



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:49 AM EST

PDB ID : 7M0R
EMDB ID : EMD-23613
Title : Cryo-EM structure of the Sema3A/PlexinA4/Neuropilin 1 complex
Authors : Lu, D.; Shang, G.; He, X.; Bai, X.; Zhang, X.
Deposited on : 2021-03-11
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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

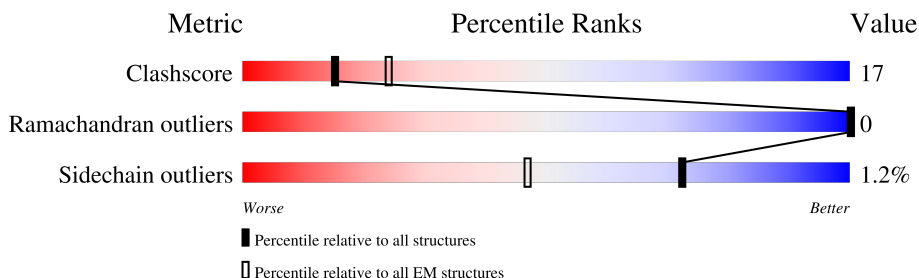
1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	E	567	
1	F	567	
2	C	614	
2	D	614	
3	A	1194	
3	B	1194	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 30898 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 Neuropilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	458	Total	C	N	O	S	0	0
			2915	1823	514	566	12		
1	F	458	Total	C	N	O	S	0	0
			2915	1823	514	566	12		

- Molecule 2 is a protein called Semaphorin-3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	588	Total	C	N	O	S	0	0
			4492	2843	782	842	25		
2	D	588	Total	C	N	O	S	0	0
			4492	2843	782	842	25		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	106	LYS	ALA	engineered mutation	UNP O08665
C	475	VAL	ILE	conflict	UNP O08665
C	551	ALA	ARG	engineered mutation	UNP O08665
C	555	ALA	ARG	engineered mutation	UNP O08665
D	106	LYS	ALA	engineered mutation	UNP O08665
D	475	VAL	ILE	conflict	UNP O08665
D	551	ALA	ARG	engineered mutation	UNP O08665
D	555	ALA	ARG	engineered mutation	UNP O08665

- Molecule 3 is a protein called Plexin-A4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1133	Total	C	N	O	S	0	0
			8040	5103	1362	1511	64		
3	B	1133	Total	C	N	O	S	0	0
			8040	5103	1362	1511	64		

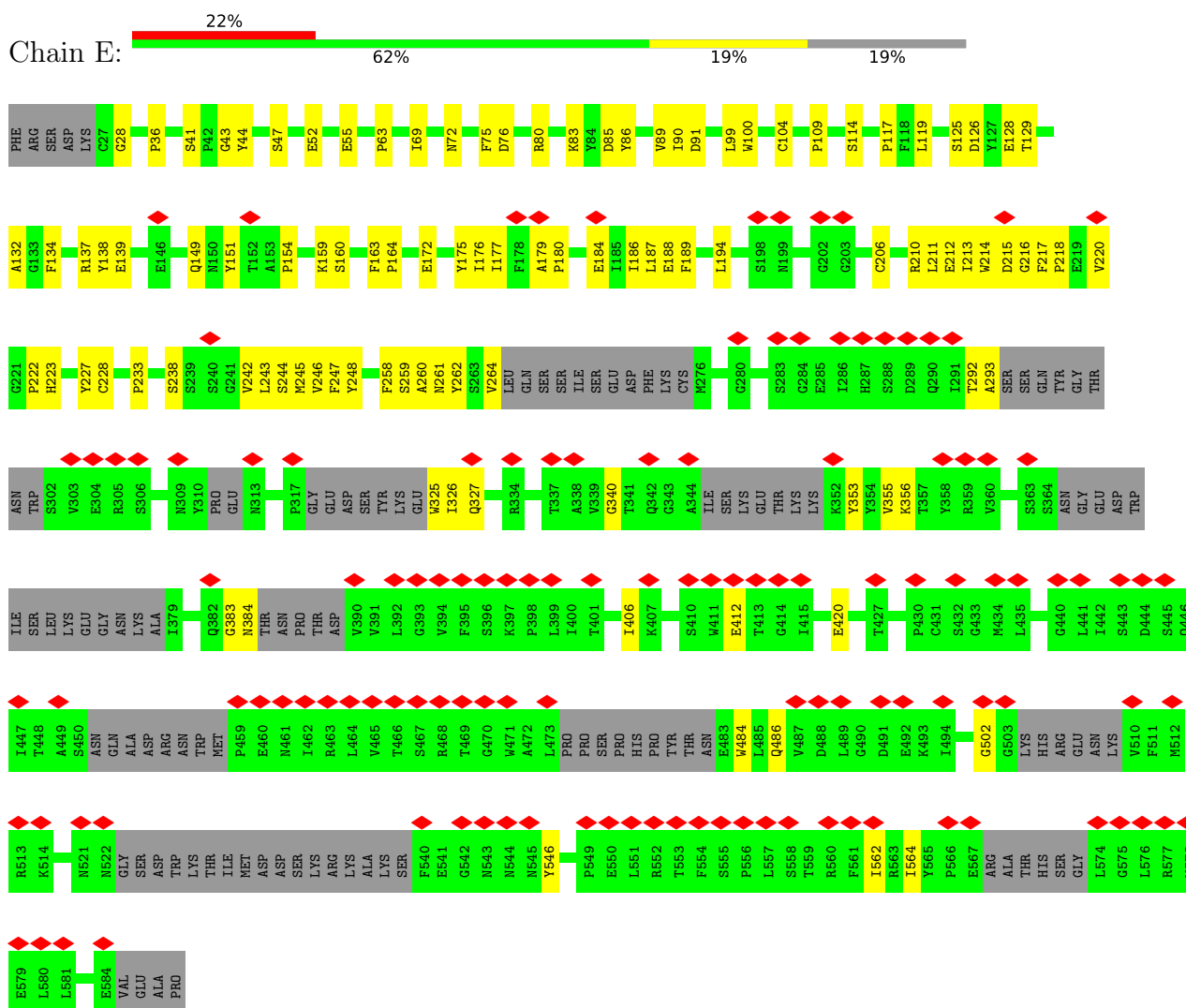
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	E	2	Total 2	Ca 2	0
4	F	2	Total 2	Ca 2	0

