:GLN:NE2	1:D:310:GLN:OE1	2.35	0.49
1:A:198:THR:OG1	1:A:199:VAL:N	2.45	0.49
1:C:632:ARG:HD3	1:D:34:ASP:HB2	1.92	0.49
1:D:535:GLU:OE2	1:D:541:ILE:HB	2.12	0.49
1:A:550:ASP:H	1:D:365:ASN:HB2	1.76	0.49
1:D:260:MET:HE3	1:D:312:PRO:HG3	1.94	0.49
1:C:390:LEU:HA	1:C:393:VAL:HG12	1.95	0.49
1:A:385:ARG:O	1:A:389:GLU:N	2.45	0.49
1:D:390:LEU:HA	1:D:393:VAL:HG12	1.95	0.49
1:A:390:LEU:HA	1:A:393:VAL:HG12	1.95	0.48
1:B:385:ARG:O	1:B:389:GLU:N	2.45	0.48
1:A:632:ARG:HD3	1:B:34:ASP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:MET:HE3	1:C:312:PRO:HG3	1.94	0.48
1:B:260:MET:HE3	1:B:312:PRO:HG3	1.94	0.48
1:D:167:LEU:HD11	1:D:189:ILE:HA	1.96	0.48
1:A:167:LEU:HD11	1:A:189:ILE:HA	1.96	0.48
1:C:365:ASN:HB2	1:D:550:ASP:H	1.78	0.48
1:B:390:LEU:HA	1:B:393:VAL:HG12	1.95	0.48
1:C:269:THR:HG22	1:C:274:THR:HG23	1.96	0.48
1:A:257:GLN:NE2	1:A:310:GLN:OE1	2.35	0.48
1:A:269:THR:HG22	1:A:274:THR:HG23	1.96	0.48
1:A:355:ARG:HD3	1:A:369:GLN:HA	1.96	0.48
1:B:167:LEU:HD11	1:B:189:ILE:HA	1.96	0.48
1:C:355:ARG:HD3	1:C:369:GLN:HA	1.96	0.48
1:D:355:ARG:HD3	1:D:369:GLN:HA	1.96	0.48
1:C:167:LEU:HD11	1:C:189:ILE:HA	1.96	0.47
1:D:49:LEU:HA	1:D:64:LEU:HD13	1.97	0.47
1:D:373:LEU:HD13	1:D:376:ALA:HB3	1.96	0.47
1:A:49:LEU:HA	1:A:64:LEU:HD13	1.97	0.47
1:C:36:GLN:HE21	1:C:78:MET:HB3	1.80	0.47
1:A:373:LEU:HD13	1:A:376:ALA:HB3	1.96	0.47
1:D:246:LEU:HA	1:D:249:VAL:HG12	1.97	0.47
1:A:36:GLN:HE21	1:A:78:MET:HB3	1.79	0.47
1:B:246:LEU:HA	1:B:249:VAL:HG12	1.97	0.47
1:D:36:GLN:HE21	1:D:78:MET:HB3	1.79	0.47
1:A:246:LEU:HA	1:A:249:VAL:HG12	1.97	0.47
1:B:47:SER:HB2	1:B:50:LEU:HB2	1.97	0.47
1:B:269:THR:HG22	1:B:274:THR:HG23	1.96	0.47
1:B:355:ARG:HD3	1:B:369:GLN:HA	1.96	0.47
1:B:373:LEU:HD13	1:B:376:ALA:HB3	1.96	0.47
1:B:632:ARG:HD3	1:C:34:ASP:HB2	1.95	0.47
1:C:246:LEU:HA	1:C:249:VAL:HG12	1.97	0.47
1:C:474:MET:HG3	1:D:492:ARG:HG3	1.96	0.47
1:A:47:SER:HB2	1:A:50:LEU:HB2	1.97	0.47
1:B:139:ARG:HA	1:B:139:ARG:HD3	1.67	0.47
1:B:81:THR:HG23	1:B:84:HIS:HD1	1.80	0.47
1:C:47:SER:HB2	1:C:50:LEU:HB2	1.97	0.47
1:D:536:LEU:HD11	1:D:544:PRO:CD	2.45	0.47
1:C:43:ARG:NH1	1:C:75:ARG:O	2.49	0.46
1:A:43:ARG:NH1	1:A:75:ARG:O	2.48	0.46
1:B:36:GLN:HE21	1:B:78:MET:HB3	1.79	0.46
1:C:373:LEU:HD13	1:C:376:ALA:HB3	1.96	0.46
1:D:397:ILE:HA	1:D:400:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ARG:NH1	1:D:75:ARG:O	2.48	0.46
1:A:397:ILE:HA	1:A:400:LEU:HB2	1.97	0.46
1:A:493:PHE:CG	1:A:573:LEU:HD13	2.51	0.46
1:B:49:LEU:HA	1:B:64:LEU:HD13	1.97	0.46
1:C:81:THR:HG23	1:C:84:HIS:HD1	1.80	0.46
1:D:269:THR:HG22	1:D:274:THR:HG23	1.96	0.46
1:C:49:LEU:HA	1:C:64:LEU:HD13	1.97	0.46
1:D:433:ALA:HA	1:D:436:VAL:HG12	1.97	0.46
1:A:165:HIS:O	1:A:168:SER:OG	2.26	0.46
1:A:420:ILE:O	1:A:483:GLN:NE2	2.49	0.46
1:B:43:ARG:NH1	1:B:75:ARG:O	2.49	0.46
1:B:397:ILE:HA	1:B:400:LEU:HB2	1.97	0.46
1:D:139:ARG:HA	1:D:139:ARG:HD3	1.67	0.46
1:B:420:ILE:O	1:B:483:GLN:NE2	2.49	0.46
1:C:321:TRP:CE2	1:C:597:ILE:HD11	2.51	0.46
1:D:522:HIS:CE1	1:D:544:PRO:HB3	2.51	0.46
1:A:564:ILE:HA	1:A:567:THR:HG22	1.98	0.46
1:A:610:ARG:NH1	1:A:613:TRP:O	2.49	0.46
1:B:321:TRP:CE2	1:B:597:ILE:HD11	2.51	0.46
1:B:564:ILE:HA	1:B:567:THR:HG22	1.98	0.46
1:B:569:LEU:O	1:B:573:LEU:N	2.45	0.46
1:C:564:ILE:HA	1:C:567:THR:HG22	1.98	0.46
1:D:47:SER:HB2	1:D:50:LEU:HB2	1.97	0.46
1:D:321:TRP:CE2	1:D:597:ILE:HD11	2.51	0.46
1:D:564:ILE:HA	1:D:567:THR:HG22	1.98	0.46
1:A:59:GLN:HA	1:A:62:ASN:HD22	1.81	0.46
1:B:312:PRO:HG2	1:B:313:VAL:HG23	1.98	0.46
1:D:59:GLN:HA	1:D:62:ASN:HD22	1.81	0.46
1:C:139:ARG:HA	1:C:139:ARG:HD3	1.67	0.45
1:C:312:PRO:HG2	1:C:313:VAL:HG23	1.98	0.45
1:C:610:ARG:NH1	1:C:613:TRP:O	2.49	0.45
