



Full wwPDB EM Validation Report ⓘ

Mar 21, 2026 – 03:49 PM UTC

PDB ID : 8FGW / pdb_00008fgw
EMDB ID : EMD-29073
Title : Human IFT-A complex structures provide molecular insights into ciliary transport
Authors : Jiang, M.; Palicharla, V.R.; Miller, D.; Hwang, S.H.; Zhu, H.; Hixson, P.; Mukhopadhyay, S.; Sun, J.
Deposited on : 2022-12-12
Resolution : 3.70 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

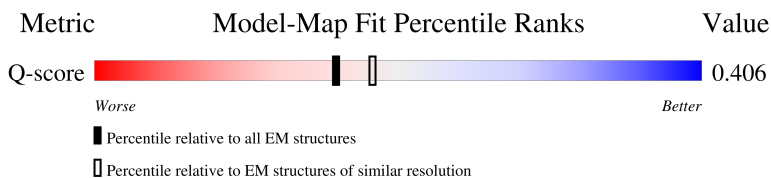
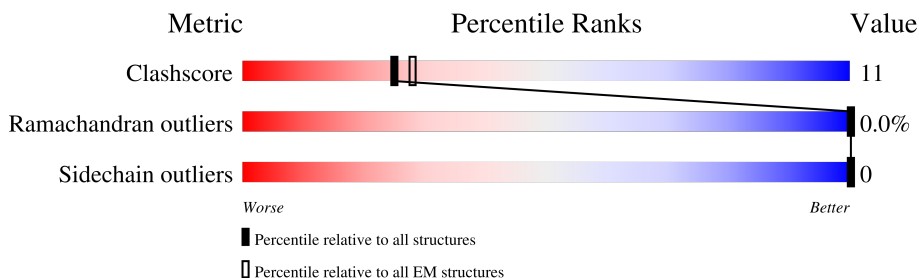
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1181	
2	B	1241	
3	C	1342	
4	D	1316	

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Mol	Chain	Length	Quality of chain
5	E	1462	22%29%12%59%
6	F	208	5%23%11%66%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43527 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 WD repeat-containing protein 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1081	Total	C	N	O	S	0	0
			8435	5402	1427	1552	54		

- Molecule 2 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1152	Total	C	N	O	S	0	0
			8941	5724	1534	1625	58		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	238	ASP	GLU	conflict	UNP Q9HBG6

- Molecule 3 is a protein called WD repeat-containing protein 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1342	Total	C	N	O	S	0	0
			10313	6545	1757	1939	72		

- Molecule 4 is a protein called Tetratricopeptide repeat protein 21B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1315	Total	C	N	O	S	0	0
			10502	6662	1807	1963	70		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	201	MET	VAL	variant	UNP Q7Z4L5
D	276	ALA	THR	variant	UNP Q7Z4L5

- Molecule 5 is a protein called Intraflagellar transport protein 140 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	603	Total	C	N	O	S	0	0
			4790	3034	841	881	34		

- Molecule 6 is a protein called Intraflagellar transport protein 43 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	71	Total	C	N	O	S	0	0
			541	343	90	107	1		

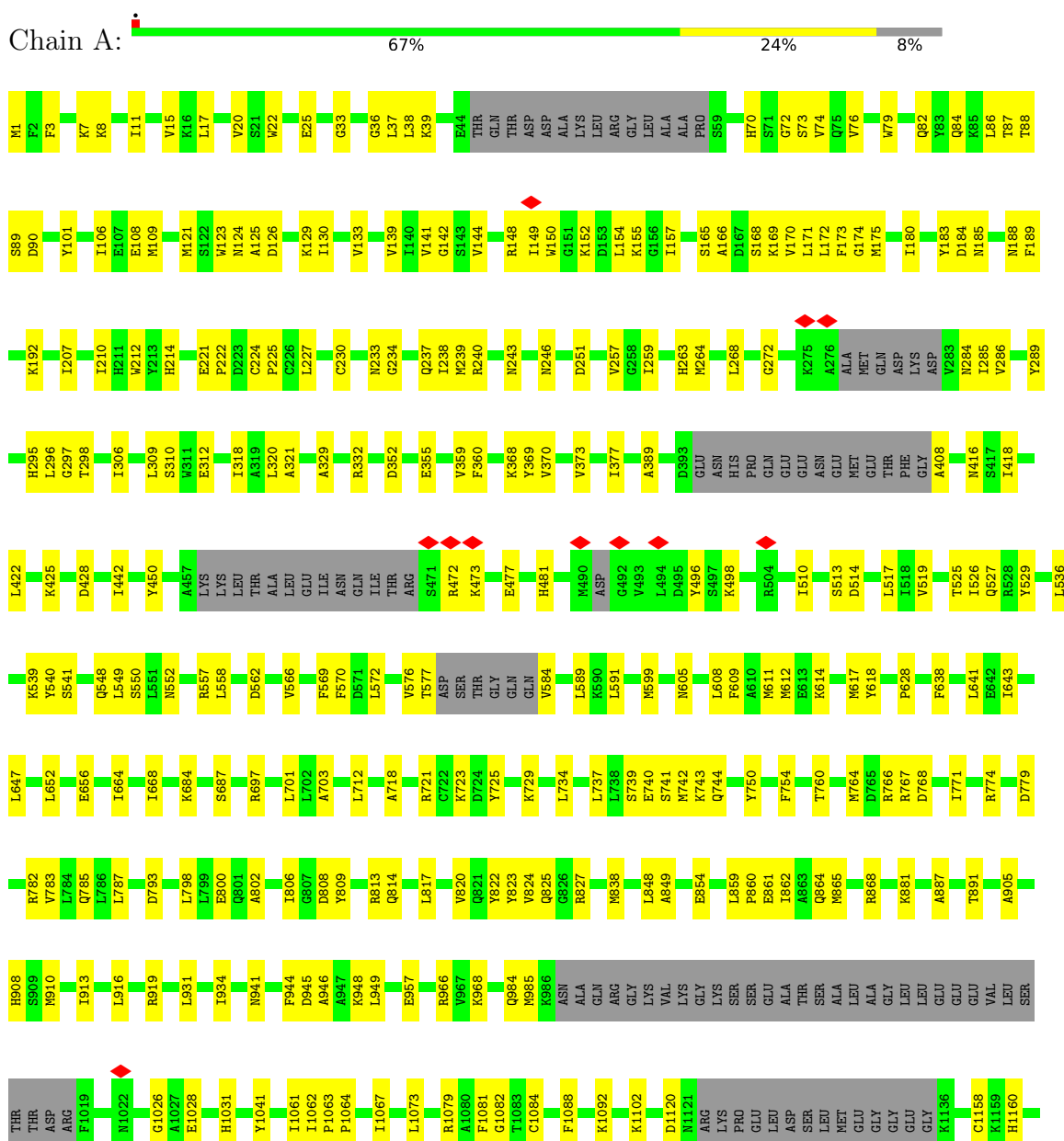
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Zn	0
			1	1	
7	B	2	Total	Zn	0
			2	2	
7	C	2	Total	Zn	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.

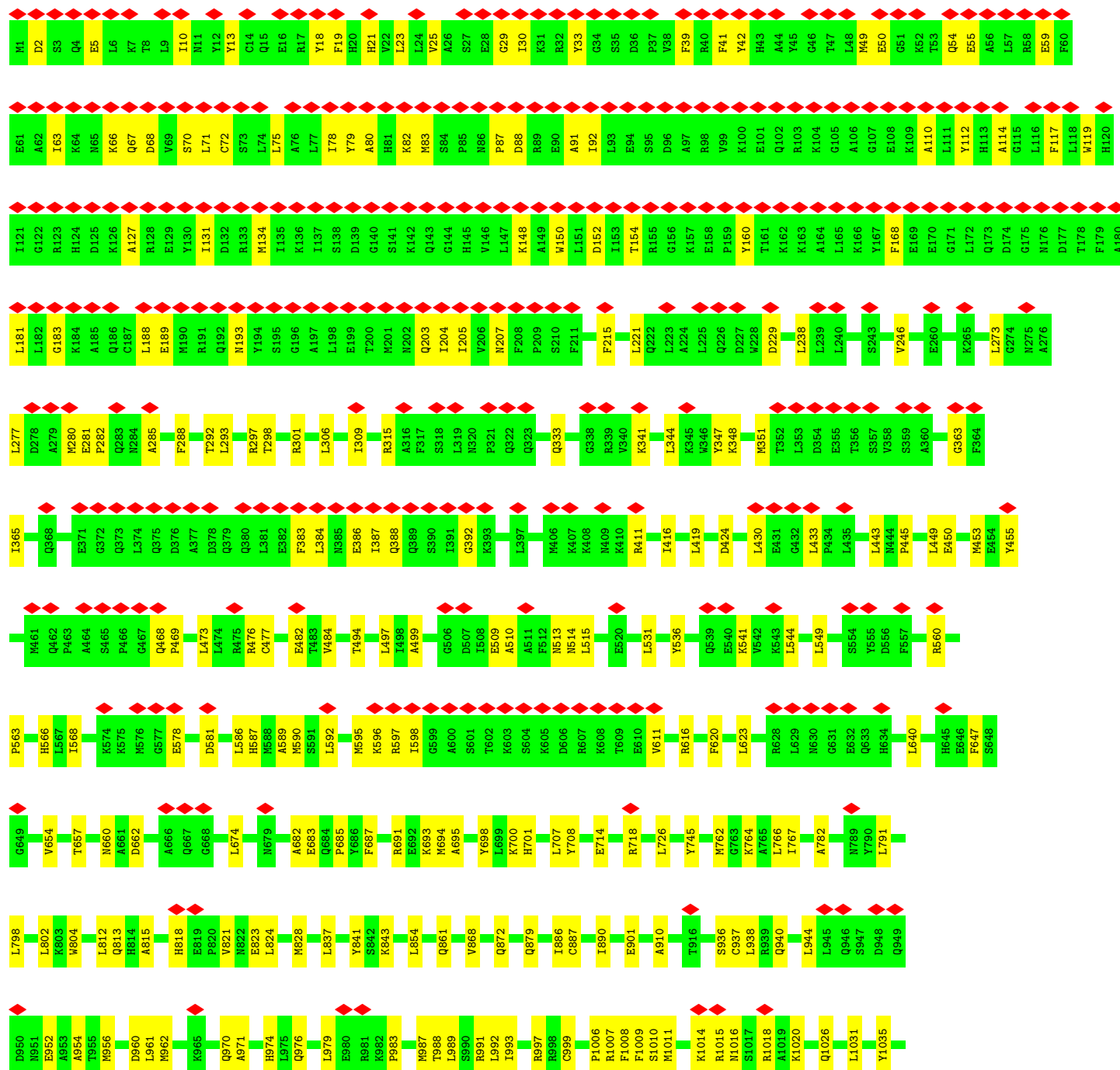
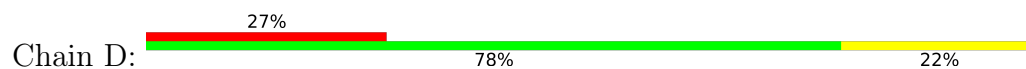
• Molecule 1: WD repeat-containing protein 35

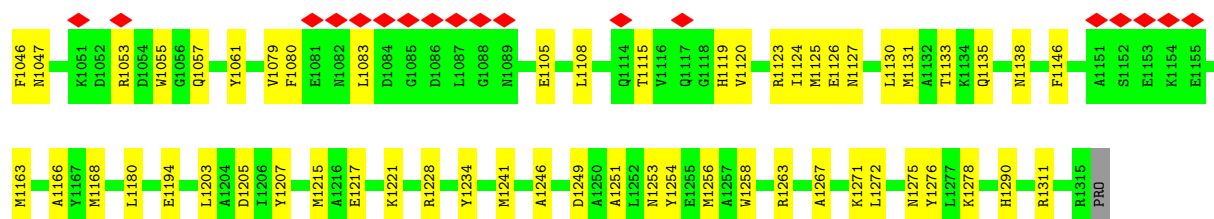


H1155	S1156	V1160	G1167	D1168	H1169	M1170	K1171	L1176	V1179	N1182	F1186	L1194	T1197	H1202	R1203	L1206	K1207	A1214	A1215	H1216	L1217	R1218	R1219	F1220	E1221	Y1222	R1223	S1224	D1227	A1228	K1229	K1231	K1232	K1233	I1234	E1235	G1236	M1237	V1238	R1239	R1240	F1241	D1242	I1243	S1244	E1245															
L1044	K1045	P1047	S1048	S1049	E1050	D1051	N1052	I1055	I1059	E1060	T1061	V1062	G1063	Q1064	A1065	L1069	L1070	D1076	L1079	G1080	E1081	N1082	D1083	G1084	M1085	P1086	K1087	Y1091	L1092	F1093	M1097	A1098	L1099	K1100	R1103	Q1117	R1123	F1130	S1131	M1132	E1135	K1140	L1154																		
G965	D966	Y967	G968	S969	A970	I971	Q972	F973	L974	V975	C979	N980	N981	E982	A983	F984	T985	L986	A987	Q988	Q989	H990	N991	K992	M993	E994	I995	Y996	A997	D998	I999	G1000	S1002	E1003	T1005	T1006	N1007	E1008	D1009	Y1010	E1020	K1021	R1022	Y1023	F1029	F1030	L1031	L1032	C1033	R1038	A1039	L1040	K1041								
G636	F637	L638	S639	N640	L641	K642	D643	T644	G645	D646	E647	E648	R661	F662	E667	B670	A682	L686	E690	Y698	R699	V704	M708	L726	A727	M728	Y733	A749	M752	L756	Q757	H758	M759	I777	A782	L785	M793	A794	L796	A796	L888																				
H797	Y798	G804	D805	E811	A815	R820	R821	R822	R823	R824	G825	D826	I827	G830	H831	R832	Q833	A834	R836	H837	P838	L842	K843	R844	D845	T849	L850	E851	N852	R853	K854	Q855	F856	L862	R865	G866	L867	Y868	Y876	I877	R878	S879	K880	V885	G886	D887	L888														
L889	P890	H891	V892	S893	S894	P895	L899	A902	K905	E906	A907	D908	G909	R910	E913	A914	A917	Y918	E919	I920	A921	K922	Q923	W924	L932	D933	H934	L935	N936	I937	P938	E939	K940	A941	V942	N943	I944	V945	R946	E947	T948	Q949	S950	L951	D952	Y957	F960	F961	L962	Q963	L964										
G965	D966	Y967	G968	S969	A970	I971	Q972	F973	L974	V975	C979	N980	N981	E982	A983	F984	T985	L986	A987	Q988	Q989	H990	N991	K992	M993	E994	I995	Y996	A997	D998	I999	G1000	S1002	E1003	T1005	T1006	N1007	E1008	D1009	Y1010	E1020	K1021	R1022	Y1023	F1029	F1030	L1031	L1032	C1033	R1038	A1039	L1040	K1041								
L1044	K1045	P1047	S1048	S1049	E1050	D1051	N1052	I1055	I1059	E1060	T1061	V1062	G1063	Q1064	A1065	L1069	L1070	D1076	L1079	G1080	E1081	N1082	D1083	G1084	M1085	P1086	K1087	Y1091	L1092	F1093	M1097	A1098	L1099	K1100	R1103	Q1117	R1123	F1130	S1131	M1132	E1135	K1140	L1154																		
H1155	S1156	V1160	G1167	D1168	H1169	M1170	K1171	L1176	V1179	N1182	F1186	L1194	T1197	H1202	R1203	L1206	K1207	A1214	A1215	H1216	L1217	R1218	R1219	F1220	E1221	Y1222	R1223	S1224	D1227	A1228	K1229	K1231	K1232	K1233	I1234	E1235	G1236	M1237	V1238	R1239	R1240	F1241	D1242	I1243	S1244	E1245															
L121	L122	I123	Y124	N125	H126	Q127	T128	S129	R130	K131	I132	P133	V134	L135	G136	K137	H138	T139	K140	R141	I142	T143	C144	G145	C146	W147	N148	A149	E150	N151	L152	L153	A154	L155	G156	G157	E158	D159	K160	M161	I162	T163	V164	S165	M166	Q167	E168	G169	D170	T171	I172	R173	Q174	T175	Q176	V177	K178	S179	E180	G119	N120
P181	S182	N183	M184	Q185	F186	F187	L188	M189	K190	M191	D192	D193	R194	T195	S196	A197	A198	E199	S200	M201	I202	S203	V204	V205	L206	G207	K208	K209	T210	L211	F212	F213	L214	N215	L216	N217	E218	P219	D220	N221	A223	D224	L225	F227	Q228	Q229	D230	F231	G232	N233	I234	V235	Y237	N238	W239	Y240					
G241	D242	G243	R244	I245	M246	I247	G248	F249	S250	C251	G252	H253	F254	V255	V256	I257	S258	T259	H260	T261	G262	E263	L264	G265	Q266	E267	I268	F269	Q270	A271	R272	H273	H274	K275	D276	N277	L278	T279	S280	I281	A282	V283	S284	Q285	E286	L287	N288	K289	V290	A291	T292	C293	G294	D295	N296	C297	I298	K299	I300		
Q301	D302	L303	V304	D305	L306	K307	D308	M309	Y310	V311	I312	L313	N314	L315	D316	E317	E318	N319	K320	G321	L322	G323	L324	L325	S326	W327	T328	D329	D330	G331	Q332	L333	L334	A335	L336	S337	T338	Q339	R340	G341	S342	L343	H344	V345	F346	L347	T348	K349	R360	L368	L380	V386	D387	N391							
F392	V393	L397	V402	G403	M404	N405	N406	R407	A408	W409	F410	Y411	V412	E415	M416	A417	V418	K419	K420	L421	K422	D423	M424	E425	Y426	L427	V430	D438	F444	H451	E454	S455	E456	I457	L458	D459	A460	Q461	E462	K463	R464	R467	P470	D473	D474	I478															
Y490	D493	Q498	Y501	I502	E503	D504	W505	N509	D510	V515	S516	K519	I520	L529	V530	K535	V540	Y541	C542	P543	V544	N545	D546	S555	L558	K559	D569	A575	K588	D589	T590	G593	F606	A607	H608	P610	N615	C620	G625																						
Q301	D302	L303	V304	D305	L306	K307	D308	M309	Y310	V311	I312	L313	N314	L315	D316	E317	E318	N319	K320	G321	L322	G323	L324	L325	S326	W327	T328	D329	D330	G331	Q332	L333	L334	A335	L336	S337	T338	Q339	R340	G341	S342	L343	H344	V345	F346	L347	T348	K349	R360	L368	L380	V386	D387	N391							
G241	D242	G243	R244	I245	M246	I247	G248	F249	S250	C251	G252	H253	F254	V255	V256	I257	S258	T259	H260	T261	G262	E263	L264	G265	Q266	E267	I268	F269	Q270	A271	R272	H273	H274	K275	D276	N277	L278	T279	S280	I281	A282	V283	S284	Q285	E286	L287	N288	K289	V290	A291	T292	C293	G294	D295	N296	C297	I298	K299	I300		
P181	S182	N183	M184	Q185	F186	F187	L188	M189	K190	M191	D192	D193	R194	T195	S196	A197	A198	E199	S200	M201	I202	S203	V204	V205	L206	G207	K208	K209	T210	L211	F212	F213	L214	N215	L216	N217	E218	P219	D220	N221	A223	D224	L225	F227	Q228	Q229	D230	F231	G232	N233	I234	V235	Y237	N238	W239	Y240					
L121	L122	I123	Y124	N125	H126	Q127	T128	S129	R130	K131	I132	P133	V134	L135	G136	K137	H138	T139	K140	R141	I142	T143	C144	G145	C146	W147	N148	A149	E150	N151	L152	L153	A154	L155	G156	G157	E158	D159	K160	M161	I162	T163	V164	S165	M166	Q167	E168	G169	D170	T171	I172	R173	Q174	T175	Q176	V177	K178	S179	E180	G119	N120
D61	W62	D63	K64	D65	G66	D67	V68	L69	A70	V71	I72	A73	E74	K75	S76	S77	C78	I79	Y80	L81	W82	D83	A84	N85	T86	N87	K88	T89	S90	Q91	L92	D93	N94	G95	M96	R97	D98	Q99	M100	S101	F102	L103	L104	W105	S106	K107	V108	G109	S110	F111	L112	A113	G115	T116	V117	K118	G119	N120			