3 Residue-property plots

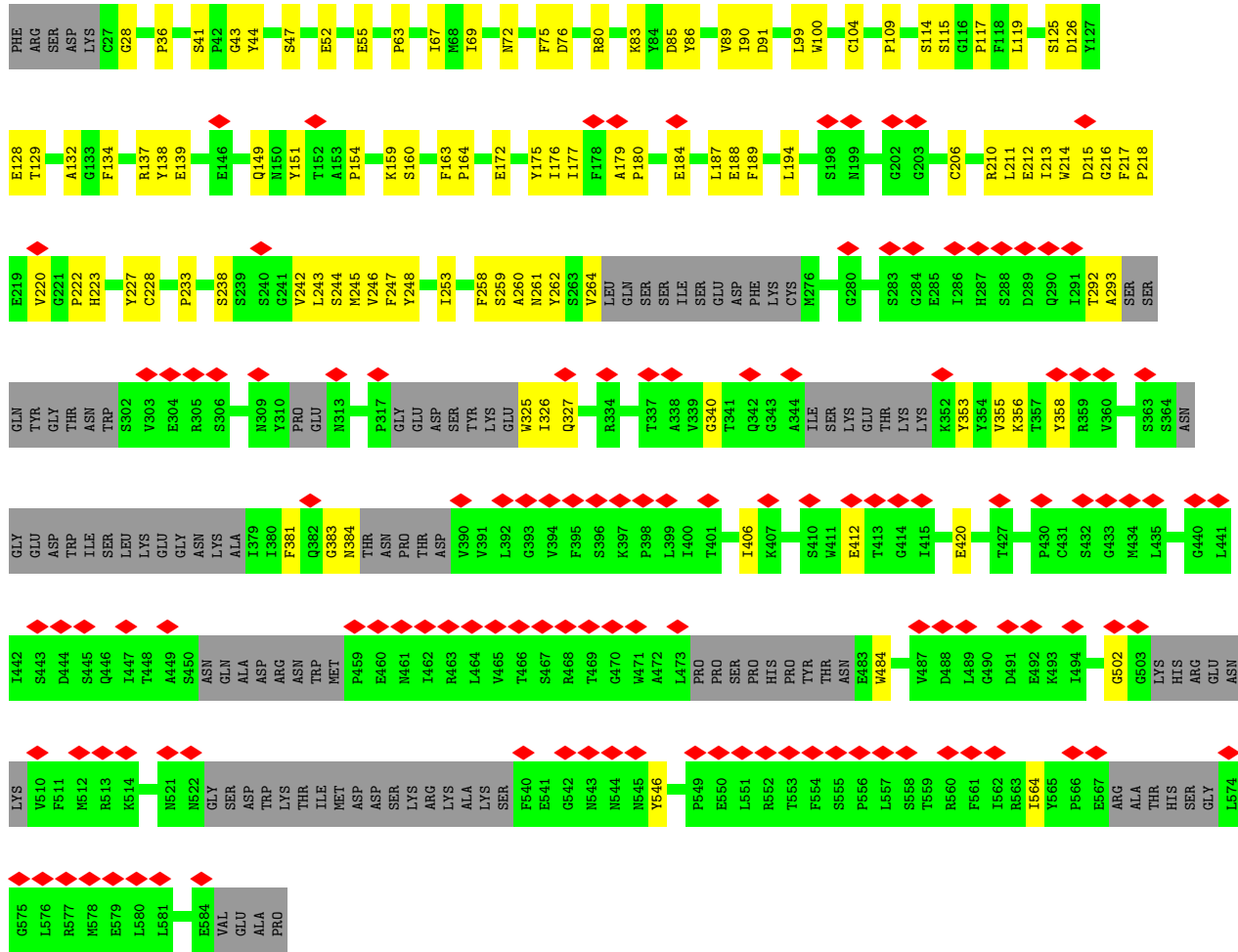
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Neuropilin-1

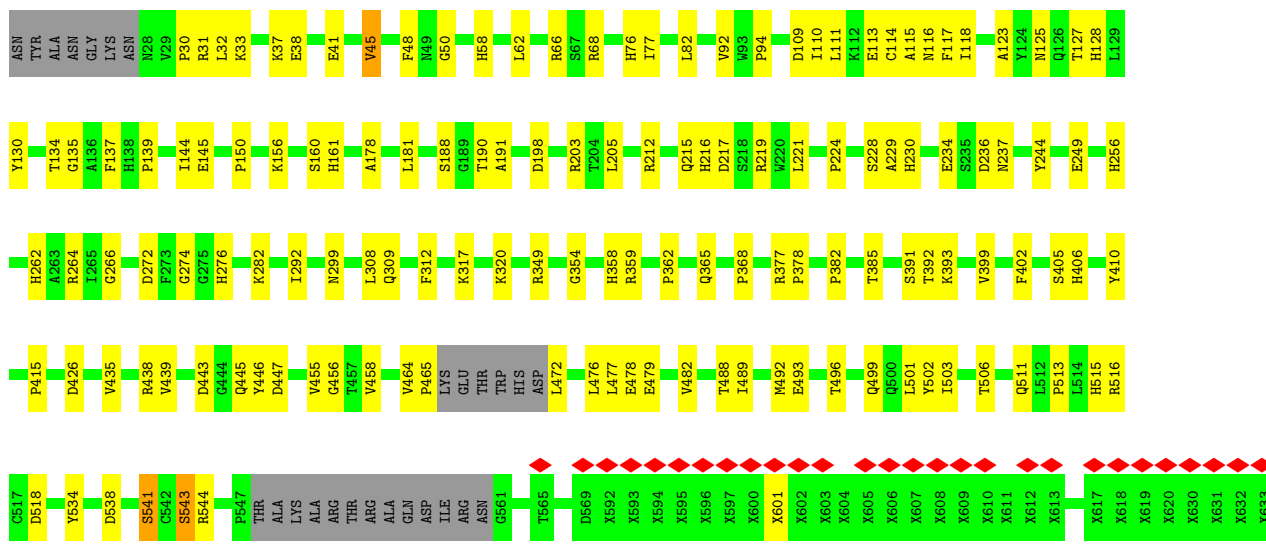
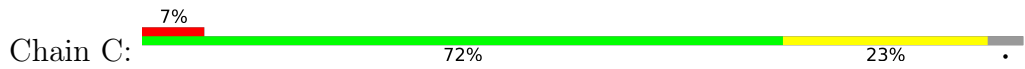