1:A:81:THR:HG23	1:A:84:HIS:HD1	1.80	0.45
1:A:321:TRP:CE2	1:A:597:ILE:HD11	2.51	0.45
1:A:433:ALA:HA	1:A:436:VAL:HG12	1.97	0.45
1:B:493:PHE:CG	1:B:573:LEU:HD13	2.51	0.45
1:D:420:ILE:O	1:D:483:GLN:NE2	2.49	0.45
1:D:610:ARG:NH1	1:D:613:TRP:O	2.49	0.45
1:B:610:ARG:NH1	1:B:613:TRP:O	2.49	0.45
1:C:493:PHE:CG	1:C:573:LEU:HD13	2.51	0.45
1:D:493:PHE:CG	1:D:573:LEU:HD13	2.51	0.45
1:C:59:GLN:HA	1:C:62:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ILE:HA	1:C:400:LEU:HB2	1.97	0.45
1:C:420:ILE:O	1:C:483:GLN:NE2	2.49	0.45
1:A:312:PRO:HG2	1:A:313:VAL:HG23	1.98	0.45
1:C:569:LEU:O	1:C:573:LEU:N	2.45	0.45
1:D:81:THR:HG23	1:D:84:HIS:HD1	1.80	0.45
1:D:307:ILE:HD12	1:D:307:ILE:HA	1.88	0.45
1:B:433:ALA:HA	1:B:436:VAL:HG12	1.97	0.45
1:D:312:PRO:HG2	1:D:313:VAL:HG23	1.98	0.45
1:B:59:GLN:HA	1:B:62:ASN:HD22	1.81	0.45
1:A:492:ARG:HG3	1:D:474:MET:HG3	1.98	0.45
1:A:542:ASP:O	1:D:541:ILE:HA	2.16	0.45
1:B:182:LEU:H	1:B:182:LEU:HG	1.51	0.45
1:C:165:HIS:O	1:C:168:SER:OG	2.26	0.45
1:C:217:ASN:OD1	1:C:217:ASN:N	2.50	0.45
1:D:217:ASN:OD1	1:D:217:ASN:N	2.50	0.45
1:C:433:ALA:HA	1:C:436:VAL:HG12	1.97	0.44
1:A:619:CYS:SG	1:A:629:TRP:NE1	2.91	0.44
1:B:497:MET:HE1	1:B:534:PHE:HE1	1.83	0.44
1:B:544:PRO:HG2	1:B:555:TYR:OH	2.17	0.44
1:C:270:TYR:HB3	1:C:273:LEU:HG	1.99	0.44
1:A:350:ARG:C	1:A:385:ARG:HH22	2.25	0.44
1:A:497:MET:HE1	1:A:534:PHE:HE1	1.83	0.44
1:B:350:ARG:C	1:B:385:ARG:HH22	2.25	0.44
1:D:302:ARG:HA	1:D:302:ARG:HD3	1.73	0.44
1:D:619:CYS:SG	1:D:629:TRP:NE1	2.91	0.44
1:B:270:TYR:HB3	1:B:273:LEU:HG	1.99	0.44
1:B:420:ILE:HA	1:B:424:PRO:HB3	1.99	0.44
1:B:619:CYS:SG	1:B:629:TRP:NE1	2.91	0.44
1:A:569:LEU:O	1:A:573:LEU:N	2.46	0.44
1:C:619:CYS:SG	1:C:629:TRP:NE1	2.91	0.44
1:D:350:ARG:C	1:D:385:ARG:HH22	2.25	0.44
1:D:420:ILE:HA	1:D:424:PRO:HB3	1.99	0.44
1:A:474:MET:HG3	1:B:492:ARG:HG3	1.99	0.44
1:B:217:ASN:N	1:B:217:ASN:OD1	2.50	0.44
1:C:350:ARG:C	1:C:385:ARG:HH22	2.25	0.44
1:C:497:MET:HE1	1:C:534:PHE:HE1	1.83	0.44
1:A:544:PRO:HG2	1:A:555:TYR:OH	2.17	0.44
1:A:270:TYR:HB3	1:A:273:LEU:HG	1.99	0.44
1:A:535:GLU:OE1	1:A:541:ILE:HB	2.18	0.44
1:A:302:ARG:HA	1:A:302:ARG:HD3	1.73	0.43
1:A:420:ILE:HA	1:A:424:PRO:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:HD13	1:A:571:LEU:HA	1.83	0.43
1:C:193:ASP:OD1	1:C:196:GLY:N	2.51	0.43
1:A:217:ASN:OD1	1:A:217:ASN:N	2.50	0.43
1:B:535:GLU:OE1	1:B:541:ILE:HB	2.18	0.43
1:B:570:MET:HA	1:B:573:LEU:HB3	2.00	0.43
1:D:270:TYR:HB3	1:D:273:LEU:HG	1.99	0.43
1:D:497:MET:HE1	1:D:534:PHE:HE1	1.83	0.43
1:D:570:MET:HA	1:D:573:LEU:HB3	2.01	0.43
1:B:132:LEU:HA	1:B:135:ALA:HB3	2.01	0.43
1:D:132:LEU:HA	1:D:135:ALA:HB3	2.01	0.43
1:D:165:HIS:O	1:D:168:SER:OG	2.26	0.43
1:A:193:ASP:OD1	1:A:196:GLY:N	2.51	0.43
1:B:403:GLU:HA	1:B:406:ASP:HB3	2.00	0.43
1:D:193:ASP:OD1	1:D:196:GLY:N	2.51	0.43
1:D:536:LEU:CD1	1:D:544:PRO:HD3	2.48	0.43
1:D:571:LEU:HD13	1:D:571:LEU:HA	1.84	0.43
1:A:403:GLU:HA	1:A:406:ASP:HB3	2.00	0.43
1:A:570:MET:HA	1:A:573:LEU:HB3	2.01	0.43
1:A:132:LEU:HA	1:A:135:ALA:HB3	2.01	0.43
1:C:330:CYS:O	1:C:334:ALA:N	2.51	0.43
1:B:193:ASP:OD1	1:B:196:GLY:N	2.51	0.43
1:C:132:LEU:HA	1:C:135:ALA:HB3	2.01	0.43
1:D:403:GLU:HA	1:D:406:ASP:HB3	2.00	0.43
1:C:420:ILE:HA	1:C:424:PRO:HB3	1.99	0.43
1:C:570:MET:HA	1:C:573:LEU:HB3	2.00	0.43
1:A:536:LEU:HD11	1:A:559:TYR:HE1	1.83	0.42
1:B:330:CYS:O	1:B:334:ALA:N	2.51	0.42
1:C:403:GLU:HA	1:C:406:ASP:HB3	2.00	0.42
1:D:543:GLY:HA3	1:D:559:TYR:OH	2.19	0.42
1:B:474:MET:HG3	1:C:492:ARG:HG3	2.01	0.42
1:C:474:MET:O	1:D:492:ARG:NH1	2.46	0.42
1:B:425:PHE:HB3	1:B:464:ASN:HD21	1.85	0.42
1:C:182:LEU:H	1:C:182:LEU:HG	1.52	0.42
1:C:536:LEU:HD11	1:C:559:TYR:HE1	1.83	0.42