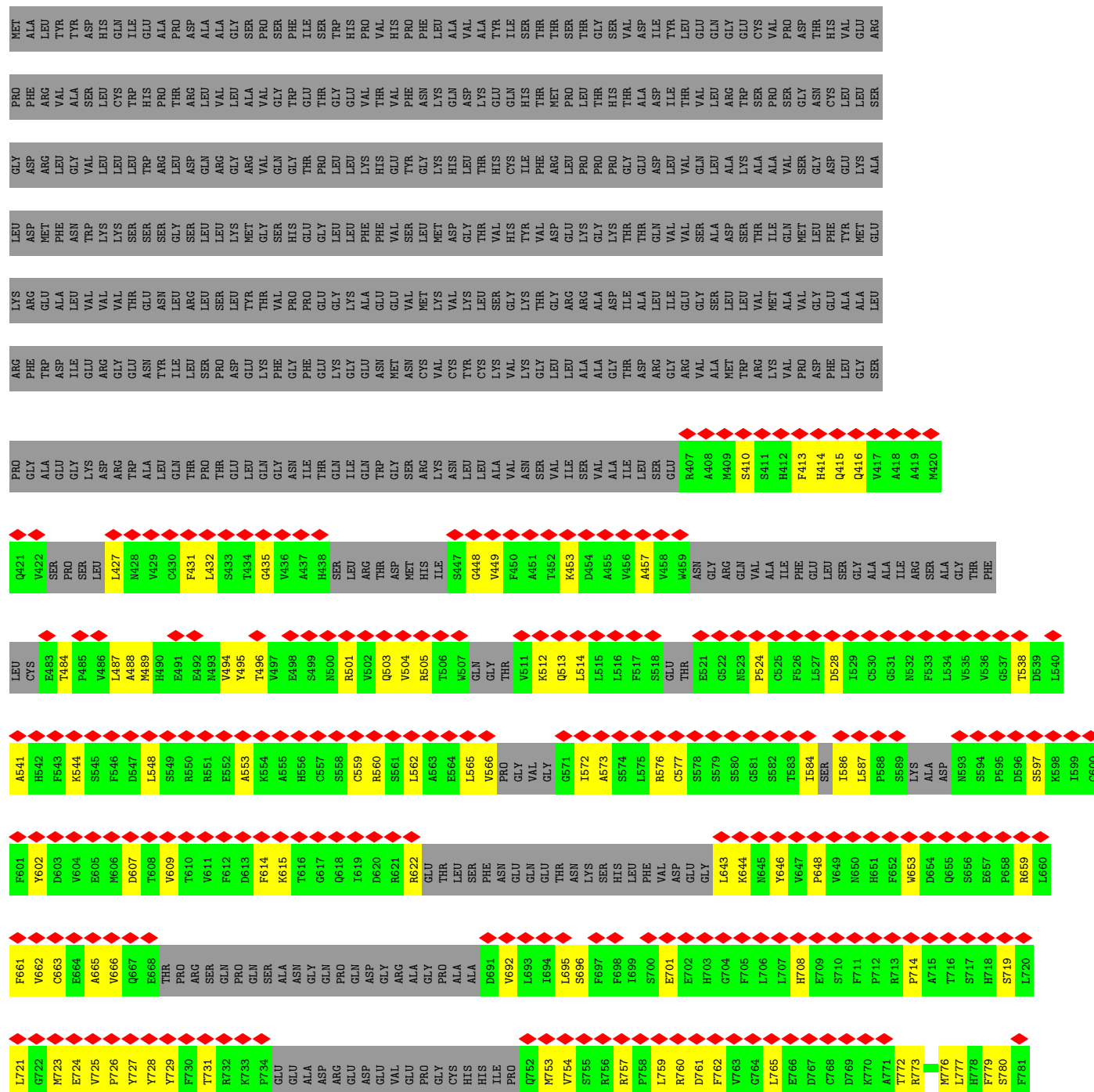


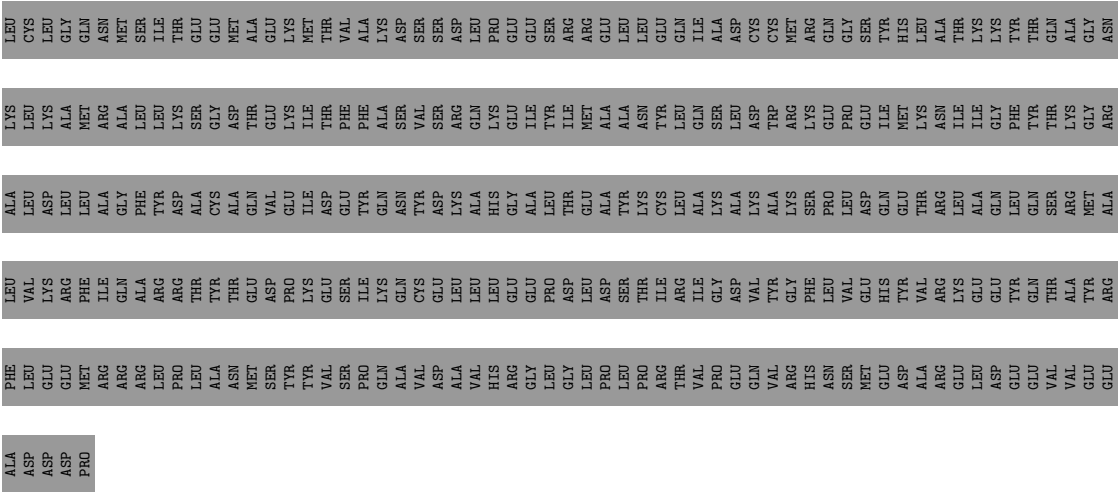
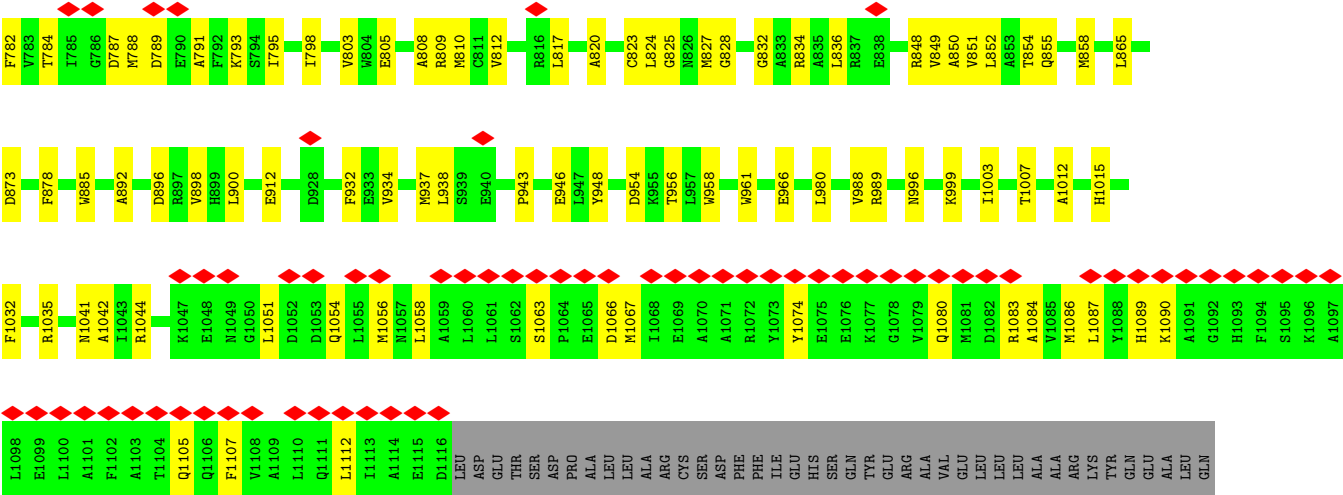
● Molecule 4: Tetratricopeptide repeat protein 21B



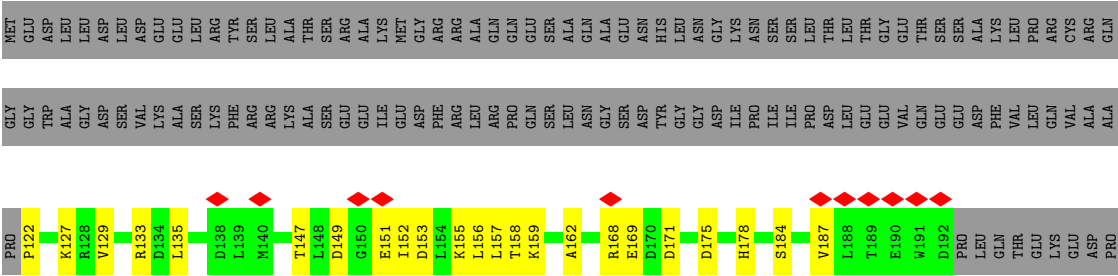


• Molecule 5: Intraflagellar transport protein 140 homolog





• Molecule 6: Intraflagellar transport protein 43 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67560	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.053	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	710.4, 710.4, 710.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.48, 1.48, 1.48	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/8613	0.34	0/11675
2	B	0.17	0/9142	0.32	0/12394
3	C	0.13	0/10522	0.29	0/14280
4	D	0.11	0/10692	0.27	0/14429
5	E	0.12	0/4889	0.31	0/6598
6	F	0.10	0/551	0.25	0/751
All	All	0.14	0/44409	0.31	0/60127

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	770	MET	Peptide

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	8435	0	8233	202	0
2	B	8941	0	8669	190	0
3	C	10313	0	10005	210	0
4	D	10502	0	10501	191	0
5	E	4790	0	4608	130	0
6	F	541	0	493	19	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
All	All	43527	0	42509	907	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 11.