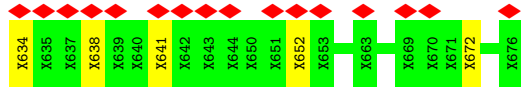
• Molecule 1: Neuropilin-1



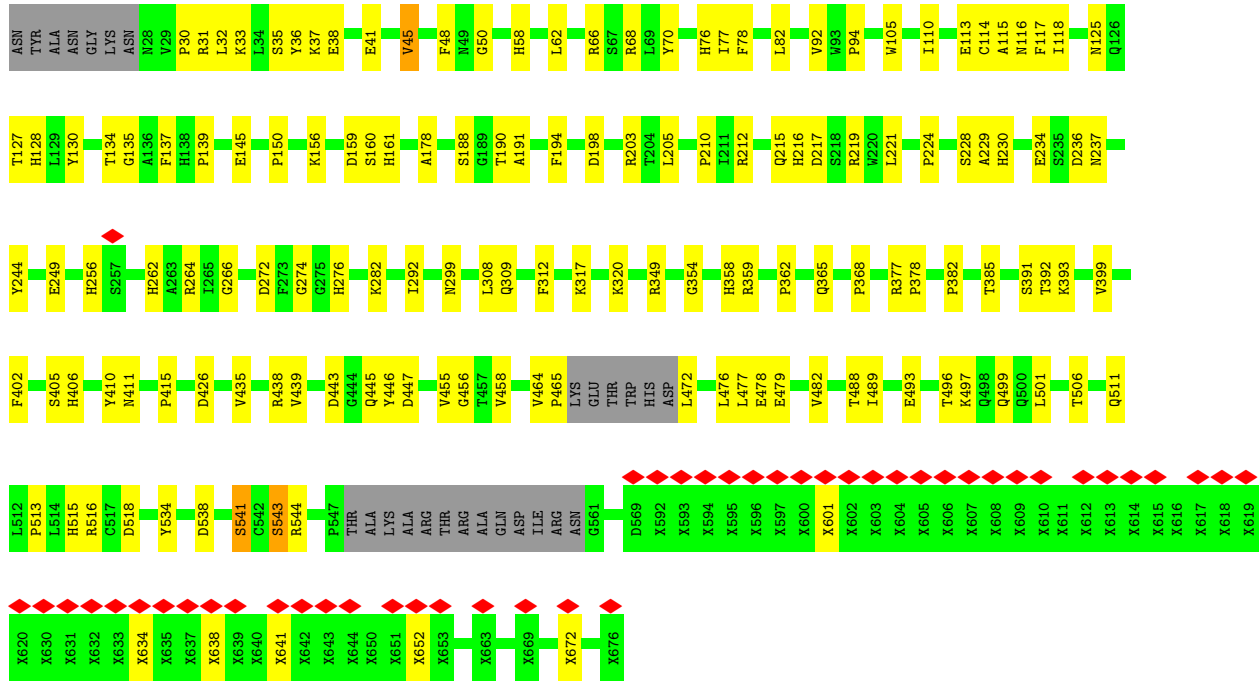
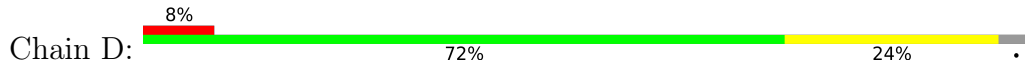


