



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:57 AM UTC

PDB ID : 8EKI / pdb_00008eki
EMDB ID : EMD-28204
Title : CryoEM structure of the Dsl1 complex bound to SNAREs Sec20 and Use1
Authors : DAmico, K.A.; Jeffrey, P.D.; Hughson, F.M.
Deposited on : 2022-09-21
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

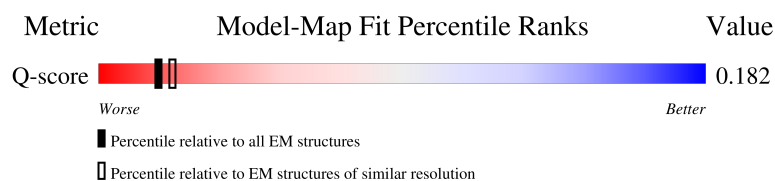
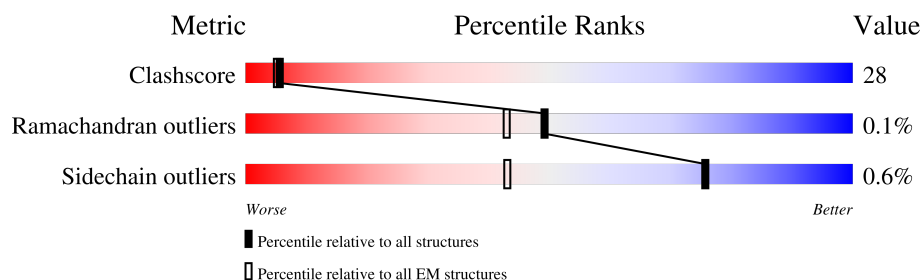
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	275	 10% 34% 28% 38%
2	B	212	 25% 16% 60%
3	C	701	 10% 46% 54%
4	D	709	 45% 50% . .

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Mol	Chain	Length	Quality of chain
5	E	783	16% 42% 40% 18%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18792 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 Protein transport protein SEC20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	170	Total	C	N	O	S	0	0
			1437	914	241	276	6		

- Molecule 2 is a protein called Protein transport protein USE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	85	Total	C	N	O	S	0	0
			714	440	131	142	1		

- Molecule 3 is a protein called Protein transport protein TIP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	701	Total	C	N	O	S	0	0
			5724	3653	952	1103	16		

- Molecule 4 is a protein called Protein transport protein SEC39.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	684	Total	C	N	O	S	0	0
			5609	3606	895	1084	24		

- Molecule 5 is a protein called Protein transport protein DSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	643	Total	C	N	O	S	0	0
			5308	3407	875	1002	24		

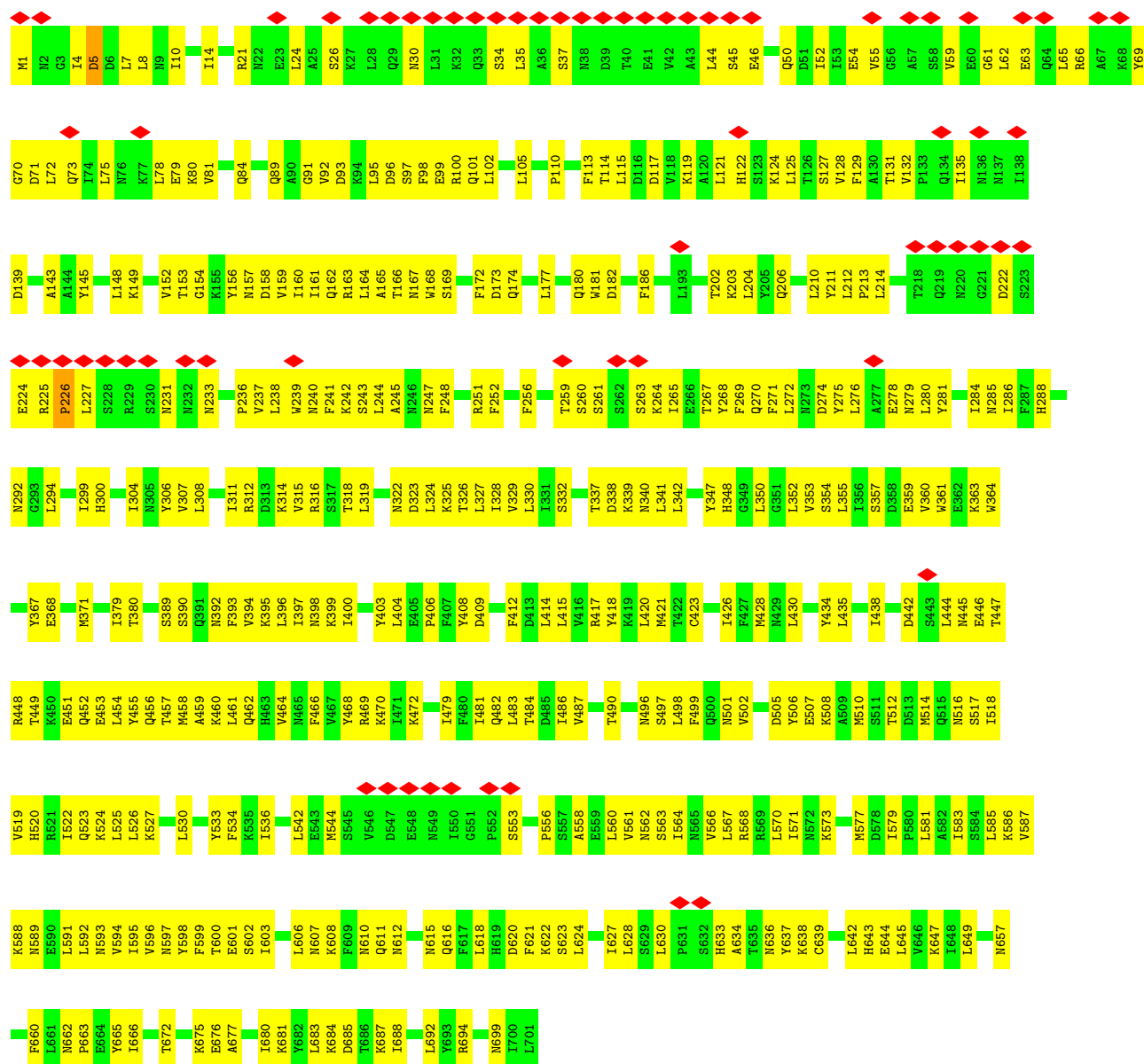
There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-28	MET	-	initiating methionine	UNP P53847
E	-27	LYS	-	expression tag	UNP P53847
E	-26	HIS	-	expression tag	UNP P53847

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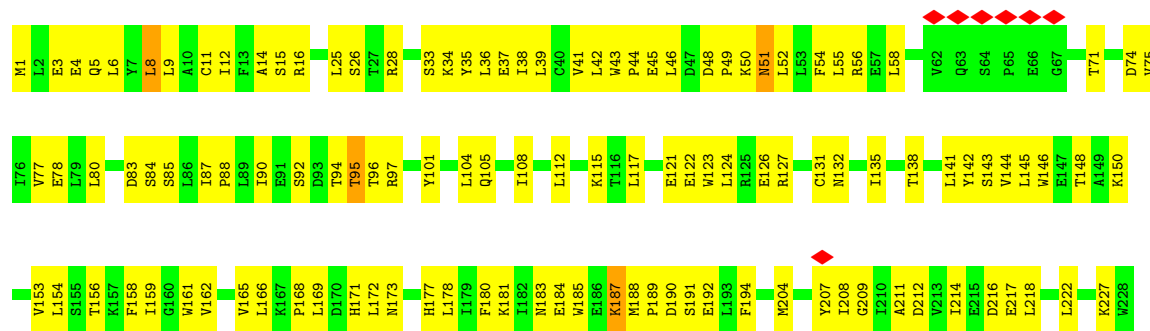
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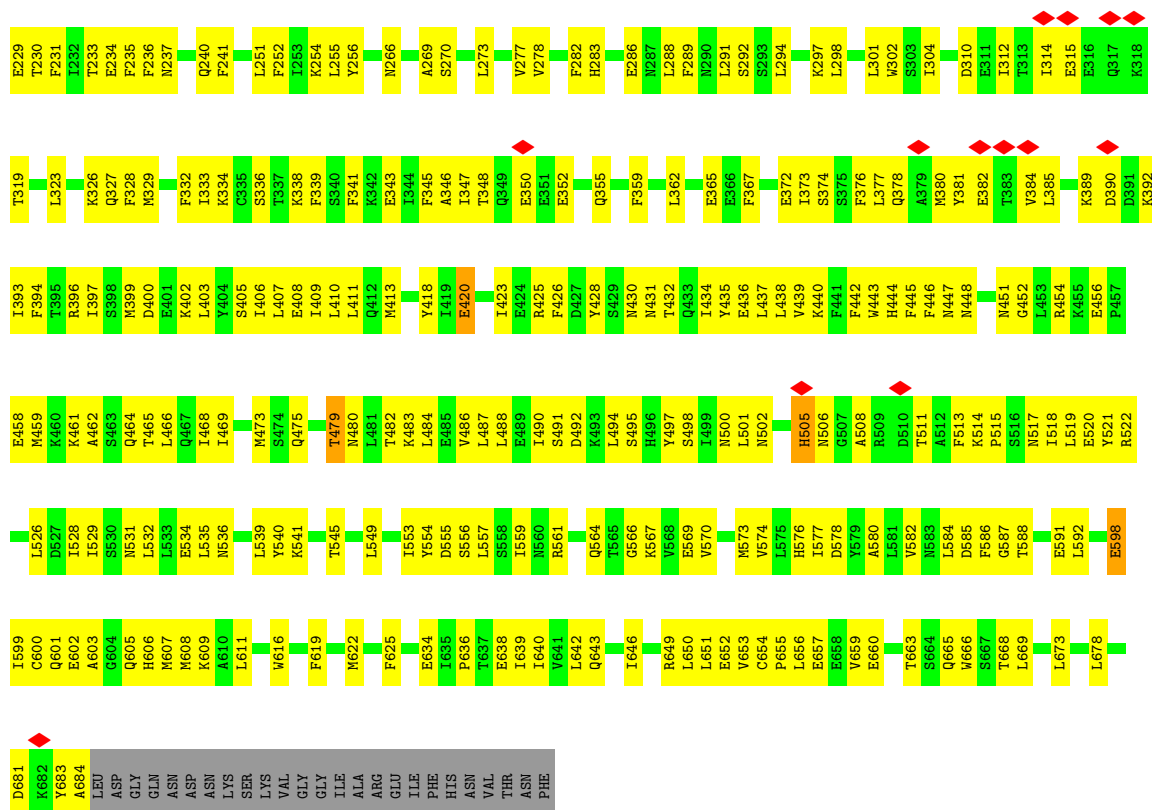
Chain	Residue	Modelled	Actual	Comment	Reference
E	-25	HIS	-	expression tag	UNP P53847
E	-24	HIS	-	expression tag	UNP P53847
E	-23	HIS	-	expression tag	UNP P53847
E	-22	HIS	-	expression tag	UNP P53847
E	-21	HIS	-	expression tag	UNP P53847
E	-20	HIS	-	expression tag	UNP P53847
E	-19	GLY	-	expression tag	UNP P53847
E	-18	ALA	-	expression tag	UNP P53847
E	-17	ALA	-	expression tag	UNP P53847
E	-16	GLY	-	expression tag	UNP P53847
E	-15	THR	-	expression tag	UNP P53847
E	-14	SER	-	expression tag	UNP P53847
E	-13	LEU	-	expression tag	UNP P53847
E	-12	TYR	-	expression tag	UNP P53847
E	-11	LYS	-	expression tag	UNP P53847
E	-10	LYS	-	expression tag	UNP P53847
E	-9	ALA	-	expression tag	UNP P53847
E	-8	GLY	-	expression tag	UNP P53847
E	-7	GLU	-	expression tag	UNP P53847
E	-6	ASN	-	expression tag	UNP P53847
E	-5	LEU	-	expression tag	UNP P53847
E	-4	TYR	-	expression tag	UNP P53847
E	-3	PHE	-	expression tag	UNP P53847
E	-2	GLN	-	expression tag	UNP P53847
E	-1	GLY	-	expression tag	UNP P53847
E	0	SER	-	expression tag	UNP P53847



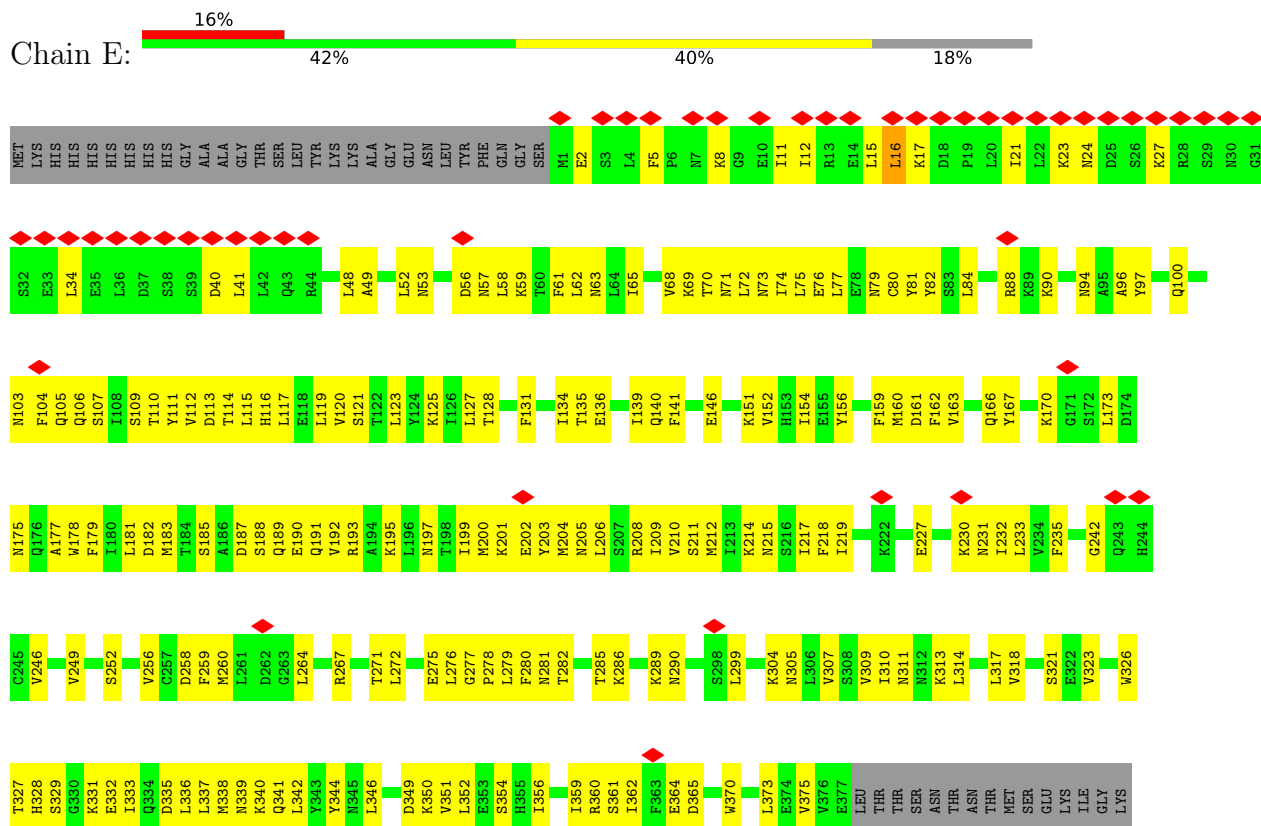
• Molecule 4: Protein transport protein SEC39

Chain D: 45% 50%





• Molecule 5: Protein transport protein DSL1



I747	A680	K608	M532	ASN	ASN
R748	K681	L609	M532	ALA	ASP
G749		L610		TRP	SER
T750	K687	P611	C535	ASP	ASP
A751	K689	Y612	F539	GLU	VAL
L752		K615		ALA	GLN
D753	F692	E616	C544	TRP	ASN
D754	A693	L617	Q545	ALA	GLU
	T694	R619	L546	ILE	LYS
	M695	P620	Y547	GLU	GLU
	G696	L621	F547	ASN	HIS
	K697	K622	M550	ILE	LEU
	F698	Q623	R551	ASP	ASN
	L699	L624	Y552	ASP	ALA
	P700	R625	L553	SER	LYS
	L701	E628	L554	LEU	ASP
	H702	R631	E555	GLU	ASP
	L703	P632	R556	ASN	ASP
	K704	L633	D557	GLY	TRP
	E705		L560	LYS	ASN
	I706	L637		GLU	TRP
	M707	N638	L563	HIS	GLU
	E708	F639	K584	LEU	VAL
	M709	L640	E565	ALA	GLU
	F710	Y641	L566	HIS	ASP
	Y711	N642	T567	ASP	ASP
	N712	D643	L570	VAL	ALA
	G713	C644	L571	GLY	ASP
	D714	V645	E572	SER	ALA
	F715	T646	T573	LEU	TRP
	Y716		K574	ASP	GLY
	L717	L649	K574	LYS	ASP
	F718	L650	L575	ASP	GLU
	A719	K651		ILE	ILE
	T720	W652		ASP	ASP
	D721		K578	ASP	ASP
	E722	L716	E491	VAL	ASP
	L723	L717	V492	ASN	ASN
	I724	F718	T493	ILE	ILE
	Q725	A719	Q494	ASP	ASP
	W726	T720		ASP	ASP
		D721	K497	ASP	GLU
		E722	L498	GLU	GLU
		L723	F499	LYS	LYS
		I724	L500	LYS	GLN
		Q725	Q504	ASN	ASN
		W726		GLN	GLU
			S509	LYS	LYS
		L730	F510	GLY	LYS
		F731	A511	GLY	LYS
		A732	D512	GLU	GLY
		D733	S513	PRO	PRO
			H514	GLU	GLU
		T734		GLU	GLU
		F735	K523	GLY	GLY
		L736	Q528		
		R737			
		R738			
		N739			
		A740			
		I741			
		D742			
		D743			
		I744			
		Y745			
		F746			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49947	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; correction was performed using the Patch CTF Estimation tool in CryoSPARC	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.372	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.186	Depositor
Map size ($\text{\AA}$)	445.59998, 445.59998, 445.59998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.114, 1.114, 1.114	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/1463	0.41	0/1966
2	B	0.27	0/726	0.42	0/973
3	C	0.24	0/5828	0.43	1/7888 (0.0%)
4	D	0.28	0/5722	0.46	0/7732
5	E	0.26	0/5409	0.47	2/7300 (0.0%)
All	All	0.26	0/19148	0.45	3/25859 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	16	LEU	CA-C-N	-5.09	113.06	120.29
5	E	16	LEU	C-N-CA	-5.09	113.06	120.29
3	C	677	ALA	N-CA-C	-5.05	108.86	114.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1437	0	1416	72	0
2	B	714	0	691	33	0
3	C	5724	0	5742	368	0
4	D	5609	0	5576	345	0
5	E	5308	0	5339	283	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18792	0	18764	1033	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 28.