All (907) 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:131:ILE:HG21	4:D:148:LYS:HB3	1.59	0.83
1:A:154:LEU:HD23	1:A:157:ILE:HD11	1.61	0.82
1:A:814:GLN:HG2	2:B:563:GLN:HB3	1.62	0.80
1:A:737:LEU:HD21	1:A:742:MET:HB3	1.66	0.78
3:C:213:PHE:HB2	3:C:223:ALA:HB3	1.66	0.76
3:C:189:MET:HB3	3:C:191:MET:HE3	1.68	0.75
2:B:755:ALA:HB2	2:B:770:MET:HG2	1.69	0.75
2:B:1068:ASN:ND2	2:B:1073:VAL:O	2.20	0.75
5:E:759:LEU:HB3	5:E:762:PHE:HB2	1.68	0.75
1:A:15:VAL:HG21	1:A:37:LEU:HD13	1.68	0.74
4:D:416:ILE:HG12	4:D:473:LEU:HD11	1.70	0.74
5:E:851:VAL:O	5:E:855:GLN:NE2	2.20	0.74
1:A:124:ASN:HD22	1:A:129:LYS:HD3	1.52	0.74
1:A:259:ILE:HG23	1:A:268:LEU:HD11	1.68	0.73
3:C:981:ASN:O	3:C:985:THR:N	2.21	0.73
3:C:240:TYR:O	3:C:244:ARG:HB2	1.89	0.73
3:C:1009:ASP:HA	3:C:1033:CYS:HB2	1.69	0.73
5:E:597:SER:HA	5:E:648:PRO:HD2	1.71	0.72
2:B:469:MET:HE2	2:B:492:LEU:HD21	1.72	0.71
4:D:152:ASP:HB3	4:D:160:TYR:HB3	1.73	0.71
3:C:733:TYR:OH	5:E:828:GLY:O	2.08	0.71
1:A:767:ARG:HH12	1:A:787:LEU:HD23	1.55	0.71
3:C:849:ILE:HG22	3:C:853:MET:HE1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:OD1	1:A:125:ALA:N	2.23	0.70
2:B:469:MET:HE1	2:B:498:LEU:HD12	1.73	0.70
4:D:745:TYR:HB3	4:D:762:MET:HE1	1.72	0.70
2:B:882:GLN:NE2	2:B:894:ALA:O	2.24	0.70
4:D:1249:ASP:O	4:D:1253:ASN:ND2	2.23	0.70
1:A:741:SER:OG	3:C:1340:GLU:OE1	2.10	0.69
3:C:1289:TRP:HD1	3:C:1329:ILE:HB	1.57	0.69
5:E:832:GLY:HA2	5:E:855:GLN:HG2	1.74	0.69
1:A:251:ASP:OD1	1:A:289:TYR:OH	2.09	0.68
1:A:285:ILE:HG23	1:A:298:THR:HG23	1.76	0.68
1:A:905:ALA:HB2	1:A:913:ILE:HD13	1.74	0.68
2:B:1074:CYS:SG	2:B:1075:ILE:N	2.65	0.68
2:B:362:ARG:NH2	2:B:421:ASP:O	2.27	0.68
5:E:584:ILE:HG22	5:E:586:ILE:HD11	1.75	0.67
2:B:285:CYS:SG	2:B:327:CYS:N	2.67	0.67
4:D:616:ARG:HG2	4:D:647:PHE:HZ	1.58	0.67
5:E:996:ASN:HB3	5:E:999:LYS:HZ1	1.60	0.67
3:C:782:ALA:HB2	3:C:797:HIS:HB2	1.76	0.67
4:D:285:ALA:HA	4:D:288:PHE:HD2	1.60	0.67
1:A:800:GLU:OE2	3:C:1219:ARG:NH2	2.27	0.67
4:D:215:PHE:HB2	4:D:238:LEU:HD21	1.76	0.66
5:E:513:GLN:NE2	5:E:553:ALA:O	2.28	0.66
4:D:1180:LEU:HB3	4:D:1203:LEU:HD22	1.77	0.66
3:C:530:VAL:HG22	3:C:540:VAL:HG22	1.77	0.66
1:A:760:THR:O	1:A:764:MET:HG2	1.97	0.65
2:B:666:PHE:O	2:B:670:GLN:N	2.29	0.65
4:D:449:LEU:HD22	4:D:497:LEU:HD12	1.77	0.65
4:D:388:GLN:NE2	4:D:392:GLY:O	2.29	0.65
1:A:1:MET:HA	1:A:332:ARG:O	1.96	0.65
4:D:861:GLN:NE2	4:D:879:GLN:OE1	2.30	0.65
5:E:659:ARG:HH12	5:E:701:GLU:HG3	1.62	0.65
3:C:148:ASN:HB2	3:C:199:GLU:HB2	1.79	0.64
4:D:598:ILE:HG13	4:D:616:ARG:HH11	1.63	0.64
2:B:990:PRO:HG2	2:B:993:ILE:HD12	1.79	0.64
5:E:496:THR:HG21	5:E:505:ARG:HE	1.61	0.64
3:C:990:HIS:O	3:C:990:HIS:ND1	2.30	0.64
3:C:1295:CYS:HB3	3:C:1317:CYS:HB3	1.78	0.64
2:B:154:GLY:HA2	2:B:179:ILE:HG13	1.79	0.64
1:A:239:MET:HB3	1:A:246:ASN:HD22	1.63	0.63
1:A:129:LYS:HG2	1:A:148:ARG:HD3	1.80	0.63
2:B:194:TRP:O	2:B:197:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:301:ARG:NH2	4:D:450:GLU:OE2	2.31	0.63
1:A:549:LEU:HB3	1:A:558:LEU:HD11	1.81	0.62
1:A:148:ARG:HH21	1:A:149:ILE:HD12	1.63	0.62
3:C:125:ASN:O	3:C:129:SER:N	2.33	0.62
4:D:1131:MET:HE1	4:D:1166:ALA:HA	1.81	0.62
1:A:1026:GLY:HA2	1:A:1061:ILE:HD13	1.79	0.62
1:A:1092:LYS:O	1:A:1102:LYS:NZ	2.31	0.62
3:C:179:SER:HB3	3:C:206:LEU:HB3	1.80	0.62
2:B:171:ARG:NH1	2:B:264:SER:OG	2.32	0.62
3:C:406:ASN:ND2	3:C:425:GLU:OE2	2.32	0.62
4:D:411:ARG:NH1	4:D:683:GLU:O	2.32	0.62
3:C:463:GLU:HG2	3:C:464:ARG:HD2	1.80	0.62
5:E:413:PHE:HB2	5:E:721:LEU:HG	1.80	0.62
6:F:147:THR:HG22	6:F:153:ASP:HA	1.82	0.62
3:C:393:VAL:HG22	3:C:402:VAL:HG12	1.81	0.62
3:C:520:ILE:HB	3:C:529:LEU:HD11	1.80	0.62
3:C:749:ALA:O	3:C:752:MET:HG3	2.00	0.62
4:D:1123:ARG:O	4:D:1127:ASN:ND2	2.33	0.61
6:F:151:GLU:HG2	6:F:152:ILE:HG13	1.82	0.61
2:B:620:PRO:HB2	2:B:636:ILE:HG21	1.81	0.61
1:A:793:ASP:O	3:C:1182:ASN:ND2	2.26	0.61
2:B:437:ASN:N	2:B:449:CYS:O	2.33	0.61
4:D:78:ILE:HG22	4:D:82:LYS:HE3	1.83	0.61
4:D:956:MET:HE3	4:D:987:MET:HG3	1.80	0.61
5:E:487:LEU:HD21	5:E:494:VAL:HG23	1.82	0.61
5:E:708:HIS:HE1	5:E:759:LEU:HD11	1.65	0.61
3:C:850:LEU:HD12	3:C:855:GLN:HB2	1.81	0.61
2:B:399:ASN:O	2:B:400:ARG:NH1	2.29	0.61
1:A:377:ILE:N	1:A:389:ALA:O	2.34	0.61
2:B:1229:CYS:HB3	2:B:1232:CYS:O	2.01	0.61
3:C:461:GLN:HG3	3:C:464:ARG:HD3	1.83	0.61
4:D:449:LEU:HD21	4:D:494:THR:HG22	1.82	0.61
4:D:682:ALA:HB2	4:D:718:ARG:HD2	1.83	0.60
1:A:184:ASP:OD2	1:A:188:ASN:ND2	2.32	0.60
2:B:567:MET:HE3	2:B:636:ILE:HD12	1.83	0.60
5:E:501:ARG:NH1	5:E:503:GLN:OE1	2.30	0.60
3:C:644:THR:HG23	3:C:648:GLU:HB2	1.83	0.60
1:A:38:LEU:HD22	1:A:88:THR:HG21	1.83	0.60
2:B:360:LYS:O	2:B:598:ASN:ND2	2.33	0.60
4:D:348:LYS:HA	4:D:351:MET:HE2	1.83	0.60
1:A:934:ILE:HG23	1:A:946:ALA:HB1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:HIS:HB3	2:B:850:ALA:HB2	1.83	0.60
3:C:895:PRO:HB3	3:C:921:ALA:HA	1.84	0.60
2:B:701:SER:OG	2:B:725:MET:SD	2.52	0.60
2:B:479:ILE:O	2:B:526:ARG:NH2	2.35	0.60
3:C:1206:LEU:HA	3:C:1245:GLU:HG3	1.84	0.60
5:E:565:LEU:HD13	5:E:609:VAL:HB	1.84	0.60
2:B:578:ILE:HD13	2:B:615:VAL:HG13	1.83	0.60
5:E:597:SER:HB2	5:E:614:PHE:HB2	1.84	0.60
3:C:98:ASP:HB2	3:C:116:THR:HG21	1.84	0.59
4:D:956:MET:HE1	4:D:988:THR:HA	1.83	0.59
5:E:501:ARG:HH22	5:E:514:LEU:HD22	1.67	0.59
1:A:237:GLN:OE1	1:A:246:ASN:ND2	2.35	0.59
1:A:548:GLN:HG2	1:A:599:MET:HE2	1.84	0.59
4:D:1241:MET:HB3	4:D:1246:ALA:HB3	1.84	0.59
3:C:1307:MET:HE1	3:C:1315:PRO:HD3	1.84	0.59
2:B:1184:LYS:HD3	2:B:1195:PHE:HE2	1.68	0.59
1:A:108:GLU:HG2	1:A:109:MET:HG3	1.85	0.59
1:A:529:TYR:HD1	1:A:536:LEU:HA	1.67	0.59
2:B:882:GLN:NE2	2:B:898:LEU:HB2	2.17	0.59
5:E:646:TYR:HB3	5:E:665:ALA:HB1	1.84	0.59
1:A:1062:ILE:HB	1:A:1067:ILE:HD11	1.85	0.59
5:E:696:SER:OG	5:E:708:HIS:ND1	2.35	0.58
5:E:759:LEU:HD23	5:E:761:ASP:H	1.68	0.58
1:A:957:GLU:OE2	1:A:966:ARG:NH2	2.36	0.58
3:C:430:VAL:HA	3:C:444:PHE:HB3	1.85	0.58
4:D:75:LEU:HD12	4:D:114:ALA:HB1	1.85	0.58
1:A:33:GLY:HA3	1:A:37:LEU:HB3	1.86	0.58
3:C:35:ASP:OD2	3:C:39:LYS:NZ	2.36	0.58
1:A:87:THR:HG22	1:A:121:MET:HE1	1.85	0.58
3:C:509:ASN:ND2	3:C:543:PRO:HB3	2.18	0.58
4:D:560:ARG:O	4:D:566:HIS:NE2	2.37	0.58
4:D:960:ASP:OD2	4:D:991:ARG:NH1	2.37	0.58
3:C:83:ASP:O	3:C:87:ASN:N	2.37	0.58
5:E:662:VAL:HB	5:E:723:MET:HE1	1.84	0.58
1:A:221:GLU:HG3	1:A:222:PRO:HD2	1.86	0.58
1:A:576:VAL:O	1:A:584:VAL:N	2.37	0.58
3:C:406:ASN:HA	3:C:430:VAL:HG23	1.86	0.58
1:A:525:THR:HA	1:A:541:SER:HA	1.84	0.57
2:B:28:ILE:HD12	2:B:61:TYR:HE1	1.69	0.57
3:C:287:LEU:HD21	3:C:349:LYS:HB2	1.85	0.57
4:D:989:LEU:O	4:D:993:ILE:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:341:LYS:HA	4:D:344:LEU:HD12	1.85	0.57
4:D:1130:LEU:O	4:D:1133:THR:OG1	2.20	0.57
4:D:1168:MET:HE3	4:D:1168:MET:O	2.04	0.57
3:C:139:THR:OG1	3:C:159:ASP:OD2	2.20	0.57
4:D:18:TYR:HB3	4:D:21:HIS:HB2	1.85	0.57
1:A:1171:SER:N	6:F:171:ASP:OD2	2.37	0.57
2:B:885:PHE:HB3	2:B:894:ALA:HB2	1.87	0.57
4:D:1020:LYS:O	4:D:1026:GLN:NE2	2.34	0.57
5:E:666:VAL:HG22	5:E:692:VAL:HG22	1.85	0.57
3:C:728:MET:HE1	5:E:834:ARG:HE	1.70	0.57
3:C:822:ILE:HG13	3:C:830:GLY:HA3	1.87	0.57
4:D:59:GLU:O	4:D:63:ILE:HG12	2.03	0.57
4:D:983:PRO:HG2	4:D:1015:ARG:HD2	1.87	0.57
1:A:481:HIS:ND1	1:A:498:LYS:O	2.38	0.57
2:B:313:ARG:NH2	2:B:316:THR:OG1	2.38	0.57
2:B:789:TRP:HB3	2:B:792:MET:HE3	1.86	0.57
3:C:610:PRO:HA	3:C:620:CYS:HA	1.87	0.57
2:B:478:VAL:HG12	2:B:480:GLY:H	1.69	0.57
3:C:289:LYS:HG2	3:C:302:ASP:HA	1.87	0.57
5:E:576:ARG:HB3	5:E:653:TRP:HD1	1.70	0.57
5:E:824:LEU:HA	5:E:827:MET:HG2	1.87	0.57
1:A:3:PHE:HZ	1:A:297:GLY:HA3	1.69	0.56
4:D:29:GLY:O	4:D:33:TYR:N	2.34	0.56
5:E:544:LYS:HE2	5:E:559:CYS:HB2	1.87	0.56
5:E:934:VAL:HG13	5:E:938:LEU:HD13	1.86	0.56
2:B:27:LEU:HD23	2:B:40:THR:HG22	1.87	0.56
2:B:579:LYS:HG3	2:B:585:VAL:HG12	1.87	0.56
2:B:602:ILE:HB	2:B:613:VAL:HB	1.87	0.56
2:B:771:TYR:HE2	2:B:783:ILE:HG13	1.70	0.56
2:B:571:SER:HB3	2:B:594:VAL:HG23	1.87	0.56
4:D:430:LEU:HD11	4:D:443:LEU:HA	1.87	0.56
4:D:1115:THR:O	4:D:1119:HIS:ND1	2.35	0.56
2:B:882:GLN:HE21	2:B:898:LEU:HB2	1.71	0.56
5:E:966:GLU:OE2	5:E:989:ARG:NH2	2.38	0.56
1:A:808:ASP:OD1	1:A:823:TYR:OH	2.17	0.56
2:B:1078:ARG:HB2	2:B:1163:PHE:HB2	1.88	0.56
3:C:509:ASN:HD22	3:C:543:PRO:HB3	1.69	0.56
3:C:1265:LEU:HD21	3:C:1276:TYR:HB3	1.87	0.56
4:D:119:TRP:HZ2	4:D:154:THR:HG21	1.70	0.56
2:B:698:ASP:OD1	2:B:713:TYR:OH	2.23	0.56
1:A:150:TRP:CD1	1:A:152:LYS:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:ILE:HD11	2:B:446:ILE:HD12	1.88	0.56
3:C:850:LEU:O	3:C:854:LYS:N	2.39	0.56
5:E:432:LEU:HD11	5:E:754:VAL:HG11	1.87	0.56
2:B:632:GLU:O	2:B:636:ILE:HG12	2.06	0.56
4:D:189:GLU:HG2	4:D:221:LEU:HD21	1.88	0.56
5:E:576:ARG:HB3	5:E:653:TRP:CD1	2.41	0.56
1:A:233:ASN:OD1	1:A:234:GLY:N	2.39	0.56
1:A:944:PHE:HE1	1:A:948:LYS:HE3	1.71	0.56
1:A:1082:GLY:HA3	1:A:1120:ASP:HB2	1.86	0.56
3:C:1194:LEU:HB3	3:C:1217:LEU:HD21	1.88	0.56
5:E:988:VAL:HG21	5:E:1012:ALA:HB1	1.88	0.56
6:F:168:ARG:HH11	6:F:168:ARG:HA	1.70	0.56
2:B:146:TYR:HE1	2:B:166:LYS:HG3	1.71	0.55
2:B:877:ARG:O	2:B:881:ALA:N	2.39	0.55
3:C:498:GLN:NE2	3:C:510:ASP:OD2	2.34	0.55
4:D:767:ILE:HD11	4:D:798:LEU:HD13	1.87	0.55
2:B:561:ASN:HB3	2:B:564:CYS:O	2.07	0.55
3:C:844:ARG:O	3:C:844:ARG:NH1	2.39	0.55
4:D:79:TYR:HA	4:D:82:LYS:HD2	1.89	0.55
6:F:175:ASP:HB3	6:F:178:HIS:HD2	1.72	0.55
3:C:827:ILE:HD11	3:C:850:LEU:HD11	1.88	0.55
5:E:573:ALA:HB3	5:E:587:LEU:HB2	1.89	0.55
5:E:892:ALA:HA	5:E:896:ASP:HB2	1.88	0.55
2:B:438:LEU:HB2	2:B:449:CYS:HB3	1.89	0.55
3:C:148:ASN:HD21	3:C:150:GLU:HB2	1.71	0.55
3:C:843:LYS:HG2	3:C:865:LYS:HE3	1.89	0.55
1:A:605:ASN:HB3	1:A:608:LEU:HB2	1.89	0.55
4:D:510:ALA:O	4:D:514:ASN:ND2	2.40	0.55
1:A:782:ARG:NH1	1:A:785:GLN:OE1	2.39	0.55
1:A:813:ARG:HE	2:B:668:ARG:HH21	1.54	0.55
1:A:1028:GLU:OE2	1:A:1160:HIS:NE2	2.40	0.54
3:C:144:CYS:SG	3:C:183:ASN:N	2.80	0.54
1:A:741:SER:HA	1:A:744:GLN:HB2	1.89	0.54
3:C:142:ILE:HD11	3:C:155:LEU:HB3	1.90	0.54
4:D:181:LEU:HB3	4:D:204:ILE:HG12	1.88	0.54
3:C:467:ARG:HB2	3:C:505:TRP:HZ2	1.73	0.54
4:D:578:GLU:HB3	4:D:581:ASP:HB2	1.90	0.54
3:C:1041:LYS:O	3:C:1045:LYS:N	2.40	0.54
4:D:1007:ARG:O	4:D:1010:SER:OG	2.16	0.54
2:B:541:TYR:HA	2:B:548:LEU:HA	1.90	0.54
2:B:647:ARG:NH2	2:B:671:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:667:GLU:OE2	3:C:670:ARG:NH2	2.33	0.54
2:B:438:LEU:HD13	2:B:476:ILE:HG22	1.90	0.54
3:C:759:TRP:HE3	3:C:777:ILE:HG23	1.72	0.54
3:C:1171:LYS:NZ	3:C:1303:GLU:OE1	2.30	0.54
1:A:166:ALA:HA	1:A:214:HIS:HD2	1.73	0.54
1:A:1158:CYS:O	1:A:1160:HIS:ND1	2.39	0.54
2:B:647:ARG:O	2:B:651:MET:HG2	2.08	0.54
4:D:962:MET:HE1	4:D:970:GLN:HB3	1.89	0.54
2:B:1195:PHE:CD2	2:B:1213:MET:HE1	2.43	0.54
3:C:1216:MET:HG3	3:C:1219:ARG:CZ	2.38	0.54
5:E:541:ALA:HA	5:E:572:ILE:HD11	1.89	0.54
1:A:697:ARG:HH12	1:A:701:LEU:HB2	1.73	0.53
1:A:861:GLU:HG3	1:A:865:MET:HE2	1.91	0.53
3:C:98:ASP:OD2	3:C:120:ASN:ND2	2.30	0.53
1:A:750:TYR:HA	2:B:673:ARG:HH12	1.73	0.53
5:E:762:PHE:HZ	5:E:777:LEU:HG	1.74	0.53
3:C:1062:VAL:HG12	3:C:1099:LEU:HD21	1.90	0.53
4:D:188:LEU:HD22	4:D:193:ASN:HD22	1.73	0.53
2:B:136:ILE:HD11	2:B:152:PHE:HD1	1.73	0.53
4:D:67:GLN:HA	4:D:70:SER:OG	2.07	0.53
1:A:562:ASP:OD1	1:A:566:VAL:N	2.42	0.53
1:A:802:ALA:O	1:A:806:ILE:HG13	2.08	0.53
3:C:1176:LEU:HB3	3:C:1197:THR:HG23	1.91	0.53
4:D:13:TYR:CD2	4:D:21:HIS:HB3	2.44	0.53
5:E:1080:GLN:HB3	5:E:1083:ARG:HD2	1.90	0.53
6:F:168:ARG:HA	6:F:168:ARG:NH1	2.24	0.53
1:A:931:LEU:HD13	6:F:184:SER:HB2	1.90	0.53
2:B:928:ILE:HG13	2:B:938:MET:HE1	1.91	0.53
2:B:1214:PHE:HB2	2:B:1219:TYR:HB2	1.90	0.53
4:D:80:ALA:HA	4:D:83:MET:SD	2.49	0.53
4:D:687:PHE:HE1	4:D:691:ARG:HH21	1.56	0.53
5:E:643:LEU:HD22	5:E:695:LEU:HD11	1.90	0.53
1:A:165:SER:HB3	1:A:170:VAL:HG22	1.90	0.53
4:D:824:LEU:HG	4:D:828:MET:HE1	1.90	0.53
1:A:20:VAL:HG23	1:A:321:ALA:HB2	1.90	0.53
5:E:958:TRP:CE3	5:E:980:LEU:HB3	2.44	0.53
2:B:79:ILE:HB	2:B:88:LEU:HB2	1.91	0.52
2:B:1082:ILE:HG22	2:B:1091:LEU:HD12	1.91	0.52
4:D:549:LEU:HD11	4:D:568:ILE:HG22	1.91	0.52
1:A:257:VAL:HG23	1:A:272:GLY:HA2	1.91	0.52
1:A:359:VAL:HG22	1:A:370:VAL:HG22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:LEU:HD11	1:A:742:MET:HG3	1.91	0.52
1:A:908:HIS:HB2	1:A:910:MET:HE1	1.90	0.52
2:B:512:LYS:NZ	2:B:513:GLN:O	2.41	0.52
3:C:100:MET:HA	3:C:116:THR:HG22	1.91	0.52
4:D:449:LEU:O	4:D:453:MET:HG2	2.09	0.52
4:D:1146:PHE:HB3	4:D:1163:MET:HB3	1.90	0.52
5:E:782:PHE:HB2	5:E:791:ALA:HB2	1.91	0.52
2:B:18:ILE:HG22	2:B:29:LEU:HD23	1.92	0.52
2:B:525:SER:OG	2:B:565:GLU:OE2	2.27	0.52
2:B:597:TYR:CD1	2:B:602:ILE:HD13	2.45	0.52
1:A:472:ARG:HG3	1:A:473:LYS:H	1.73	0.52
3:C:1176:LEU:HD13	3:C:1197:THR:HA	1.90	0.52
1:A:418:ILE:HG23	2:B:642:THR:HG22	1.91	0.52
2:B:1091:LEU:HD22	2:B:1204:ILE:HG12	1.91	0.52
3:C:941:ALA:O	3:C:945:VAL:HG23	2.09	0.52
2:B:513:GLN:HG2	2:B:514:ALA:H	1.75	0.52
1:A:124:ASN:ND2	1:A:129:LYS:HD3	2.24	0.52
5:E:565:LEU:HB3	5:E:609:VAL:HG11	1.90	0.52
4:D:282:PRO:O	4:D:315:ARG:NH2	2.38	0.52
1:A:968:LYS:HE2	1:A:1031:HIS:HB2	1.92	0.52
5:E:484:THR:HG21	5:E:487:LEU:HB2	1.92	0.52
2:B:908:GLU:OE1	2:B:910:ARG:NE	2.39	0.51
3:C:138:HIS:ND1	3:C:161:MET:SD	2.83	0.51
3:C:360:ARG:NH1	3:C:397:LEU:O	2.42	0.51
5:E:1056:MET:SD	5:E:1083:ARG:HD3	2.50	0.51
2:B:113:SER:HA	2:B:134:LYS:HG3	1.93	0.51
1:A:133:VAL:HG12	1:A:139:VAL:HG22	1.92	0.51
1:A:148:ARG:HE	1:A:149:ILE:HG13	1.75	0.51
2:B:28:ILE:HG12	2:B:37:VAL:HG22	1.91	0.51
3:C:83:ASP:O	3:C:87:ASN:HA	2.11	0.51
5:E:760:ARG:NH2	5:E:761:ASP:OD1	2.34	0.51
2:B:1036:GLU:HB2	3:C:544:VAL:HG21	1.92	0.51
3:C:63:ASP:HB3	3:C:105:TRP:CD1	2.45	0.51
2:B:882:GLN:HE22	2:B:894:ALA:C	2.18	0.51
3:C:21:TRP:HE1	3:C:335:ALA:HB2	1.76	0.51
3:C:83:ASP:O	3:C:87:ASN:CA	2.59	0.51