1:B:165:HIS:O	1:B:168:SER:OG	2.26	0.42
1:D:536:LEU:HD11	1:D:559:TYR:HE1	1.83	0.42
1:A:283:ILE:HG23	1:A:292:LEU:HD23	2.02	0.42
1:A:425:PHE:HB3	1:A:464:ASN:HD21	1.85	0.42
1:C:200:LEU:HD22	1:C:200:LEU:HA	1.89	0.42
1:C:283:ILE:HG23	1:C:292:LEU:HD23	2.02	0.42
1:B:536:LEU:HD11	1:B:559:TYR:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:HA3	1:A:111:THR:OG1	2.20	0.42
1:C:425:PHE:HB3	1:C:464:ASN:HD21	1.85	0.42
1:D:425:PHE:HB3	1:D:464:ASN:HD21	1.85	0.42
1:D:536:LEU:HD12	1:D:544:PRO:HD3	2.02	0.42
1:C:296:ILE:HG12	1:C:307:ILE:HG21	2.02	0.42
1:D:283:ILE:HG23	1:D:292:LEU:HD23	2.02	0.42
1:D:330:CYS:O	1:D:334:ALA:N	2.51	0.42
1:B:283:ILE:HG23	1:B:292:LEU:HD23	2.02	0.41
1:D:569:LEU:O	1:D:573:LEU:N	2.46	0.41
1:C:396:ALA:O	1:C:400:LEU:N	2.53	0.41
1:D:256:PHE:CG	1:D:307:ILE:HD11	2.55	0.41
1:D:296:ILE:HG12	1:D:307:ILE:HG21	2.02	0.41
1:B:256:PHE:CG	1:B:307:ILE:HD11	2.55	0.41
1:C:256:PHE:CG	1:C:307:ILE:HD11	2.55	0.41
1:B:367:LEU:HG	1:C:516:ASP:HB3	2.01	0.41
1:C:359:ARG:H	1:C:359:ARG:HD3	1.86	0.41
1:C:581:THR:HG21	1:D:575:ILE:HG12	2.02	0.41
1:D:79:GLY:HA3	1:D:111:THR:OG1	2.20	0.41
1:C:286:SER:O	1:C:288:ASP:N	2.49	0.41
1:C:571:LEU:HD13	1:C:571:LEU:HA	1.84	0.41
1:D:57:ASP:O	1:D:61:LEU:N	2.54	0.41
1:D:359:ARG:H	1:D:359:ARG:HD3	1.86	0.41
1:A:57:ASP:O	1:A:61:LEU:N	2.54	0.41
1:B:557:ILE:O	1:B:561:ALA:N	2.45	0.41
1:C:57:ASP:O	1:C:61:LEU:N	2.54	0.41
1:C:535:GLU:CD	1:C:541:ILE:HB	2.46	0.41
1:D:80:GLU:HG3	1:D:110:MET:HE3	2.03	0.41
1:D:308:LEU:HD21	1:D:598:VAL:HG21	2.02	0.41
1:A:256:PHE:CG	1:A:307:ILE:HD11	2.55	0.41
1:A:139:ARG:HA	1:A:139:ARG:HD3	1.67	0.41
1:A:330:CYS:O	1:A:334:ALA:N	2.51	0.41
1:B:79:GLY:HA3	1:B:111:THR:OG1	2.20	0.41
1:C:557:ILE:O	1:C:561:ALA:N	2.46	0.41
1:A:296:ILE:HG12	1:A:307:ILE:HG21	2.02	0.41
1:A:359:ARG:H	1:A:359:ARG:HD3	1.86	0.41
1:A:367:LEU:HG	1:B:516:ASP:HB3	2.03	0.41
1:A:429:ILE:HD12	1:A:429:ILE:HA	1.97	0.41
1:B:57:ASP:O	1:B:61:LEU:N	2.54	0.41
1:B:296:ILE:HG12	1:B:307:ILE:HG21	2.03	0.41
1:B:307:ILE:HD12	1:B:307:ILE:HA	1.88	0.41
1:B:308:LEU:HD21	1:B:598:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:GLY:CA	1:B:559:TYR:OH	2.69	0.41
1:C:79:GLY:HA3	1:C:111:THR:OG1	2.20	0.41
1:C:308:LEU:HD21	1:C:598:VAL:HG21	2.02	0.41
1:C:321:TRP:CZ2	1:C:326:ARG:HB3	2.56	0.41
1:C:610:ARG:HA	1:C:610:ARG:HD2	1.94	0.41
1:D:182:LEU:HD12	1:D:183:ILE:HG23	2.03	0.41
1:D:428:LEU:HD12	1:D:460:LEU:HB2	2.03	0.41
1:B:359:ARG:H	1:B:359:ARG:HD3	1.86	0.41
1:C:490:LEU:O	1:C:494:CYS:N	2.52	0.41
1:B:321:TRP:CZ2	1:B:326:ARG:HB3	2.56	0.40
1:C:80:GLU:HG3	1:C:110:MET:HE3	2.03	0.40
1:C:541:ILE:HG23	1:C:543:GLY:H	1.86	0.40
1:A:182:LEU:HD12	1:A:183:ILE:HG23	2.03	0.40
1:A:321:TRP:CZ2	1:A:326:ARG:HB3	2.56	0.40
1:A:428:LEU:HD12	1:A:460:LEU:HB2	2.03	0.40
1:B:182:LEU:HD12	1:B:183:ILE:HG23	2.03	0.40
1:B:541:ILE:HG23	1:B:543:GLY:H	1.86	0.40
1:C:81:THR:HG23	1:C:84:HIS:ND1	2.36	0.40
1:C:428:LEU:HD12	1:C:460:LEU:HB2	2.03	0.40
1:D:321:TRP:CZ2	1:D:326:ARG:HB3	2.56	0.40
1:A:302:ARG:HB3	1:A:305:ARG:HH21	1.86	0.40
1:A:490:LEU:O	1:A:494:CYS:N	2.52	0.40
1:A:80:GLU:HG3	1:A:110:MET:HE3	2.03	0.40
1:A:308:LEU:HD21	1:A:598:VAL:HG21	2.02	0.40
1:C:182:LEU:HD12	1:C:183:ILE:HG23	2.03	0.40
1:D:40:GLN:HE22	1:D:80:GLU:CD	2.30	0.40
1:C:50:LEU:HD13	1:C:50:LEU:HA	1.97	0.40
1:C:363:ARG:HD3	1:C:365:ASN:ND2	2.37	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	609/742 (82%)	541 (89%)	65 (11%)	3 (0%)	24	62
1	B	609/742 (82%)	540 (89%)	66 (11%)	3 (0%)	24	62
1	C	609/742 (82%)	541 (89%)	64 (10%)	4 (1%)	18	55
1	D	609/742 (82%)	540 (89%)	66 (11%)	3 (0%)	24	62
All	All	2436/2968 (82%)	2162 (89%)	261 (11%)	13 (0%)	26	62