All (1033) 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)
4:D:606:HIS:ND1	4:D:607:MET:HE2	1.41	1.32
2:B:33:GLN:O	2:B:36:SER:HB2	1.28	1.28
4:D:606:HIS:ND1	4:D:607:MET:CE	2.09	1.15
3:C:46:GLU:O	3:C:50:GLN:HB2	1.58	1.03
2:B:33:GLN:O	2:B:36:SER:CB	2.07	1.02
3:C:50:GLN:HE21	3:C:54:GLU:CD	1.76	0.94
3:C:50:GLN:HE21	3:C:54:GLU:CG	1.81	0.94
5:E:669:LEU:O	5:E:673:ASN:HB2	1.71	0.90
4:D:601:GLN:HE22	4:D:649:ARG:HH21	1.20	0.90
3:C:158:ASP:HA	3:C:162:GLN:HB2	1.55	0.89
3:C:46:GLU:O	3:C:50:GLN:CB	2.23	0.87
3:C:102:LEU:HB3	3:C:160:ILE:HD11	1.56	0.86
4:D:204:MET:HE2	4:D:209:GLY:HA3	1.55	0.85
3:C:212:LEU:HD12	3:C:213:PRO:HD2	1.57	0.84
3:C:50:GLN:NE2	3:C:54:GLU:HG3	1.93	0.82
3:C:156:TYR:HA	3:C:160:ILE:HD13	1.59	0.82
4:D:420:GLU:HA	4:D:423:ILE:HG22	1.60	0.82
4:D:377:LEU:HA	4:D:380:MET:HE3	1.64	0.80
4:D:601:GLN:HA	4:D:608:MET:HE1	1.64	0.80
4:D:536:ASN:HB3	4:D:539:LEU:HD23	1.64	0.79
4:D:606:HIS:CE1	4:D:607:MET:CE	2.65	0.79
3:C:583:ILE:HA	3:C:586:LYS:HE2	1.62	0.79
5:E:200:MET:HA	5:E:204:MET:HB3	1.64	0.79
5:E:258:ASP:OD1	5:E:313:LYS:NZ	2.14	0.78
4:D:80:LEU:HB2	4:D:87:ILE:HG12	1.64	0.78
4:D:657:GLU:OE1	4:D:657:GLU:N	2.15	0.78
4:D:183:ASN:O	4:D:187:LYS:HB2	1.84	0.77
3:C:169:SER:HB2	3:C:239:TRP:HB2	1.66	0.77
2:B:33:GLN:HA	2:B:36:SER:OG	1.85	0.77
3:C:444:LEU:HD21	3:C:452:GLN:HB3	1.67	0.77
3:C:114:THR:H	3:C:117:ASP:HB2	1.48	0.77
3:C:161:ILE:HD13	3:C:211:TYR:HA	1.67	0.75
5:E:134:ILE:HG12	5:E:139:ILE:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:160:MET:HA	5:E:163:VAL:HG22	1.67	0.75
4:D:522:ARG:NH2	4:D:557:LEU:O	2.20	0.74
2:B:48:ARG:HA	2:B:51:HIS:HB2	1.69	0.74
5:E:134:ILE:HG23	5:E:139:ILE:HG12	1.70	0.74
4:D:282:PHE:HD1	4:D:341:PHE:HE2	1.36	0.73
5:E:277:GLY:HA3	5:E:326:TRP:CE2	2.23	0.73
4:D:606:HIS:CE1	4:D:607:MET:HE1	2.23	0.72
5:E:117:LEU:HD11	5:E:188:SER:HB2	1.71	0.72
1:A:31:GLU:HG3	1:A:155:ARG:HD3	1.69	0.72
5:E:125:LYS:HA	5:E:128:THR:HG22	1.70	0.72
4:D:435:TYR:HA	4:D:438:LEU:HD12	1.72	0.72
3:C:50:GLN:NE2	3:C:54:GLU:CG	2.50	0.71
5:E:210:VAL:HG13	5:E:276:LEU:HD21	1.71	0.71
3:C:225:ARG:HH22	3:C:417:ARG:C	1.97	0.71
4:D:465:THR:HA	4:D:468:ILE:HD12	1.72	0.71
5:E:88:ARG:NH2	5:E:113:ASP:OD1	2.20	0.71
5:E:127:LEU:HD23	5:E:203:TYR:CG	2.25	0.71
4:D:501:LEU:HG	4:D:531:ASN:HD22	1.56	0.71
5:E:71:ASN:HA	5:E:74:ILE:HG12	1.71	0.71
4:D:327:GLN:HE21	4:D:389:LYS:HE2	1.56	0.70
3:C:34:SER:HB2	5:E:27:LYS:HB2	1.72	0.70
3:C:102:LEU:HD22	3:C:160:ILE:HG12	1.73	0.70
3:C:542:LEU:HB3	3:C:610:ASN:HD21	1.57	0.70
4:D:41:VAL:HG21	4:D:108:ILE:HG23	1.73	0.70
1:A:175:TYR:HE1	3:C:285:ASN:HA	1.57	0.70
4:D:519:LEU:HA	4:D:557:LEU:HD21	1.74	0.70
3:C:115:LEU:HD22	3:C:203:LYS:HG3	1.74	0.70
4:D:333:ILE:HG13	4:D:334:LYS:HG3	1.73	0.70
5:E:58:LEU:HA	5:E:61:PHE:HD1	1.56	0.70
5:E:669:LEU:O	5:E:673:ASN:CB	2.39	0.70
3:C:37:SER:CB	5:E:24:ASN:O	2.40	0.69
3:C:92:VAL:HG23	3:C:145:TYR:HD2	1.56	0.69
4:D:380:MET:O	4:D:385:LEU:N	2.26	0.69
3:C:66:ARG:HD3	3:C:75:LEU:HD22	1.75	0.69
3:C:451:GLU:HA	3:C:454:LEU:HD12	1.73	0.69
3:C:110:PRO:HB2	3:C:167:ASN:HD22	1.58	0.69
4:D:678:LEU:HD12	5:E:580:ARG:HD2	1.75	0.69
4:D:447:ASN:HD22	5:E:193:ARG:HD3	1.57	0.68
4:D:491:SER:O	4:D:495:SER:OG	2.11	0.68
3:C:276:LEU:HD12	3:C:280:LEU:HB2	1.74	0.68
3:C:599:PHE:HA	3:C:603:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:ASP:HB3	4:D:51:ASN:HB2	1.74	0.68
1:A:120:ILE:HD11	3:C:681:LYS:HD3	1.75	0.68
5:E:212:MET:HG2	5:E:235:PHE:CE2	2.28	0.68
4:D:501:LEU:HD11	4:D:528:ILE:HA	1.75	0.68
2:B:44:GLU:O	2:B:48:ARG:HB2	1.94	0.67
4:D:339:PHE:HA	4:D:343:GLU:OE1	1.94	0.67
4:D:44:PRO:O	4:D:127:ARG:NH2	2.27	0.67
5:E:199:ILE:HA	5:E:203:TYR:HD2	1.59	0.67
4:D:458:GLU:HA	4:D:461:LYS:HD2	1.75	0.67
3:C:115:LEU:O	3:C:119:LYS:HB2	1.95	0.66
3:C:98:PHE:O	3:C:102:LEU:HG	1.96	0.66
4:D:288:LEU:HA	4:D:291:LEU:HD23	1.78	0.66
4:D:283:HIS:NE2	4:D:315:GLU:OE2	2.20	0.66
5:E:307:VAL:HA	5:E:310:ILE:HD12	1.78	0.65
3:C:125:LEU:HD23	3:C:212:LEU:HD23	1.77	0.65
4:D:423:ILE:HG13	4:D:428:TYR:HB2	1.79	0.65
5:E:68:VAL:O	5:E:72:LEU:HG	1.97	0.65
4:D:508:ALA:HB2	5:E:170:LYS:HB3	1.78	0.65
5:E:578:LYS:HD2	5:E:617:ILE:HG12	1.78	0.65
4:D:500:ASN:H	4:D:531:ASN:HD21	1.45	0.65
5:E:606:ILE:HA	5:E:610:LEU:HD12	1.79	0.65
3:C:268:TYR:O	3:C:272:LEU:HG	1.97	0.65
3:C:66:ARG:NH1	3:C:79:GLU:OE2	2.29	0.64
1:A:152:HIS:CD2	1:A:155:ARG:HH22	2.15	0.64
3:C:71:ASP:HA	3:C:75:LEU:HD13	1.79	0.64
4:D:50:LYS:HG3	4:D:51:ASN:H	1.61	0.64
1:A:62:LEU:O	1:A:66:ILE:HG12	1.98	0.64
4:D:444:HIS:CE1	4:D:448:ASN:HD21	2.15	0.64
4:D:483:LYS:HB3	4:D:556:SER:HA	1.80	0.64
5:E:328:HIS:HE1	5:E:333:ILE:HD13	1.63	0.64
5:E:590:LEU:HD13	5:E:652:TRP:HE1	1.62	0.64
3:C:556:PRO:HA	3:C:616:GLN:HE22	1.62	0.64
4:D:235:PHE:HA	4:D:240:GLN:HG3	1.79	0.63
5:E:90:LYS:O	5:E:94:ASN:N	2.22	0.63
1:A:145:VAL:HA	1:A:148:ILE:HG22	1.81	0.63
4:D:348:THR:HG22	4:D:393:ILE:HA	1.78	0.63
5:E:58:LEU:HA	5:E:61:PHE:CD1	2.33	0.63
3:C:160:ILE:O	3:C:164:LEU:HB2	1.98	0.63
3:C:312:ARG:HG2	3:C:352:LEU:HD13	1.80	0.63
4:D:402:LYS:O	4:D:406:ILE:HG12	1.99	0.63
4:D:408:GLU:HA	4:D:411:LEU:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:458:MET:HG3	3:C:577:MET:HE3	1.80	0.63
3:C:657:ASN:HB3	3:C:660:PHE:HE1	1.62	0.63
4:D:43:TRP:HB3	4:D:127:ARG:HH12	1.64	0.63
5:E:127:LEU:HD11	5:E:159:PHE:HE1	1.62	0.63
5:E:177:ALA:O	5:E:181:LEU:CB	2.47	0.63
4:D:501:LEU:HB2	4:D:513:PHE:HE1	1.64	0.63
5:E:698:PHE:HB2	5:E:706:ILE:HD12	1.79	0.63
2:B:23:ASN:OD1	2:B:26:ARG:NH2	2.28	0.63
3:C:260:SER:OG	3:C:318:THR:HB	1.99	0.63
3:C:65:LEU:HD23	3:C:69:TYR:CD2	2.34	0.62
3:C:392:ASN:HA	3:C:395:LYS:HD2	1.81	0.62
4:D:407:LEU:HD13	4:D:434:ILE:HD13	1.81	0.62
4:D:112:LEU:O	4:D:115:LYS:HD3	1.99	0.62
4:D:222:LEU:HA	4:D:227:LYS:HB2	1.81	0.62
5:E:53:ASN:O	5:E:57:ASN:ND2	2.19	0.62
3:C:340:ASN:HD22	3:C:341:LEU:HD12	1.64	0.62
4:D:236:PHE:HA	4:D:241:PHE:HE2	1.63	0.62
3:C:14:ILE:HD11	5:E:56:ASP:HA	1.82	0.62
4:D:117:LEU:HD21	4:D:123:TRP:HD1	1.65	0.62
2:B:26:ARG:O	2:B:30:VAL:HG22	2.00	0.62
5:E:173:LEU:HD13	5:E:175:ASN:ND2	2.15	0.62
3:C:65:LEU:HD23	3:C:69:TYR:HD2	1.64	0.62
3:C:390:SER:O	3:C:393:PHE:HB3	1.98	0.62
5:E:373:LEU:HD23	5:E:373:LEU:H	1.63	0.62
3:C:566:VAL:O	3:C:570:LEU:HG	1.99	0.61
5:E:120:VAL:HG21	5:E:192:VAL:HG23	1.81	0.61
5:E:195:LYS:O	5:E:199:ILE:HG12	2.00	0.61
3:C:616:GLN:NE2	3:C:620:ASP:OD2	2.34	0.61
5:E:621:LEU:HB3	5:E:633:LEU:HG	1.81	0.61
3:C:308:LEU:HA	3:C:311:ILE:HD12	1.80	0.61
4:D:241:PHE:HZ	4:D:255:LEU:HD12	1.66	0.61
3:C:248:PHE:HB2	3:C:275:TYR:CZ	2.36	0.61
4:D:301:LEU:HA	4:D:304:ILE:HD12	1.80	0.61
1:A:22:LYS:O	1:A:26:ILE:HG12	2.01	0.61
4:D:606:HIS:HA	4:D:609:LYS:HD2	1.83	0.61
3:C:361:TRP:CZ2	3:C:415:LEU:HD21	2.36	0.61
5:E:500:LEU:O	5:E:504:GLN:HG2	2.01	0.61
4:D:302:TRP:HH2	4:D:326:LYS:HE3	1.66	0.61
4:D:380:MET:HB3	4:D:385:LEU:HG	1.82	0.61
5:E:628:GLU:HG2	5:E:631:ARG:HH12	1.65	0.61
2:B:32:LYS:O	2:B:36:SER:OG	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:SER:O	3:C:101:GLN:HG2	1.99	0.60
4:D:132:ASN:HA	4:D:135:ILE:HB	1.83	0.60
5:E:703:LEU:HD23	5:E:736:LEU:HG	1.83	0.60
3:C:7:LEU:HA	3:C:10:ILE:HB	1.84	0.60
5:E:547:TYR:CZ	5:E:571:LEU:HD22	2.37	0.60
5:E:560:LEU:HB3	5:E:563:ILE:HB	1.82	0.60
3:C:62:LEU:HD23	3:C:65:LEU:HD12	1.82	0.60
3:C:121:LEU:HA	3:C:124:LYS:HD2	1.84	0.60
4:D:6:LEU:HB2	4:D:25:LEU:HD11	1.82	0.60
4:D:169:LEU:O	4:D:173:ASN:ND2	2.35	0.60
4:D:347:ILE:O	4:D:355:GLN:NE2	2.33	0.60
2:B:24:ARG:NH1	4:D:46:LEU:HB3	2.17	0.60
3:C:156:TYR:HE2	3:C:212:LEU:HB3	1.66	0.60
3:C:45:SER:OG	3:C:46:GLU:N	2.33	0.60
3:C:694:ARG:HG2	3:C:699:ASN:HB2	1.82	0.60
5:E:121:SER:O	5:E:125:LYS:HG2	2.01	0.60
3:C:316:ARG:HB2	3:C:355:LEU:HB2	1.84	0.59
3:C:259:THR:O	3:C:264:LYS:NZ	2.35	0.59
4:D:456:GLU:HG3	4:D:459:MET:H	1.67	0.59
4:D:529:ILE:HA	4:D:532:LEU:HD12	1.84	0.59
5:E:305:ASN:O	5:E:309:VAL:HG23	2.03	0.59
3:C:325:LYS:HD2	3:C:367:TYR:OH	2.02	0.59
3:C:65:LEU:HA	3:C:69:TYR:HD2	1.67	0.59
4:D:570:VAL:HA	4:D:573:MET:HE3	1.83	0.59
5:E:111:TYR:O	5:E:115:LEU:HG	2.02	0.59
4:D:407:LEU:O	4:D:411:LEU:HG	2.01	0.59
5:E:697:LYS:O	5:E:700:PRO:HD2	2.02	0.59
3:C:105:LEU:HB2	3:C:113:PHE:CZ	2.38	0.59
3:C:527:LYS:HD3	3:C:530:LEU:HD12	1.84	0.59
3:C:662:ASN:OD1	3:C:665:TYR:HB3	2.03	0.59
3:C:442:ASP:OD1	3:C:448:ARG:NH2	2.35	0.59
4:D:378:GLN:HA	4:D:381:TYR:CD2	2.38	0.59
3:C:657:ASN:HB3	3:C:660:PHE:CE1	2.38	0.58
3:C:666:ILE:HG12	3:C:692:LEU:HD22	1.84	0.58
4:D:211:ALA:HA	4:D:214:ILE:HD11	1.86	0.58
5:E:27:LYS:HB3	5:E:34:LEU:HD21	1.85	0.58
5:E:81:TYR:CE1	5:E:166:GLN:HB3	2.38	0.58
3:C:294:LEU:HD13	3:C:299:ILE:HD11	1.85	0.58
3:C:460:LYS:O	3:C:464:VAL:HG23	2.03	0.58
5:E:612:TYR:O	5:E:616:GLU:HB2	2.03	0.58
1:A:107:LEU:HD11	1:A:135:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:580:ALA:O	4:D:584:LEU:N	2.37	0.58
4:D:660:GLU:OE1	5:E:523:LYS:NZ	2.37	0.58
2:B:26:ARG:HB2	2:B:49:TYR:CZ	2.39	0.58
3:C:611:GLN:NE2	3:C:615:ASN:OD1	2.36	0.58
4:D:431:ASN:OD1	4:D:432:THR:N	2.37	0.58
4:D:435:TYR:O	4:D:439:VAL:HG23	2.03	0.58
5:E:664:GLY:O	5:E:668:SER:OG	2.20	0.58
4:D:171:HIS:HB3	4:D:217:GLU:OE2	2.04	0.58
5:E:671:VAL:HG13	5:E:692:PHE:HD2	1.67	0.58
4:D:54:PHE:O	4:D:58:LEU:HG	2.04	0.58
4:D:251:LEU:O	4:D:255:LEU:HG	2.03	0.58
5:E:317:LEU:O	5:E:321:SER:OG	2.21	0.58
1:A:91:LEU:HA	1:A:111:LYS:O	2.03	0.58
1:A:133:GLN:HB2	2:B:26:ARG:NE	2.18	0.58
3:C:172:PHE:CE2	3:C:240:ASN:HB3	2.38	0.58
3:C:458:MET:HB2	3:C:577:MET:HG2	1.85	0.58
4:D:588:THR:O	4:D:592:LEU:HG	2.04	0.58
5:E:375:VAL:HG22	5:E:491:GLU:HG2	1.85	0.58
5:E:645:VAL:O	5:E:649:ILE:HG12	2.04	0.58
4:D:598:GLU:O	4:D:602:GLU:HG3	2.03	0.58
5:E:140:GLN:HB2	5:E:232:ILE:HG12	1.86	0.57
5:E:560:LEU:HD13	5:E:563:ILE:HD12	1.85	0.57
1:A:89:PRO:HB3	3:C:637:TYR:CD2	2.39	0.57
1:A:175:TYR:CE1	3:C:285:ASN:HA	2.39	0.57
3:C:227:LEU:HG	3:C:417:ARG:HB3	1.86	0.57
3:C:300:HIS:CE1	3:C:347:TYR:HA	2.39	0.57
4:D:143:SER:HA	4:D:146:TRP:CE2	2.39	0.57
4:D:486:VAL:O	4:D:490:ILE:HG22	2.04	0.57
4:D:569:GLU:HG2	4:D:573:MET:HE2	1.86	0.57
3:C:139:ASP:HB3	3:C:143:ALA:HB2	1.86	0.57
5:E:119:LEU:O	5:E:123:LEU:HG	2.05	0.57
5:E:650:LEU:O	5:E:725:GLN:NE2	2.38	0.57
3:C:526:LEU:HD21	3:C:595:ILE:HG22	1.87	0.57
4:D:502:ASN:ND2	4:D:511:THR:OG1	2.37	0.57
5:E:671:VAL:O	5:E:689:ARG:NH2	2.37	0.57
3:C:114:THR:HB	3:C:117:ASP:H	1.70	0.57
3:C:350:LEU:HD11	3:C:354:SER:HB3	1.87	0.57
4:D:171:HIS:NE2	4:D:212:ASP:OD2	2.37	0.57
4:D:465:THR:O	4:D:469:ILE:HG12	2.04	0.57
3:C:161:ILE:O	3:C:165:ALA:CB	2.52	0.57
4:D:506:ASN:HD21	5:E:170:LYS:C	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:652:GLU:O	5:E:360:ARG:NE	2.38	0.57
3:C:281:TYR:O	3:C:285:ASN:ND2	2.38	0.57
4:D:346:ALA:O	4:D:350:GLU:N	2.38	0.57
5:E:200:MET:O	5:E:205:ASN:N	2.37	0.57
3:C:304:ILE:HA	3:C:307:VAL:HG22	1.87	0.56
3:C:394:VAL:HG13	3:C:470:LYS:HG2	1.86	0.56
5:E:200:MET:HG2	5:E:205:ASN:ND2	2.20	0.56
3:C:46:GLU:O	3:C:50:GLN:N	2.37	0.56
5:E:134:ILE:HG22	5:E:208:ARG:HH11	1.70	0.56
5:E:161:ASP:HA	5:E:267:ARG:NH2	2.20	0.56
5:E:532:MET:HG2	5:E:550:MET:HE1	1.86	0.56
5:E:746:GLU:O	5:E:750:THR:HG23	2.04	0.56
4:D:355:GLN:OE1	4:D:396:ARG:HB2	2.05	0.56
5:E:252:SER:O	5:E:256:VAL:HG23	2.05	0.56
5:E:734:THR:HG23	5:E:737:ARG:H	1.69	0.56
1:A:157:LEU:HA	1:A:160:ASN:HD21	1.69	0.56
4:D:162:VAL:HA	4:D:166:LEU:HD13	1.86	0.56
4:D:501:LEU:HB2	4:D:513:PHE:CE1	2.41	0.56
3:C:7:LEU:HD23	5:E:65:ILE:HD12	1.88	0.56
3:C:455:TYR:CE1	3:C:573:LYS:HG2	2.41	0.56
5:E:566:LEU:O	5:E:570:LEU:HG	2.06	0.56
4:D:52:LEU:O	4:D:55:LEU:HG	2.06	0.56
3:C:311:ILE:O	3:C:315:VAL:HG22	2.05	0.56
3:C:379:ILE:HG13	3:C:380:THR:HG23	1.86	0.56
3:C:645:LEU:O	3:C:649:LEU:HG	2.05	0.56
5:E:127:LEU:HB3	5:E:203:TYR:CE1	2.40	0.56
2:B:44:GLU:O	2:B:48:ARG:CB	2.54	0.56
3:C:225:ARG:CZ	3:C:417:ARG:HB2	2.36	0.56
5:E:702:HIS:O	5:E:706:ILE:HG12	2.06	0.56
2:B:24:ARG:HH12	4:D:46:LEU:HB3	1.70	0.56
3:C:267:THR:O	3:C:270:GLN:NE2	2.39	0.56
4:D:41:VAL:HG11	4:D:112:LEU:HG	1.88	0.56
3:C:105:LEU:HB2	3:C:113:PHE:HZ	1.71	0.55
4:D:83:ASP:OD1	4:D:85:SER:OG	2.21	0.55
4:D:94:THR:OG1	4:D:95:THR:N	2.39	0.55
3:C:62:LEU:O	3:C:75:LEU:HD21	2.07	0.55
3:C:66:ARG:HB3	3:C:75:LEU:HD13	1.88	0.55
3:C:157:ASN:OD1	3:C:161:ILE:HD12	2.07	0.55
3:C:399:LYS:O	3:C:403:TYR:N	2.37	0.55
3:C:618:LEU:HD11	3:C:622:LYS:HE3	1.89	0.55
4:D:252:PHE:HZ	4:D:277:VAL:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:532:MET:SD	5:E:563:ILE:HA	2.46	0.55
3:C:237:VAL:HB	3:C:239:TRP:CD1	2.41	0.55
3:C:412:PHE:HD2	3:C:415:LEU:HD13	1.70	0.55
3:C:683:LEU:HD11	3:C:687:LYS:HB3	1.88	0.55
4:D:101:TYR:OH	4:D:105:GLN:NE2	2.40	0.55
4:D:359:PHE:CZ	4:D:402:LYS:HB3	2.41	0.55
5:E:11:ILE:O	5:E:15:LEU:HG	2.06	0.55
4:D:352:GLU:HA	4:D:396:ARG:HB3	1.88	0.55
4:D:526:LEU:HD23	4:D:526:LEU:H	1.70	0.55
3:C:122:HIS:HE2	3:C:212:LEU:HD13	1.72	0.55
5:E:193:ARG:O	5:E:197:ASN:ND2	2.38	0.55
1:A:77:LEU:HD11	1:A:135:VAL:HG12	1.88	0.55
3:C:672:THR:HA	3:C:675:LYS:HG2	1.88	0.55
3:C:672:THR:HA	3:C:675:LYS:HE3	1.89	0.55
3:C:592:LEU:O	3:C:596:VAL:HG23	2.07	0.55
4:D:26:SER:HA	4:D:35:TYR:CZ	2.41	0.55
3:C:225:ARG:HE	3:C:417:ARG:HH21	1.53	0.55
5:E:314:LEU:O	5:E:318:VAL:HG23	2.07	0.55
4:D:45:GLU:OE1	4:D:45:GLU:N	2.38	0.54
4:D:168:PRO:HA	4:D:217:GLU:HG2	1.88	0.54
4:D:651:LEU:HD11	4:D:659:VAL:HG23	1.88	0.54
5:E:177:ALA:O	5:E:181:LEU:HB3	2.06	0.54
5:E:16:LEU:HD11	5:E:23:LYS:HD2	1.90	0.54
3:C:315:VAL:O	3:C:319:LEU:N	2.41	0.54
1:A:14:ASP:O	1:A:18:ASN:ND2	2.31	0.54
3:C:8:LEU:HA	5:E:62:LEU:HD13	1.89	0.54
3:C:394:VAL:HG12	3:C:398:ASN:HD21	1.72	0.54
5:E:278:PRO:HG3	5:E:326:TRP:HB3	1.89	0.54
4:D:517:ASN:O	4:D:520:GLU:HB2	2.08	0.54
5:E:127:LEU:HD11	5:E:159:PHE:CE1	2.41	0.54
1:A:67:GLU:HA	1:A:70:VAL:HG12	1.89	0.54
5:E:349:ASP:HA	5:E:352:LEU:HD12	1.88	0.54
1:A:132:LEU:HD11	2:B:50:GLN:HE22	1.73	0.54
5:E:365:ASP:HB3	5:E:370:TRP:HE1	1.73	0.54
3:C:224:GLU:HG3	3:C:225:ARG:H	1.72	0.54
3:C:238:LEU:H	3:C:242:LYS:NZ	2.05	0.54
3:C:486:ILE:O	3:C:490:THR:N	2.41	0.54
4:D:376:PHE:CD2	4:D:380:MET:HE2	2.43	0.54
2:B:18:GLN:HA	2:B:21:ASN:HD22	1.73	0.53
4:D:446:PHE:HE2	4:D:519:LEU:HD11	1.73	0.53
1:A:78:LYS:O	1:A:82:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLU:O	1:A:151:GLN:HB2	2.09	0.53
3:C:89:GLN:NE2	3:C:93:ASP:OD2	2.41	0.53
3:C:222:ASP:HB2	3:C:226:PRO:HG3	1.91	0.53
3:C:157:ASN:HA	3:C:161:ILE:HB	1.90	0.53
3:C:315:VAL:HG21	3:C:352:LEU:HD12	1.90	0.53
1:A:100:ARG:NH2	1:A:102:ASP:OD2	2.35	0.53
3:C:124:LYS:O	3:C:128:VAL:HG23	2.08	0.53
4:D:605:GLN:HA	4:D:608:MET:HG2	1.90	0.53
4:D:92:SER:HB2	4:D:97:ARG:HD3	1.90	0.53
4:D:606:HIS:CE1	4:D:607:MET:HE2	2.26	0.53
4:D:355:GLN:CD	4:D:396:ARG:HB2	2.34	0.53
4:D:431:ASN:HB3	4:D:434:ILE:HG22	1.91	0.53
4:D:574:VAL:HA	4:D:577:ILE:HD12	1.91	0.53
3:C:523:GLN:O	3:C:527:LYS:HG2	2.09	0.53
5:E:159:PHE:HA	5:E:162:PHE:CE1	2.44	0.53
3:C:499:PHE:C	3:C:501:ASN:H	2.16	0.53
4:D:104:LEU:O	4:D:108:ILE:HG12	2.09	0.53
4:D:162:VAL:HA	4:D:166:LEU:HB2	1.91	0.53
4:D:236:PHE:HZ	4:D:256:TYR:HB2	1.74	0.53
3:C:417:ARG:HG3	3:C:418:TYR:N	2.24	0.52
4:D:236:PHE:HA	4:D:241:PHE:CE2	2.44	0.52
4:D:608:MET:HB3	4:D:653:VAL:HG21	1.89	0.52
4:D:654:CYS:O	5:E:360:ARG:NH2	2.40	0.52
5:E:141:PHE:O	5:E:231:ASN:ND2	2.42	0.52
5:E:227:GLU:HB2	5:E:230:LYS:HB2	1.91	0.52
5:E:304:LYS:HG3	5:E:337:LEU:HD22	1.90	0.52
3:C:389:SER:O	3:C:390:SER:C	2.50	0.52
4:D:50:LYS:HE3	4:D:144:VAL:HG21	1.91	0.52
4:D:488:LEU:HA	4:D:491:SER:OG	2.09	0.52
5:E:200:MET:HA	5:E:204:MET:CB	2.37	0.52
3:C:78:LEU:HD11	5:E:2:GLU:O	2.09	0.52
3:C:449:THR:HG23	3:C:452:GLN:H	1.74	0.52
4:D:323:LEU:HD13	4:D:392:LYS:HE2	1.92	0.52
5:E:159:PHE:O	5:E:163:VAL:HG13	2.09	0.52