• Molecule 2: Semaphorin-3A

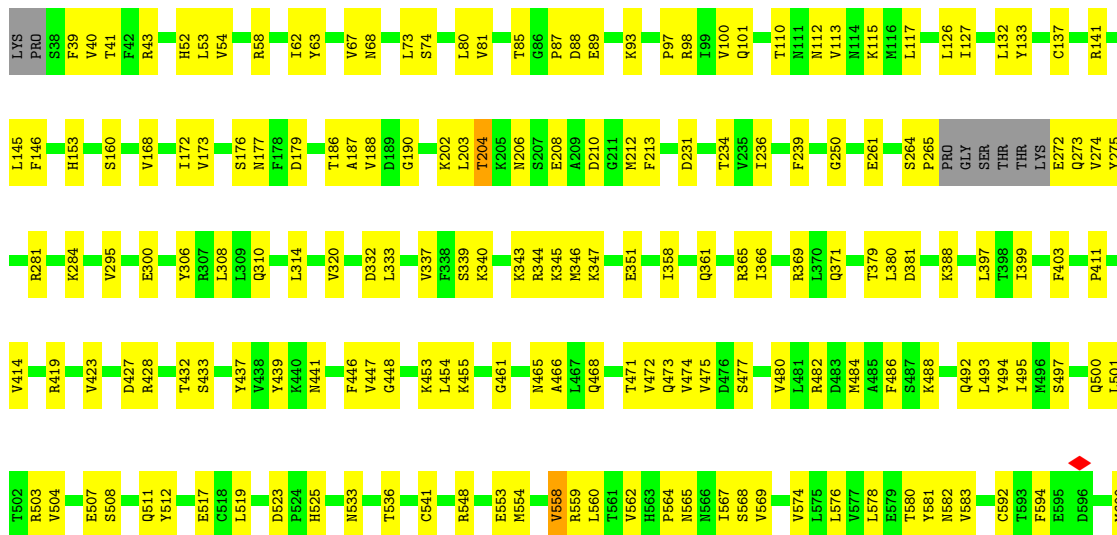


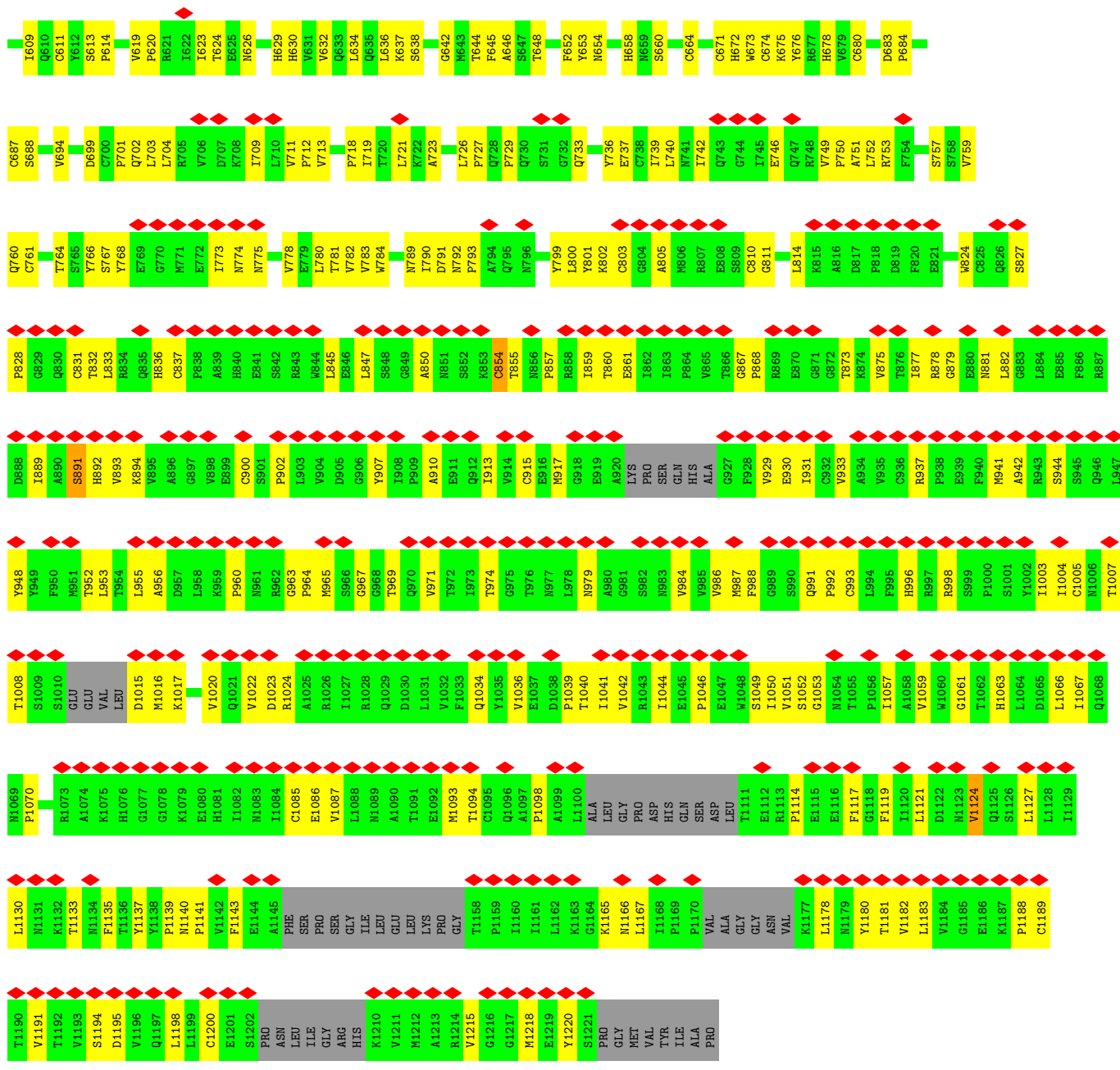


• Molecule 2: Semaphorin-3A

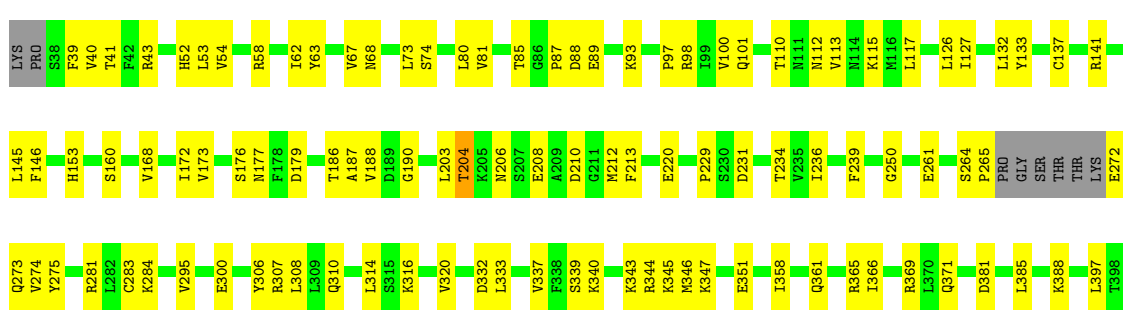


• Molecule 3: Plexin-A4





● Molecule 3: Plexin-A4



L1178	L1179	Y1180	T1181	V1182	L1183	V1184	G1185	E1186	K1187	P1188	C1189	T1190	V1191	T1192	V1193	S1194	D1195	V1196	Q1197	L1198	L1199	C1200	E1201	S1202	PRO	ASN	LEU	PRO	ILE	GLY	GLY	ILE	ARG	HIS	K1210	V1211	M1212	A1213	V1214	V1215	G1216	G1217	M1218	E1219	Y1220	S1221	PRO	GLY	MET	VAL	TYR	ILE	ALA	PRO	K1177																									
G1118	F1119	L1120	L1121	D1122	M1123	V1124	Q1125	S1126	L1127	I1128	I1129	L1130	M1131	K1132	T1133	M1134	F1135	T1136	Y1137	Y1138	P1139	M1140	P1141	F1143	E1144	A1145	PHE	SER	PRO	LEU	GLY	GLY	ILE	LEU	LEU	M1089	A1090	L1091	PRO	GLY	T1158	P1159	I1160	I1161	L1162	K1163	G1164	K1165	M1166	L1167	I1168	P1169	P1170	VAL	ALA	GLY	GLY	ASN	VAL	K1177																				
A1058	V1059	W1060	G1061	T1062	H1063	L1064	D1065	L1066	I1067	Q1068	M1069	P1070	Q1071	I1072	R1073	A1074	K1075	H1076	G1077	G1078	K1079	E1080	M1081	I1082	M1083	I1084	C1085	E1086	V1087	L1088	M1089	A1090	L1091	E1092	M1093	T1094	C1095	Q1096	A1097	P1098	A1099	L1100	ALA	LEU	GLY	PRO	ASP	HIS	GLN	GLN	ASP	LEU	T1111	I1112	R1113	P1114	E1115	E1116	F1117																					
R987	R988	S989	P1000	S1001	Y1002	I1003	I1004	C1005	M1006	T1007	T1008	S1009	G1010	GLU	GLU	VAL	LEU	D1015	M1016	K1017	V1020	Q1021	V1022	D1023	R1024	A1025	R1026	I1027	R1028	Q1029	D1030	L1031	V1032	F1033	Q1034	Y1035	V1036	E1037	D1038	P1039	T1040	I1041	V1042	R1043	I1044	E1045	P1046	E1047	W1048	S1049	I1050	V1051	S1052	M1054	T1055	P1056	I1057																							
R937	P938	E939	F940	M941	A942	R943	S944	S945	R946	L947	Y948	Y949	F950	M951	T952	L953	T954	L955	A956	D957	L958	K959	P960	M961	R962	P964	M965	S966	G967	G968	T969	Q970	M971	T972	R973	T974	G975	T976	M977	L978	N979	A980	G981	S982	M983	V984	V985	N986	N987	F988	G989	S990	Q991	P992	C993	L994	F995	H996																						
R877	R878	C879	E880	N881	L882	G883	L884	E885	F886	R887	D888	L889	A890	S891	H892	L893	M894	K895	A896	G897	V898	E899	C900	P902	L903	V904	D905	L845	E946	L847	S948	R949	G949	A950	M951	S952	K953	C954	T955	N956	P957	R958	K959	L960	M961	C962	M963	R964	S965	A966	G967	R968	E969	C970	M971	S972	R973	V914	C915	E916	M917	G918	E919	A920	LYS	PRO	SER	GLN	HIS	ALA	G927	F928	V929	E930	I931	C932	V933	A934	V935	C936