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	VAL
1	B	585	VAL
1	C	585	VAL
1	D	585	VAL
1	C	545	ALA
1	A	373	LEU
1	A	584	ARG
1	B	373	LEU
1	C	373	LEU
1	D	373	LEU
1	B	584	ARG
1	C	584	ARG
1	D	584	ARG

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	529/645 (82%)	500 (94%)	29 (6%)	19	42
1	B	529/645 (82%)	500 (94%)	29 (6%)	19	42
1	C	529/645 (82%)	500 (94%)	29 (6%)	19	42
1	D	529/645 (82%)	500 (94%)	29 (6%)	19	42
All	All	2116/2580 (82%)	2000 (94%)	116 (6%)	21	42

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	51	LEU
1	A	81	THR
1	A	136	LEU
1	A	139	ARG
1	A	144	SER
1	A	153	ARG
1	A	160	ILE
1	A	182	LEU
1	A	190	ARG
1	A	200	LEU
1	A	229	LEU
1	A	315	GLU
1	A	352	LEU
1	A	359	ARG
1	A	398	ILE
1	A	400	LEU
1	A	421	LEU
1	A	452	VAL
1	A	480	ILE
1	A	520	LEU
1	A	554	MET
1	A	556	SER
1	A	564	ILE
1	A	571	LEU
1	A	573	LEU
1	A	592	LEU
1	A	604	LEU
1	A	608	LEU
1	B	34	ASP
1	B	51	LEU
1	B	81	THR
1	B	136	LEU
1	B	139	ARG
1	B	144	SER
1	B	153	ARG
1	B	160	ILE
1	B	182	LEU
1	B	190	ARG
1	B	200	LEU
1	B	229	LEU
1	B	315	GLU
1	B	352	LEU

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Mol	Chain	Res	Type
1	B	359	ARG
1	B	398	ILE
1	B	400	LEU
1	B	421	LEU
1	B	452	VAL
1	B	480	ILE
1	B	520	LEU
1	B	554	MET
1	B	556	SER
1	B	564	ILE
1	B	571	LEU
1	B	573	LEU
1	B	592	LEU
1	B	604	LEU
1	B	608	LEU
1	C	34	ASP
1	C	51	LEU
1	C	81	THR
1	C	136	LEU
1	C	139	ARG
1	C	144	SER
1	C	153	ARG
1	C	160	ILE
1	C	182	LEU
1	C	190	ARG
1	C	200	LEU
1	C	229	LEU
1	C	315	GLU
1	C	352	LEU
1	C	359	ARG
1	C	398	ILE
1	C	400	LEU
1	C	421	LEU
1	C	452	VAL
1	C	480	ILE
1	C	520	LEU
1	C	554	MET
1	C	556	SER
1	C	564	ILE
1	C	571	LEU
1	C	573	LEU
1	C	592	LEU

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Mol	Chain	Res	Type
1	C	604	LEU
1	C	608	LEU
1	D	34	ASP
1	D	51	LEU
1	D	81	THR
1	D	136	LEU
1	D	139	ARG
1	D	144	SER
1	D	153	ARG
1	D	160	ILE
1	D	182	LEU
1	D	190	ARG
1	D	200	LEU
1	D	229	LEU
1	D	315	GLU
1	D	352	LEU
1	D	359	ARG
1	D	398	ILE
1	D	400	LEU
1	D	421	LEU
1	D	452	VAL
1	D	480	ILE
1	D	520	LEU
1	D	554	MET
1	D	556	SER
1	D	564	ILE
1	D	571	LEU
1	D	573	LEU
1	D	592	LEU
1	D	604	LEU
1	D	608	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	127	ASN
1	A	165	HIS
1	A	206	GLN
1	A	208	ASN
1	A	369	GLN
1	A	370	GLN

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Mol	Chain	Res	Type
1	A	418	GLN
1	A	464	ASN
1	A	546	ASN
1	B	56	ASN
1	B	127	ASN
1	B	165	HIS
1	B	206	GLN
1	B	208	ASN
1	B	369	GLN
1	B	370	GLN
1	B	418	GLN
1	B	464	ASN
1	B	546	ASN
1	C	56	ASN
1	C	127	ASN
1	C	165	HIS
1	C	206	GLN
1	C	208	ASN
1	C	369	GLN
1	C	370	GLN
1	C	418	GLN
1	C	464	ASN
1	C	522	HIS
1	C	546	ASN
1	D	56	ASN
1	D	127	ASN
1	D	165	HIS
1	D	206	GLN
1	D	208	ASN
1	D	369	GLN
1	D	370	GLN
1	D	418	GLN
1	D	464	ASN
1	D	546	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FZ4	A	801	-	17,18,18	0.76	0	18,22,22	1.51	2 (11%)
2	FZ4	B	801	-	17,18,18	0.75	0	18,22,22	1.50	2 (11%)
2	FZ4	C	801	-	17,18,18	0.76	0	18,22,22	1.52	2 (11%)
2	FZ4	D	801	-	17,18,18	0.77	0	18,22,22	1.51	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FZ4	A	801	-	-	7/12/12/12	0/2/2/2
2	FZ4	B	801	-	-	7/12/12/12	0/2/2/2
2	FZ4	C	801	-	-	7/12/12/12	0/2/2/2
2	FZ4	D	801	-	-	7/12/12/12	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FZ4	C13-C08-C09	3.18	120.51	116.86
2	D	801	FZ4	C13-C08-C09	3.16	120.49	116.86
2	A	801	FZ4	C13-C08-C09	3.16	120.48	116.86
2	B	801	FZ4	C13-C08-C09	3.15	120.48	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FZ4	C07-C02-C03	3.13	120.46	116.86
2	C	801	FZ4	C07-C02-C03	3.13	120.45	116.86
2	A	801	FZ4	C07-C02-C03	3.11	120.43	116.86
2	B	801	FZ4	C07-C02-C03	3.09	120.41	116.86