5:E:946:GLU:HB3	5:E:961:TRP:CZ2	2.45	0.51
1:A:25:GLU:HB3	1:A:84:GLN:HE22	1.76	0.51
3:C:509:ASN:ND2	3:C:541:TYR:OH	2.33	0.51
4:D:1080:PHE:HD1	4:D:1083:LEU:HD12	1.76	0.51
1:A:168:SER:O	1:A:168:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:764:PRO:HG2	2:B:789:TRP:HH2	1.75	0.51
5:E:779:PHE:CD1	5:E:791:ALA:HB1	2.46	0.51
5:E:851:VAL:O	5:E:854:THR:OG1	2.22	0.51
3:C:805:ASP:OD1	3:C:805:ASP:N	2.44	0.51
6:F:122:PRO:HG2	6:F:127:LYS:HE2	1.93	0.51
1:A:230:CYS:CB	1:A:259:ILE:HD11	2.41	0.50
4:D:365:ILE:HD12	4:D:384:LEU:HD12	1.93	0.50
1:A:536:LEU:HD21	1:A:539:LYS:HE3	1.92	0.50
3:C:811:GLU:HB3	3:C:837:HIS:HE2	1.76	0.50
4:D:1047:ASN:HB2	6:F:135:LEU:HD11	1.92	0.50
3:C:1052:ASN:HA	3:C:1055:ILE:HD12	1.92	0.50
5:E:780:SER:O	5:E:784:THR:HG23	2.11	0.50
1:A:286:VAL:HG21	1:A:320:LEU:HD22	1.93	0.50
1:A:774:ARG:NH1	1:A:779:ASP:OD2	2.43	0.50
2:B:928:ILE:HG13	2:B:938:MET:CE	2.42	0.50
3:C:386:VAL:HG11	3:C:402:VAL:HG21	1.93	0.50
4:D:999:CYS:HA	4:D:1228:ARG:HH21	1.75	0.50
4:D:563:PRO:HG2	4:D:611:VAL:HG13	1.93	0.50
5:E:782:PHE:HB3	5:E:787:ASP:HB3	1.94	0.50
5:E:873:ASP:OD1	5:E:873:ASP:N	2.44	0.50
5:E:989:ARG:HG3	5:E:1015:HIS:NE2	2.26	0.50
1:A:966:ARG:HH21	6:F:187:VAL:HG22	1.77	0.50
1:A:1041:TYR:OH	6:F:162:ALA:O	2.21	0.50
5:E:1051:LEU:HB3	5:E:1054:GLN:HB2	1.92	0.50
3:C:322:LEU:HD13	3:C:336:LEU:HD21	1.94	0.50
3:C:558:ILE:HG21	3:C:575:ALA:HB1	1.92	0.50
1:A:7:LYS:HG2	1:A:8:LYS:H	1.77	0.50
1:A:240:ARG:HG2	1:A:243:ASN:HD21	1.76	0.50
2:B:972:GLU:HG3	2:B:1009:LEU:HD21	1.94	0.50
3:C:1005:THR:HG23	3:C:1006:THR:HG22	1.93	0.50
4:D:119:TRP:CH2	4:D:150:TRP:HB3	2.47	0.50
4:D:976:GLN:HG3	4:D:1008:PHE:HE1	1.76	0.50
1:A:860:PRO:O	1:A:864:GLN:HG2	2.12	0.50
2:B:536:ASP:HB3	2:B:555:ALA:H	1.77	0.50
2:B:557:SER:O	2:B:570:PHE:HA	2.11	0.50
4:D:854:LEU:HB3	4:D:890:ILE:HG12	1.94	0.50
5:E:528:ASP:OD2	5:E:577:CYS:N	2.42	0.50
5:E:765:LEU:HD12	5:E:776:MET:SD	2.52	0.50
5:E:1089:HIS:CE1	5:E:1112:LEU:HB3	2.46	0.50
6:F:156:LEU:O	6:F:159:LYS:NZ	2.45	0.50
1:A:124:ASN:OD1	1:A:168:SER:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:ALA:HB3	2:B:534:GLU:HG3	1.94	0.49
4:D:246:VAL:HG13	4:D:273:LEU:HD11	1.93	0.49
1:A:73:SER:OG	1:A:74:VAL:N	2.45	0.49
1:A:985:MET:HE3	1:A:985:MET:HA	1.94	0.49
3:C:1123:ARG:NH2	3:C:1318:SER:OG	2.45	0.49
1:A:149:ILE:HB	1:A:150:TRP:HE3	1.78	0.49
1:A:172:LEU:HD23	1:A:172:LEU:H	1.76	0.49
2:B:374:VAL:HG12	2:B:422:MET:HE1	1.94	0.49
2:B:984:SER:OG	2:B:1072:ASN:OD1	2.29	0.49
3:C:1233:LYS:O	3:C:1237:MET:HG3	2.12	0.49
1:A:787:LEU:HD21	1:A:798:LEU:HD23	1.94	0.49
2:B:537:THR:HA	2:B:552:GLU:O	2.12	0.49
3:C:885:VAL:O	3:C:889:LEU:HG	2.13	0.49
4:D:443:LEU:HD21	4:D:484:VAL:HG22	1.94	0.49
1:A:76:VAL:HG23	1:A:121:MET:HE2	1.94	0.49
5:E:765:LEU:HB2	5:E:776:MET:HE1	1.95	0.49
1:A:37:LEU:HD21	1:A:39:LYS:HG3	1.93	0.49
1:A:174:GLY:C	1:A:175:MET:HE2	2.37	0.49
1:A:569:PHE:HB3	1:A:589:LEU:HD12	1.95	0.49
1:A:638:PHE:CD1	1:A:643:ILE:HG12	2.47	0.49
1:A:817:LEU:H	1:A:820:VAL:HG23	1.78	0.49
4:D:383:PHE:O	4:D:386:GLU:HG2	2.12	0.49
4:D:997:ARG:NH2	4:D:1194:GLU:OE2	2.45	0.49
5:E:772:THR:HG23	5:E:798:ILE:HG12	1.93	0.49
5:E:1086:MET:HE2	5:E:1090:LYS:HG2	1.94	0.49
1:A:809:TYR:O	1:A:813:ARG:HD3	2.12	0.49
3:C:493:ASP:HA	3:C:516:SER:HB2	1.94	0.49
3:C:519:LYS:NZ	3:C:559:LYS:O	2.45	0.49
4:D:21:HIS:CE1	4:D:280:MET:HE3	2.47	0.49
4:D:416:ILE:HG23	4:D:473:LEU:HD21	1.94	0.49
1:A:428:ASP:HB2	1:A:496:TYR:CE1	2.48	0.49
5:E:808:ALA:HB2	5:E:823:CYS:SG	2.53	0.49
1:A:510:ILE:HG22	1:A:519:VAL:HG22	1.95	0.49
1:A:859:LEU:HD13	1:A:881:LYS:HG2	1.94	0.49
2:B:784:CYS:O	2:B:788:GLY:N	2.45	0.49
2:B:1209:SER:OG	2:B:1232:CYS:SG	2.70	0.48
4:D:68:ASP:HA	4:D:110:ALA:HB2	1.94	0.48
4:D:1251:ALA:HB1	4:D:1276:TYR:CE1	2.48	0.48
1:A:175:MET:HE2	1:A:175:MET:N	2.28	0.48
1:A:849:ALA:HB2	1:A:862:ILE:HG21	1.95	0.48
2:B:181:SER:HB3	2:B:257:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1195:PHE:HD2	2:B:1213:MET:HE1	1.78	0.48
4:D:2:ASP:HB3	4:D:5:GLU:HG3	1.94	0.48
4:D:23:LEU:HD11	4:D:50:GLU:HG3	1.95	0.48
4:D:815:ALA:O	4:D:818:HIS:ND1	2.43	0.48
3:C:211:LEU:HD23	3:C:225:LEU:HD12	1.94	0.48
3:C:968:GLY:O	3:C:971:ILE:HG22	2.13	0.48
4:D:384:LEU:O	4:D:388:GLN:HG2	2.14	0.48
4:D:384:LEU:HD23	4:D:387:ILE:HD11	1.95	0.48
5:E:817:LEU:HD22	5:E:848:ARG:HG2	1.94	0.48
1:A:221:GLU:HB3	1:A:224:CYS:HB3	1.95	0.48
1:A:3:PHE:CZ	1:A:297:GLY:HA3	2.48	0.48
1:A:526:ILE:HG12	1:A:540:TYR:HB2	1.94	0.48
2:B:471:SER:HB3	2:B:494:ASN:HB2	1.95	0.48
1:A:822:TYR:C	1:A:824:VAL:H	2.21	0.48
4:D:112:TYR:HB2	4:D:134:MET:HE1	1.96	0.48
4:D:937:CYS:SG	4:D:961:LEU:HD11	2.52	0.48
4:D:1108:LEU:HD13	4:D:1126:GLU:HG2	1.94	0.48
2:B:747:THR:O	2:B:751:ILE:HG12	2.14	0.48
3:C:71:VAL:HB	3:C:80:TYR:HB2	1.95	0.48
5:E:431:PHE:O	5:E:435:GLY:N	2.47	0.48
2:B:865:TYR:HD2	2:B:888:ALA:HB2	1.78	0.48
3:C:615:ASN:OD1	3:C:661:ARG:NH2	2.42	0.48
4:D:482:GLU:OE2	4:D:872:GLN:NE2	2.43	0.48
4:D:1057:GLN:HG2	4:D:1061:TYR:CZ	2.49	0.48
2:B:970:ARG:NH1	2:B:973:THR:OG1	2.46	0.48
3:C:41:PHE:CD1	3:C:47:LYS:HA	2.49	0.48
4:D:1016:ASN:HD21	4:D:1018:ARG:HB2	1.79	0.48
2:B:18:ILE:HD12	2:B:337:VAL:HG13	1.96	0.48
2:B:473:ILE:HG23	2:B:490:VAL:HG13	1.96	0.48
3:C:1117:GLN:HG3	3:C:1154:LEU:HD21	1.96	0.48
4:D:1267:ALA:O	4:D:1271:LYS:HG2	2.14	0.48
5:E:789:ASP:O	5:E:793:LYS:HG2	2.14	0.48
1:A:76:VAL:HG22	1:A:89:SER:HB2	1.95	0.47
2:B:171:ARG:NE	2:B:258:ASP:OD2	2.47	0.47
3:C:7:LEU:HD12	3:C:343:LEU:HD23	1.96	0.47
3:C:246:MET:SD	3:C:290:VAL:HG21	2.54	0.47
3:C:590:THR:OG1	3:C:593:GLY:O	2.32	0.47
5:E:648:PRO:HB3	5:E:663:CYS:SG	2.54	0.47
1:A:284:ASN:HB3	1:A:306:ILE:HD11	1.97	0.47
3:C:412:VAL:HG23	3:C:421:LEU:HD11	1.96	0.47
3:C:1314:CYS:HB3	3:C:1317:CYS:SG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:414:HIS:CE1	5:E:415:GLN:HG3	2.48	0.47
5:E:427:LEU:HD21	5:E:449:VAL:HG21	1.96	0.47
1:A:82:GLN:HE21	1:A:126:ASP:C	2.21	0.47
2:B:982:LEU:HD13	2:B:999:LEU:HD21	1.95	0.47
5:E:494:VAL:O	5:E:504:VAL:HA	2.14	0.47
1:A:173:PHE:HE2	1:A:183:TYR:CG	2.33	0.47
1:A:618:TYR:CE2	1:A:628:PRO:HG3	2.49	0.47
1:A:854:GLU:OE1	3:C:1239:ARG:NH1	2.47	0.47
2:B:449:CYS:SG	2:B:473:ILE:HB	2.55	0.47
3:C:823:ARG:C	3:C:824:MET:HE2	2.39	0.47
3:C:905:LYS:O	3:C:909:GLY:N	2.44	0.47
5:E:560:ARG:NH2	5:E:607:ASP:OD2	2.48	0.47
1:A:721:ARG:NH2	2:B:761:ILE:HG22	2.28	0.47
1:A:767:ARG:HH12	1:A:787:LEU:HA	1.78	0.47
3:C:256:VAL:HG12	3:C:268:ILE:HD12	1.95	0.47
4:D:1207:TYR:CD2	4:D:1215:MET:HG3	2.49	0.47
5:E:727:TYR:HB2	5:E:729:TYR:CZ	2.49	0.47
1:A:513:SER:OG	1:A:514:ASP:N	2.46	0.47
1:A:570:PHE:HD2	1:A:572:LEU:HD23	1.80	0.47
1:A:848:LEU:HD22	1:A:862:ILE:HD11	1.96	0.47
3:C:686:LEU:HD22	3:C:726:LEU:HD22	1.95	0.47
4:D:203:GLN:NE2	4:D:207:ASN:OD1	2.48	0.47
4:D:1006:PRO:O	4:D:1009:PHE:HB2	2.15	0.47
4:D:1234:TYR:CZ	4:D:1256:MET:HG2	2.49	0.47
2:B:277:ARG:HH12	2:B:312:VAL:HG22	1.79	0.47
2:B:985:LEU:HD12	2:B:986:PRO:HD2	1.97	0.47
3:C:279:THR:HG23	3:C:294:GLY:HA2	1.96	0.47
4:D:824:LEU:HD21	4:D:868:VAL:HG22	1.97	0.47
4:D:1011:MET:HA	4:D:1014:LYS:HB2	1.96	0.47
1:A:1081:PHE:HA	1:A:1084:CYS:HB3	1.97	0.47
3:C:117:VAL:HG13	3:C:141:ARG:HB2	1.95	0.47
1:A:157:ILE:HD12	1:A:175:MET:SD	2.55	0.47
4:D:687:PHE:HZ	4:D:718:ARG:HH21	1.61	0.47
5:E:719:SER:OG	5:E:731:THR:OG1	2.22	0.47
3:C:11:THR:HB	3:C:35:ASP:HB3	1.97	0.47
3:C:899:LEU:HD13	3:C:923:GLN:HG3	1.96	0.47
4:D:695:ALA:HB1	4:D:708:TYR:CD1	2.50	0.47
1:A:734:LEU:HD11	1:A:743:LYS:HA	1.96	0.46
2:B:960:ARG:NH1	2:B:964:ASP:OD1	2.48	0.46
3:C:114:VAL:HG23	3:C:122:LEU:HB3	1.98	0.46
3:C:997:ALA:HA	3:C:1000:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:ALA:O	4:D:131:ILE:HG12	2.15	0.46
4:D:509:GLU:OE2	4:D:513:ASN:ND2	2.49	0.46
4:D:1217:GLU:OE2	4:D:1221:LYS:NZ	2.32	0.46
5:E:817:LEU:HA	5:E:820:ALA:HB3	1.96	0.46
5:E:1074:TYR:HB2	5:E:1084:ALA:HB2	1.97	0.46
2:B:282:ASP:OD2	4:D:1290:HIS:NE2	2.42	0.46
2:B:305:SER:OG	2:B:313:ARG:NH1	2.48	0.46
2:B:440:VAL:HB	2:B:447:ILE:HB	1.97	0.46
3:C:296:ASN:HD21	3:C:320:LYS:HA	1.80	0.46
3:C:1001:GLY:HA2	3:C:1005:THR:HB	1.97	0.46
5:E:489:MET:HE1	5:E:494:VAL:HG23	1.98	0.46
5:E:943:PRO:O	5:E:946:GLU:HG3	2.15	0.46
2:B:405:LEU:HD12	2:B:408:LYS:HE2	1.98	0.46
2:B:755:ALA:HB1	2:B:771:TYR:CD1	2.50	0.46
3:C:215:ASN:OD1	3:C:218:GLU:N	2.47	0.46
3:C:795:LEU:HB2	3:C:820:MET:HB3	1.97	0.46
4:D:782:ALA:HB1	4:D:791:LEU:HD13	1.96	0.46
4:D:802:LEU:HD12	4:D:804:TRP:HD1	1.80	0.46
5:E:504:VAL:O	5:E:512:LYS:N	2.29	0.46
2:B:58:CYS:SG	2:B:99:VAL:HG12	2.55	0.46
2:B:771:TYR:HD2	2:B:780:ALA:HA	1.81	0.46
1:A:36:GLY:N	1:A:72:GLY:O	2.48	0.46
1:A:70:HIS:HA	1:A:90:ASP:OD2	2.15	0.46
3:C:831:VAL:O	3:C:835:LEU:HG	2.15	0.46
3:C:1278:ILE:HG21	3:C:1297:PHE:HB3	1.96	0.46
4:D:956:MET:CE	4:D:987:MET:HG3	2.45	0.46
1:A:712:LEU:HD21	1:A:734:LEU:HD23	1.95	0.46
2:B:619:ALA:HB3	2:B:620:PRO:HD3	1.97	0.46
3:C:237:TYR:HB2	3:C:247:ILE:HG12	1.98	0.46
4:D:662:ASP:N	4:D:693:LYS:HZ1	2.13	0.46
4:D:1008:PHE:HA	4:D:1011:MET:SD	2.56	0.46
3:C:515:VAL:HG21	3:C:535:LYS:HE3	1.98	0.46
3:C:1230:TYR:O	3:C:1234:ILE:HG12	2.15	0.46
4:D:347:TYR:CZ	4:D:363:GLY:HA3	2.51	0.46
5:E:1086:MET:HE3	5:E:1086:MET:O	2.16	0.46
6:F:169:GLU:OE1	6:F:169:GLU:N	2.49	0.46
1:A:740:GLU:C	1:A:742:MET:H	2.24	0.46
2:B:1036:GLU:OE1	3:C:588:LYS:NZ	2.44	0.46
2:B:1097:TYR:O	2:B:1168:VAL:HG12	2.16	0.46
4:D:936:SER:O	4:D:940:GLN:HG2	2.15	0.46
1:A:408:ALA:N	1:A:428:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:SER:O	1:A:558:LEU:HD12	2.15	0.46
2:B:282:ASP:H	2:B:300:SER:HB3	1.79	0.46
3:C:876:TYR:O	3:C:880:LYS:N	2.49	0.46
4:D:586:LEU:HD13	4:D:623:LEU:HA	1.97	0.46
1:A:11:ILE:HG13	1:A:17:LEU:HD11	1.98	0.46
1:A:109:MET:HE1	1:A:144:VAL:O	2.16	0.46
3:C:94:ASN:HD22	3:C:96:MET:HE2	1.81	0.46
3:C:106:SER:HB2	3:C:111:PHE:HB2	1.98	0.46
3:C:239:TRP:CH2	3:C:259:THR:HG21	2.51	0.46
3:C:555:SER:HB3	3:C:558:ILE:HG13	1.97	0.46
3:C:1218:MET:HE1	3:C:1235:GLU:HA	1.98	0.46
4:D:10:ILE:HG21	4:D:42:TYR:CD2	2.51	0.46
4:D:19:PHE:CE1	4:D:49:MET:HE3	2.51	0.46
4:D:75:LEU:HD23	4:D:78:ILE:HD12	1.96	0.46
4:D:764:LYS:O	4:D:767:ILE:HG22	2.15	0.45
4:D:813:GLN:NE2	4:D:841:TYR:OH	2.47	0.45
4:D:1053:ARG:HA	6:F:155:LYS:HZ3	1.82	0.45
3:C:662:PHE:HE2	3:C:690:GLU:HG3	1.81	0.45
3:C:212:PHE:CE2	3:C:214:LEU:HB2	2.52	0.45
4:D:119:TRP:HH2	4:D:150:TRP:HE3	1.63	0.45
4:D:766:LEU:HD23	4:D:766:LEU:HA	1.81	0.45
1:A:129:LYS:HG2	1:A:148:ARG:CD	2.47	0.45
1:A:813:ARG:NE	2:B:668:ARG:HH21	2.15	0.45
4:D:938:LEU:HG	4:D:961:LEU:HD13	1.99	0.45
1:A:22:TRP:CZ2	1:A:312:GLU:HG3	2.51	0.45
1:A:169:LYS:O	1:A:185:ASN:HB2	2.17	0.45
1:A:225:PRO:HB2	1:A:238:ILE:HG22	1.98	0.45
1:A:612:MET:HE2	1:A:617:MET:HG3	1.97	0.45
2:B:489:LEU:HG	2:B:520:LEU:HD13	1.98	0.45
4:D:419:LEU:HD13	4:D:455:TYR:HE1	1.81	0.45
4:D:952:GLU:O	4:D:956:MET:HG2	2.16	0.45
5:E:524:PRO:HA	5:E:538:THR:HG22	1.99	0.45
1:A:154:LEU:HB3	1:A:155:LYS:H	1.57	0.45
1:A:608:LEU:HA	1:A:608:LEU:HD23	1.82	0.45
2:B:606:HIS:O	2:B:609:SER:OG	2.20	0.45
2:B:1054:VAL:HG11	2:B:1063:ASN:HB3	1.98	0.45
4:D:411:ARG:HH22	4:D:685:PRO:HG3	1.81	0.45
3:C:39:LYS:HB3	3:C:41:PHE:CE1	2.52	0.45
5:E:488:ALA:O	5:E:489:MET:HE2	2.17	0.45
2:B:35:LEU:HB2	2:B:49:LEU:HB2	1.99	0.45
5:E:615:LYS:HA	5:E:644:LYS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:708:HIS:CE1	5:E:759:LEU:HD11	2.48	0.45
3:C:32:THR:HB	3:C:38:VAL:HG22	1.99	0.45
3:C:281:ILE:HG12	3:C:292:THR:HG22	1.99	0.45
3:C:902:ALA:HB2	3:C:917:ALA:HB3	1.98	0.45
4:D:515:LEU:HD11	4:D:531:LEU:HG	1.98	0.45
4:D:970:GLN:O	4:D:974:HIS:ND1	2.50	0.45
4:D:1135:GLN:OE1	4:D:1138:ASN:ND2	2.50	0.45
5:E:812:VAL:HG11	5:E:858:MET:SD	2.57	0.45
5:E:849:VAL:HB	5:E:865:LEU:HD21	1.98	0.45
1:A:352:ASP:OD1	1:A:352:ASP:N	2.50	0.45
2:B:401:LEU:HB3	2:B:412:TYR:HB2	1.98	0.45
3:C:125:ASN:O	3:C:129:SER:CA	2.64	0.45
4:D:277:LEU:HD12	4:D:281:GLU:HB2	1.99	0.45
5:E:453:LYS:HA	5:E:453:LYS:HD3	1.79	0.45
5:E:566:VAL:HG13	5:E:622:ARG:HH12	1.81	0.45
5:E:753:MET:HE2	5:E:753:MET:HA	1.99	0.45
1:A:416:ASN:ND2	1:A:422:LEU:HD21	2.31	0.44
1:A:905:ALA:HA	1:A:910:MET:HE2	1.98	0.44
5:E:812:VAL:HG22	5:E:852:LEU:HD22	1.98	0.44
2:B:463:LYS:NZ	2:B:466:GLU:OE1	2.41	0.44
2:B:913:ASP:OD1	2:B:1233:ARG:NH2	2.42	0.44
2:B:1016:ARG:NH2	2:B:1045:LYS:O	2.50	0.44
4:D:205:ILE:HG12	4:D:215:PHE:CE1	2.51	0.44
4:D:887:CYS:HB2	4:D:910:ALA:HB2	1.99	0.44
4:D:1031:LEU:HD23	4:D:1046:PHE:HZ	1.82	0.44
5:E:708:HIS:HA	5:E:784:THR:HG22	1.99	0.44
1:A:609:PHE:HE2	1:A:611:MET:HB3	1.82	0.44
2:B:18:ILE:HG23	2:B:326:THR:HG21	1.99	0.44
2:B:1209:SER:O	2:B:1210:CYS:SG	2.75	0.44
3:C:1130:PHE:HB2	3:C:1316:MET:HE3	2.00	0.44
3:C:1288:ASP:HB3	3:C:1300:LEU:HD22	1.97	0.44
3:C:61:ASP:HB3	3:C:105:TRP:CE3	2.52	0.44
3:C:272:ARG:HH11	3:C:275:LYS:HA	1.82	0.44
3:C:501:TYR:CZ	3:C:503:GLU:HB3	2.52	0.44
3:C:815:ALA:HB2	3:C:837:HIS:CE1	2.53	0.44
4:D:430:LEU:HA	4:D:433:LEU:HD12	1.98	0.44
4:D:455:TYR:HD2	4:D:477:CYS:SG	2.41	0.44
5:E:1003:ILE:O	5:E:1007:THR:OG1	2.30	0.44
1:A:76:VAL:HG21	1:A:121:MET:HG3	1.99	0.44
1:A:481:HIS:HB2	1:A:498:LYS:HB3	1.99	0.44
5:E:414:HIS:ND1	5:E:415:GLN:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:MET:CE	1:A:243:ASN:H	2.29	0.44
3:C:899:LEU:HD12	3:C:918:TYR:HE1	1.83	0.44
4:D:640:LEU:HD21	4:D:660:ASN:HA	1.99	0.44
1:A:368:LYS:NZ	1:A:656:GLU:O	2.34	0.44
1:A:442:ILE:HG12	1:A:517:LEU:HD11	1.99	0.44
1:A:764:MET:HE3	3:C:1340:GLU:OE2	2.17	0.44
2:B:977:ILE:HG12	2:B:1088:TYR:CD1	2.52	0.44
3:C:932:LEU:HB2	3:C:957:VAL:HG12	1.99	0.44
4:D:812:LEU:HD13	4:D:837:LEU:HA	1.99	0.44
1:A:309:LEU:HD22	1:A:318:ILE:HD11	2.00	0.44
3:C:1093:PHE:CE2	3:C:1132:MET:HG2	2.52	0.44
3:C:1214:ALA:HB1	3:C:1234:ILE:HG23	1.99	0.44
5:E:560:ARG:HG3	5:E:602:TYR:CZ	2.53	0.44
1:A:360:PHE:HB2	1:A:369:TYR:HB2	2.00	0.44
1:A:754:PHE:HE1	2:B:672:LEU:HD22	1.83	0.44