A816	D817	P818	D819	F820	E821	W824	C825	Q826	S827	P828	G829	Q830	C831	T832	L833	R834	Q835	H836	C837	P838	A839	H840	E841	S842	R843	W844	L845	E946	L847	S848	R949	A950	M951	S952	K953	C954	T955	N956	P957	R958	K959	L960	M961	C962	M963	R964	S965	A966	G967	R968	E969	C970	M971	S972	R973	V914	C915	E916	M917	G918	E919	A920	LYS	PRO	SER	GLN	HIS	ALA	G927	F928	V929	E930	I931	C932	V933	A934	V935	C936		
A751	L752	C679	F754	S757	S758	Q760	C761	Q762	N763	T764	S765	T766	Y767	Y768	E769	G770	M771	E772	I773	N774	W775	Y778	E779	L780	W781	W782	W783	W784	N785	G786	N789	I790	D791	N792	P793	A794	Q795	N796	Y799	L800	Y801	K802	C803	N804	A805	M806	R807	E808	I745	E746	Q747	R748	V749	P750																										
R677	H678	C680	D683	P684	C687	S688	V694	D699	C700	I609	Q610	C611	C612	S613	L614	V619	P620	R621	I622	I623	T624	E625	M626	H629	H630	L634	Q635	L636	K637	S638	T644	F645	A646	S647	T648	F652	Y653	M654	N655	I656	L657	M658	S659	V660	C664	C671	H672	W673	C674	K675	Y676																													
L493	Y494	L495	M496	C497	L498	M499	V500	E501	S502	R503	F504	E507	S508	Q511	Y512	E517	C518	L519	S521	G522	K440	D523	F524	H525	H526	H527	H528	H529	H530	H531	H532	H533	H534	C535	T536	C541	E546	P547	R548	R549	E553	M554	V558	R559	L560	V562	M565	I566	S567	M568	M569	V574	L575	V577																										
L399	F403	Y404	M496	L406	D407	M408	V414	R419	V423	D427	R428	S433	Y437	G520	V438	Y439	G522	K440	M441	F446	V447	G448	K453	L454	K455	G461	M465	A466	L467	Q468	T471	Q472	Q473	V474	V475	S477	W480	L481	R482	M483	M484	A485	E486	S487	K488	Q492																																		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	26741	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	302.40002, 302.40002, 302.40002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.27	0/2965	0.46	0/4045
1	F	0.27	0/2965	0.46	0/4045
2	C	0.34	0/4281	0.45	1/5809 (0.0%)
2	D	0.34	0/4281	0.46	1/5809 (0.0%)
3	A	0.29	0/8211	0.47	0/11236
3	B	0.29	0/8211	0.47	0/11236
All	All	0.30	0/30914	0.47	2/42180 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	465	PRO	N-CA-CB	5.92	110.41	103.30
2	D	465	PRO	N-CA-CB	5.92	110.40	103.30