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FZ4	O14-B01-C02-C03
2	A	801	FZ4	O14-B01-C02-C07
2	A	801	FZ4	C02-B01-O14-C15
2	A	801	FZ4	C08-B01-O14-C15
2	A	801	FZ4	O14-C15-C16-N17
2	B	801	FZ4	O14-B01-C02-C03
2	B	801	FZ4	O14-B01-C02-C07
2	B	801	FZ4	C02-B01-O14-C15
2	B	801	FZ4	C08-B01-O14-C15
2	B	801	FZ4	O14-C15-C16-N17
2	C	801	FZ4	O14-B01-C02-C03
2	C	801	FZ4	O14-B01-C02-C07
2	C	801	FZ4	C02-B01-O14-C15
2	C	801	FZ4	C08-B01-O14-C15
2	C	801	FZ4	O14-C15-C16-N17
2	D	801	FZ4	O14-B01-C02-C03
2	D	801	FZ4	O14-B01-C02-C07
2	D	801	FZ4	C02-B01-O14-C15
2	D	801	FZ4	C08-B01-O14-C15
2	D	801	FZ4	O14-C15-C16-N17
2	A	801	FZ4	C08-B01-C02-C03
2	B	801	FZ4	C08-B01-C02-C03
2	C	801	FZ4	C08-B01-C02-C03
2	D	801	FZ4	C08-B01-C02-C03
2	A	801	FZ4	C08-B01-C02-C07
2	B	801	FZ4	C08-B01-C02-C07
2	C	801	FZ4	C08-B01-C02-C07
2	D	801	FZ4	C08-B01-C02-C07

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	544:PRO	C	545:ALA	N	1.73
1	C	540:ILE	C	541:ILE	N	1.10

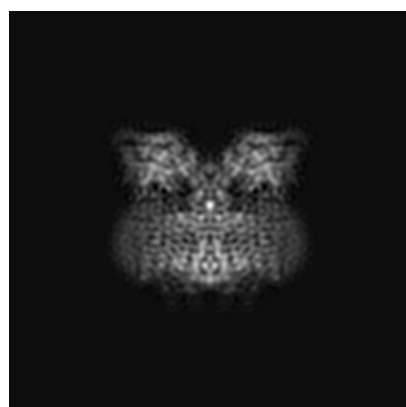
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7825. These allow visual inspection of the internal detail of the map and identification of artifacts.

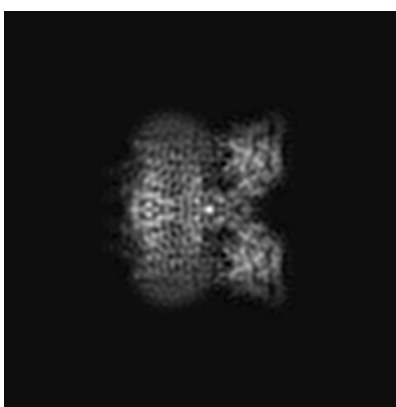
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

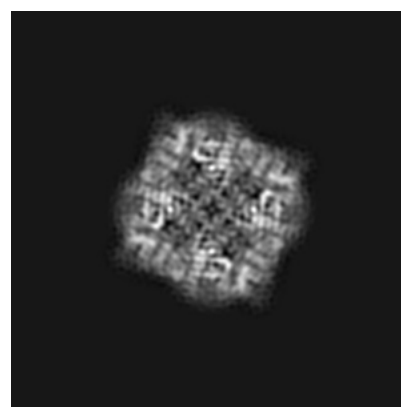
6.1.1 Primary map



X



Y



Z

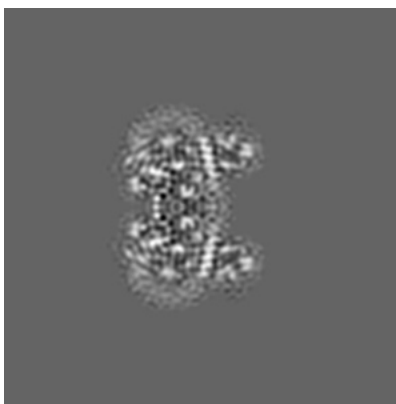
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 102



Y Index: 102



Z Index: 102

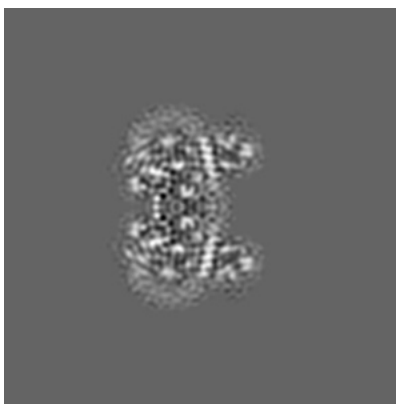
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 102



Y Index: 102

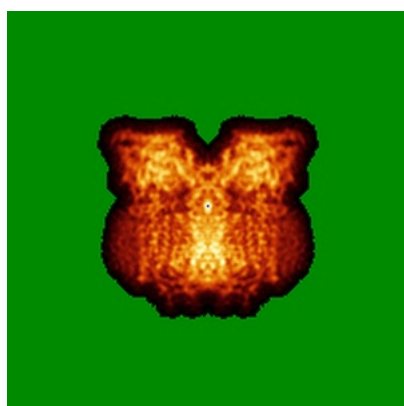


Z Index: 122

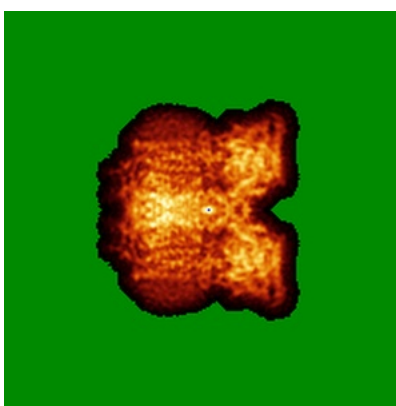
The images above show the largest variance slices of the map in three orthogonal directions.