5:E:182:ASP:HB2	5:E:183:MET:HE2	1.91	0.52
1:A:128:LEU:HA	1:A:131:VAL:HG22	1.90	0.52
5:E:332:GLU:HG2	5:E:333:ILE:HD12	1.91	0.52
5:E:314:LEU:HD22	5:E:328:HIS:CG	2.44	0.52
4:D:5:GLN:HB3	4:D:90:ILE:HD11	1.91	0.52
4:D:482:THR:O	4:D:486:VAL:HG22	2.10	0.52
5:E:311:ASN:OD1	5:E:328:HIS:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:LEU:HG	5:E:62:LEU:HB2	1.91	0.52
3:C:412:PHE:CE2	3:C:414:LEU:HB3	2.45	0.52
3:C:464:VAL:HG13	3:C:506:TYR:CD1	2.45	0.52
4:D:117:LEU:HD11	4:D:123:TRP:HB2	1.91	0.52
5:E:605:THR:HA	5:E:609:LEU:HB3	1.92	0.52
2:B:45:GLU:OE2	2:B:48:ARG:NH2	2.42	0.52
3:C:274:ASP:OD2	3:C:275:TYR:N	2.42	0.52
4:D:464:GLN:O	4:D:468:ILE:HG13	2.10	0.52
4:D:500:ASN:ND2	4:D:511:THR:O	2.43	0.52
4:D:600:CYS:HA	4:D:603:ALA:HB3	1.91	0.52
4:D:643:GLN:HA	4:D:646:ILE:HD12	1.92	0.52
1:A:88:TYR:HE1	1:A:120:ILE:HG22	1.75	0.52
2:B:24:ARG:HH21	4:D:48:ASP:HA	1.75	0.52
3:C:110:PRO:CB	3:C:167:ASN:HD22	2.22	0.52
4:D:461:LYS:O	4:D:465:THR:HG23	2.10	0.52
5:E:277:GLY:HA2	5:E:280:PHE:HB2	1.91	0.52
4:D:144:VAL:HG23	4:D:145:LEU:HD12	1.92	0.52
1:A:101:TYR:CE2	3:C:496:ASN:HA	2.45	0.51
3:C:239:TRP:HA	3:C:242:LYS:HB2	1.91	0.51
4:D:252:PHE:CZ	4:D:277:VAL:HG23	2.44	0.51
5:E:76:GLU:HG2	5:E:79:ASN:HB2	1.92	0.51
5:E:211:SER:HA	5:E:214:LYS:HG2	1.91	0.51
3:C:512:THR:O	3:C:516:ASN:ND2	2.44	0.51
4:D:14:ALA:HB3	4:D:42:LEU:HD22	1.92	0.51
5:E:695:MET:HA	5:E:698:PHE:CD1	2.45	0.51
3:C:37:SER:HB3	5:E:24:ASN:O	2.10	0.51
3:C:95:LEU:HB3	3:C:152:VAL:HG11	1.92	0.51
3:C:322:ASN:HB3	3:C:327:LEU:HD21	1.91	0.51
4:D:234:GLU:O	4:D:237:ASN:ND2	2.43	0.51
3:C:206:GLN:O	3:C:210:LEU:HG	2.10	0.51
4:D:207:TYR:HB3	4:D:254:LYS:HZ1	1.76	0.51
4:D:425:ARG:HD3	4:D:426:PHE:CZ	2.45	0.51
3:C:169:SER:HB2	3:C:239:TRP:CB	2.37	0.51
3:C:315:VAL:O	3:C:319:LEU:HG	2.11	0.51
3:C:394:VAL:HA	3:C:397:ILE:HD12	1.92	0.51
5:E:217:ILE:O	5:E:219:ILE:HD12	2.10	0.51
1:A:16:LEU:HD13	1:A:141:TYR:CZ	2.46	0.51
3:C:5:ASP:OD1	3:C:5:ASP:N	2.40	0.51
3:C:72:LEU:HD23	3:C:75:LEU:HD12	1.92	0.51
3:C:132:VAL:HG21	3:C:145:TYR:OH	2.11	0.51
4:D:122:GLU:CD	4:D:122:GLU:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:380:MET:O	4:D:385:LEU:HB2	2.11	0.51
4:D:445:PHE:HA	4:D:448:ASN:HD22	1.76	0.51
4:D:454:ARG:HG2	4:D:492:ASP:OD2	2.11	0.51
4:D:545:THR:O	4:D:549:LEU:HG	2.10	0.51
1:A:2:VAL:HB	3:C:633:HIS:HB3	1.93	0.51
3:C:211:TYR:CZ	3:C:213:PRO:HA	2.46	0.51
3:C:403:TYR:HD2	3:C:404:LEU:HD12	1.75	0.51
4:D:298:LEU:HB3	4:D:333:ILE:HG22	1.92	0.51
4:D:480:ASN:O	4:D:484:LEU:HG	2.11	0.51
4:D:519:LEU:O	4:D:522:ARG:HB2	2.11	0.51
4:D:601:GLN:NE2	4:D:649:ARG:HH21	2.00	0.51
5:E:575:LEU:HA	5:E:578:LYS:HE2	1.93	0.51
5:E:667:VAL:HG13	5:E:692:PHE:CE2	2.46	0.51
5:E:669:LEU:HA	5:E:672:ASN:HB3	1.93	0.51
5:E:260:MET:SD	5:E:272:LEU:HD22	2.50	0.50
3:C:322:ASN:OD1	3:C:323:ASP:N	2.44	0.50
4:D:580:ALA:HB1	4:D:585:ASP:HB3	1.94	0.50
1:A:142:ARG:HA	1:A:145:VAL:HG22	1.93	0.50
3:C:522:ILE:HD13	3:C:525:LEU:HD21	1.93	0.50
4:D:526:LEU:HA	4:D:529:ILE:HG22	1.92	0.50
5:E:286:LYS:O	5:E:290:ASN:ND2	2.44	0.50
5:E:304:LYS:HA	5:E:307:VAL:HG12	1.92	0.50
5:E:615:LYS:HA	5:E:619:ARG:HD2	1.93	0.50
3:C:159:VAL:HB	3:C:160:ILE:HD12	1.94	0.50
3:C:304:ILE:HD13	3:C:347:TYR:HB2	1.93	0.50
3:C:451:GLU:OE2	3:C:455:TYR:OH	2.22	0.50
4:D:5:GLN:O	4:D:9:LEU:HG	2.11	0.50
4:D:143:SER:HA	4:D:146:TRP:CZ2	2.46	0.50
4:D:165:VAL:C	4:D:168:PRO:HD2	2.37	0.50
4:D:514:LYS:O	4:D:517:ASN:ND2	2.44	0.50
4:D:554:TYR:HA	4:D:559:ILE:HD12	1.94	0.50
5:E:695:MET:O	5:E:699:LEU:HG	2.12	0.50
2:B:79:GLN:O	2:B:83:LYS:HG2	2.11	0.50
3:C:444:LEU:O	3:C:448:ARG:NH2	2.45	0.50
4:D:6:LEU:HA	4:D:9:LEU:HD12	1.94	0.50
4:D:278:VAL:HG21	4:D:312:ILE:HG12	1.92	0.50
5:E:135:THR:C	5:E:208:ARG:HH12	2.20	0.50
4:D:43:TRP:HB3	4:D:127:ARG:NH1	2.26	0.50
4:D:52:LEU:HD23	4:D:54:PHE:CE2	2.47	0.50
4:D:181:LYS:HZ2	4:D:184:GLU:N	2.10	0.50
4:D:328:PHE:HB2	4:D:329:MET:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:225:ARG:NH2	3:C:421:MET:SD	2.85	0.50
3:C:542:LEU:HB3	3:C:610:ASN:ND2	2.26	0.50
5:E:173:LEU:O	5:E:173:LEU:HD12	2.12	0.50
3:C:240:ASN:O	3:C:244:LEU:HG	2.12	0.50
4:D:25:LEU:HD12	4:D:28:ARG:HB2	1.92	0.50
5:E:71:ASN:HB3	5:E:80:CYS:SG	2.52	0.50
3:C:14:ILE:HD11	5:E:59:LYS:HB2	1.93	0.50
4:D:48:ASP:CB	4:D:51:ASN:HB2	2.40	0.50
5:E:183:MET:HB2	5:E:189:GLN:CD	2.37	0.50
5:E:586:ILE:HG21	5:E:644:CYS:O	2.12	0.50
1:A:156:ASP:O	1:A:160:ASN:ND2	2.45	0.49
3:C:21:ARG:HD2	5:E:49:ALA:HA	1.94	0.49
3:C:326:THR:O	3:C:330:LEU:HG	2.12	0.49
3:C:66:ARG:HA	3:C:70:GLY:C	2.37	0.49
3:C:323:ASP:OD2	3:C:326:THR:N	2.44	0.49
4:D:517:ASN:O	4:D:521:TYR:HD1	1.95	0.49
5:E:199:ILE:HA	5:E:203:TYR:CD2	2.45	0.49
3:C:281:TYR:HA	3:C:284:ILE:HB	1.94	0.49
3:C:408:TYR:HB3	3:C:479:ILE:HG21	1.93	0.49
3:C:544:MET:HB2	3:C:612:ASN:CG	2.37	0.49
3:C:561:VAL:HA	3:C:564:ILE:HD12	1.93	0.49
1:A:164:ARG:HG2	3:C:348:HIS:CE1	2.47	0.49
3:C:601:GLU:O	3:C:606:LEU:HG	2.12	0.49
4:D:185:TRP:HA	4:D:188:MET:HE3	1.94	0.49
4:D:479:THR:O	4:D:482:THR:HB	2.12	0.49
5:E:71:ASN:O	5:E:75:LEU:N	2.46	0.49
5:E:84:LEU:HD23	5:E:116:HIS:CD2	2.48	0.49
3:C:84:GLN:NE2	3:C:135:ILE:HG21	2.27	0.49
3:C:127:SER:O	3:C:131:THR:HG23	2.13	0.49
4:D:410:LEU:HD21	4:D:418:TYR:HB2	1.93	0.49
5:E:365:ASP:HB3	5:E:370:TRP:NE1	2.28	0.49
1:A:164:ARG:HD3	3:C:348:HIS:CG	2.47	0.49
3:C:102:LEU:HB3	3:C:160:ILE:CD1	2.35	0.49
3:C:227:LEU:HG	3:C:417:ARG:CB	2.43	0.49
3:C:420:LEU:HD23	3:C:483:LEU:HD22	1.94	0.49
4:D:214:ILE:HA	4:D:218:LEU:HB3	1.95	0.49
4:D:508:ALA:CB	5:E:170:LYS:HB3	2.43	0.49
1:A:68:SER:O	1:A:71:SER:OG	2.23	0.49
4:D:181:LYS:N	4:D:184:GLU:OE2	2.33	0.49
4:D:640:ILE:HG23	4:D:669:LEU:HD12	1.94	0.49
1:A:132:LEU:HA	1:A:135:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:180:PHE:CD1	4:D:188:MET:HE1	2.47	0.49
4:D:241:PHE:CZ	4:D:255:LEU:HD12	2.48	0.49
4:D:663:THR:O	4:D:666:TRP:HB3	2.13	0.49
5:E:370:TRP:H	5:E:370:TRP:CD1	2.30	0.49
1:A:67:GLU:O	1:A:70:VAL:HG12	2.12	0.49
1:A:101:TYR:CZ	3:C:496:ASN:HA	2.48	0.49
3:C:359:GLU:O	3:C:363:LYS:HG2	2.13	0.49
4:D:181:LYS:HZ2	4:D:184:GLU:H	1.60	0.49
5:E:277:GLY:HA3	5:E:326:TRP:CZ2	2.48	0.49
3:C:261:SER:H	3:C:264:LYS:HB2	1.78	0.48
4:D:380:MET:HB3	4:D:385:LEU:CG	2.43	0.48
1:A:13:GLN:HG3	1:A:137:TRP:CZ2	2.47	0.48
3:C:4:ILE:H	5:E:107:SER:HB2	1.78	0.48
3:C:602:SER:HA	3:C:606:LEU:HD12	1.95	0.48
4:D:55:LEU:HA	4:D:58:LEU:HD12	1.94	0.48
4:D:216:ASP:OD1	4:D:217:GLU:HG3	2.13	0.48
3:C:35:LEU:HD22	5:E:34:LEU:HD13	1.95	0.48
3:C:50:GLN:HE21	3:C:54:GLU:HG3	1.48	0.48
4:D:566:GLY:O	4:D:570:VAL:HG23	2.13	0.48
5:E:242:GLY:O	5:E:246:VAL:HG23	2.12	0.48
2:B:17:LYS:NZ	4:D:41:VAL:O	2.47	0.48
3:C:225:ARG:NH2	3:C:417:ARG:HE	2.12	0.48
3:C:265:ILE:HG13	3:C:330:LEU:HD22	1.96	0.48
4:D:665:GLN:O	4:D:668:THR:HB	2.13	0.48
5:E:81:TYR:CZ	5:E:166:GLN:HB3	2.49	0.48
3:C:14:ILE:CD1	5:E:59:LYS:HB2	2.43	0.48
3:C:238:LEU:O	3:C:241:PHE:N	2.47	0.48
4:D:294:LEU:O	4:D:298:LEU:HG	2.13	0.48
4:D:400:ASP:OD1	4:D:428:TYR:OH	2.26	0.48
4:D:573:MET:HE1	4:D:599:ILE:HD13	1.96	0.48
5:E:131:PHE:CD1	5:E:156:TYR:HB2	2.48	0.48
3:C:113:PHE:CD2	3:C:164:LEU:HD11	2.49	0.48
3:C:644:GLU:CD	3:C:680:ILE:HG13	2.38	0.48
4:D:39:LEU:O	4:D:43:TRP:HB2	2.14	0.48
4:D:365:GLU:OE1	5:E:103:ASN:HB3	2.13	0.48
4:D:681:ASP:HB3	4:D:684:ALA:HB2	1.95	0.48
5:E:201:LYS:O	5:E:206:LEU:N	2.47	0.48
5:E:338:MET:O	5:E:341:GLN:NE2	2.36	0.48
3:C:59:VAL:O	3:C:63:GLU:HG3	2.13	0.48
3:C:202:THR:OG1	3:C:292:ASN:OD1	2.32	0.48
3:C:564:ILE:HG23	3:C:627:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:LYS:O	4:D:38:ILE:HG22	2.14	0.48
5:E:218:PHE:HA	5:E:249:VAL:HG21	1.95	0.48
5:E:565:GLU:HG3	5:E:566:LEU:N	2.28	0.48
3:C:110:PRO:HA	3:C:113:PHE:HD2	1.79	0.48
3:C:526:LEU:HG	3:C:530:LEU:HD11	1.95	0.48
4:D:43:TRP:HD1	4:D:127:ARG:NH2	2.12	0.48
1:A:4:THR:HA	3:C:633:HIS:CD2	2.49	0.48
3:C:102:LEU:HA	3:C:105:LEU:HG	1.96	0.48
3:C:428:MET:HE2	3:C:498:LEU:HB3	1.94	0.48
3:C:630:LEU:HD13	3:C:634:ALA:HB3	1.95	0.48
5:E:123:LEU:O	5:E:127:LEU:HD13	2.14	0.48
5:E:314:LEU:HD22	5:E:328:HIS:CD2	2.49	0.48
5:E:667:VAL:O	5:E:671:VAL:HG22	2.14	0.48
3:C:182:ASP:HA	3:C:286:ILE:HD13	1.95	0.48
3:C:516:ASN:HA	3:C:519:VAL:HG22	1.94	0.48
3:C:593:ASN:OD1	3:C:638:LYS:HG3	2.13	0.48
2:B:65:HIS:CE1	2:B:69:LYS:HG3	2.49	0.47
4:D:74:ASP:O	4:D:78:GLU:HG3	2.13	0.47
4:D:456:GLU:CB	4:D:459:MET:HE3	2.44	0.47
3:C:263:SER:O	3:C:267:THR:HG23	2.14	0.47
5:E:209:ILE:HG13	5:E:210:VAL:N	2.29	0.47
5:E:528:GLN:O	5:E:532:MET:HG3	2.14	0.47
4:D:26:SER:HA	4:D:35:TYR:CE2	2.49	0.47
4:D:158:PHE:O	4:D:162:VAL:HG23	2.14	0.47
4:D:292:SER:O	4:D:297:LYS:NZ	2.32	0.47
4:D:394:PHE:CD1	4:D:397:ILE:HD11	2.48	0.47
5:E:578:LYS:O	5:E:582:VAL:HG12	2.14	0.47
5:E:642:ASN:HA	5:E:646:THR:HB	1.97	0.47
5:E:665:GLU:O	5:E:669:LEU:HG	2.14	0.47
2:B:50:GLN:O	2:B:54:GLN:HG2	2.14	0.47
3:C:623:SER:O	3:C:627:ILE:HG13	2.13	0.47
4:D:380:MET:O	4:D:385:LEU:CA	2.62	0.47
4:D:384:VAL:HG12	4:D:385:LEU:HD23	1.97	0.47
5:E:233:LEU:HD13	5:E:259:PHE:HB2	1.95	0.47
5:E:610:LEU:HD21	5:E:670:LEU:HD22	1.96	0.47
2:B:12:TYR:OH	4:D:16:ARG:NH2	2.44	0.47
3:C:96:ASP:O	3:C:100:ARG:HG3	2.15	0.47
3:C:153:THR:HG22	3:C:157:ASN:HD21	1.78	0.47
4:D:194:PHE:HB3	4:D:235:PHE:CE2	2.48	0.47
4:D:461:LYS:HA	4:D:464:GLN:OE1	2.14	0.47
5:E:667:VAL:HG13	5:E:692:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:567:LEU:HB3	3:C:627:ILE:HG21	1.96	0.47
4:D:367:PHE:HE1	4:D:376:PHE:HD2	1.62	0.47
4:D:515:PRO:O	4:D:518:ILE:HG12	2.15	0.47
5:E:106:GLN:O	5:E:109:SER:OG	2.29	0.47
5:E:134:ILE:HG22	5:E:208:ARG:NH1	2.28	0.47
5:E:185:SER:O	5:E:189:GLN:HB2	2.14	0.47
1:A:149:LEU:HD13	3:C:481:ILE:HD13	1.97	0.47
1:A:160:ASN:O	1:A:164:ARG:HG3	2.14	0.47
3:C:7:LEU:HB2	5:E:104:PHE:CZ	2.48	0.47
3:C:161:ILE:O	3:C:165:ALA:HB2	2.14	0.47
5:E:687:LYS:O	5:E:717:LEU:HD13	2.15	0.47
3:C:264:LYS:HB3	3:C:268:TYR:CZ	2.49	0.47
4:D:314:ILE:HD11	4:D:319:THR:HA	1.95	0.47
5:E:70:THR:HA	5:E:73:ASN:HD22	1.78	0.47
5:E:551:ARG:NH2	5:E:624:ILE:O	2.47	0.47
1:A:119:ASP:OD1	1:A:120:ILE:N	2.45	0.47
3:C:459:ALA:O	3:C:462:GLN:HG2	2.15	0.47
4:D:84:SER:HA	4:D:87:ILE:HG13	1.96	0.47
4:D:432:THR:O	4:D:436:GLU:HG3	2.14	0.47
4:D:636:PRO:O	4:D:640:ILE:HG13	2.14	0.47
5:E:65:ILE:HA	5:E:68:VAL:HG22	1.97	0.47
5:E:359:ILE:HA	5:E:362:ILE:HD12	1.95	0.47
5:E:640:LEU:HA	5:E:644:CYS:SG	2.55	0.47
5:E:699:LEU:HB2	5:E:700:PRO:HD3	1.97	0.47
3:C:227:LEU:HG	3:C:417:ARG:HD2	1.97	0.47
3:C:417:ARG:HG3	3:C:418:TYR:H	1.80	0.47
3:C:510:MET:HA	3:C:514:MET:SD	2.55	0.47
3:C:630:LEU:HB3	3:C:634:ALA:HB3	1.96	0.46
4:D:376:PHE:HD2	4:D:380:MET:HE2	1.78	0.46
4:D:587:GLY:O	4:D:591:GLU:HG2	2.15	0.46
5:E:545:GLN:HB2	5:E:623:LYS:NZ	2.30	0.46
3:C:466:PHE:HA	3:C:469:ARG:HH11	1.80	0.46
3:C:560:LEU:HD12	3:C:563:SER:HB2	1.97	0.46
4:D:1:MET:HE3	4:D:97:ARG:HH22	1.80	0.46
4:D:399:MET:HE2	4:D:402:LYS:HZ2	1.80	0.46
5:E:227:GLU:O	5:E:231:ASN:N	2.47	0.46
5:E:572:GLU:HA	5:E:575:LEU:HG	1.97	0.46
5:E:621:LEU:HA	5:E:624:ILE:HG12	1.97	0.46
3:C:353:VAL:HG23	3:C:361:TRP:HZ2	1.81	0.46
4:D:181:LYS:O	4:D:184:GLU:HG2	2.15	0.46
5:E:285:THR:O	5:E:289:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD11	1:A:141:TYR:CE2	2.50	0.46
1:A:88:TYR:CZ	1:A:124:LEU:HB2	2.50	0.46
1:A:121:TYR:O	1:A:125:VAL:HG23	2.16	0.46
3:C:526:LEU:HD13	3:C:567:LEU:HD21	1.98	0.46
4:D:619:PHE:HB3	4:D:650:LEU:HD13	1.98	0.46
3:C:7:LEU:HD13	5:E:104:PHE:HZ	1.79	0.46
4:D:447:ASN:O	4:D:514:LYS:NZ	2.34	0.46
3:C:78:LEU:HA	3:C:81:VAL:HG22	1.97	0.46
4:D:52:LEU:HA	4:D:54:PHE:CE2	2.51	0.46
4:D:328:PHE:CE1	4:D:393:ILE:HG13	2.49	0.46
4:D:518:ILE:HG13	4:D:519:LEU:N	2.30	0.46
5:E:346:LEU:O	5:E:350:LYS:HG2	2.16	0.46
1:A:175:TYR:O	1:A:180:GLN:NE2	2.49	0.46
3:C:238:LEU:HB3	3:C:241:PHE:HD2	1.81	0.46
4:D:442:PHE:CZ	4:D:484:LEU:HD22	2.50	0.46
5:E:59:LYS:NZ	5:E:63:ASN:HD21	2.14	0.46
1:A:117:ASN:O	1:A:121:TYR:N	2.44	0.46
1:A:153:HIS:CE1	3:C:482:GLN:NE2	2.83	0.46
3:C:21:ARG:HG2	5:E:48:LEU:HB3	1.97	0.46
3:C:91:GLY:O	3:C:95:LEU:HD12	2.16	0.46
3:C:157:ASN:ND2	3:C:214:LEU:HG	2.30	0.46
4:D:405:SER:O	4:D:409:ILE:HG13	2.15	0.46
5:E:178:TRP:HB2	5:E:182:ASP:OD2	2.15	0.46
2:B:71:MET:SD	4:D:88:PRO:HB2	2.55	0.46
3:C:44:LEU:HD23	3:C:44:LEU:HA	1.81	0.46
3:C:278:GLU:HG3	3:C:279:ASN:ND2	2.31	0.46
3:C:364:TRP:O	3:C:368:GLU:HG2	2.16	0.46
4:D:8:LEU:HA	4:D:11:CYS:SG	2.56	0.46
4:D:540:TYR:OH	4:D:541:LYS:HE3	2.16	0.46
4:D:578:ASP:O	4:D:582:VAL:HG23	2.16	0.46
5:E:535:CYS:O	5:E:539:PHE:N	2.49	0.46
5:E:579:TYR:HA	5:E:582:VAL:HG12	1.97	0.46
5:E:688:MET:HE3	5:E:688:MET:HB2	1.73	0.46
3:C:269:PHE:CG	3:C:337:THR:HG21	2.51	0.46
3:C:445:ASN:O	3:C:448:ARG:NE	2.46	0.46
3:C:596:VAL:HG11	3:C:638:LYS:HB3	1.98	0.46
4:D:345:PHE:O	4:D:348:THR:OG1	2.32	0.46
4:D:399:MET:HA	4:D:402:LYS:HD2	1.98	0.46
5:E:12:ILE:O	5:E:16:LEU:HG	2.16	0.46
1:A:160:ASN:OD1	1:A:161:ASP:N	2.49	0.45
3:C:158:ASP:O	3:C:163:ARG:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:324:LEU:H	3:C:324:LEU:HD12	1.80	0.45
4:D:452:GLY:O	4:D:492:ASP:HA	2.16	0.45
4:D:554:TYR:HD1	4:D:559:ILE:HD12	1.81	0.45
1:A:16:LEU:O	1:A:20:LEU:HG	2.16	0.45
5:E:200:MET:HG2	5:E:205:ASN:HD21	1.81	0.45
5:E:260:MET:HE1	5:E:272:LEU:HD13	1.98	0.45
1:A:72:ASP:C	1:A:75:SER:HG	2.24	0.45
3:C:231:ASN:ND2	3:C:233:ASN:OD1	2.49	0.45
3:C:245:ALA:HB2	3:C:307:VAL:HG12	1.98	0.45
3:C:520:HIS:HB3	3:C:524:LYS:NZ	2.31	0.45
3:C:533:TYR:HA	3:C:536:ILE:HG13	1.98	0.45
4:D:189:PRO:HD2	4:D:192:GLU:OE2	2.16	0.45
4:D:327:GLN:OE1	4:D:392:LYS:N	2.36	0.45
4:D:394:PHE:HB3	4:D:397:ILE:CG1	2.46	0.45
5:E:277:GLY:HA3	5:E:326:TRP:CD2	2.51	0.45
1:A:139:TYR:CZ	1:A:143:LEU:HD11	2.52	0.45
3:C:502:VAL:HG12	3:C:506:TYR:CE2	2.51	0.45
3:C:643:HIS:O	3:C:647:LYS:HG2	2.17	0.45
4:D:173:ASN:O	4:D:177:HIS:N	2.47	0.45
4:D:191:SER:OG	4:D:192:GLU:N	2.49	0.45
5:E:152:VAL:HG13	5:E:154:ILE:HD11	1.99	0.45
5:E:336:LEU:HA	5:E:339:ASN:HD22	1.81	0.45
3:C:616:GLN:HE21	3:C:620:ASP:CG	2.25	0.45
4:D:430:ASN:CG	4:D:475:GLN:HB2	2.42	0.45
4:D:636:PRO:HD2	4:D:639:ILE:HD12	1.98	0.45
3:C:124:LYS:O	3:C:127:SER:OG	2.28	0.45
4:D:172:LEU:HB3	4:D:217:GLU:OE1	2.16	0.45
4:D:616:TRP:CD1	4:D:655:PRO:HG2	2.51	0.45
3:C:37:SER:OG	5:E:24:ASN:HB3	2.16	0.45
3:C:72:LEU:H	3:C:75:LEU:HD12	1.80	0.45
3:C:154:GLY:HA2	3:C:214:LEU:HD21	1.98	0.45
3:C:240:ASN:OD1	3:C:241:PHE:N	2.44	0.45
4:D:46:LEU:HD21	4:D:135:ILE:HD11	1.99	0.45
5:E:697:LYS:O	5:E:701:LEU:HG	2.17	0.45
1:A:175:TYR:CE1	3:C:284:ILE:HG22	2.52	0.45
3:C:341:LEU:O	3:C:347:TYR:N	2.47	0.45
5:E:15:LEU:HD22	5:E:21:ILE:HD13	1.99	0.45
3:C:501:ASN:O	3:C:505:ASP:N	2.36	0.45
3:C:587:VAL:O	3:C:591:LEU:HD13	2.17	0.45
5:E:112:VAL:O	5:E:116:HIS:HD2	2.00	0.45
3:C:299:ILE:HD13	3:C:299:ILE:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:GLU:HG2	4:D:4:GLU:N	2.32	0.45
5:E:256:VAL:O	5:E:260:MET:HG2	2.17	0.45
5:E:323:VAL:HG21	5:E:326:TRP:CE2	2.52	0.45
5:E:590:LEU:HD22	5:E:652:TRP:HZ2	1.82	0.45
5:E:720:THR:O	5:E:724:ILE:HG12	2.17	0.45
1:A:28:ARG:HA	1:A:31:GLU:HB2	1.98	0.44
1:A:30:LYS:HE2	1:A:155:ARG:HH11	1.81	0.44
3:C:160:ILE:HD12	3:C:160:ILE:N	2.31	0.44
3:C:329:VAL:HA	3:C:332:SER:OG	2.17	0.44
3:C:553:SER:O	3:C:553:SER:OG	2.35	0.44
3:C:95:LEU:HD21	3:C:129:PHE:CE1	2.52	0.44
3:C:156:TYR:O	3:C:160:ILE:HB	2.17	0.44
3:C:271:PHE:HA	3:C:274:ASP:OD1	2.17	0.44
4:D:3:GLU:HG2	4:D:4:GLU:H	1.81	0.44
4:D:373:ILE:HG22	4:D:377:LEU:CD1	2.47	0.44
4:D:390:ASP:N	4:D:390:ASP:OD1	2.44	0.44
4:D:634:GLU:HG3	4:D:683:TYR:OH	2.17	0.44
5:E:16:LEU:HD22	5:E:23:LYS:H	1.82	0.44
5:E:160:MET:HE2	5:E:160:MET:HB2	1.78	0.44
5:E:639:PHE:O	5:E:643:ASP:HB2	2.17	0.44
3:C:534:PHE:HB2	3:C:598:TYR:OH	2.17	0.44