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	E	2915	0	2144	70	0
1	F	2915	0	2144	72	0
2	C	4492	0	4067	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4492	0	4067	95	0
3	A	8040	0	7294	323	0
3	B	8040	0	7294	326	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
All	All	30898	0	27010	963	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 17.

All (963) 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)
3:A:986:VAL:HG23	3:A:993:CYS:HB3	1.54	0.90
3:B:986:VAL:HG23	3:B:993:CYS:HB3	1.54	0.89
3:B:857:PRO:HB2	3:B:942:ALA:HB2	1.57	0.86
1:E:353:TYR:HA	1:E:412:GLU:O	1.76	0.86
1:F:353:TYR:HA	1:F:412:GLU:O	1.76	0.85
3:B:882:LEU:HB2	3:B:910:ALA:H	1.42	0.84
3:A:857:PRO:HB2	3:A:942:ALA:HB2	1.57	0.84
2:C:464:VAL:O	2:C:472:LEU:HA	1.78	0.83
3:A:882:LEU:HB2	3:A:910:ALA:H	1.42	0.83
2:D:464:VAL:O	2:D:472:LEU:HA	1.78	0.83
3:A:559:ARG:HB2	3:A:581:TYR:HB2	1.63	0.81
1:E:187:LEU:HD13	1:E:262:TYR:HB3	1.63	0.79
3:A:859:ILE:HB	3:A:944:SER:HA	1.64	0.79
3:B:559:ARG:HB2	3:B:581:TYR:HB2	1.63	0.79
3:B:859:ILE:HB	3:B:944:SER:HA	1.64	0.78
1:F:187:LEU:HD13	1:F:262:TYR:HB3	1.63	0.78
3:B:824:TRP:HA	3:B:831:CYS:HA	1.65	0.78
3:B:475:VAL:HG12	3:B:477:SER:H	1.50	0.77
3:A:824:TRP:HA	3:A:831:CYS:HA	1.65	0.76
1:F:217:PHE:HB3	1:F:220:VAL:HB	1.68	0.76
3:A:726:LEU:HD12	3:A:753:ARG:HG3	1.68	0.76
3:B:726:LEU:HD12	3:B:753:ARG:HG3	1.67	0.76
1:E:217:PHE:HB3	1:E:220:VAL:HB	1.68	0.75
3:A:492:GLN:HG2	3:A:503:ARG:HH11	1.51	0.74
3:B:492:GLN:HG2	3:B:503:ARG:HH11	1.51	0.74
3:A:475:VAL:HG12	3:A:477:SER:H	1.50	0.74
3:B:578:LEU:H	3:B:609:ILE:H	1.35	0.74
3:A:53:LEU:HD12	3:A:62:ILE:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:810:CYS:SG	3:A:881:ASN:ND2	2.61	0.74
3:B:810:CYS:SG	3:B:881:ASN:ND2	2.61	0.73
2:C:354:GLY:O	2:C:377:ARG:NH2	2.22	0.73
3:B:984:VAL:HG12	3:B:1022:VAL:HG13	1.71	0.73
2:C:256:HIS:HE1	2:D:365:GLN:HG2	1.51	0.73
2:D:354:GLY:O	2:D:377:ARG:NH2	2.22	0.73
3:A:578:LEU:H	3:A:609:ILE:H	1.35	0.73
3:A:43:ARG:HD3	3:A:500:GLN:HB3	1.71	0.72
3:B:1063:HIS:HB3	3:B:1066:LEU:HD21	1.70	0.72
3:B:580:THR:HB	3:B:583:VAL:HG11	1.71	0.72
3:A:984:VAL:HG12	3:A:1022:VAL:HG13	1.71	0.72
3:B:53:LEU:HD12	3:B:62:ILE:HD11	1.70	0.72
3:B:868:PRO:HA	3:B:952:THR:HA	1.72	0.72
3:A:580:THR:HB	3:A:583:VAL:HG11	1.71	0.71
3:A:569:VAL:HG21	3:A:623:ILE:HD13	1.72	0.71
3:B:1050:ILE:HD13	3:B:1178:LEU:HD21	1.71	0.71
3:A:1063:HIS:HB3	3:A:1066:LEU:HD21	1.70	0.71
2:D:217:ASP:OD2	2:D:219:ARG:NH1	2.21	0.71
3:B:320:VAL:H	3:B:441:ASN:HB3	1.56	0.71
3:A:1050:ILE:HD13	3:A:1178:LEU:HD21	1.71	0.71
3:B:308:LEU:HB2	3:B:339:SER:HB3	1.72	0.71
3:B:43:ARG:HD3	3:B:500:GLN:HB3	1.71	0.70
3:A:273:GLN:HB2	3:A:344:ARG:HH12	1.57	0.70
3:A:308:LEU:HB2	3:A:339:SER:HB3	1.72	0.70
3:A:446:PHE:HB3	3:A:454:LEU:HD11	1.72	0.70
3:B:569:VAL:HG21	3:B:623:ILE:HD13	1.72	0.70
3:B:964:PRO:HG3	3:B:1066:LEU:HD13	1.74	0.70
3:A:320:VAL:H	3:A:441:ASN:HB3	1.56	0.70
3:A:533:ASN:ND2	3:A:644:THR:O	2.24	0.70
3:A:868:PRO:HA	3:A:952:THR:HA	1.72	0.70
1:F:211:LEU:HD11	1:F:245:MET:HB3	1.75	0.69
3:B:87:PRO:HA	3:B:110:THR:O	1.93	0.69
3:B:533:ASN:ND2	3:B:644:THR:O	2.24	0.69
3:B:446:PHE:HB3	3:B:454:LEU:HD11	1.72	0.69
3:A:87:PRO:HA	3:A:110:THR:O	1.93	0.69
3:A:964:PRO:HG3	3:A:1066:LEU:HD13	1.74	0.69
3:A:1215:VAL:HG23	3:A:1218:MET:HB3	1.75	0.69
1:E:211:LEU:HD11	1:E:245:MET:HB3	1.74	0.69
3:A:1067:ILE:HG23	3:A:1070:PRO:HG3	1.75	0.69
3:B:273:GLN:HB2	3:B:344:ARG:HH12	1.57	0.69
3:B:1182:VAL:H	3:B:1191:VAL:HG11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:THR:HA	2:D:139:PRO:HA	1.74	0.69
3:B:703:LEU:H	3:B:793:PRO:HD2	1.57	0.69
3:A:153:HIS:NE2	3:A:210:ASP:OD1	2.26	0.69
3:B:721:LEU:HB2	3:B:759:VAL:HB	1.75	0.69
3:B:1215:VAL:HG23	3:B:1218:MET:HB3	1.75	0.69
3:A:953:LEU:HD22	3:A:1020:VAL:HG11	1.75	0.68
3:A:1182:VAL:H	3:A:1191:VAL:HG11	1.57	0.68
3:B:719:ILE:HB	3:B:761:CYS:HB2	1.75	0.68
2:D:92:VAL:HG12	2:D:94:PRO:HD3	1.76	0.68
3:A:475:VAL:HG13	3:A:500:GLN:HE21	1.59	0.68
3:A:704:LEU:H	3:A:723:ALA:HA	1.59	0.68
3:A:508:SER:O	3:A:511:GLN:NE2	2.23	0.68
3:A:703:LEU:H	3:A:793:PRO:HD2	1.57	0.68
3:A:1194:SER:H	3:A:1198:LEU:HD21	1.59	0.68
2:C:92:VAL:HG12	2:C:94:PRO:HD3	1.76	0.68
3:B:953:LEU:HD22	3:B:1020:VAL:HG11	1.75	0.68
3:B:704:LEU:H	3:B:723:ALA:HA	1.59	0.68
3:B:1194:SER:H	3:B:1198:LEU:HD21	1.59	0.68
3:A:1178:LEU:HD23	3:A:1215:VAL:HB	1.76	0.68
1:E:44:TYR:OH	1:E:72:ASN:ND2	2.27	0.67
2:C:217:ASP:OD2	2:C:219:ARG:NH1	2.21	0.67
3:B:1183:LEU:HB2	3:B:1188:PRO:HA	1.76	0.67
3:B:749:VAL:HG11	3:B:764:THR:HG21	1.76	0.67
3:A:956:ALA:HB3	3:A:974:THR:HG23	1.77	0.67
3:B:1067:ILE:HG23	3:B:1070:PRO:HG3	1.75	0.67
3:A:578:LEU:HB2	3:A:609:ILE:HB	1.75	0.67
3:A:719:ILE:HB	3:A:761:CYS:HB2	1.75	0.67
3:B:153:HIS:NE2	3:B:210:ASP:OD1	2.26	0.67