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

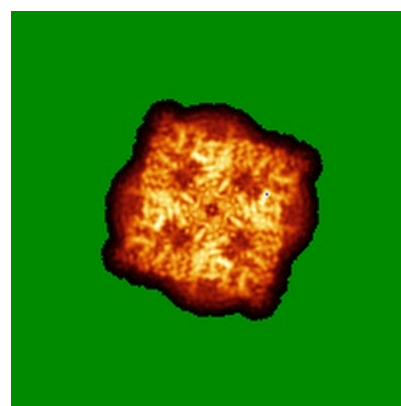
6.4.1 Primary map



X



Y

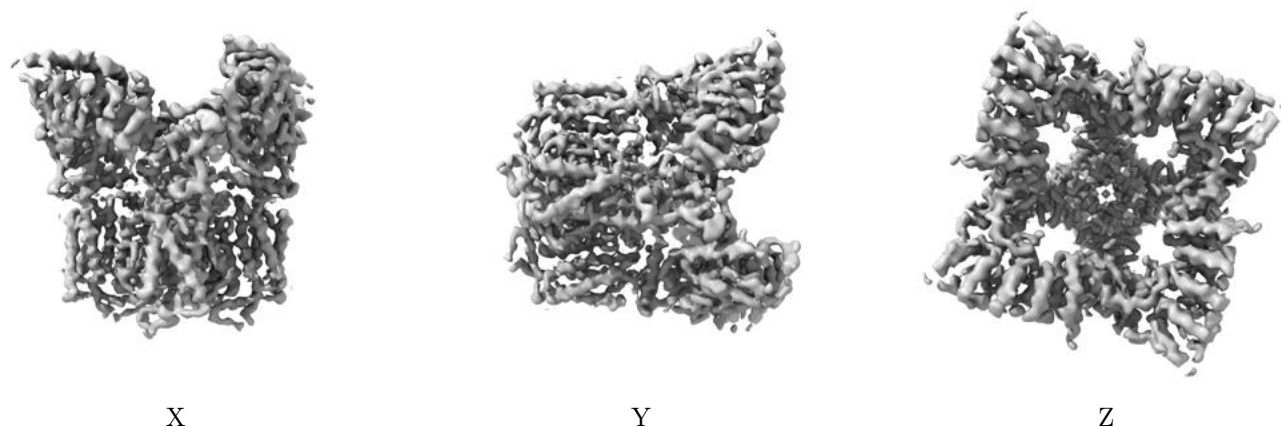


Z

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 0.0669. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

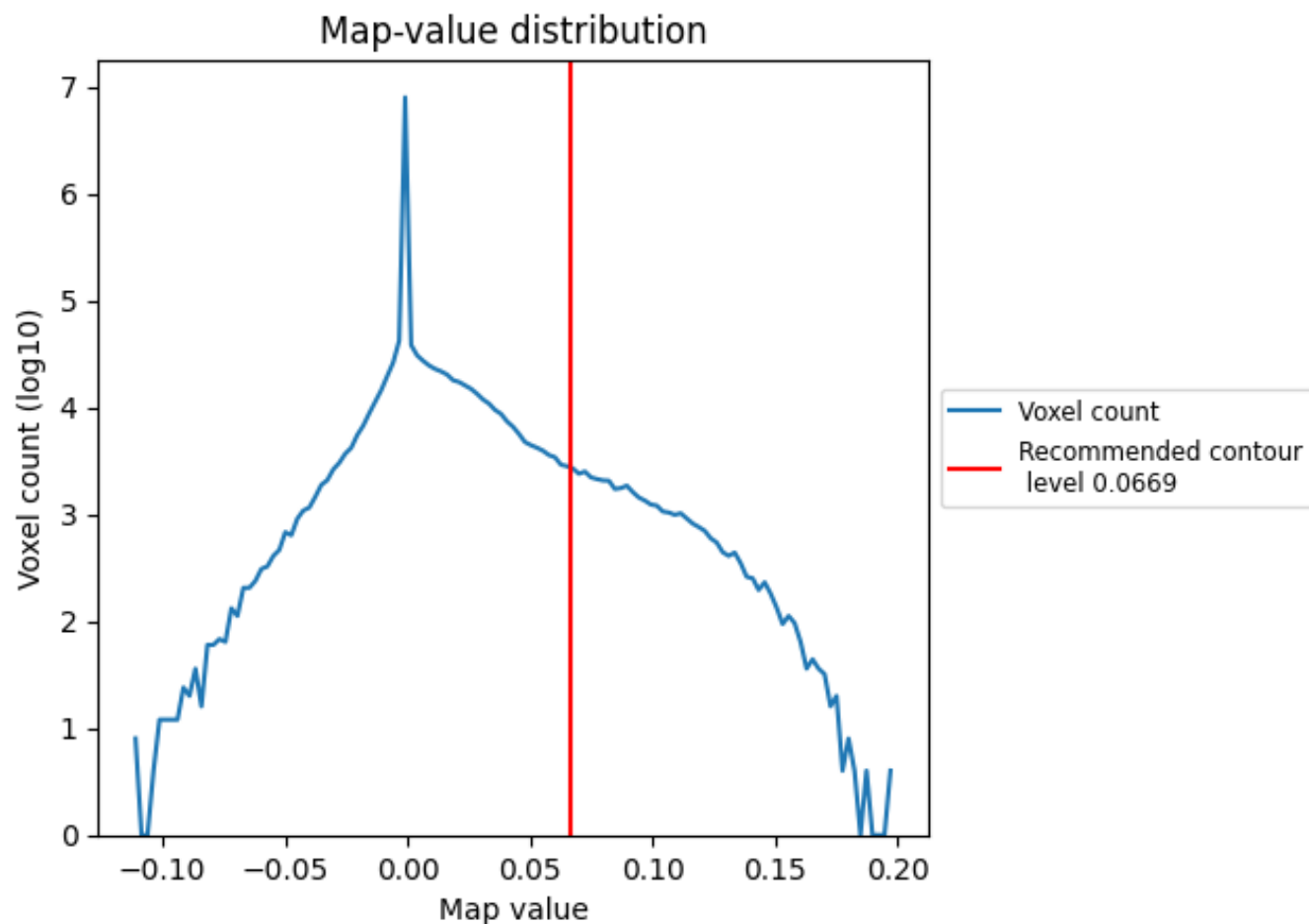
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