4:D:37:GLU:O	4:D:41:VAL:HG22	2.16	0.44
4:D:208:ILE:HG13	4:D:209:GLY:H	1.81	0.44
4:D:373:ILE:H	4:D:373:ILE:HD12	1.83	0.44
4:D:446:PHE:CE1	4:D:487:LEU:HD21	2.53	0.44
4:D:447:ASN:O	5:E:193:ARG:NH2	2.51	0.44
4:D:608:MET:O	4:D:611:LEU:HG	2.17	0.44
5:E:116:HIS:O	5:E:120:VAL:HG22	2.17	0.44
3:C:46:GLU:HB3	5:E:8:LYS:HG3	1.99	0.44
4:D:447:ASN:HB3	5:E:193:ARG:NE	2.32	0.44
4:D:451:ASN:OD1	4:D:451:ASN:N	2.51	0.44
3:C:484:THR:HA	3:C:487:VAL:HG12	2.00	0.44
4:D:12:ILE:HD11	4:D:16:ARG:NE	2.32	0.44
4:D:286:GLU:HA	4:D:289:PHE:CD2	2.53	0.44
4:D:564:GLN:O	4:D:567:LYS:HB2	2.18	0.44
5:E:278:PRO:HD3	5:E:326:TRP:CD1	2.53	0.44
1:A:93:LEU:HD11	1:A:107:LEU:HB3	2.00	0.44
1:A:153:HIS:O	1:A:157:LEU:HG	2.17	0.44
3:C:571:ILE:HD13	3:C:627:ILE:O	2.18	0.44
4:D:162:VAL:HG22	4:D:166:LEU:HD22	1.99	0.44
5:E:259:PHE:O	5:E:264:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:279:LEU:HD12	5:E:279:LEU:H	1.82	0.44
5:E:333:ILE:HA	5:E:336:LEU:HG	1.98	0.44
5:E:361:SER:HA	5:E:364:GLU:HB2	1.99	0.44
1:A:89:PRO:HG3	3:C:637:TYR:CE1	2.53	0.44
3:C:168:TRP:HB3	3:C:204:LEU:HD11	1.97	0.44
4:D:376:PHE:O	4:D:380:MET:HG3	2.18	0.44
5:E:281:ASN:ND2	5:E:327:THR:O	2.51	0.44
5:E:637:LEU:HD21	5:E:679:LEU:HD12	2.00	0.44
3:C:1:MET:SD	3:C:10:ILE:HD12	2.58	0.44
3:C:507:GLU:HA	3:C:510:MET:HE2	1.99	0.44
4:D:187:LYS:HB3	4:D:187:LYS:HE3	1.44	0.44
4:D:438:LEU:CD1	4:D:473:MET:HE3	2.47	0.44
4:D:673:LEU:HD21	5:E:573:THR:HG23	1.98	0.44
5:E:103:ASN:OD1	5:E:104:PHE:N	2.51	0.44
3:C:588:LYS:O	3:C:628:LEU:HD23	2.18	0.44
1:A:109:ILE:HG13	1:A:109:ILE:O	2.18	0.43
1:A:132:LEU:HD11	2:B:50:GLN:NE2	2.32	0.43
3:C:636:ASN:OD1	3:C:639:CYS:N	2.47	0.43
3:C:675:LYS:HG3	3:C:676:GLU:OE2	2.17	0.43
3:C:683:LEU:HG	3:C:684:LYS:O	2.18	0.43
4:D:50:LYS:HG3	4:D:51:ASN:N	2.31	0.43
4:D:131:CYS:O	4:D:135:ILE:HG12	2.17	0.43
4:D:168:PRO:HB3	4:D:217:GLU:HA	2.00	0.43
4:D:332:PHE:HA	4:D:336:SER:O	2.17	0.43
5:E:167:TYR:HE1	5:E:179:PHE:CZ	2.35	0.43
5:E:336:LEU:HD12	5:E:337:LEU:N	2.33	0.43
3:C:227:LEU:CB	3:C:417:ARG:HD2	2.47	0.43
4:D:270:SER:O	4:D:273:LEU:HG	2.18	0.43
4:D:501:LEU:HD13	4:D:528:ILE:HG12	1.99	0.43
3:C:24:LEU:HD11	5:E:41:LEU:HD22	1.99	0.43
4:D:71:THR:O	4:D:75:VAL:HG23	2.19	0.43
4:D:178:LEU:HD13	4:D:180:PHE:HE2	1.83	0.43
4:D:338:LYS:HD3	4:D:362:LEU:HD13	1.99	0.43
4:D:462:ALA:O	4:D:466:LEU:HG	2.19	0.43
5:E:356:ILE:O	5:E:359:ILE:HG22	2.18	0.43
3:C:72:LEU:O	3:C:75:LEU:HB2	2.19	0.43
4:D:638:GLU:HG2	4:D:639:ILE:H	1.83	0.43
5:E:211:SER:HA	5:E:214:LYS:HE3	2.00	0.43
5:E:544:CYS:O	5:E:548:VAL:HG13	2.18	0.43
1:A:81:ILE:O	1:A:85:THR:HG23	2.19	0.43
3:C:148:LEU:O	3:C:152:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:461:LEU:HD21	3:C:579:ILE:HG23	1.99	0.43
3:C:624:LEU:HD13	3:C:627:ILE:HD12	2.00	0.43
4:D:156:THR:HA	4:D:159:ILE:HD12	1.99	0.43
4:D:399:MET:HE2	4:D:402:LYS:NZ	2.33	0.43
4:D:446:PHE:HE1	4:D:487:LEU:HD21	1.83	0.43
5:E:88:ARG:HG3	5:E:178:TRP:HZ3	1.83	0.43
2:B:16:SER:OG	4:D:15:SER:HB2	2.19	0.43
3:C:157:ASN:O	3:C:162:GLN:N	2.51	0.43
3:C:468:TYR:O	3:C:472:LYS:HG2	2.19	0.43
4:D:439:VAL:HG12	4:D:443:TRP:CD1	2.54	0.43
5:E:79:ASN:HA	5:E:82:TYR:HD2	1.84	0.43
5:E:202:GLU:O	5:E:206:LEU:HA	2.18	0.43
5:E:492:VAL:HA	5:E:549:ASP:OD1	2.18	0.43
5:E:532:MET:HE3	5:E:550:MET:SD	2.58	0.43
5:E:610:LEU:HD13	5:E:673:ASN:CG	2.44	0.43
4:D:437:LEU:HA	4:D:440:LYS:CD	2.48	0.43
4:D:634:GLU:HG3	4:D:683:TYR:CZ	2.53	0.43
5:E:235:PHE:CD1	5:E:235:PHE:N	2.85	0.43
5:E:329:SER:C	5:E:331:LYS:H	2.27	0.43
5:E:342:LEU:C	5:E:344:TYR:H	2.26	0.43
1:A:7:GLN:HA	1:A:10:GLU:HG2	2.01	0.43
1:A:148:ILE:HD12	1:A:148:ILE:HA	1.91	0.43
2:B:9:PHE:CD2	4:D:104:LEU:HD11	2.53	0.43
3:C:211:TYR:HB2	3:C:236:PRO:HB3	2.01	0.43
3:C:252:PHE:HZ	3:C:268:TYR:HB3	1.84	0.43
3:C:327:LEU:HD23	3:C:330:LEU:HD12	2.00	0.43
3:C:406:PRO:O	3:C:409:ASP:HB2	2.19	0.43
3:C:672:THR:O	3:C:675:LYS:HG2	2.19	0.43
4:D:117:LEU:CD1	4:D:122:GLU:HG2	2.49	0.43
4:D:430:ASN:ND2	4:D:473:MET:HA	2.33	0.43
5:E:88:ARG:HH12	5:E:183:MET:HA	1.84	0.43
5:E:724:ILE:HD12	5:E:741:ILE:HG12	1.99	0.43
3:C:172:PHE:HE2	3:C:240:ASN:HB3	1.83	0.43
3:C:663:PRO:HA	3:C:666:ILE:HD12	2.00	0.43
4:D:399:MET:O	4:D:403:LEU:HG	2.18	0.43
5:E:563:ILE:O	5:E:567:THR:HG22	2.19	0.43
3:C:251:ARG:HH21	3:C:275:TYR:HD1	1.67	0.43
3:C:392:ASN:O	3:C:395:LYS:HB2	2.19	0.43
3:C:434:TYR:O	3:C:438:ILE:HG12	2.18	0.43
4:D:273:LEU:O	4:D:277:VAL:HG12	2.19	0.43
4:D:411:LEU:HD11	4:D:437:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:447:ASN:C	4:D:514:LYS:HZ1	2.23	0.43
4:D:465:THR:O	4:D:468:ILE:HB	2.19	0.43
1:A:90:GLU:HB2	1:A:113:ASP:H	1.84	0.42
3:C:292:ASN:HB2	3:C:294:LEU:HG	2.01	0.42
4:D:656:LEU:O	4:D:659:VAL:HG12	2.18	0.42
5:E:110:THR:O	5:E:114:THR:HG23	2.18	0.42
5:E:177:ALA:O	5:E:181:LEU:HB2	2.19	0.42
5:E:545:GLN:NE2	5:E:549:ASP:OD1	2.51	0.42
1:A:89:PRO:HB3	3:C:637:TYR:CG	2.55	0.42
3:C:530:LEU:HD13	3:C:598:TYR:CD2	2.54	0.42
3:C:589:ASN:HD21	3:C:636:ASN:ND2	2.17	0.42
3:C:594:VAL:HA	3:C:597:ASN:ND2	2.35	0.42
4:D:484:LEU:O	4:D:487:LEU:HB3	2.19	0.42
2:B:56:GLU:OE2	2:B:56:GLU:N	2.37	0.42
3:C:62:LEU:HB3	3:C:75:LEU:CD2	2.49	0.42
3:C:80:LYS:O	3:C:84:GLN:HG3	2.20	0.42
4:D:229:GLU:O	4:D:233:THR:OG1	2.31	0.42
5:E:135:THR:OG1	5:E:136:GLU:N	2.52	0.42
2:B:18:GLN:O	2:B:22:LEU:HD23	2.19	0.42
3:C:99:GLU:HB2	3:C:152:VAL:HG23	2.01	0.42
3:C:357:SER:OG	3:C:360:VAL:HG23	2.18	0.42
3:C:423:CYS:SG	3:C:498:LEU:HD13	2.60	0.42
3:C:597:ASN:O	3:C:601:GLU:HG2	2.19	0.42
4:D:4:GLU:OE2	4:D:97:ARG:NE	2.52	0.42
4:D:409:ILE:O	4:D:413:MET:N	2.49	0.42
5:E:187:ASP:O	5:E:191:GLN:HG3	2.19	0.42
5:E:351:VAL:O	5:E:354:SER:OG	2.32	0.42
5:E:695:MET:HA	5:E:698:PHE:CE1	2.54	0.42
2:B:30:VAL:HG12	2:B:46:PHE:HE2	1.84	0.42
4:D:94:THR:O	4:D:96:THR:N	2.52	0.42
4:D:138:THR:HB	4:D:141:LEU:HG	2.00	0.42
4:D:532:LEU:O	4:D:536:ASN:N	2.48	0.42
5:E:545:GLN:HB2	5:E:623:LYS:HZ3	1.85	0.42
1:A:157:LEU:HA	1:A:160:ASN:ND2	2.33	0.42
3:C:4:ILE:HG12	5:E:111:TYR:CD1	2.55	0.42
3:C:52:ILE:HA	3:C:65:LEU:HD11	2.01	0.42
3:C:238:LEU:HB2	3:C:306:TYR:CE2	2.54	0.42
3:C:497:SER:OG	3:C:498:LEU:N	2.53	0.42
3:C:562:ASN:O	3:C:566:VAL:HG23	2.20	0.42
3:C:564:ILE:HG22	3:C:568:ARG:HH12	1.84	0.42
3:C:596:VAL:HG22	3:C:621:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:LEU:HB3	4:D:117:LEU:HD21	2.02	0.42
4:D:381:TYR:CE1	4:D:426:PHE:HZ	2.37	0.42
4:D:498:SER:OG	4:D:535:LEU:HG	2.20	0.42
4:D:500:ASN:H	4:D:531:ASN:ND2	2.16	0.42
4:D:646:ILE:O	4:D:650:LEU:HG	2.19	0.42
5:E:359:ILE:O	5:E:362:ILE:HB	2.19	0.42
5:E:638:ASN:HA	5:E:688:MET:SD	2.59	0.42
1:A:175:TYR:OH	3:C:288:HIS:HB3	2.20	0.42
3:C:4:ILE:O	3:C:8:LEU:HG	2.20	0.42
3:C:339:LYS:HE3	3:C:339:LYS:HB3	1.95	0.42
3:C:581:LEU:O	3:C:585:LEU:HG	2.20	0.42
4:D:6:LEU:O	4:D:25:LEU:HD21	2.19	0.42
4:D:43:TRP:CD2	4:D:44:PRO:HD2	2.55	0.42
4:D:121:GLU:O	4:D:124:LEU:HG	2.19	0.42
5:E:97:TYR:OH	5:E:105:GLN:HB3	2.20	0.42
2:B:33:GLN:C	2:B:36:SER:H	2.28	0.42
3:C:173:ASP:CG	3:C:243:SER:HB3	2.44	0.42
3:C:315:VAL:HG23	3:C:355:LEU:HD22	2.01	0.42
3:C:444:LEU:HD12	3:C:444:LEU:HA	1.86	0.42
3:C:514:MET:HA	3:C:517:SER:OG	2.19	0.42
3:C:596:VAL:O	3:C:600:THR:HG22	2.20	0.42
4:D:14:ALA:O	4:D:44:PRO:HD3	2.19	0.42
4:D:122:GLU:O	4:D:126:GLU:HG2	2.20	0.42
4:D:218:LEU:HD11	4:D:231:PHE:CE2	2.55	0.42
5:E:40:ASP:OD1	5:E:41:LEU:N	2.53	0.42
5:E:553:LEU:HD23	5:E:553:LEU:HA	1.87	0.42
1:A:89:PRO:HB3	3:C:637:TYR:CE2	2.54	0.42
2:B:81:SER:O	2:B:85:ARG:HB2	2.19	0.42
3:C:403:TYR:CD2	3:C:404:LEU:HD12	2.54	0.42
4:D:501:LEU:CD1	4:D:528:ILE:HA	2.48	0.42
5:E:139:ILE:HD11	5:E:212:MET:SD	2.60	0.42
5:E:722:GLU:HG2	5:E:726:TRP:CD1	2.55	0.42
1:A:102:ASP:OD1	1:A:102:ASP:N	2.51	0.42
1:A:174:ASP:O	1:A:177:LYS:HG2	2.20	0.42
3:C:174:GLN:NE2	3:C:177:LEU:HD11	2.34	0.42
3:C:238:LEU:HB2	3:C:306:TYR:CZ	2.55	0.42
3:C:396:LEU:O	3:C:400:ILE:HG12	2.20	0.42
3:C:530:LEU:HD13	3:C:598:TYR:CE2	2.55	0.42
3:C:607:ASN:OD1	3:C:608:LYS:N	2.53	0.42
4:D:586:PHE:HE2	4:D:642:LEU:HD13	1.85	0.42
5:E:299:LEU:HD13	5:E:340:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:344:TYR:CE2	5:E:514:HIS:HB2	2.55	0.42
4:D:553:ILE:O	4:D:556:SER:OG	2.34	0.41
5:E:336:LEU:HA	5:E:339:ASN:HB2	2.01	0.41
5:E:492:VAL:HG13	5:E:549:ASP:HA	2.02	0.41
5:E:494:GLN:HA	5:E:497:LYS:HE2	2.01	0.41
5:E:610:LEU:HD13	5:E:673:ASN:ND2	2.35	0.41
3:C:304:ILE:HB	3:C:347:TYR:CD1	2.55	0.41
3:C:393:PHE:CE2	3:C:397:ILE:HD11	2.55	0.41
3:C:435:LEU:HD12	3:C:506:TYR:CZ	2.55	0.41
3:C:544:MET:SD	3:C:612:ASN:ND2	2.93	0.41
4:D:172:LEU:N	4:D:217:GLU:OE2	2.53	0.41
4:D:180:PHE:HD1	4:D:188:MET:HE1	1.85	0.41
4:D:188:MET:HE3	4:D:188:MET:HB2	1.77	0.41
4:D:372:GLU:HG3	4:D:374:SER:OG	2.20	0.41
4:D:501:LEU:HD11	4:D:528:ILE:HG23	2.03	0.41
5:E:146:GLU:HB3	5:E:151:LYS:HB3	2.02	0.41
3:C:14:ILE:HG23	5:E:52:LEU:HD11	2.03	0.41
3:C:325:LYS:HD2	3:C:367:TYR:CZ	2.56	0.41
3:C:685:ASP:HA	3:C:688:ILE:HD12	2.01	0.41
4:D:141:LEU:HA	4:D:141:LEU:HD23	1.79	0.41
4:D:161:TRP:CH2	4:D:166:LEU:HD11	2.55	0.41
4:D:638:GLU:HG2	4:D:639:ILE:N	2.36	0.41
5:E:211:SER:O	5:E:212:MET:C	2.62	0.41
1:A:91:LEU:HD21	1:A:93:LEU:HB2	2.01	0.41
3:C:84:GLN:CD	3:C:135:ILE:HG12	2.46	0.41
3:C:181:TRP:CZ2	3:C:244:LEU:HD22	2.56	0.41
3:C:338:ASP:O	3:C:342:LEU:HD23	2.19	0.41
3:C:588:LYS:HD3	3:C:628:LEU:O	2.20	0.41
4:D:420:GLU:HA	4:D:423:ILE:CG2	2.43	0.41
4:D:531:ASN:O	4:D:534:GLU:HB3	2.20	0.41
4:D:622:MET:HE2	4:D:622:MET:HB2	1.81	0.41
5:E:96:ALA:O	5:E:100:GLN:HG2	2.21	0.41
5:E:698:PHE:HZ	5:E:726:TRP:CG	2.38	0.41
1:A:69:LYS:HA	1:A:69:LYS:HD3	1.83	0.41
2:B:73:SER:HA	2:B:76:GLU:HG3	2.03	0.41
3:C:10:ILE:HD13	5:E:58:LEU:HB2	2.03	0.41
3:C:248:PHE:HB2	3:C:275:TYR:CE1	2.55	0.41
3:C:434:TYR:CZ	3:C:438:ILE:HG21	2.55	0.41
3:C:453:GLU:HA	3:C:456:GLN:HE21	1.85	0.41
3:C:508:LYS:HB2	3:C:508:LYS:HE3	1.85	0.41
4:D:42:LEU:HD23	4:D:42:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:77:VAL:O	4:D:80:LEU:HG	2.20	0.41
1:A:16:LEU:HB3	1:A:141:TYR:CE2	2.56	0.41
3:C:256:PHE:HE2	3:C:271:PHE:CD2	2.38	0.41
3:C:367:TYR:CE1	3:C:371:MET:HE3	2.55	0.41
4:D:434:ILE:O	4:D:437:LEU:HG	2.20	0.41
5:E:352:LEU:HD21	5:E:523:LYS:HB3	2.02	0.41
5:E:574:LYS:HA	5:E:574:LYS:HD3	1.81	0.41
3:C:26:SER:O	3:C:30:ASN:HB2	2.20	0.41
3:C:149:LYS:O	3:C:153:THR:OG1	2.27	0.41
3:C:182:ASP:OD2	3:C:247:ASN:ND2	2.54	0.41
3:C:225:ARG:NH2	3:C:417:ARG:HB2	2.36	0.41
3:C:518:ILE:O	3:C:522:ILE:HG12	2.20	0.41
3:C:533:TYR:CD1	3:C:560:LEU:HB2	2.56	0.41
4:D:447:ASN:HB3	5:E:193:ARG:CZ	2.51	0.41
4:D:555:ASP:OD1	4:D:561:ARG:NH1	2.53	0.41
5:E:77:LEU:N	5:E:80:CYS:SG	2.80	0.41
5:E:489:HIS:HB2	5:E:625:ARG:NH1	2.36	0.41
5:E:553:LEU:O	5:E:557:ASP:N	2.48	0.41
3:C:62:LEU:HD11	5:E:5:PHE:HZ	1.86	0.41
3:C:272:LEU:HD13	3:C:311:ILE:HD13	2.03	0.41
3:C:328:ILE:HD12	3:C:403:TYR:OH	2.21	0.41
3:C:426:ILE:O	3:C:430:LEU:HB2	2.21	0.41
3:C:621:PHE:CE2	3:C:642:LEU:HD22	2.55	0.41
4:D:181:LYS:HG2	4:D:183:ASN:H	1.85	0.41
4:D:373:ILE:O	4:D:377:LEU:HD12	2.21	0.41
5:E:532:MET:HG2	5:E:550:MET:CE	2.50	0.41
5:E:610:LEU:HD22	5:E:673:ASN:HB3	2.02	0.41
5:E:710:PHE:HB2	5:E:715:PHE:HD2	1.85	0.41
1:A:164:ARG:HD3	3:C:348:HIS:CD2	2.56	0.41
3:C:24:LEU:HD12	3:C:24:LEU:HA	1.87	0.41
3:C:446:GLU:OE1	3:C:447:THR:N	2.54	0.41
3:C:526:LEU:O	3:C:530:LEU:N	2.52	0.41
3:C:672:THR:O	3:C:676:GLU:HG2	2.21	0.41
4:D:85:SER:O	4:D:88:PRO:HD2	2.21	0.41
4:D:117:LEU:HD21	4:D:123:TRP:CD1	2.50	0.41
4:D:150:LYS:HB3	4:D:153:VAL:HG11	2.03	0.41
4:D:190:ASP:OD1	4:D:190:ASP:N	2.53	0.41
4:D:222:LEU:O	4:D:227:LYS:N	2.53	0.41
4:D:505:HIS:HD2	5:E:275:GLU:OE1	2.04	0.41
4:D:514:LYS:H	4:D:517:ASN:HD21	1.68	0.41
5:E:698:PHE:HA	5:E:701:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:705:GLU:O	5:E:709:MET:HG3	2.20	0.41
5:E:724:ILE:HD12	5:E:741:ILE:HG23	2.03	0.41
5:E:749:GLY:O	5:E:752:LEU:HG	2.21	0.41
3:C:121:LEU:HD22	3:C:124:LYS:NZ	2.36	0.41
3:C:260:SER:HB3	3:C:314:LYS:NZ	2.36	0.41
3:C:394:VAL:HG12	3:C:398:ASN:ND2	2.36	0.41
3:C:454:LEU:O	3:C:457:THR:OG1	2.35	0.41
3:C:458:MET:HE2	3:C:458:MET:HB3	1.83	0.41
4:D:52:LEU:HD23	4:D:54:PHE:HE2	1.84	0.41
4:D:90:ILE:O	4:D:92:SER:N	2.53	0.41
4:D:227:LYS:HA	4:D:230:THR:HG22	2.02	0.41
4:D:540:TYR:HA	4:D:576:HIS:CE1	2.56	0.41
5:E:65:ILE:O	5:E:69:LYS:HG3	2.20	0.41
5:E:188:SER:HA	5:E:191:GLN:OE1	2.21	0.41
5:E:279:LEU:HA	5:E:282:THR:HG22	2.01	0.41
5:E:586:ILE:O	5:E:590:LEU:HG	2.21	0.41
5:E:670:LEU:O	5:E:674:THR:N	2.54	0.41
3:C:55:VAL:O	3:C:61:GLY:HA3	2.21	0.40
3:C:161:ILE:O	3:C:165:ALA:HB3	2.18	0.40
3:C:459:ALA:HA	3:C:462:GLN:HG2	2.04	0.40
3:C:644:GLU:HB3	3:C:680:ILE:HD12	2.02	0.40
4:D:56:ARG:HH22	4:D:148:THR:HG23	1.85	0.40
4:D:154:LEU:HD13	4:D:158:PHE:CE1	2.56	0.40
4:D:266:ASN:HB3	4:D:269:ALA:HB3	2.02	0.40
4:D:494:LEU:HA	4:D:497:TYR:HD2	1.86	0.40
5:E:276:LEU:HA	5:E:279:LEU:HD13	2.02	0.40
5:E:335:ASP:O	5:E:339:ASN:N	2.54	0.40
3:C:73:GLN:H	3:C:73:GLN:CD	2.29	0.40
3:C:558:ALA:O	3:C:561:VAL:HG12	2.21	0.40
4:D:48:ASP:CG	4:D:49:PRO:HD2	2.46	0.40
4:D:434:ILE:HG23	4:D:435:TYR:N	2.36	0.40
4:D:446:PHE:CE2	4:D:519:LEU:HD11	2.53	0.40
5:E:88:ARG:HG3	5:E:178:TRP:CZ3	2.56	0.40
5:E:593:PHE:HB3	5:E:652:TRP:HH2	1.86	0.40
3:C:129:PHE:CE1	3:C:149:LYS:HE3	2.56	0.40
3:C:162:GLN:O	3:C:166:THR:HG23	2.22	0.40
3:C:180:GLN:O	3:C:186:PHE:HB2	2.22	0.40
3:C:390:SER:O	3:C:394:VAL:HG23	2.22	0.40
4:D:310:ASP:OD1	4:D:310:ASP:N	2.54	0.40
4:D:625:PHE:N	4:D:643:GLN:HE22	2.20	0.40
4:D:654:CYS:O	5:E:360:ARG:NH1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:TRP:CG	5:E:179:PHE:N	2.90	0.40
5:E:214:LYS:HG3	5:E:215:ASN:N	2.36	0.40
2:B:75:TYR:CG	4:D:88:PRO:HB3	2.56	0.40
3:C:323:ASP:O	3:C:327:LEU:HG	2.22	0.40
4:D:33:SER:O	4:D:37:GLU:HG3	2.21	0.40
4:D:142:TYR:HD2	4:D:145:LEU:HD22	1.85	0.40
4:D:150:LYS:O	4:D:153:VAL:HG22	2.21	0.40
5:E:311:ASN:ND2	5:E:333:ILE:HB	2.37	0.40
5:E:604:ALA:HA	5:E:608:LYS:HD2	2.03	0.40
5:E:640:LEU:O	5:E:644:CYS:HB2	2.21	0.40
1:A:116:MET:HE1	1:A:121:TYR:HA	2.03	0.40
1:A:122:ALA:O	1:A:126:GLU:HG2	2.22	0.40
3:C:506:TYR:O	3:C:510:MET:HG2	2.22	0.40
4:D:410:LEU:HA	4:D:413:MET:HB2	2.04	0.40
4:D:540:TYR:O	4:D:576:HIS:ND1	2.51	0.40
5:E:131:PHE:O	5:E:141:PHE:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/275 (60%)	161 (97%)	5 (3%)	0	100	100
2	B	83/212 (39%)	81 (98%)	2 (2%)	0	100	100
3	C	699/701 (100%)	639 (91%)	59 (8%)	1 (0%)	48	83
4	D	682/709 (96%)	634 (93%)	46 (7%)	2 (0%)	36	71
5	E	639/783 (82%)	612 (96%)	27 (4%)	0	100	100
All	All	2269/2680 (85%)	2127 (94%)	139 (6%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	51	ASN
4	D	95	THR
3	C	226	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/258 (63%)	161 (99%)	1 (1%)	78	80
2	B	80/189 (42%)	80 (100%)	0	100	100
3	C	658/658 (100%)	657 (100%)	1 (0%)	87	85
4	D	636/657 (97%)	629 (99%)	7 (1%)	65	74
5	E	603/724 (83%)	600 (100%)	3 (0%)	81	81
All	All	2139/2486 (86%)	2127 (99%)	12 (1%)	76	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
3	C	5	ASP
4	D	8	LEU
4	D	187	LYS
4	D	382	GLU
4	D	420	GLU
4	D	479	THR
4	D	505	HIS
4	D	598	GLU
5	E	17	LYS
5	E	190	GLU
5	E	271	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	153	HIS
2	B	21	ASN
2	B	51	HIS
2	B	65	HIS
3	C	9	ASN
3	C	30	ASN
3	C	50	GLN
3	C	73	GLN
3	C	85	GLN
3	C	157	ASN
3	C	167	ASN
3	C	174	GLN
3	C	220	ASN
3	C	285	ASN
3	C	340	ASN
3	C	382	ASN
3	C	398	ASN
3	C	456	GLN
3	C	465	ASN
3	C	482	GLN
3	C	565	ASN
3	C	589	ASN
3	C	597	ASN
3	C	611	GLN
3	C	612	ASN
3	C	615	ASN
3	C	657	ASN
4	D	99	ASN
4	D	105	GLN
4	D	173	ASN
4	D	284	ASN
4	D	317	GLN
4	D	430	ASN
4	D	447	ASN
4	D	448	ASN
4	D	502	ASN
4	D	505	HIS
4	D	517	ASN
4	D	531	ASN
4	D	601	GLN
5	E	30	ASN
5	E	63	ASN