3:A:721:LEU:HB2	3:A:759:VAL:HB	1.75	0.67
3:B:475:VAL:HG13	3:B:500:GLN:HE21	1.59	0.67
3:B:629:HIS:HA	3:B:653:TYR:HA	1.77	0.67
3:A:168:VAL:HG22	3:A:186:THR:HG23	1.77	0.67
2:C:134:THR:HA	2:C:139:PRO:HA	1.74	0.66
3:B:956:ALA:HB3	3:B:974:THR:HG23	1.77	0.66
3:B:578:LEU:HB2	3:B:609:ILE:HB	1.75	0.66
3:A:749:VAL:HG11	3:A:764:THR:HG21	1.76	0.66
3:A:1183:LEU:HB2	3:A:1188:PRO:HA	1.76	0.66
3:B:713:VAL:O	3:B:836:HIS:NE2	2.28	0.66
3:B:1178:LEU:HD23	3:B:1215:VAL:HB	1.76	0.66
2:C:234:GLU:OE2	2:C:349:ARG:NE	2.28	0.66
3:A:369:ARG:HG2	3:A:414:VAL:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:713:VAL:O	3:A:836:HIS:NE2	2.28	0.66
2:D:215:GLN:HE21	2:D:216:HIS:CD2	2.14	0.66
3:B:168:VAL:HG22	3:B:186:THR:HG23	1.77	0.66
2:C:215:GLN:HE21	2:C:216:HIS:CD2	2.14	0.65
1:F:44:TYR:OH	1:F:72:ASN:ND2	2.27	0.65
2:D:320:LYS:O	2:D:349:ARG:NH2	2.29	0.65
3:A:629:HIS:HA	3:A:653:TYR:HA	1.77	0.65
3:B:369:ARG:HG2	3:B:414:VAL:HG12	1.77	0.65
3:B:963:GLY:N	3:B:1034:GLN:O	2.30	0.65
3:B:474:VAL:HG23	3:B:475:VAL:HG23	1.77	0.65
2:C:113:GLU:HB3	2:C:137:PHE:HE1	1.61	0.65
2:C:320:LYS:O	2:C:349:ARG:NH2	2.29	0.65
3:A:474:VAL:HG23	3:A:475:VAL:HG23	1.77	0.65
3:B:594:PHE:HA	3:B:634:LEU:HA	1.78	0.65
1:F:213:ILE:HG12	1:F:245:MET:HG3	1.78	0.65
3:B:1180:TYR:CE2	3:B:1182:VAL:HG23	2.32	0.65
2:C:538:ASP:OD1	2:C:541:SER:N	2.29	0.64
3:A:594:PHE:HA	3:A:634:LEU:HA	1.78	0.64
1:E:28:GLY:HA2	1:E:55:GLU:O	1.98	0.64
1:E:213:ILE:HG12	1:E:245:MET:HG3	1.78	0.64
2:D:228:SER:OG	2:D:230:HIS:NE2	2.29	0.64
2:D:234:GLU:OE2	2:D:349:ARG:NE	2.28	0.64
2:D:113:GLU:HB3	2:D:137:PHE:HE1	1.61	0.64
3:A:361:GLN:OE1	3:A:365:ARG:NH2	2.31	0.64
3:A:1180:TYR:CE2	3:A:1182:VAL:HG23	2.32	0.64
1:E:128:GLU:HG3	1:E:129:THR:H	1.62	0.64
3:B:361:GLN:OE1	3:B:365:ARG:NH2	2.31	0.64
2:D:66:ARG:HA	2:D:150:PRO:HB3	1.80	0.64
1:F:128:GLU:HG3	1:F:129:THR:H	1.62	0.63
1:F:154:PRO:HG3	1:F:180:PRO:HG2	1.81	0.63
3:A:963:GLY:N	3:A:1034:GLN:O	2.30	0.63
1:F:28:GLY:HA2	1:F:55:GLU:O	1.98	0.63
1:E:154:PRO:HG3	1:E:180:PRO:HG2	1.80	0.63
3:B:811:GLY:HA3	3:B:881:ASN:HA	1.80	0.63
2:C:66:ARG:HA	2:C:150:PRO:HB3	1.80	0.63
3:B:41:THR:OG1	3:B:500:GLN:OE1	2.16	0.63
3:A:987:MET:HA	3:A:992:PRO:HA	1.81	0.63
2:C:237:ASN:ND2	2:C:385:THR:OG1	2.31	0.62
2:D:125:ASN:HB2	2:D:128:HIS:HB2	1.81	0.62
3:A:811:GLY:HA3	3:A:881:ASN:HA	1.80	0.62
3:B:987:MET:HA	3:B:992:PRO:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:ASN:HB2	2:C:128:HIS:HB2	1.81	0.62
1:F:69:ILE:HA	1:F:137:ARG:O	2.00	0.62
1:F:52:GLU:H	1:F:125:SER:HB3	1.64	0.62
2:D:249:GLU:OE2	2:D:264:ARG:NH1	2.33	0.62
2:D:538:ASP:OD1	2:D:541:SER:N	2.29	0.62
3:B:614:PRO:HD2	3:B:652:PHE:HZ	1.65	0.62
3:B:892:HIS:CE1	3:B:931:ILE:HB	2.35	0.62
1:E:69:ILE:HA	1:E:137:ARG:O	2.00	0.61
3:A:1040:THR:HA	3:A:1127:LEU:HD21	1.82	0.61
3:B:1040:THR:HA	3:B:1127:LEU:HD21	1.82	0.61
3:B:423:VAL:HG12	3:B:466:ALA:HB2	1.83	0.61
3:B:960:PRO:HD2	3:B:971:VAL:HG13	1.81	0.61
2:D:105:TRP:CZ2	3:B:397:LEU:HD13	2.34	0.61
3:A:907:TYR:HA	3:A:913:ILE:HA	1.82	0.61
3:A:892:HIS:CE1	3:A:931:ILE:HB	2.35	0.61
3:A:960:PRO:HD2	3:A:971:VAL:HG13	1.81	0.61
3:B:562:VAL:O	3:B:565:ASN:ND2	2.34	0.61
1:E:52:GLU:H	1:E:125:SER:HB3	1.64	0.61
3:A:620:PRO:HA	3:A:623:ILE:HG12	1.83	0.61
3:A:768:TYR:OH	3:A:773:ILE:O	2.17	0.61
3:B:721:LEU:HD11	3:B:780:LEU:HD11	1.83	0.61
3:A:306:TYR:HE1	3:A:351:GLU:HG2	1.66	0.61
3:B:306:TYR:HE1	3:B:351:GLU:HG2	1.66	0.61
1:F:160:SER:HB3	1:F:258:PHE:H	1.65	0.61
3:A:423:VAL:HG12	3:A:466:ALA:HB2	1.83	0.61
1:E:160:SER:HB3	1:E:258:PHE:H	1.65	0.60
2:C:30:PRO:HA	2:C:476:LEU:HD22	1.83	0.60
3:A:300:GLU:OE2	3:A:419:ARG:NH1	2.35	0.60
2:C:249:GLU:OE2	2:C:264:ARG:NH1	2.33	0.60
3:A:562:VAL:O	3:A:565:ASN:ND2	2.34	0.60
3:A:782:VAL:HG23	3:A:790:ILE:HD13	1.83	0.60
3:A:775:ASN:HD22	3:A:801:TYR:HB3	1.66	0.60
3:B:300:GLU:OE2	3:B:419:ARG:NH1	2.35	0.60
3:B:740:LEU:O	3:B:746:GLU:HA	2.02	0.60
2:D:237:ASN:ND2	2:D:385:THR:OG1	2.31	0.60
3:B:907:TYR:HA	3:B:913:ILE:HA	1.82	0.60
3:B:768:TYR:OH	3:B:773:ILE:O	2.17	0.60
2:D:30:PRO:HA	2:D:476:LEU:HD22	1.83	0.60
3:B:775:ASN:HD22	3:B:801:TYR:HB3	1.67	0.60
3:B:52:HIS:NE2	3:B:115:LYS:O	2.35	0.59
2:C:190:THR:HG22	2:C:191:ALA:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:52:HIS:NE2	3:A:115:LYS:O	2.35	0.59
3:A:913:ILE:HG22	3:A:915:CYS:HB2	1.84	0.59
3:A:314:LEU:HD11	3:A:332:ASP:HB2	1.85	0.59
3:A:721:LEU:HD11	3:A:780:LEU:HD11	1.83	0.59
3:B:508:SER:O	3:B:511:GLN:NE2	2.23	0.59
1:E:85:ASP:OD1	1:E:126:ASP:N	2.33	0.59
2:C:228:SER:OG	2:C:230:HIS:NE2	2.29	0.59
3:A:740:LEU:O	3:A:746:GLU:HA	2.02	0.59
2:D:190:THR:HG22	2:D:191:ALA:H	1.67	0.59
3:A:614:PRO:HD2	3:A:652:PHE:HZ	1.65	0.59
3:B:351:GLU:HA	3:B:427:ASP:HA	1.85	0.59
3:B:620:PRO:HA	3:B:623:ILE:HG12	1.83	0.59