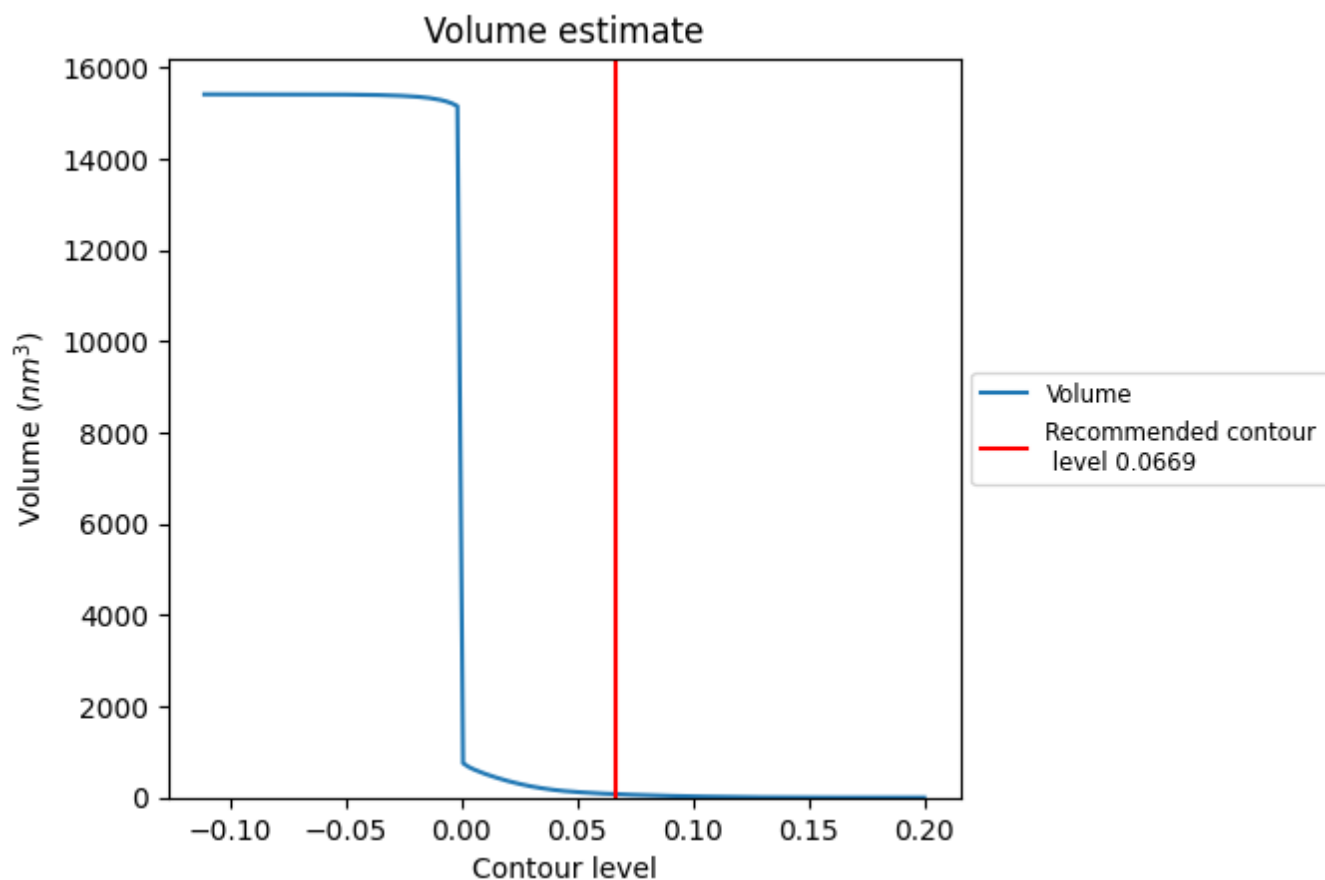
This section contains the results of statistical analysis of the map.

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.

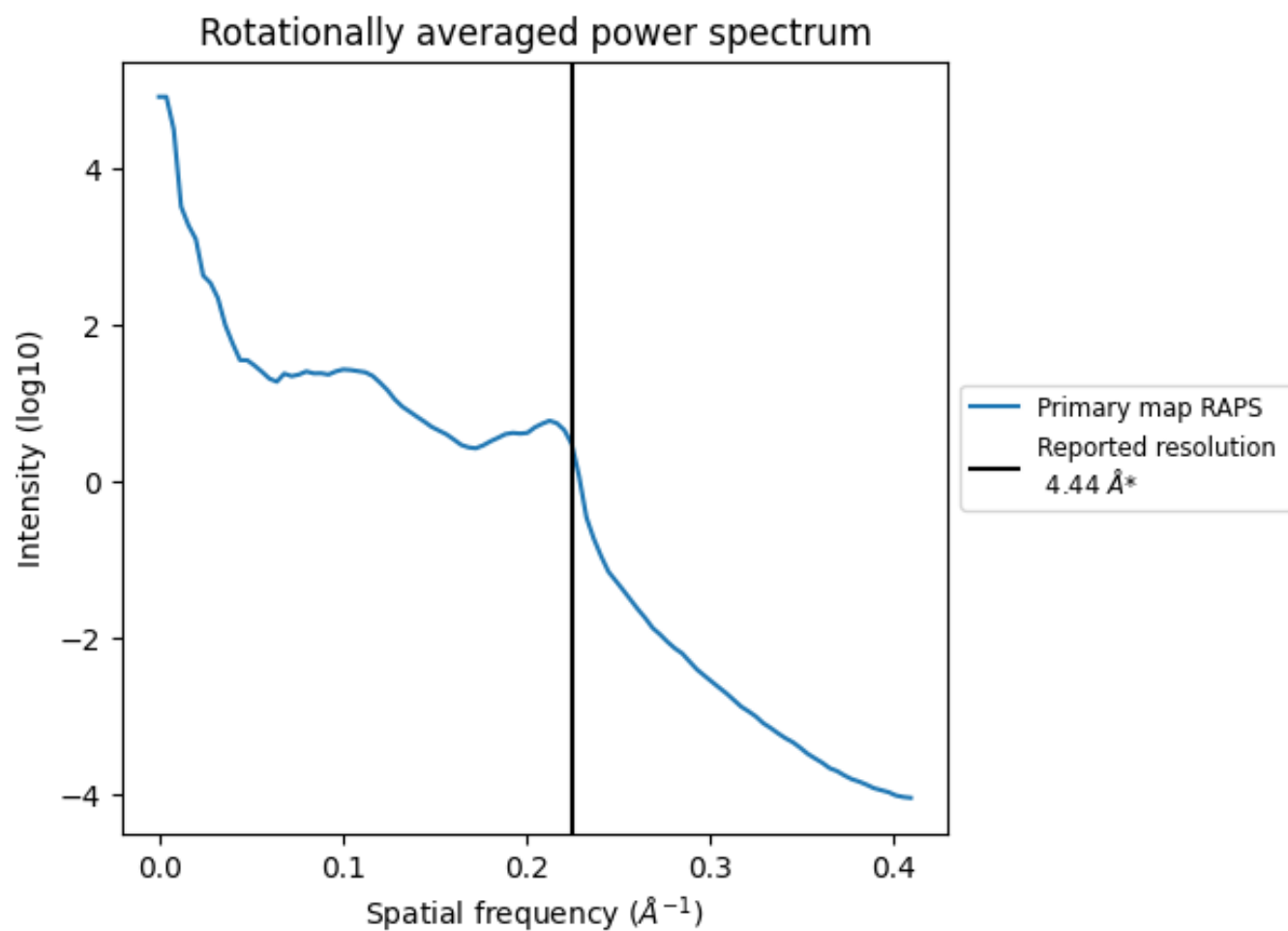
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 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 0.225 Å⁻¹