2:B:469:MET:HG3	2:B:473:ILE:HD11	2.00	0.44
3:C:1223:ARG:HD2	3:C:1223:ARG:HA	1.89	0.44
4:D:119:TRP:CH2	4:D:150:TRP:HE3	2.36	0.44
4:D:1079:VAL:HG23	4:D:1205:ASP:OD1	2.17	0.44
5:E:725:VAL:HG12	5:E:773:ARG:HH11	1.83	0.44
1:A:172:LEU:HD12	1:A:180:ILE:HG21	2.00	0.43
3:C:159:ASP:OD1	3:C:159:ASP:N	2.51	0.43
3:C:1140:LYS:HA	3:C:1140:LYS:HD3	1.81	0.43
4:D:419:LEU:HD13	4:D:455:TYR:CE1	2.52	0.43
5:E:836:LEU:HD11	5:E:852:LEU:HD12	2.00	0.43
1:A:240:ARG:HG2	1:A:243:ASN:ND2	2.33	0.43
2:B:1084:SER:OG	2:B:1087:SER:O	2.36	0.43
3:C:704:VAL:O	3:C:708:MET:HG3	2.19	0.43
3:C:967:TYR:O	3:C:970:ALA:HB3	2.18	0.43
4:D:469:PRO:HB3	4:D:726:LEU:HD22	1.99	0.43
4:D:979:LEU:HD12	4:D:992:LEU:HD22	1.99	0.43
5:E:795:ILE:HD12	5:E:803:VAL:HG11	2.00	0.43
1:A:230:CYS:HB2	1:A:259:ILE:HD11	2.00	0.43
2:B:517:VAL:HG13	2:B:531:VAL:HG13	2.01	0.43
2:B:663:LYS:HG3	2:B:678:ILE:HG21	1.99	0.43
2:B:910:ARG:HG2	5:E:932:PHE:HE2	1.83	0.43
3:C:42:ASP:HB3	3:C:48:ARG:HE	1.83	0.43
3:C:478:ILE:HD12	3:C:490:TYR:CD1	2.53	0.43
3:C:1156:SER:O	3:C:1160:VAL:HG23	2.18	0.43
4:D:21:HIS:O	4:D:25:VAL:HG23	2.19	0.43
4:D:306:LEU:HD22	4:D:333:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1042:ALA:HB1	5:E:1058:LEU:HD13	2.00	0.43
2:B:428:GLU:HG3	2:B:459:PHE:HB3	2.00	0.43
2:B:458:SER:OG	2:B:459:PHE:N	2.51	0.43
3:C:67:ASP:HA	3:C:84:ALA:HB3	2.00	0.43
3:C:862:LEU:HA	3:C:865:LYS:HD3	2.00	0.43
3:C:979:CYS:HB3	3:C:982:GLU:HG2	2.00	0.43
3:C:996:TYR:O	3:C:1000:ILE:HG23	2.19	0.43
4:D:976:GLN:HG3	4:D:1008:PHE:CE1	2.52	0.43
6:F:129:VAL:O	6:F:133:ARG:HG2	2.18	0.43
1:A:101:TYR:HB3	1:A:106:ILE:HD13	2.01	0.43
1:A:450:TYR:CE1	1:A:477:GLU:HB3	2.53	0.43
1:A:966:ARG:NH2	6:F:187:VAL:HG22	2.33	0.43
2:B:282:ASP:HB2	2:B:300:SER:HB2	1.99	0.43
2:B:910:ARG:HG2	5:E:932:PHE:CE2	2.54	0.43
5:E:415:GLN:O	5:E:453:LYS:HE2	2.18	0.43
1:A:1079:ARG:NH2	6:F:149:ASP:OD1	2.52	0.43
2:B:139:SER:HB2	2:B:182:ILE:HG13	2.00	0.43
2:B:515:THR:OG1	2:B:533:ASP:HB2	2.19	0.43
2:B:561:ASN:HB2	2:B:567:MET:HB2	2.01	0.43
3:C:3:ARG:HA	3:C:346:PHE:HA	2.00	0.43
3:C:201:MET:SD	3:C:213:PHE:HB3	2.59	0.43
3:C:933:ASP:O	3:C:936:ASN:ND2	2.51	0.43
4:D:654:VAL:O	4:D:657:THR:OG1	2.31	0.43
5:E:892:ALA:HB1	5:E:900:LEU:HA	2.00	0.43
1:A:868:ARG:NH1	2:B:544:ASP:OD2	2.39	0.43
2:B:673:ARG:O	2:B:676:GLU:HG2	2.18	0.43
2:B:1222:LEU:HD23	2:B:1222:LEU:HA	1.85	0.43
3:C:391:ASN:HB2	3:C:404:MET:HA	2.00	0.43
4:D:298:THR:HG22	4:D:445:PRO:HG2	2.01	0.43
4:D:595:MET:HG3	4:D:595:MET:O	2.18	0.43
1:A:171:LEU:O	1:A:183:TYR:HB2	2.18	0.43
1:A:189:PHE:HZ	1:A:192:LYS:HG3	1.84	0.43
1:A:355:GLU:HB2	1:A:373:VAL:O	2.19	0.43
2:B:263:VAL:HG23	2:B:277:ARG:HB2	2.01	0.43
2:B:314:LEU:HD22	2:B:390:LEU:HD13	2.01	0.43
3:C:81:LEU:HD11	3:C:92:LEU:HD22	2.00	0.43
3:C:798:TYR:HE2	3:C:820:MET:HE3	1.82	0.43
4:D:767:ILE:HD12	4:D:767:ILE:HA	1.92	0.43
4:D:1272:LEU:HD11	4:D:1276:TYR:CZ	2.53	0.43
5:E:432:LEU:HD13	5:E:729:TYR:CE1	2.54	0.43
5:E:457:ALA:HB2	5:E:489:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:LYS:O	1:A:687:SER:OG	2.35	0.43
2:B:178:PRO:O	2:B:259:TRP:N	2.49	0.43
2:B:947:ARG:HH22	2:B:986:PRO:HB3	1.82	0.43
4:D:700:LYS:HE3	4:D:701:HIS:NE2	2.34	0.43
4:D:1278:LYS:HA	4:D:1278:LYS:HD3	1.79	0.43
1:A:641:LEU:HD22	1:A:668:ILE:HD11	2.00	0.43
2:B:256:VAL:O	2:B:263:VAL:HA	2.19	0.43
2:B:258:ASP:O	2:B:283:PRO:HD2	2.19	0.43
2:B:743:ASP:N	2:B:744:PRO:HD3	2.34	0.43
3:C:175:THR:HG21	3:C:214:LEU:HD13	2.00	0.43
3:C:782:ALA:HA	3:C:785:LEU:HD12	2.01	0.43
4:D:229:ASP:OD1	4:D:229:ASP:N	2.49	0.43
4:D:1254:TYR:HB3	4:D:1272:LEU:HB2	2.01	0.43
5:E:912:GLU:HG3	5:E:937:MET:HG3	2.00	0.43
2:B:257:ALA:HB1	2:B:283:PRO:HB2	2.01	0.42
4:D:71:LEU:HB3	4:D:110:ALA:HB1	1.99	0.42
5:E:696:SER:O	5:E:708:HIS:HB3	2.19	0.42
1:A:608:LEU:HB3	1:A:638:PHE:HE2	1.83	0.42
2:B:831:MET:HE2	2:B:831:MET:HB2	1.90	0.42
2:B:850:ALA:HB3	2:B:868:TYR:HE2	1.84	0.42
3:C:411:TYR:CE2	3:C:420:LYS:HB3	2.54	0.42
5:E:723:MET:HG3	5:E:728:TYR:HA	2.01	0.42
5:E:1032:PHE:HE1	5:E:1035:ARG:HH21	1.67	0.42
1:A:527:GLN:HG2	1:A:539:LYS:HG2	2.00	0.42
1:A:916:LEU:HD22	1:A:919:ARG:HH12	1.84	0.42
1:A:941:ASN:HB3	1:A:984:GLN:OE1	2.20	0.42
1:A:1063:PRO:HA	1:A:1064:PRO:HD3	1.95	0.42
2:B:34:ARG:HH11	2:B:48:PRO:HB3	1.85	0.42
2:B:548:LEU:HD23	2:B:548:LEU:H	1.84	0.42
3:C:146:CYS:HB3	3:C:184:MET:O	2.19	0.42
3:C:569:ASP:OD2	3:C:661:ARG:NH2	2.48	0.42
3:C:837:HIS:HD2	3:C:838:PRO:HD2	1.84	0.42
4:D:707:LEU:HD23	4:D:707:LEU:HA	1.92	0.42
4:D:962:MET:HG3	4:D:971:ALA:HB2	2.00	0.42
1:A:838:MET:HE3	1:A:838:MET:HB3	1.89	0.42
2:B:102:ASN:HB3	2:B:107:GLN:H	1.84	0.42
2:B:496:GLN:HE21	2:B:509:VAL:HG13	1.84	0.42
3:C:258:SER:OG	3:C:260:HIS:ND1	2.40	0.42
3:C:1040:LEU:HD22	3:C:1070:LEU:HD23	2.01	0.42
4:D:41:PHE:HD1	4:D:63:ILE:HD12	1.84	0.42
4:D:886:ILE:O	4:D:890:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1256:MET:HE2	4:D:1256:MET:HB2	1.85	0.42
1:A:723:LYS:HD3	1:A:723:LYS:HA	1.78	0.42
1:A:737:LEU:HD23	1:A:739:SER:H	1.84	0.42
1:A:764:MET:HE2	1:A:766:ARG:HG3	2.02	0.42
1:A:825:GLN:O	1:A:827:ARG:NH1	2.51	0.42
2:B:438:LEU:HD12	2:B:449:CYS:SG	2.60	0.42
3:C:258:SER:HG	3:C:260:HIS:HD1	1.62	0.42
3:C:844:ARG:HB2	3:C:868:TYR:CZ	2.55	0.42
4:D:901:GLU:H	4:D:901:GLU:CD	2.26	0.42
2:B:5:LEU:HD21	2:B:8:ARG:HE	1.84	0.42
2:B:1206:MET:HG2	2:B:1213:MET:HG2	2.01	0.42
3:C:112:LEU:HB3	3:C:124:TYR:HB3	2.02	0.42
3:C:1169:HIS:CD2	3:C:1203:ARG:HD3	2.55	0.42
4:D:714:GLU:HB3	4:D:718:ARG:NH2	2.35	0.42
5:E:1041:ASN:OD1	5:E:1044:ARG:NH2	2.41	0.42
2:B:924:GLN:O	2:B:928:ILE:HG12	2.20	0.42
2:B:1009:LEU:HB3	2:B:1053:LEU:HD11	2.02	0.42
3:C:368:LEU:HD12	3:C:386:VAL:O	2.20	0.42
4:D:468:GLN:HE21	4:D:468:GLN:HB3	1.73	0.42
5:E:494:VAL:HG11	5:E:505:ARG:HG2	2.02	0.42
1:A:212:TRP:CD2	1:A:227:LEU:HD12	2.54	0.42
1:A:318:ILE:HG23	1:A:329:ALA:HB3	2.01	0.42
1:A:647:LEU:HD21	1:A:664:ILE:HD12	2.02	0.42
1:A:703:ALA:HB2	1:A:718:ALA:HB3	2.02	0.42
2:B:16:ASN:ND2	2:B:56:VAL:O	2.52	0.42
3:C:106:SER:HA	3:C:147:TRP:CG	2.55	0.42
3:C:426:TYR:OH	3:C:451:HIS:NE2	2.40	0.42
3:C:682:ALA:HB1	3:C:698:TYR:CE1	2.54	0.42
3:C:1059:ILE:HD11	3:C:1091:TYR:HB3	2.02	0.42
3:C:1317:CYS:SG	3:C:1319:GLU:HB2	2.59	0.42
1:A:22:TRP:H	1:A:310:SER:HB3	1.83	0.42
2:B:697:ALA:HB2	2:B:712:LEU:HB3	2.02	0.42
2:B:792:MET:O	2:B:796:ILE:HG22	2.19	0.42
2:B:977:ILE:O	2:B:981:LEU:HD23	2.20	0.42
3:C:4:ILE:HD11	3:C:347:LEU:HD13	2.01	0.42
4:D:987:MET:HA	4:D:1055:TRP:HH2	1.84	0.42
4:D:1120:VAL:O	4:D:1124:ILE:HG12	2.20	0.42
5:E:725:VAL:HA	5:E:726:PRO:HA	1.76	0.42
2:B:498:LEU:CD2	2:B:509:VAL:HA	2.50	0.42
2:B:1064:ASN:OD1	2:B:1074:CYS:HA	2.20	0.42
2:B:1065:PRO:HB2	2:B:1067:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:CYS:SG	4:D:117:PHE:HB2	2.59	0.42
4:D:87:PRO:HB2	4:D:92:ILE:HD11	2.00	0.42
4:D:536:TYR:CE2	4:D:544:LEU:HB3	2.55	0.42
5:E:1063:SER:OG	5:E:1066:ASP:OD2	2.32	0.42
1:A:33:GLY:N	1:A:37:LEU:O	2.49	0.41
1:A:212:TRP:CE3	1:A:227:LEU:HD12	2.55	0.41
1:A:263:HIS:NE2	1:A:264:MET:HG3	2.34	0.41
1:A:771:ILE:HG21	1:A:798:LEU:HD21	2.02	0.41
2:B:1184:LYS:HD2	2:B:1213:MET:HE3	2.02	0.41
3:C:279:THR:HG21	3:C:322:LEU:HB2	2.01	0.41
3:C:409:TRP:CD1	3:C:423:ASP:HB3	2.55	0.41
3:C:542:CYS:O	3:C:546:ASP:N	2.53	0.41
4:D:997:ARG:HD3	4:D:1035:TYR:CG	2.54	0.41
4:D:1105:GLU:HA	4:D:1108:LEU:HD12	2.02	0.41
5:E:541:ALA:HB1	5:E:562:LEU:HB3	2.02	0.41
5:E:762:PHE:CG	5:E:776:MET:HE3	2.54	0.41
1:A:779:ASP:O	1:A:783:VAL:HG23	2.21	0.41
2:B:143:ASP:OD2	2:B:250:ARG:NH2	2.47	0.41
2:B:677:LEU:HD22	2:B:702:TYR:CD2	2.55	0.41
3:C:277:ASN:N	3:C:295:ASP:OD1	2.51	0.41
3:C:606:PHE:O	3:C:608:HIS:ND1	2.49	0.41
4:D:698:TYR:CD2	4:D:707:LEU:HB3	2.55	0.41
4:D:1271:LYS:O	4:D:1275:ASN:ND2	2.46	0.41
5:E:487:LEU:HD23	5:E:488:ALA:N	2.35	0.41
1:A:887:ALA:O	1:A:891:THR:HG23	2.20	0.41
2:B:99:VAL:HG23	2:B:110:SER:HB3	2.02	0.41
2:B:732:PHE:CZ	2:B:754:GLN:HA	2.55	0.41
3:C:21:TRP:CE3	3:C:29:LEU:HB2	2.55	0.41
3:C:756:LEU:HB3	3:C:758:HIS:ND1	2.36	0.41
3:C:845:ASP:O	3:C:849:ILE:HG13	2.20	0.41
4:D:424:ASP:OD1	4:D:476:ARG:NH2	2.38	0.41
4:D:596:LYS:HA	4:D:596:LYS:HD3	1.90	0.41
4:D:616:ARG:HE	4:D:620:PHE:HE2	1.68	0.41
4:D:979:LEU:HD11	4:D:989:LEU:HA	2.02	0.41
4:D:1258:TRP:HE1	4:D:1263:ARG:HH21	1.67	0.41
5:E:850:ALA:O	5:E:854:THR:HG23	2.19	0.41
5:E:934:VAL:HG11	5:E:948:TYR:CD2	2.55	0.41
2:B:158:ILE:HB	2:B:167:VAL:HG12	2.02	0.41
3:C:300:ILE:O	3:C:310:TYR:HB3	2.20	0.41
3:C:322:LEU:HA	3:C:338:THR:HA	2.03	0.41
4:D:54:GLN:HG2	4:D:55:GLU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:416:GLN:HG2	5:E:724:GLU:CD	2.45	0.41
5:E:836:LEU:HD21	5:E:852:LEU:HD12	2.02	0.41
1:A:207:ILE:HG21	1:A:210:ILE:HG13	2.02	0.41
1:A:234:GLY:O	1:A:251:ASP:HB2	2.19	0.41
1:A:295:HIS:CD2	1:A:296:LEU:H	2.39	0.41
1:A:945:ASP:O	1:A:949:LEU:HG	2.20	0.41
2:B:143:ASP:CG	2:B:250:ARG:HH22	2.27	0.41
2:B:272:GLN:NE2	2:B:276:ASP:OD1	2.51	0.41
2:B:412:TYR:CE2	2:B:426:VAL:HG22	2.55	0.41
3:C:161:MET:HE2	3:C:161:MET:HB2	2.00	0.41
3:C:284:SER:O	3:C:288:ASN:N	2.54	0.41
4:D:293:LEU:O	4:D:297:ARG:HG2	2.21	0.41
4:D:762:MET:HA	4:D:762:MET:HE2	2.02	0.41
4:D:1061:TYR:HA	4:D:1125:MET:HE1	2.02	0.41
1:A:142:GLY:HA2	1:A:148:ARG:H	1.85	0.41
1:A:868:ARG:HH12	2:B:544:ASP:CG	2.26	0.41
2:B:1232:CYS:O	2:B:1234:ARG:N	2.51	0.41
3:C:1085:MET:O	3:C:1085:MET:HG2	2.21	0.41
3:C:1179:VAL:HG13	3:C:1186:PHE:CE1	2.56	0.41
4:D:88:ASP:HB2	4:D:91:ALA:HB3	2.01	0.41
4:D:536:TYR:CD2	4:D:544:LEU:HB3	2.55	0.41
4:D:1251:ALA:HB1	4:D:1276:TYR:HE1	1.86	0.41
5:E:714:PRO:HG3	5:E:757:ARG:HH21	1.85	0.41
2:B:771:TYR:HB3	2:B:780:ALA:HB2	2.03	0.41
3:C:815:ALA:HB1	3:C:842:LEU:HD13	2.03	0.41
5:E:653:TRP:CZ3	5:E:661:PHE:HB2	2.56	0.41
1:A:577:THR:O	1:A:577:THR:OG1	2.37	0.41
1:A:1073:LEU:HD11	6:F:158:THR:HG22	2.03	0.41
2:B:8:ARG:HH11	2:B:344:THR:HG21	1.86	0.41
3:C:699:ARG:HD3	5:E:885:TRP:HE1	1.86	0.41
4:D:66:LYS:O	4:D:70:SER:N	2.53	0.41
5:E:762:PHE:HA	5:E:776:MET:CE	2.51	0.41
5:E:954:ASP:C	5:E:956:THR:H	2.29	0.41
1:A:552:ASN:ND2	1:A:557:ARG:HG2	2.36	0.41
1:A:638:PHE:CE1	1:A:643:ILE:HG12	2.56	0.41
1:A:725:TYR:CE2	1:A:729:LYS:HD2	2.55	0.41
1:A:737:LEU:HD21	1:A:742:MET:CB	2.44	0.41
1:A:827:ARG:HG2	3:C:1219:ARG:NE	2.36	0.41
2:B:143:ASP:N	2:B:143:ASP:OD1	2.53	0.41
2:B:536:ASP:O	2:B:555:ALA:N	2.54	0.41
2:B:665:ALA:O	2:B:669:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:VAL:HG22	3:C:141:ARG:HG3	2.02	0.41
4:D:515:LEU:HD21	4:D:531:LEU:HB3	2.03	0.41
5:E:854:THR:HG22	5:E:878:PHE:HE2	1.86	0.41
5:E:896:ASP:C	5:E:898:VAL:H	2.28	0.41
1:A:141:VAL:HG21	1:A:150:TRP:CH2	2.56	0.41
2:B:103:PRO:HD3	2:B:140:TRP:HB3	2.03	0.41
3:C:252:GLY:HA2	3:C:278:LEU:HB2	2.04	0.41
3:C:1176:LEU:HD23	3:C:1176:LEU:HA	1.97	0.41
4:D:215:PHE:CB	4:D:238:LEU:HD21	2.47	0.41
5:E:495:TYR:OH	5:E:548:LEU:HD21	2.21	0.41
5:E:788:MET:HG3	5:E:810:MET:HE1	2.03	0.41
5:E:1105:GLN:HE21	5:E:1107:PHE:HE2	1.69	0.41
1:A:768:ASP:CG	3:C:1266:LEU:HD22	2.47	0.40
1:A:1084:CYS:SG	1:A:1088:PHE:HE2	2.44	0.40
2:B:181:SER:OG	2:B:286:ILE:HG22	2.21	0.40
2:B:263:VAL:HG13	2:B:279:LEU:HD11	2.02	0.40
2:B:569:CYS:SG	2:B:594:VAL:HG21	2.61	0.40
2:B:952:TYR:OH	2:B:991:SER:O	2.23	0.40
3:C:467:ARG:HD2	3:C:505:TRP:HE1	1.86	0.40
3:C:785:LEU:HD13	3:C:793:ASN:HB2	2.03	0.40
3:C:971:ILE:HG23	3:C:983:ALA:HB1	2.03	0.40
3:C:984:PHE:HD1	3:C:987:ALA:HB3	1.85	0.40
3:C:1097:MET:HE2	3:C:1135:GLU:HG3	2.02	0.40
4:D:292:THR:HB	4:D:309:ILE:HG23	2.02	0.40
5:E:805:GLU:O	5:E:809:ARG:HG3	2.21	0.40
5:E:1067:MET:HB2	5:E:1087:LEU:HB3	2.03	0.40
5:E:1074:TYR:CB	5:E:1084:ALA:HB2	2.51	0.40
1:A:123:TRP:CE3	1:A:130:ILE:HB	2.56	0.40
1:A:569:PHE:CE2	1:A:591:LEU:HD23	2.56	0.40
2:B:1033:LYS:HA	2:B:1033:LYS:HD3	1.83	0.40
3:C:1284:MET:HE3	3:C:1285:LEU:H	1.86	0.40
4:D:30:ILE:HG13	4:D:39:PHE:HB3	2.03	0.40
4:D:674:LEU:O	4:D:694:MET:HE1	2.20	0.40
4:D:843:LYS:HD3	4:D:843:LYS:HA	1.95	0.40
4:D:944:LEU:HD23	4:D:954:ALA:HB2	2.03	0.40
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.87	0.40
2:B:259:TRP:CZ3	4:D:1311:ARG:HG2	2.57	0.40
2:B:383:VAL:HG21	2:B:422:MET:HB3	2.03	0.40
3:C:53:LEU:HD13	3:C:73:ALA:HB2	2.02	0.40
3:C:922:LYS:HA	3:C:924:TRP:CZ3	2.57	0.40
4:D:499:ALA:HB2	4:D:514:ASN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:587:HIS:O	4:D:590:MET:HB2	2.21	0.40
4:D:821:VAL:HG12	4:D:823:GLU:H	1.86	0.40
1:A:1088:PHE:CZ	6:F:157:LEU:HD11	2.57	0.40
2:B:63:LYS:HE3	2:B:63:LYS:HB3	1.84	0.40
2:B:277:ARG:HD3	2:B:277:ARG:HA	1.83	0.40
2:B:772:ILE:HG12	2:B:796:ILE:HD12	2.04	0.40
3:C:201:MET:HB2	3:C:215:ASN:HD22	1.87	0.40
3:C:470:PRO:HD3	3:C:478:ILE:HD11	2.03	0.40
3:C:1194:LEU:HD23	3:C:1194:LEU:HA	1.90	0.40
4:D:168:PHE:CZ	4:D:183:GLY:HA3	2.56	0.40
4:D:597:ARG:N	4:D:616:ARG:HH12	2.20	0.40
5:E:410:SER:HB2	5:E:448:GLY:HA2	2.04	0.40
5:E:823:CYS:C	5:E:825:GLY:H	2.29	0.40
5:E:824:LEU:HD21	5:E:836:LEU:HD12	2.04	0.40
1:A:79:TRP:CZ3	1:A:86:LEU:HB2	2.56	0.40
1:A:425:LYS:HE2	1:A:425:LYS:HB2	1.78	0.40
2:B:496:GLN:NE2	2:B:498:LEU:HD21	2.36	0.40
2:B:726:TYR:HE2	2:B:738:PHE:CE1	2.39	0.40
2:B:866:MET:N	2:B:867:PRO:HD2	2.37	0.40
3:C:298:ILE:HD11	3:C:336:LEU:HD22	2.03	0.40
4:D:541:LYS:HG2	4:D:544:LEU:HD12	2.03	0.40
4:D:589:ALA:HA	4:D:592:LEU:HG	2.03	0.40
5:E:782:PHE:O	5:E:787:ASP:N	2.54	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	1063/1181 (90%)	995 (94%)	67 (6%)	1 (0%)	48	78
2	B	1144/1241 (92%)	1093 (96%)	51 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	1340/1342 (100%)	1281 (96%)	58 (4%)	1 (0%)	48	78
4	D	1313/1316 (100%)	1283 (98%)	30 (2%)	0	100	100
5	E	579/1462 (40%)	559 (96%)	20 (4%)	0	100	100
6	F	69/208 (33%)	66 (96%)	3 (4%)	0	100	100
All	All	5508/6750 (82%)	5277 (96%)	229 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	LYS
3	C	989	GLN