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Mol	Chain	Res	Type
5	E	73	ASN
5	E	106	GLN
5	E	116	HIS
5	E	137	ASN
5	E	175	ASN
5	E	205	ASN
5	E	228	ASN
5	E	231	ASN
5	E	290	ASN
5	E	339	ASN
5	E	514	HIS
5	E	545	GLN
5	E	642	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

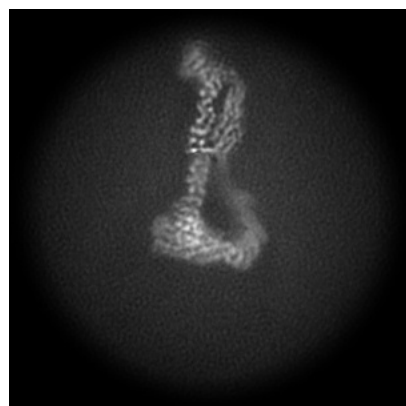
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28204. These allow visual inspection of the internal detail of the map and identification of artifacts.

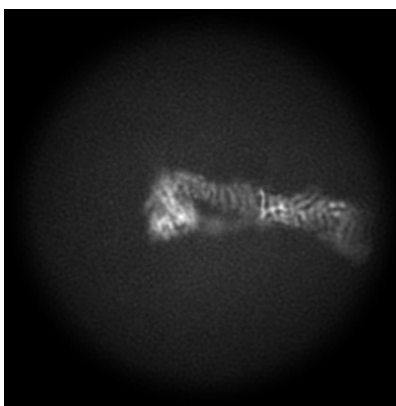
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