8 Fourier-Shell correlation

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

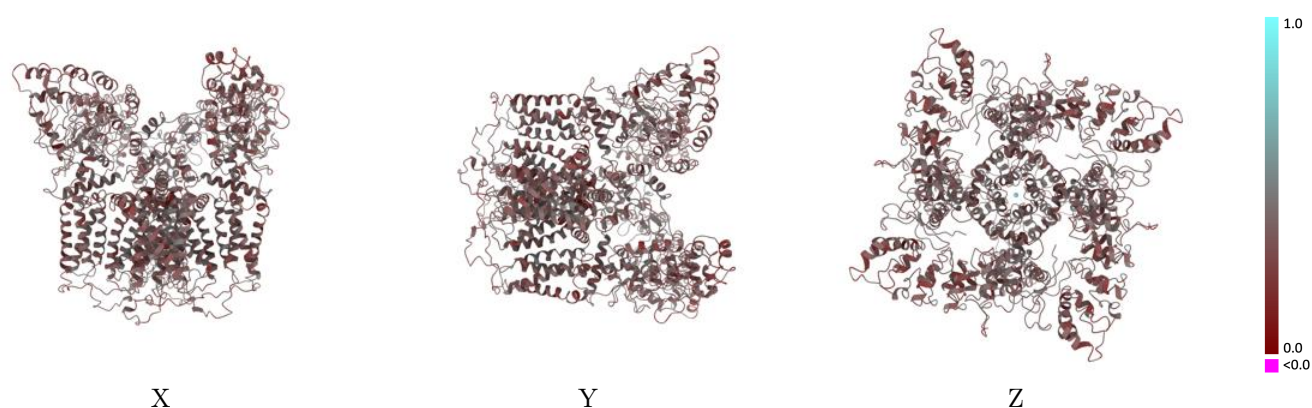
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7825 and PDB model 6D7T. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

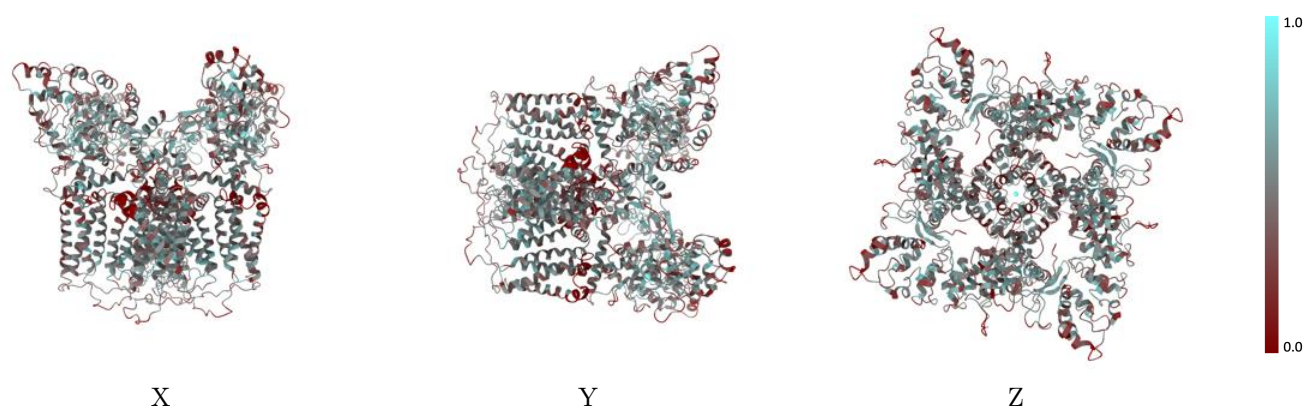
This section was not generated.

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



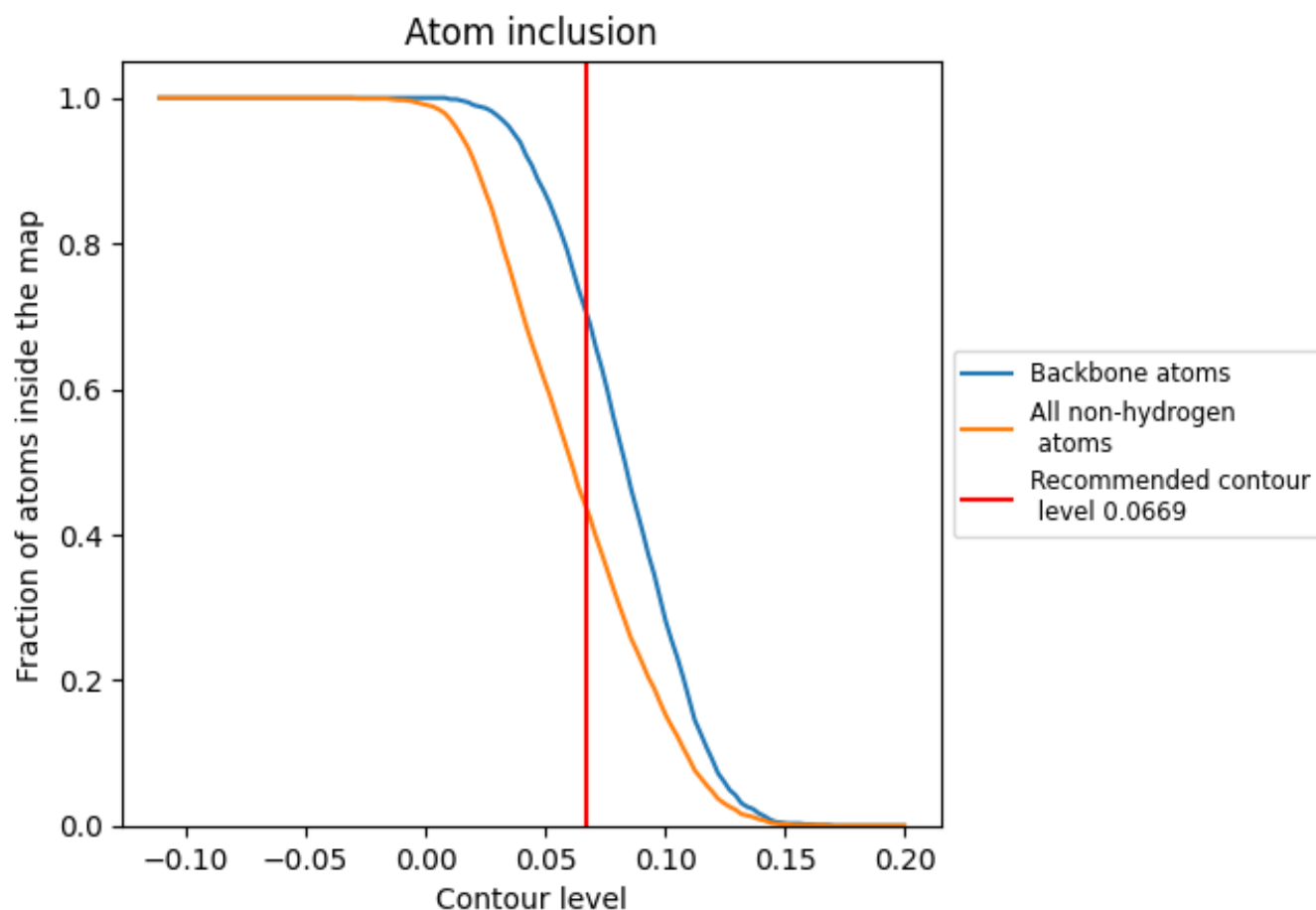
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0669).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 44% 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 (0.0669) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4380	0.3540
A	0.4380	0.3540
B	0.4380	0.3540
C	0.4390	0.3530
D	0.4370	0.3540