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	885/1018 (87%)	885 (100%)	0	100	100
2	B	927/1091 (85%)	927 (100%)	0	100	100
3	C	1080/1156 (93%)	1080 (100%)	0	100	100
4	D	1115/1136 (98%)	1115 (100%)	0	100	100
5	E	502/1246 (40%)	502 (100%)	0	100	100
6	F	54/181 (30%)	54 (100%)	0	100	100
All	All	4563/5828 (78%)	4563 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	80	ASN
1	A	246	ASN

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Mol	Chain	Res	Type
1	A	543	ASN
1	A	818	ASN
1	A	1039	GLN
2	B	92	HIS
2	B	145	GLN
2	B	303	GLN
2	B	1005	GLN
3	C	238	ASN
3	C	296	ASN
3	C	332	GLN
3	C	734	ASN
3	C	881	ASN
3	C	925	GLN
3	C	1052	ASN
3	C	1072	ASN
3	C	1126	HIS
3	C	1294	HIS
3	C	1325	GLN
4	D	4	GLN
4	D	193	ASN
4	D	203	GLN
4	D	207	ASN
4	D	388	GLN
4	D	513	ASN
4	D	514	ASN
4	D	834	GLN
4	D	881	HIS
4	D	1047	ASN
4	D	1057	GLN
4	D	1082	ASN
4	D	1138	ASN
4	D	1209	GLN
5	E	667	GLN
5	E	855	GLN
5	E	895	HIS
5	E	991	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