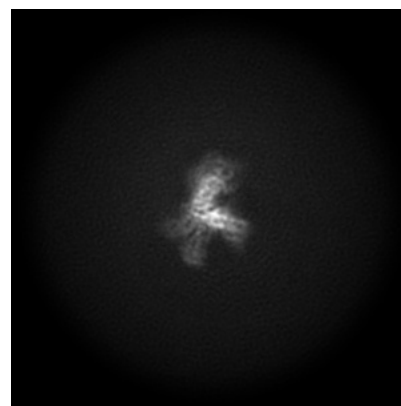
6.1.1 Primary map



X

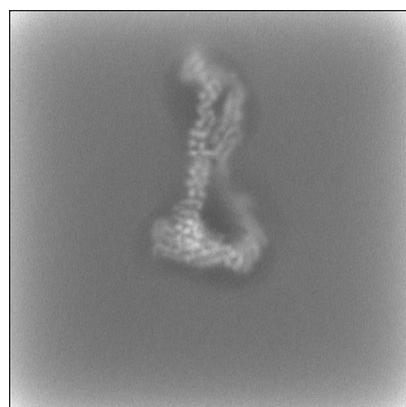


Y

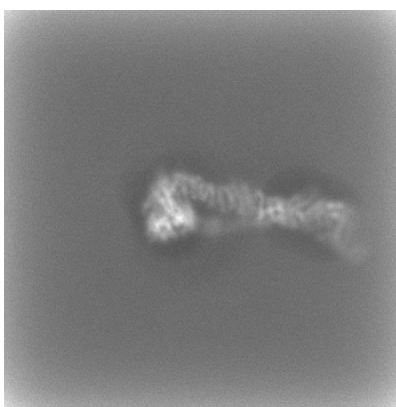


Z

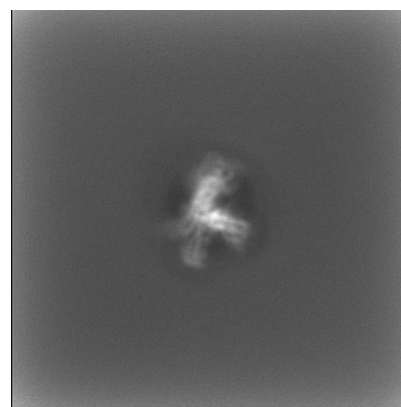
6.1.2 Raw map



X



Y



Z

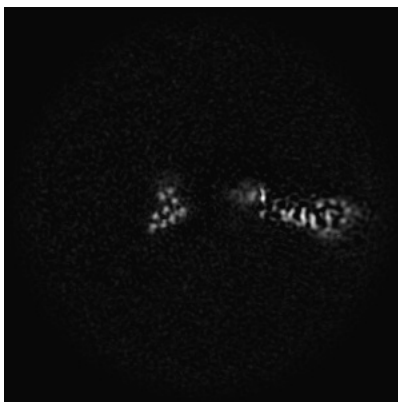
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