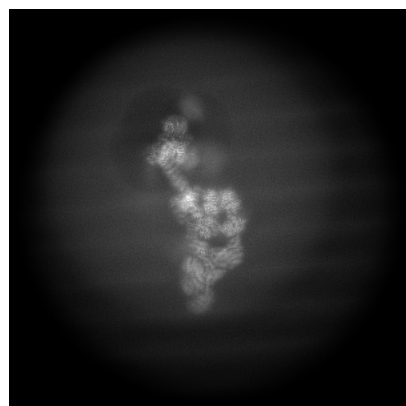
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29073. These allow visual inspection of the internal detail of the map and identification of artifacts.

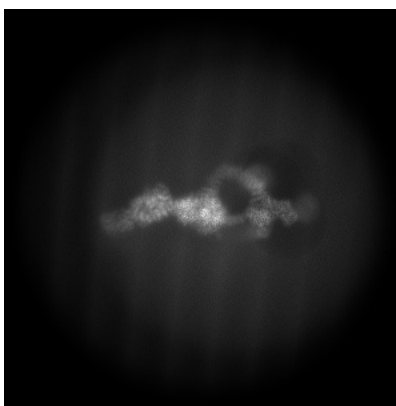
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

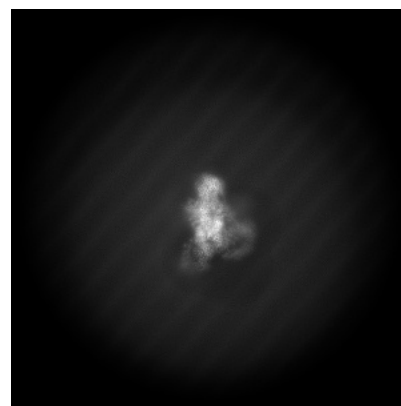
6.1.1 Primary map



X

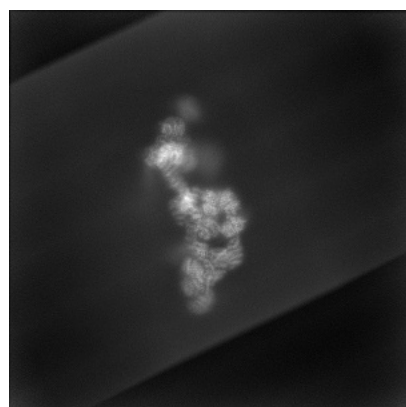


Y

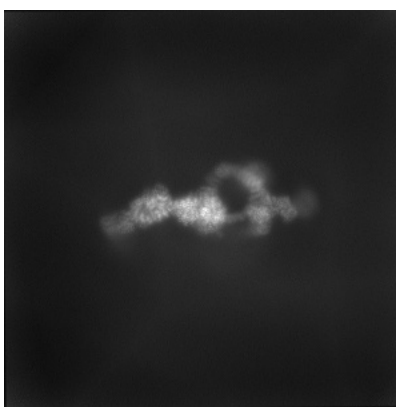


Z

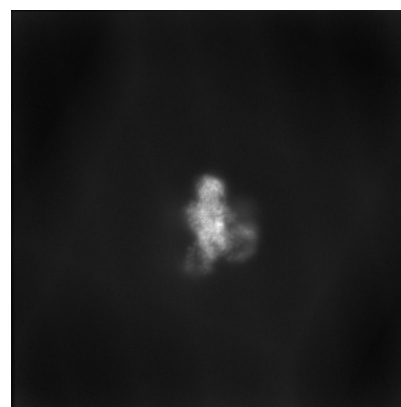
6.1.2 Raw map



X



Y

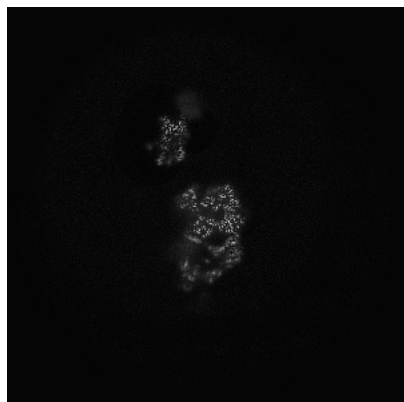


Z

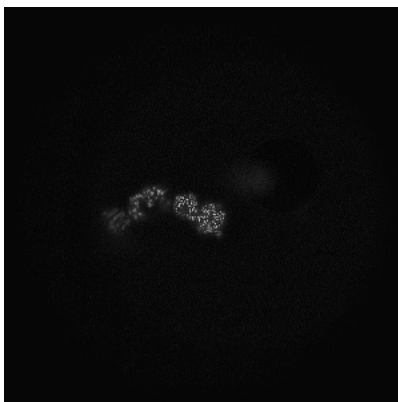
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

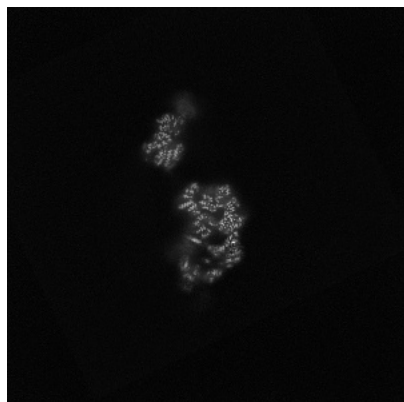


Y Index: 240



Z Index: 240

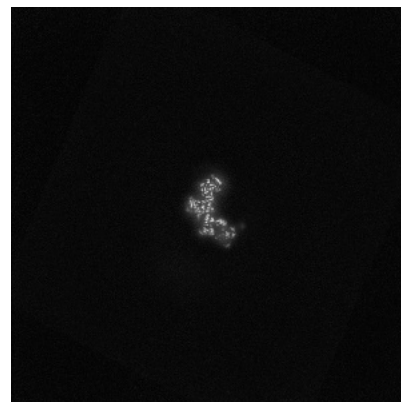
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

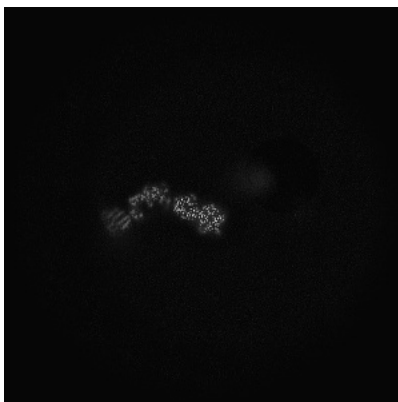
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

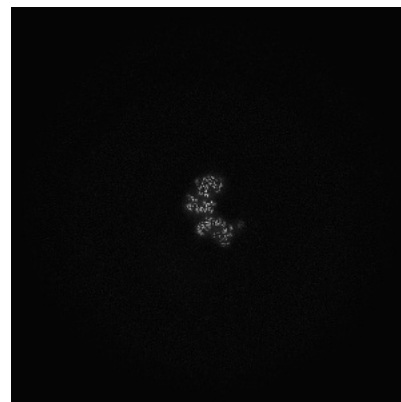
6.3.1 Primary map



X Index: 231

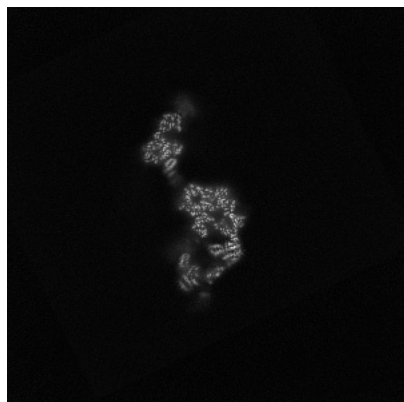


Y Index: 238

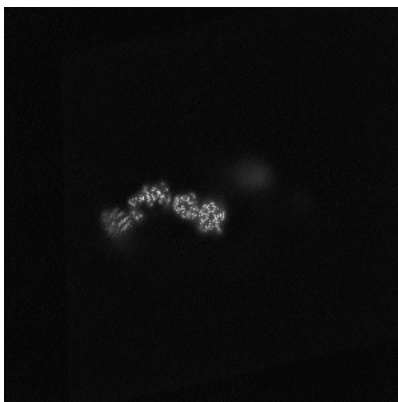


Z Index: 244

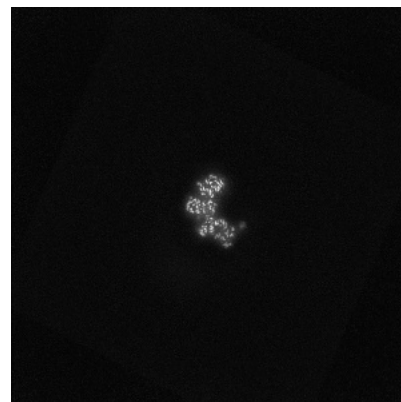
6.3.2 Raw map



X Index: 236



Y Index: 237

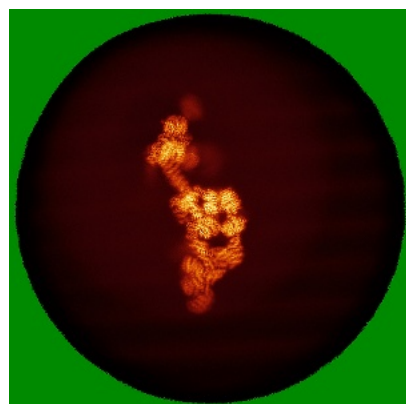


Z Index: 242

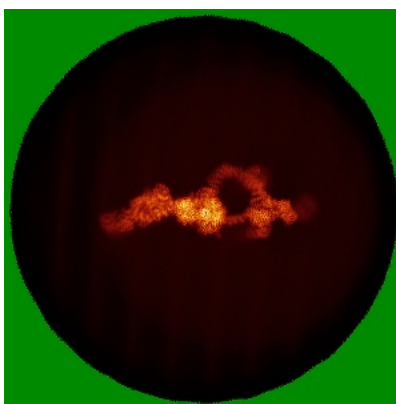
The images above show the largest variance slices of the map in three orthogonal directions.

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

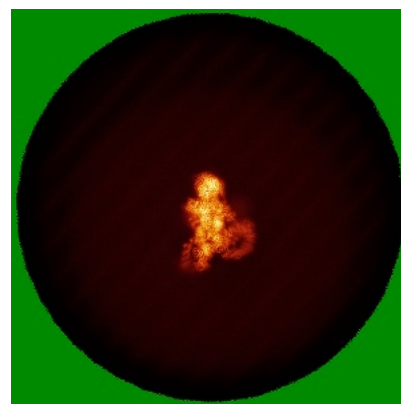
6.4.1 Primary map



X

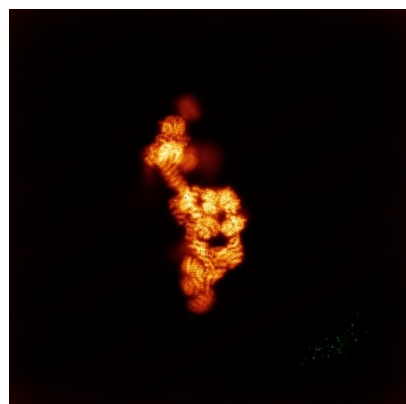


Y

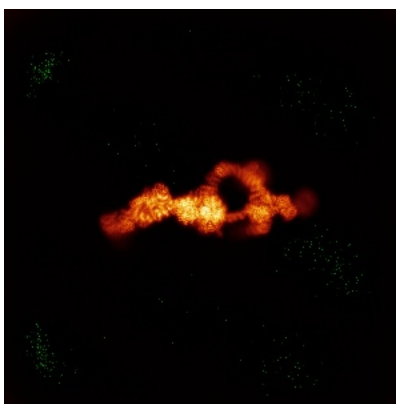


Z

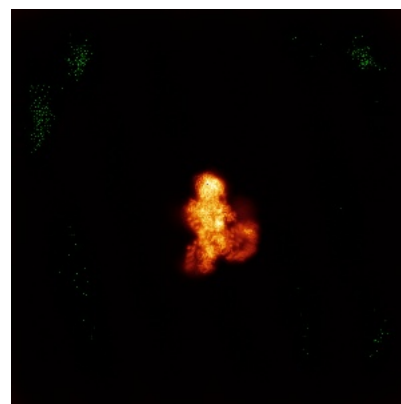
6.4.2 Raw map



X



Y

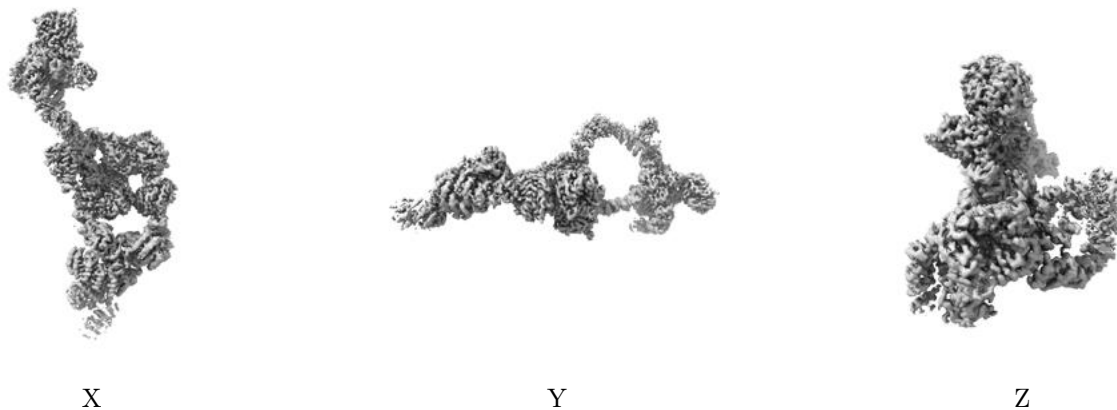


Z

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 1.0. 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.

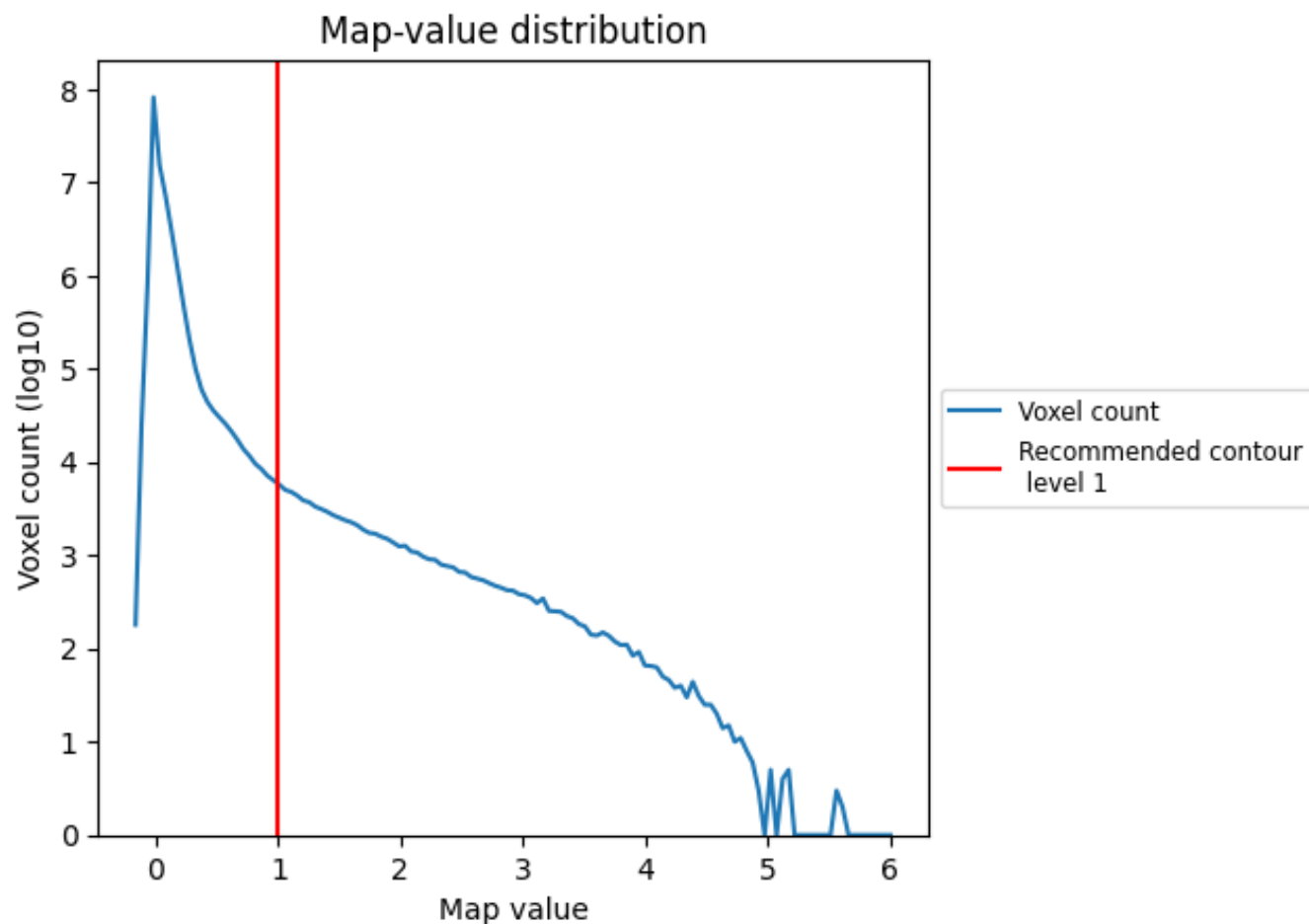
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

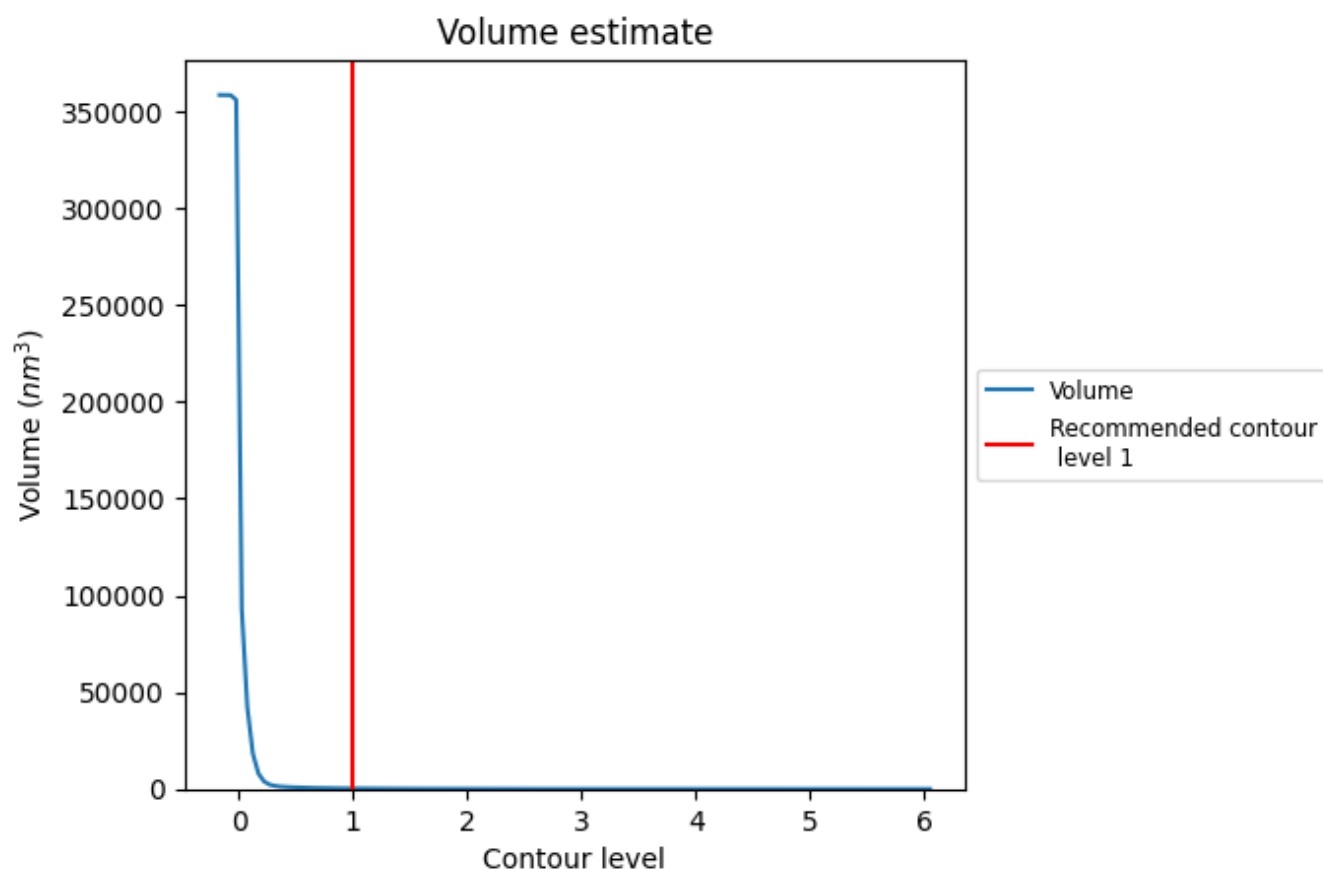
This section contains the results of statistical analysis of the map.

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.

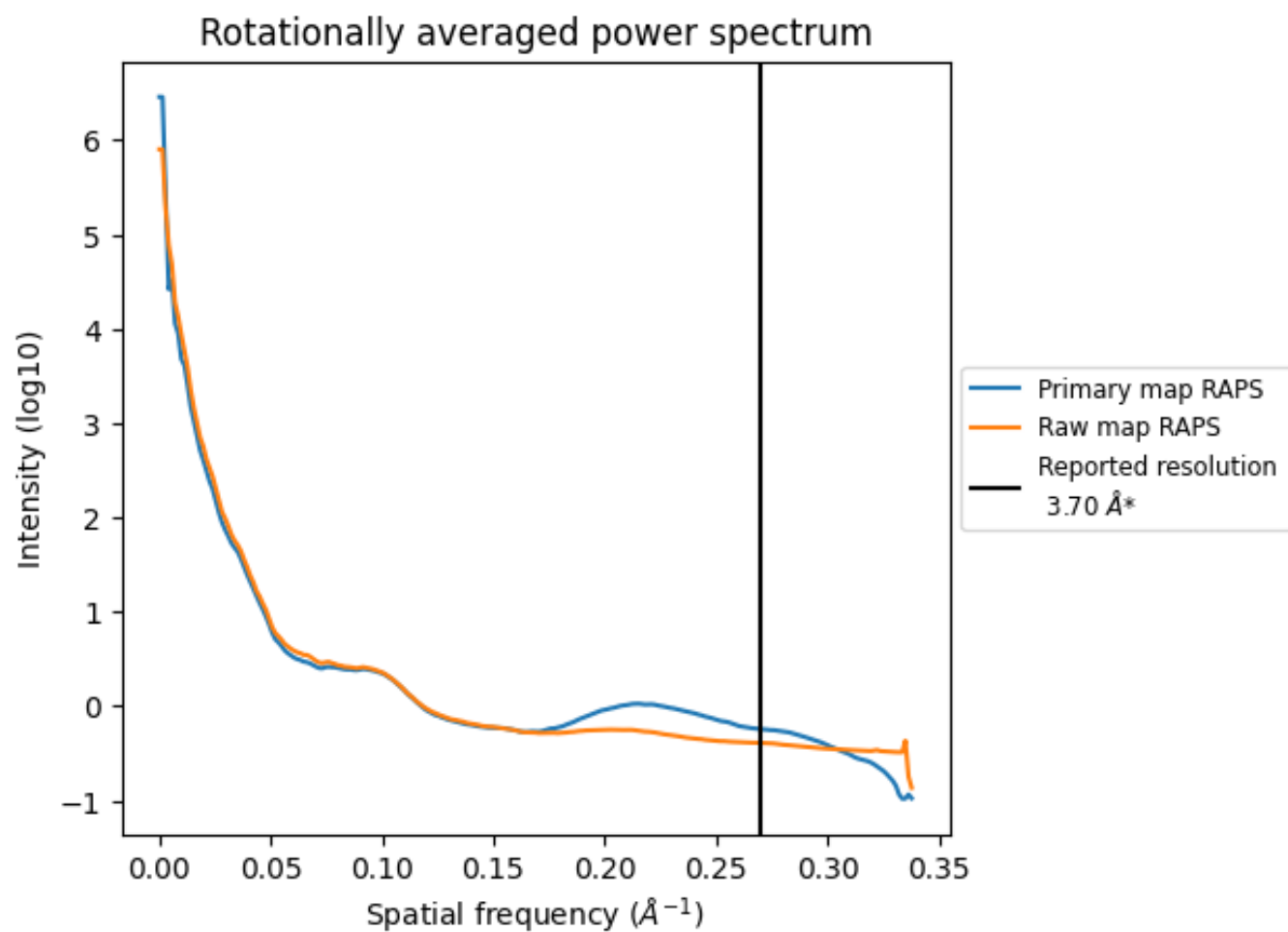
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm^3 ; this corresponds to an approximate mass of 234 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 ⓘ

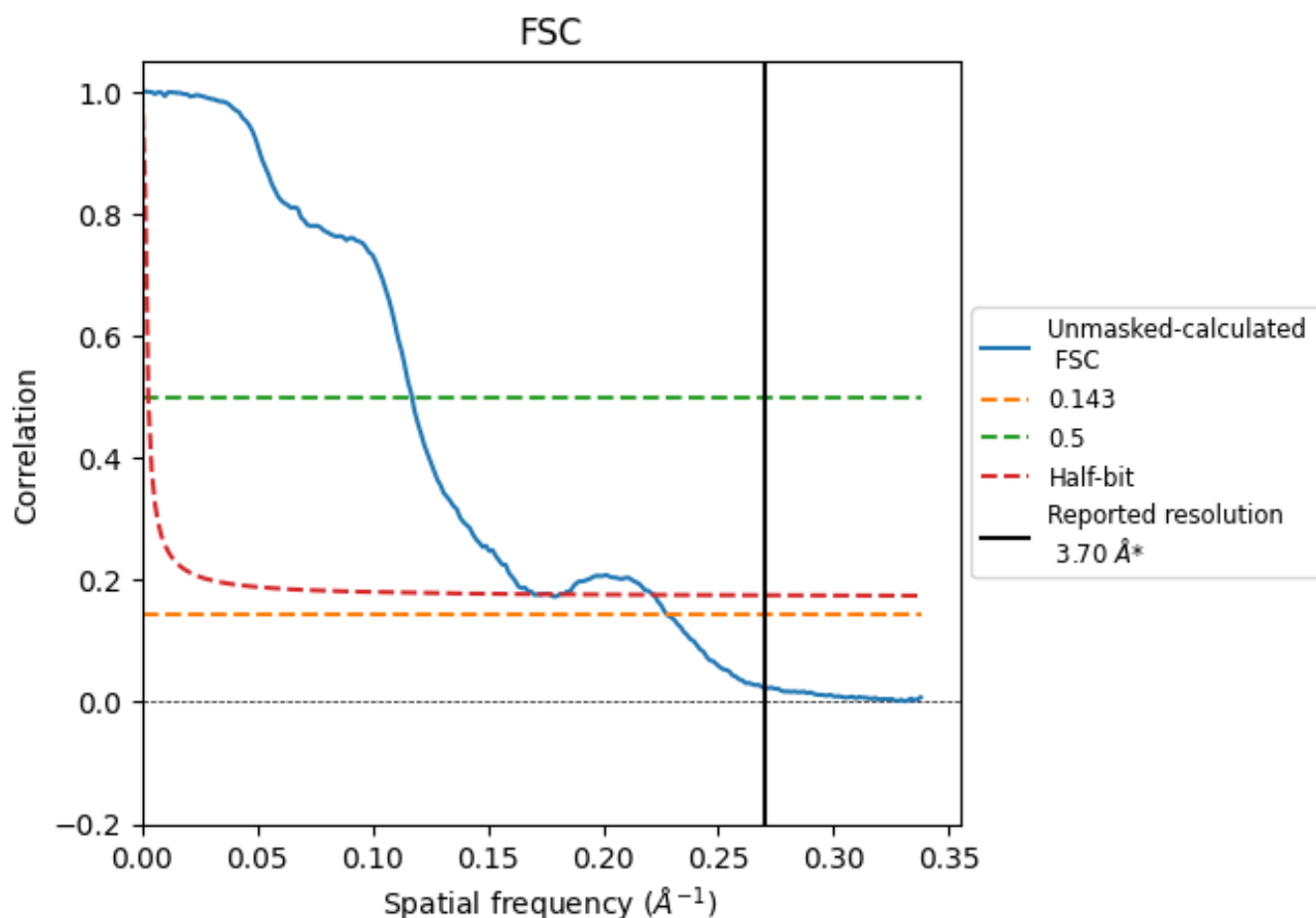


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

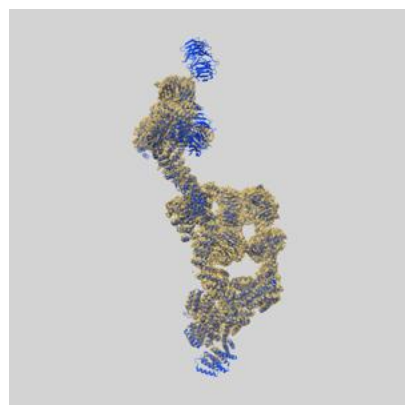
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.39	8.54	5.88

*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 4.39 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29073 and PDB model 8FGW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

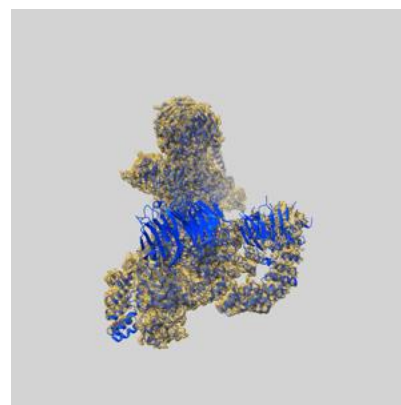
9.1 Map-model overlay [i](#)



X



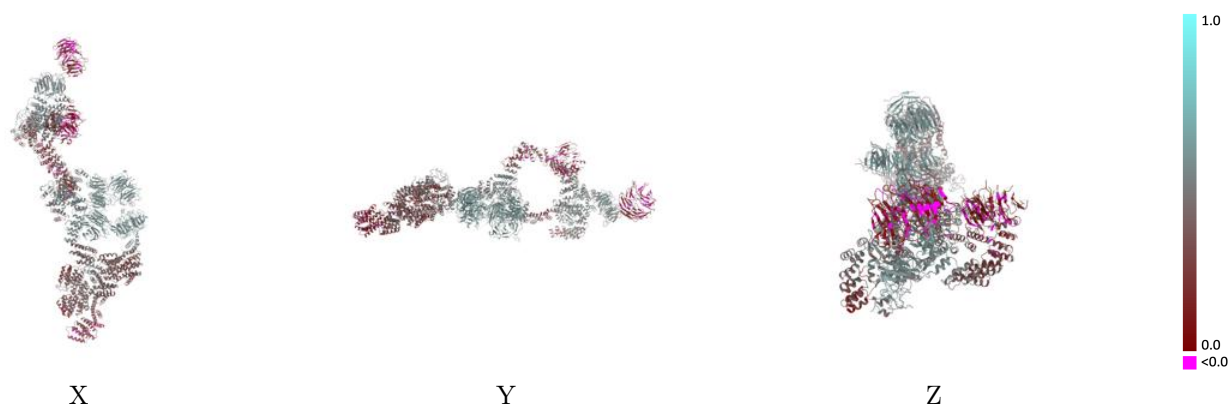
Y



Z

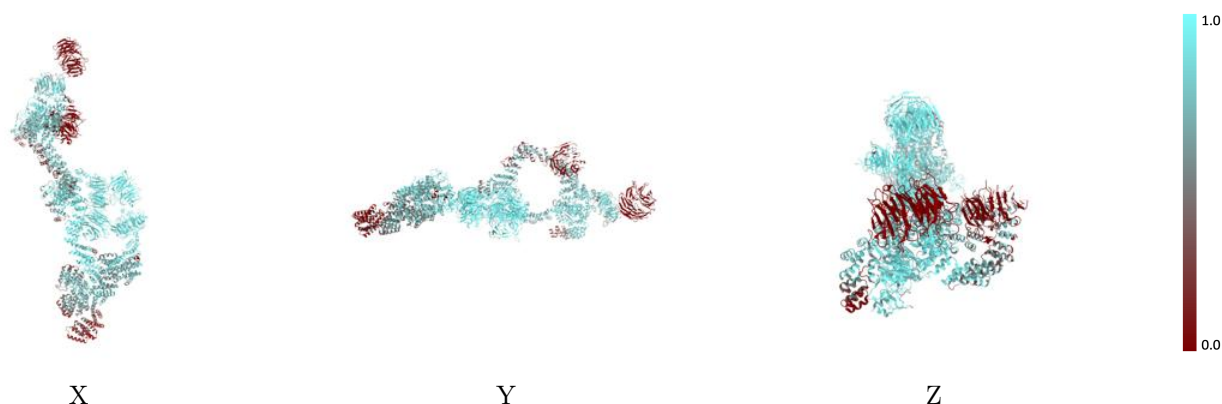
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



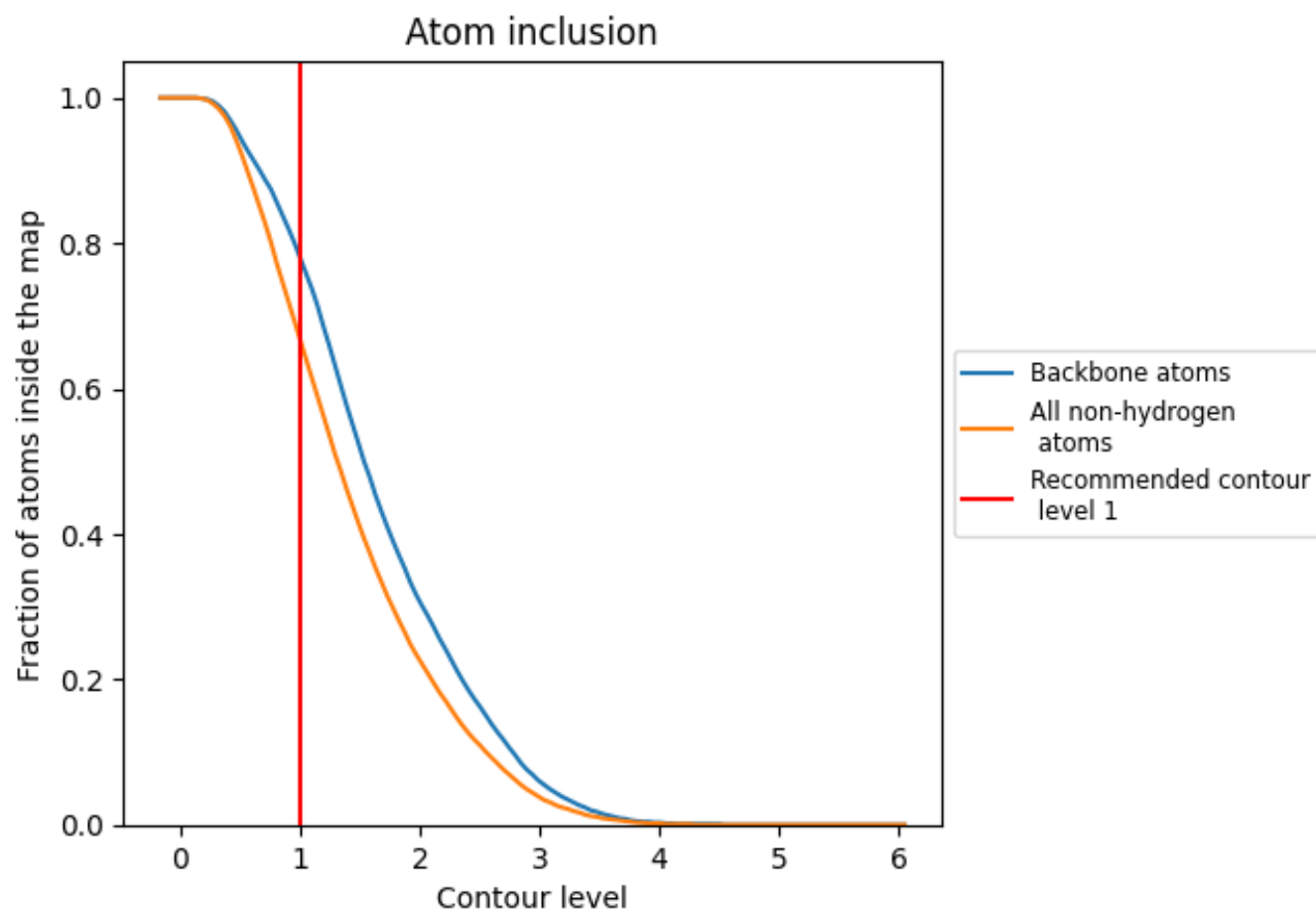
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6680	0.4060
A	0.9210	0.5150
B	0.8940	0.5230
C	0.5010	0.3570
D	0.5590	0.3170
E	0.3940	0.2980
F	0.6910	0.3760

1.0

0.0

<0.0