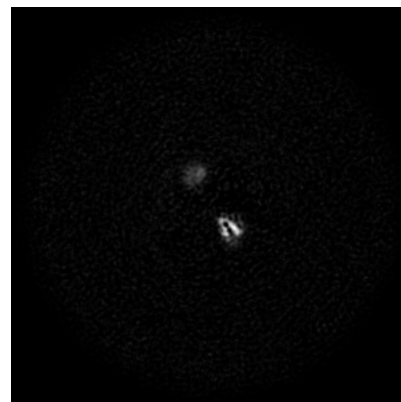
6.2.1 Primary map



X Index: 200

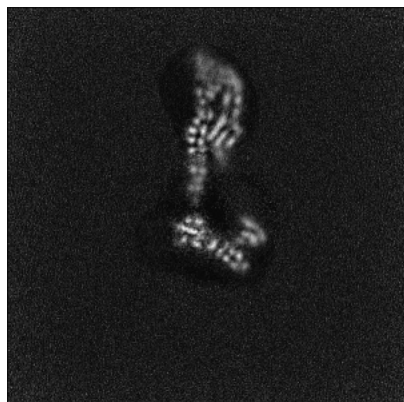


Y Index: 200

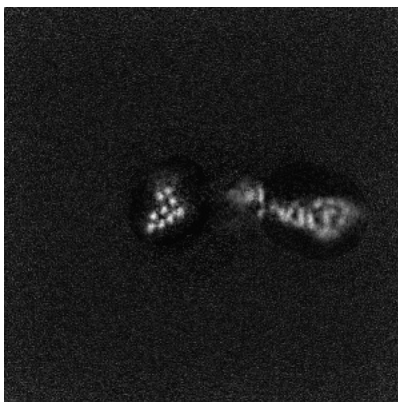


Z Index: 200

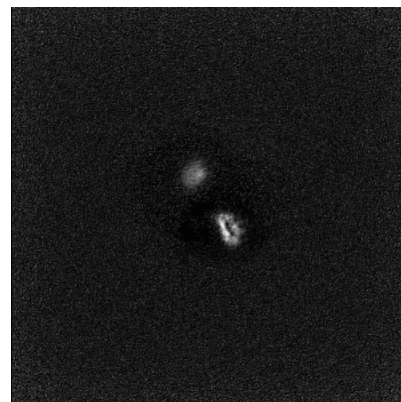
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

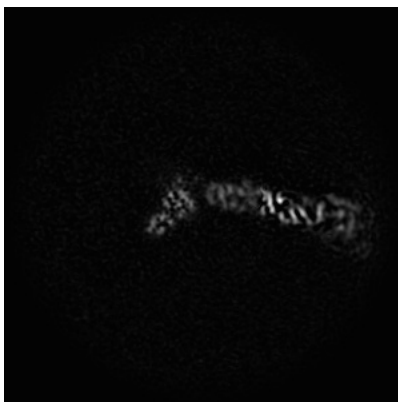
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

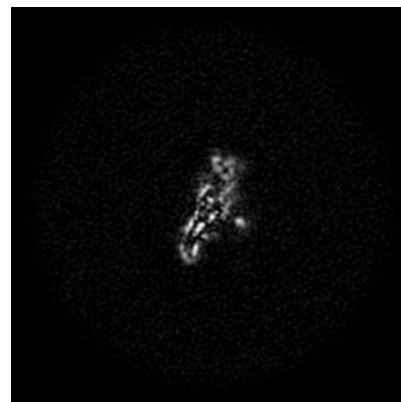
6.3.1 Primary map



X Index: 200

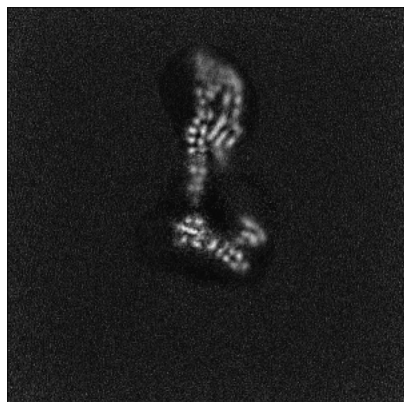


Y Index: 192

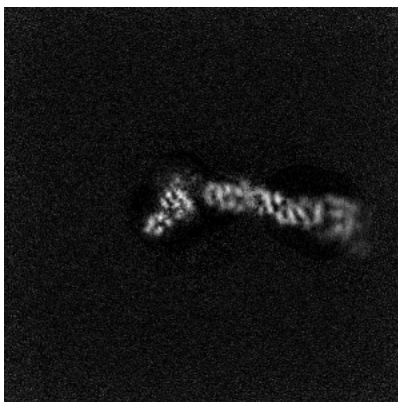


Z Index: 164

6.3.2 Raw map



X Index: 200



Y Index: 192

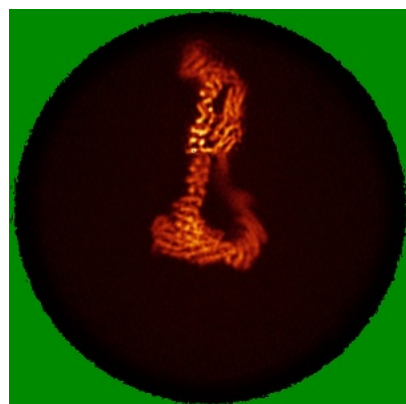


Z Index: 161

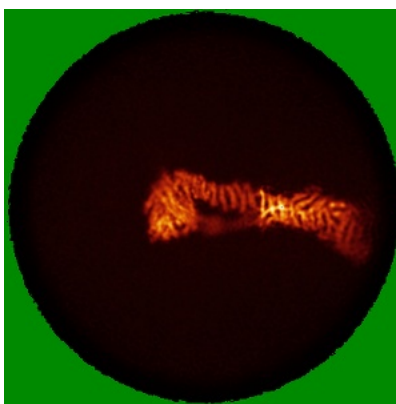
The images above show the largest variance slices of the map in three orthogonal directions.

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

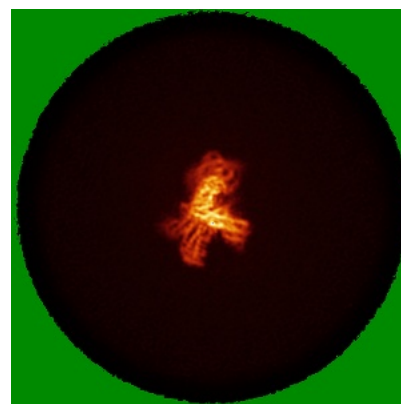
6.4.1 Primary map



X

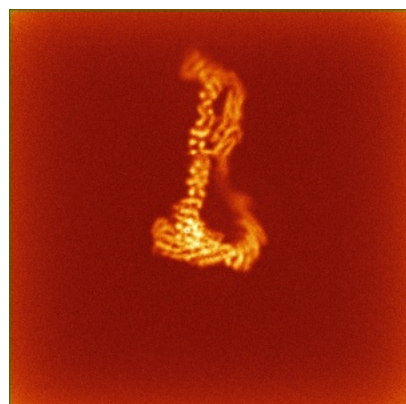


Y

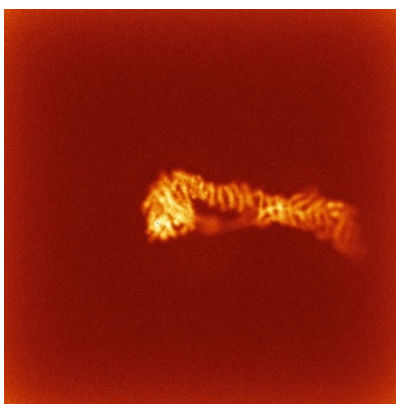


Z

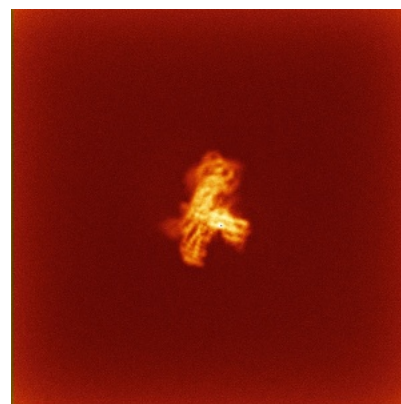
6.4.2 Raw map



X



Y

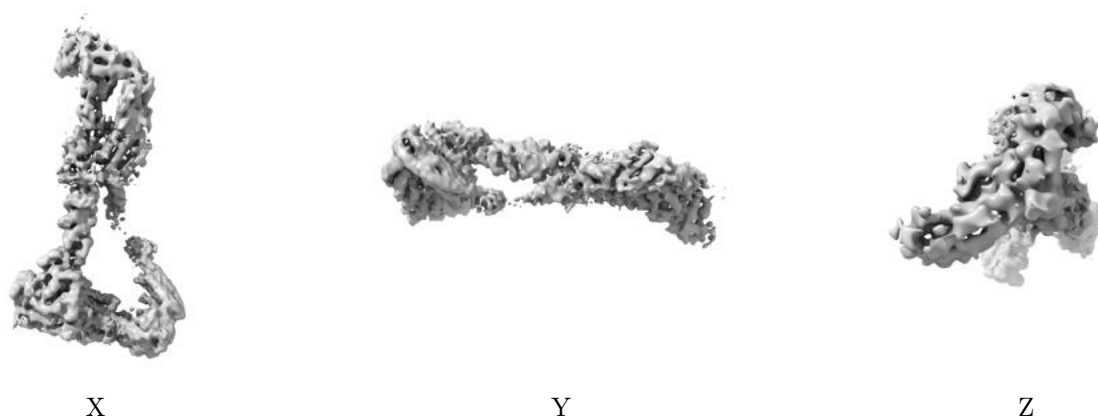


Z

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

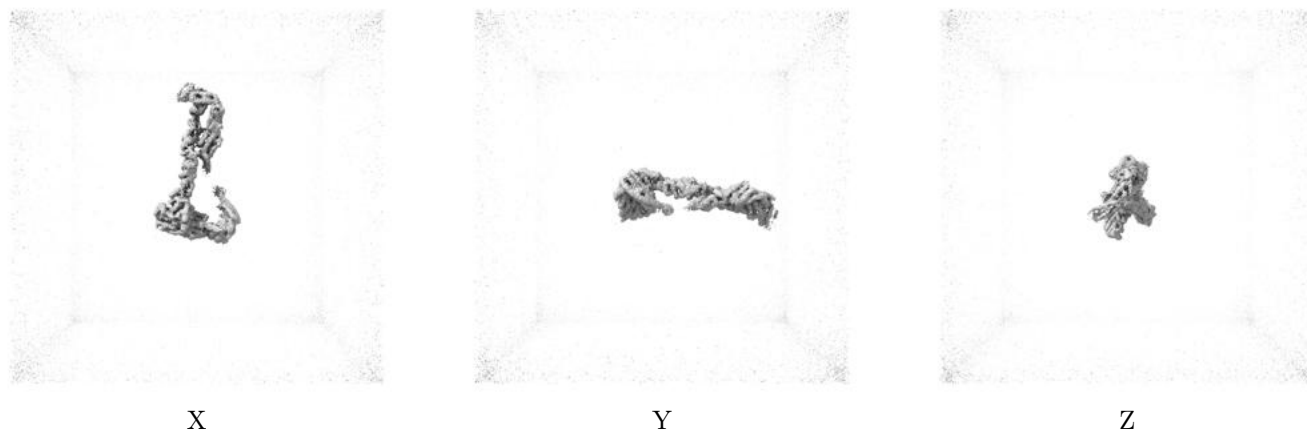
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.186. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

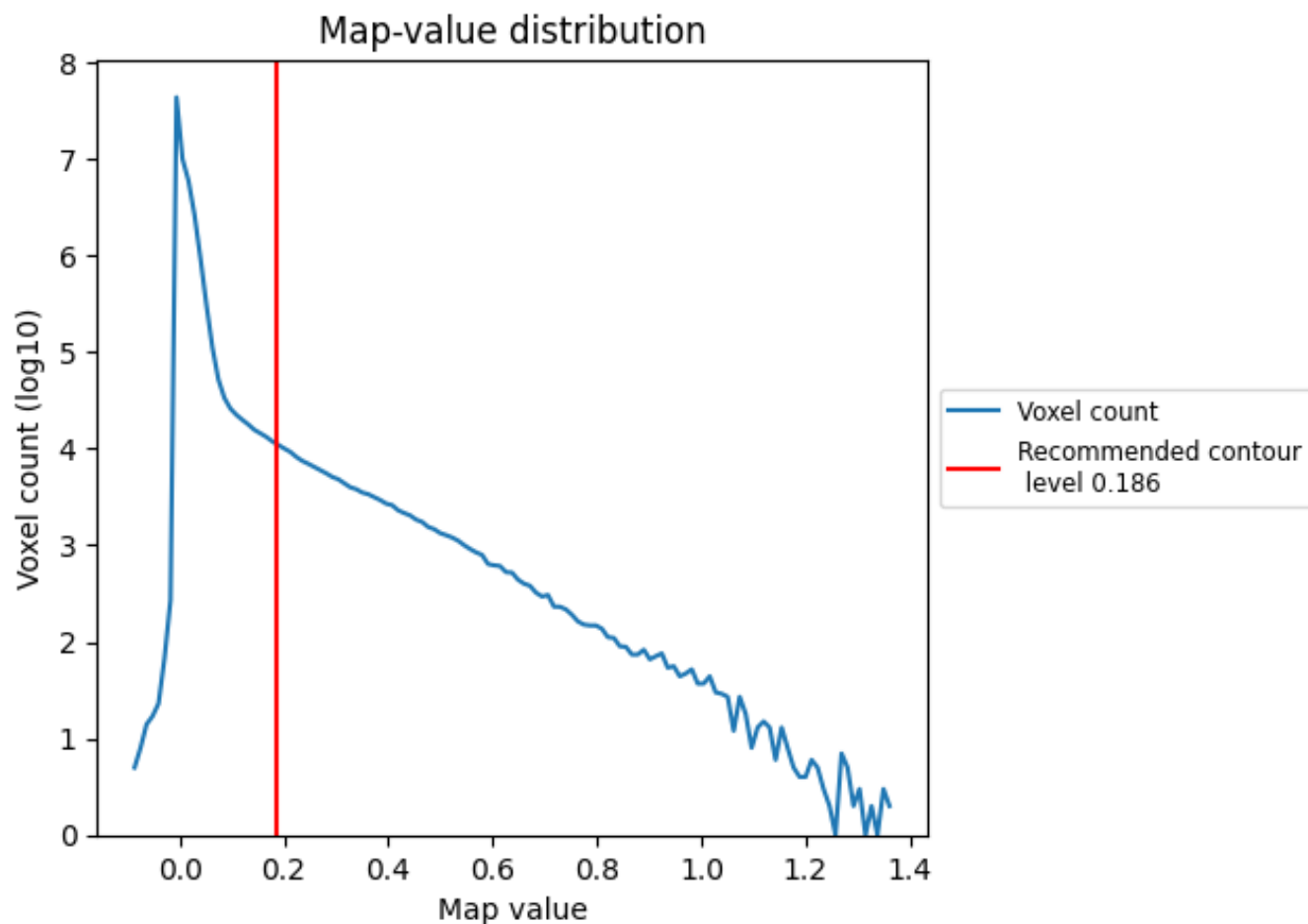
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

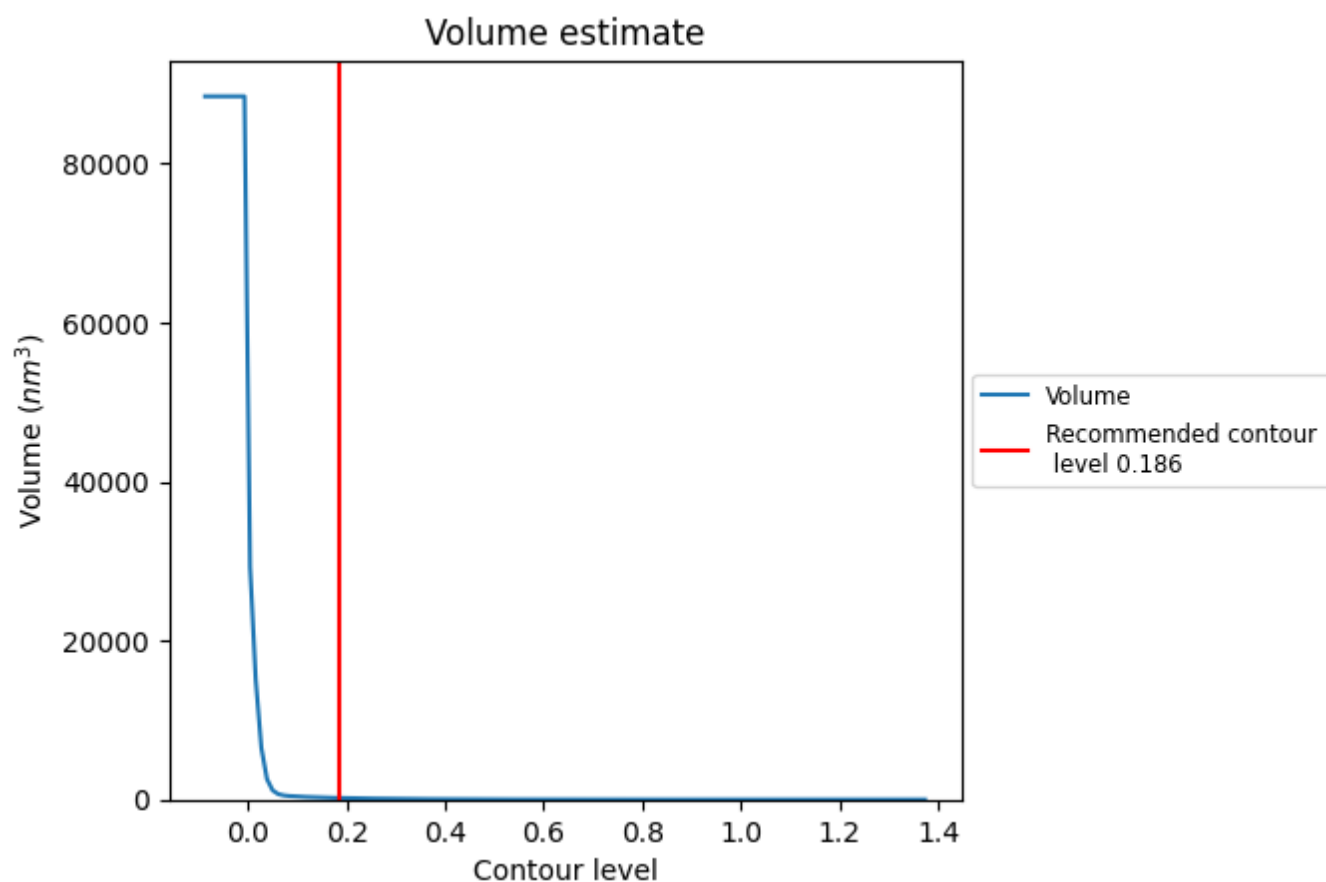
This section contains the results of statistical analysis of the map.

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.

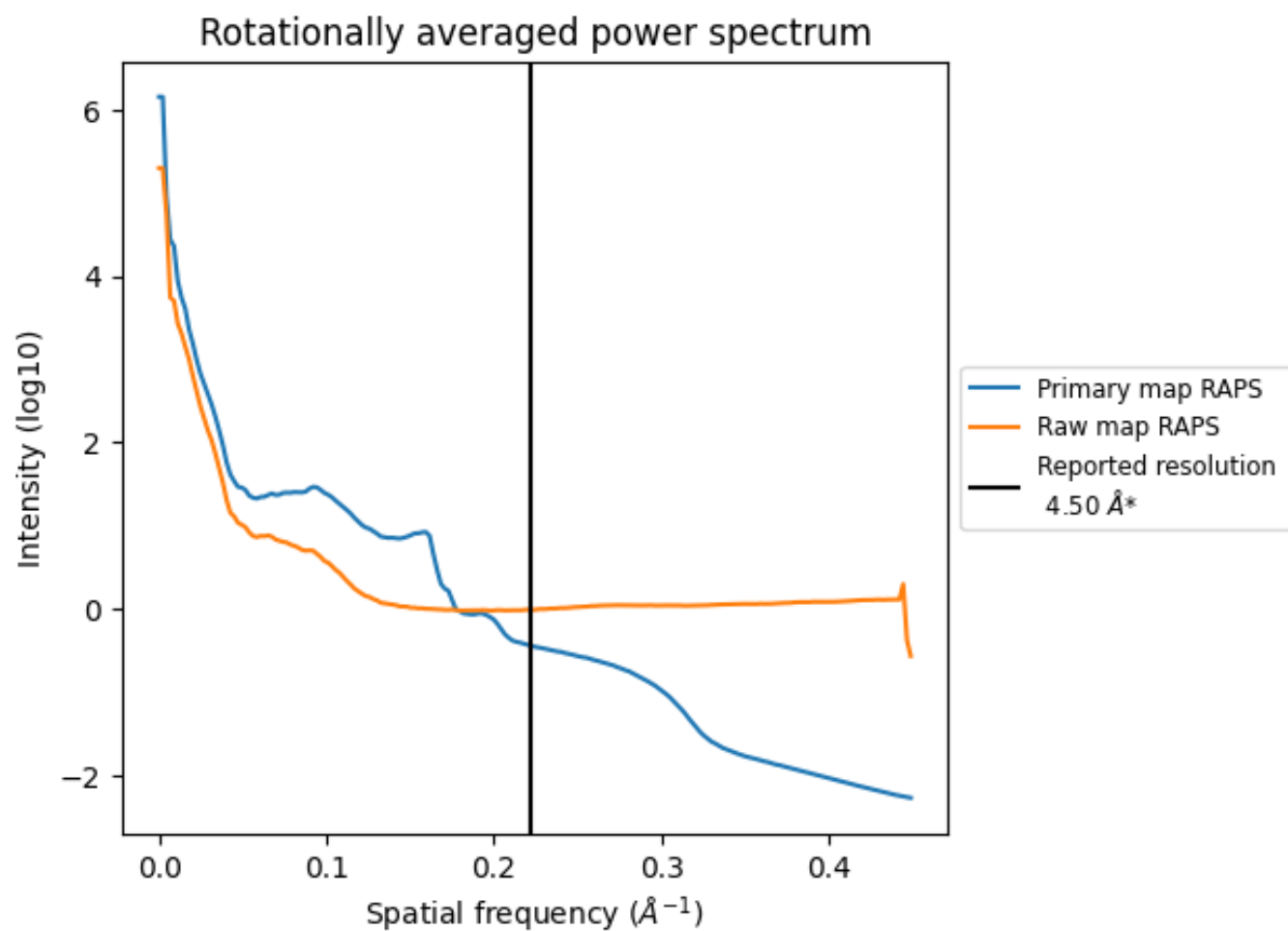
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 200 nm³; this corresponds to an approximate mass of 181 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 ⓘ

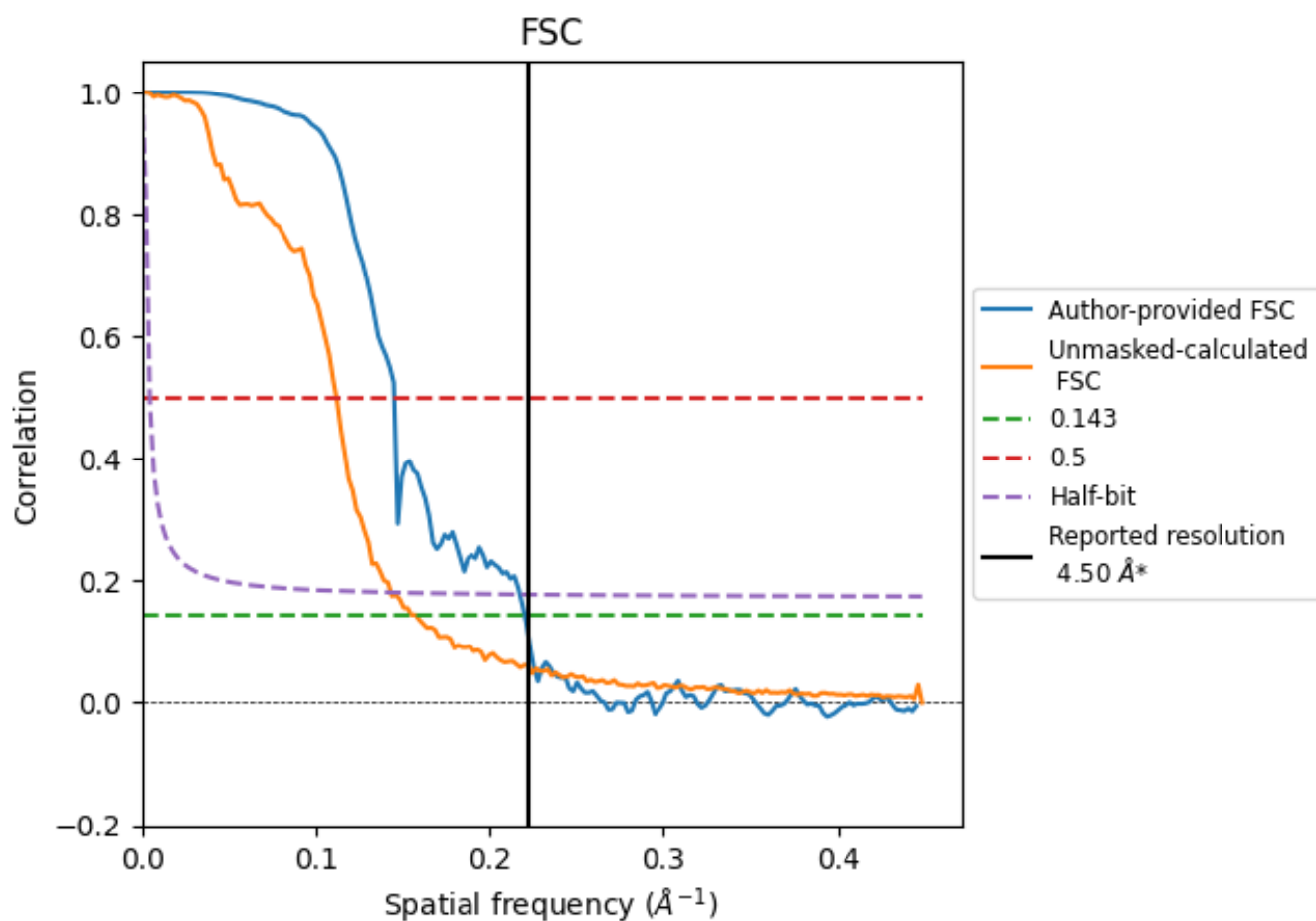


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

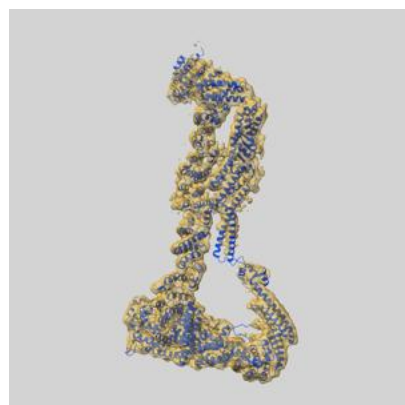
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.54	6.90	4.60
Unmasked-calculated*	6.35	8.94	6.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.35 differs from the reported value 4.5 by more than 10 %

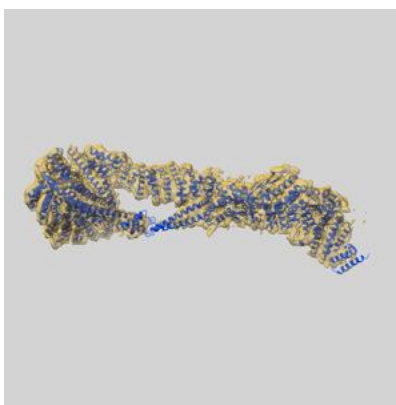
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28204 and PDB model 8EKI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

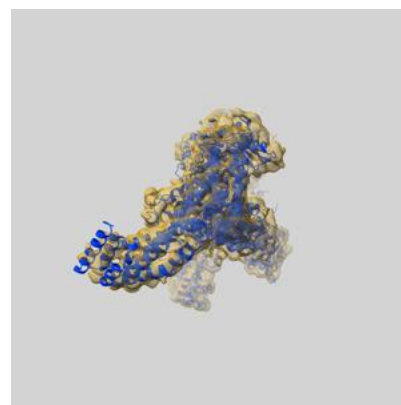
9.1 Map-model overlay [i](#)



X



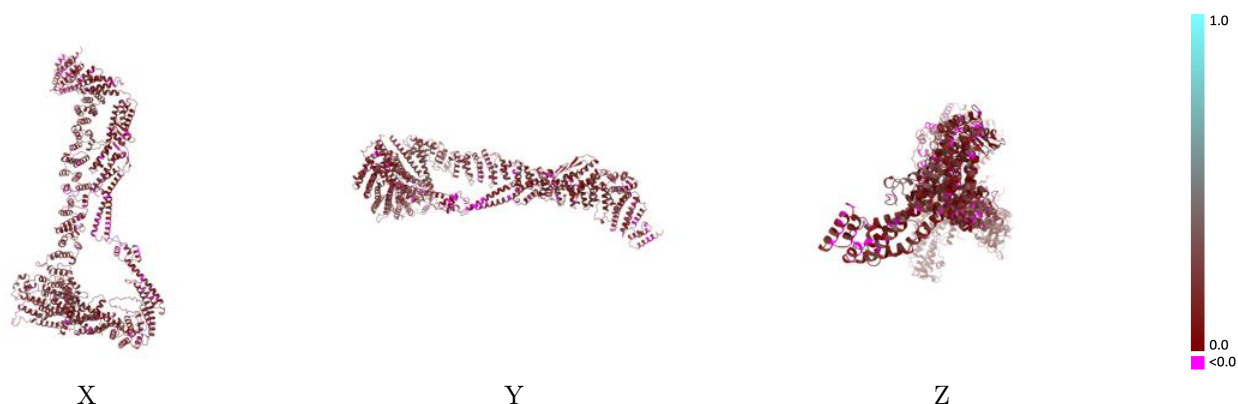
Y



Z

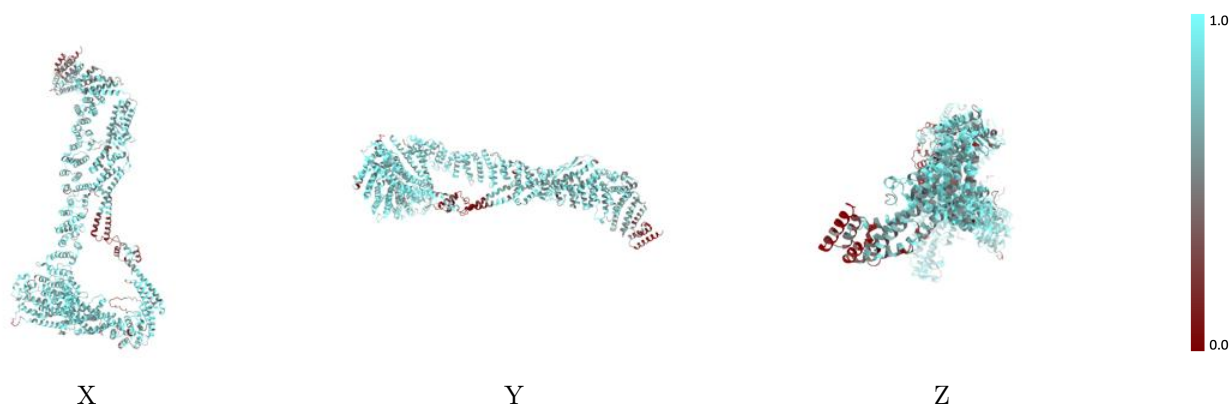
The images above show the 3D surface view of the map at the recommended contour level 0.186 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



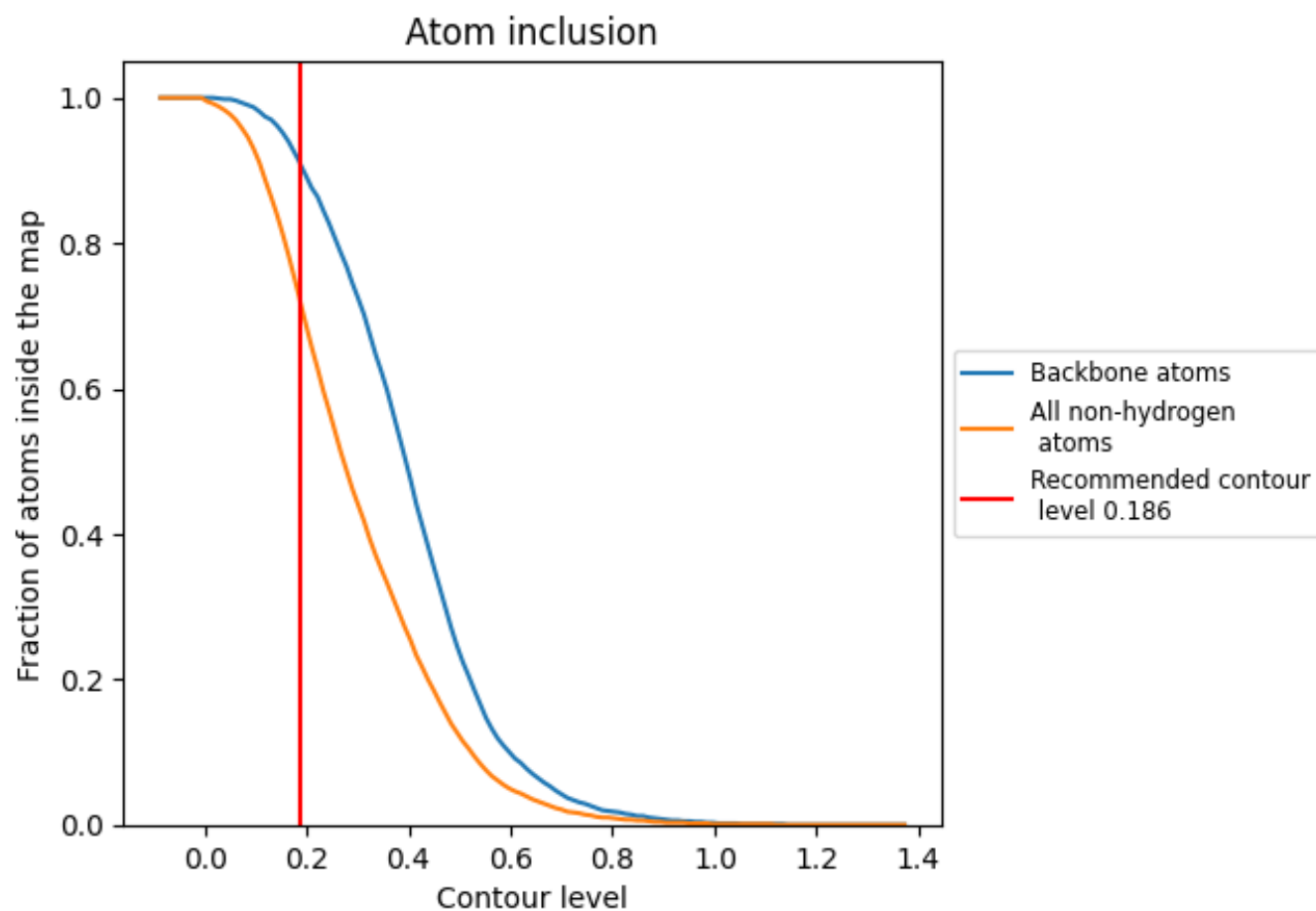
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.186).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 72% 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 (0.186) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.1820
A	0.7600	0.2240
B	0.7940	0.2100
C	0.7540	0.1870
D	0.7710	0.1960
E	0.6270	0.1460