3:B:913:ILE:HG22	3:B:915:CYS:HB2	1.84	0.59
3:B:1180:TYR:HE2	3:B:1182:VAL:HG23	1.68	0.59
3:A:1180:TYR:HE2	3:A:1182:VAL:HG23	1.68	0.59
3:A:674:CYS:O	3:A:678:HIS:N	2.35	0.59
2:D:203:ARG:NH2	2:D:272:ASP:O	2.34	0.59
3:A:41:THR:OG1	3:A:500:GLN:OE1	2.16	0.59
3:A:351:GLU:HA	3:A:427:ASP:HA	1.85	0.59
3:B:314:LEU:HD11	3:B:332:ASP:HB2	1.85	0.59
3:B:782:VAL:HG23	3:B:790:ILE:HD13	1.83	0.59
2:C:234:GLU:O	2:C:320:LYS:NZ	2.36	0.58
2:D:116:ASN:HA	2:D:135:GLY:HA2	1.85	0.58
2:C:116:ASN:HA	2:C:135:GLY:HA2	1.85	0.58
2:D:234:GLU:O	2:D:320:LYS:NZ	2.36	0.58
3:B:674:CYS:O	3:B:678:HIS:N	2.35	0.58
3:A:984:VAL:HA	3:A:1022:VAL:HA	1.86	0.58
3:A:673:TRP:HE3	3:A:680:CYS:HB2	1.69	0.58
3:A:703:LEU:HD21	3:A:782:VAL:HG22	1.86	0.58
3:B:824:TRP:HB3	3:B:845:LEU:HB3	1.86	0.58
3:A:824:TRP:HB3	3:A:845:LEU:HB3	1.86	0.58
3:B:673:TRP:HE3	3:B:680:CYS:HB2	1.69	0.58
3:B:984:VAL:HA	3:B:1022:VAL:HA	1.86	0.58
3:A:784:TRP:CD1	3:A:790:ILE:HD11	2.39	0.57
3:A:381:ASP:HA	3:A:388:LYS:HD2	1.86	0.57
3:B:784:TRP:CD1	3:B:790:ILE:HD11	2.39	0.57
1:E:63:PRO:HA	1:E:117:PRO:HG3	1.85	0.57
1:F:80:ARG:O	1:F:83:LYS:NZ	2.35	0.57
1:F:184:GLU:HA	1:F:238:SER:O	2.04	0.57
3:A:1130:LEU:O	3:A:1133:THR:OG1	2.22	0.57
3:B:703:LEU:HD21	3:B:782:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:480:VAL:HB	3:A:495:ILE:HD11	1.87	0.57
1:E:355:VAL:O	1:E:384:ASN:N	2.38	0.57
2:C:31:ARG:HB3	2:C:477:LEU:O	2.04	0.57
3:B:231:ASP:HA	3:B:234:THR:HG22	1.87	0.57
3:B:433:SER:OG	3:B:484:MET:SD	2.63	0.57
1:F:151:TYR:HB2	1:F:177:ILE:HG12	1.87	0.57
3:B:701:PRO:HB2	3:B:790:ILE:HG23	1.87	0.56
2:C:160:SER:OG	2:C:161:HIS:ND1	2.37	0.56
2:D:160:SER:OG	2:D:161:HIS:ND1	2.37	0.56
1:F:63:PRO:HA	1:F:117:PRO:HG3	1.85	0.56
2:D:31:ARG:HB3	2:D:477:LEU:O	2.04	0.56
3:A:1139:PRO:HB2	3:A:1166:ASN:HB3	1.87	0.56
3:B:784:TRP:HD1	3:B:790:ILE:HD11	1.71	0.56
3:B:687:CYS:SG	3:B:688:SER:N	2.78	0.56
1:E:184:GLU:HA	1:E:238:SER:O	2.04	0.56
3:B:1124:VAL:HG23	3:B:1127:LEU:HB2	1.88	0.56
3:A:433:SER:OG	3:A:484:MET:SD	2.63	0.56
3:B:480:VAL:HB	3:B:495:ILE:HD11	1.87	0.56
3:B:1141:PRO:HB3	3:B:1167:LEU:HA	1.87	0.56
1:F:355:VAL:O	1:F:384:ASN:N	2.38	0.56
3:A:261:GLU:HB3	3:A:274:VAL:HG23	1.88	0.56
3:A:868:PRO:HG2	3:A:1024:ARG:H	1.70	0.56
3:B:68:ASN:OD1	3:B:112:ASN:N	2.35	0.56
3:A:1141:PRO:HB3	3:A:1167:LEU:HA	1.88	0.56
3:A:701:PRO:HB2	3:A:790:ILE:HG23	1.87	0.56
3:A:1124:VAL:HG23	3:A:1127:LEU:HB2	1.88	0.56
2:C:37:LYS:NZ	2:C:38:GLU:OE2	2.37	0.55
3:A:814:LEU:HD22	3:A:847:LEU:HB2	1.88	0.55
3:B:512:TYR:HH	3:B:521:SER:HG	1.54	0.55
3:B:814:LEU:HD22	3:B:847:LEU:HB2	1.88	0.55
3:A:371:GLN:HA	3:A:399:ILE:HD13	1.88	0.55
3:A:687:CYS:SG	3:A:688:SER:N	2.78	0.55
3:B:371:GLN:HA	3:B:399:ILE:HD13	1.88	0.55
3:B:381:ASP:HA	3:B:388:LYS:HD2	1.86	0.55
2:C:652:UNK:O	2:C:672:UNK:N	2.39	0.55
3:A:231:ASP:HA	3:A:234:THR:HG22	1.87	0.55
3:B:868:PRO:HG2	3:B:1024:ARG:H	1.70	0.55
1:F:292:THR:N	1:F:327:GLN:O	2.37	0.55
3:A:784:TRP:HD1	3:A:790:ILE:HD11	1.71	0.55
3:B:711:VAL:HG11	3:B:766:TYR:HD2	1.71	0.55
3:B:173:VAL:HG21	3:B:284:LYS:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:TYR:HB2	1:E:177:ILE:HG12	1.87	0.55
2:D:652:UNK:O	2:D:672:UNK:N	2.39	0.55
3:B:1139:PRO:HB2	3:B:1166:ASN:HB3	1.87	0.55
3:B:548:ARG:HE	3:B:582:ASN:HA	1.72	0.55
3:B:574:VAL:HG22	3:B:613:SER:HB3	1.89	0.55
1:F:151:TYR:N	1:F:176:ILE:O	2.39	0.55
3:A:986:VAL:O	3:A:993:CYS:N	2.40	0.55
1:F:253:ILE:HD12	2:D:497:LYS:NZ	2.21	0.55
3:A:711:VAL:HG11	3:A:766:TYR:HD2	1.71	0.55
3:B:1182:VAL:O	3:B:1189:CYS:HB3	2.07	0.55
3:A:574:VAL:HG22	3:A:613:SER:HB3	1.89	0.54
3:B:576:LEU:HD11	3:B:611:CYS:HB3	1.89	0.54
3:A:845:LEU:CD1	3:A:855:THR:H	2.21	0.54
1:E:151:TYR:N	1:E:176:ILE:O	2.39	0.54
1:E:206:CYS:O	1:E:210:ARG:HB3	2.08	0.54
3:A:1087:VAL:HA	3:A:1093:MET:HB2	1.89	0.54
3:B:261:GLU:HB3	3:B:274:VAL:HG23	1.88	0.54
1:F:206:CYS:O	1:F:210:ARG:HB3	2.08	0.54
2:D:496:THR:O	2:D:499:GLN:NE2	2.41	0.54
3:A:115:LYS:HE2	3:A:160:SER:HB3	1.90	0.54
3:B:986:VAL:O	3:B:993:CYS:N	2.40	0.54
3:A:703:LEU:HD13	3:A:723:ALA:HB2	1.89	0.54
3:B:845:LEU:CD1	3:B:855:THR:H	2.21	0.54
3:B:955:LEU:HD11	3:B:1020:VAL:HB	1.89	0.54
3:A:173:VAL:HG21	3:A:284:LYS:HG2	1.89	0.54
2:C:438:ARG:HB3	2:C:445:GLN:HE21	1.72	0.54
1:F:90:ILE:HA	1:F:99:LEU:HA	1.90	0.54
2:D:105:TRP:CH2	3:B:397:LEU:HD13	2.43	0.54
3:A:955:LEU:HD11	3:A:1020:VAL:HB	1.89	0.54
3:A:1039:PRO:HB3	3:A:1063:HIS:HB2	1.90	0.54
3:B:1087:VAL:HA	3:B:1093:MET:HB2	1.90	0.54
1:E:292:THR:N	1:E:327:GLN:O	2.37	0.54
3:A:1182:VAL:O	3:A:1189:CYS:HB3	2.08	0.54
1:F:325:TRP:HA	1:F:406:ILE:O	2.08	0.54
1:E:325:TRP:HA	1:E:406:ILE:O	2.08	0.53
2:D:359:ARG:HH21	2:D:362:PRO:HA	1.73	0.53
3:A:160:SER:HB2	3:A:186:THR:HG21	1.90	0.53
3:A:433:SER:HB2	3:A:482:ARG:HA	1.90	0.53
3:B:996:HIS:N	3:B:1004:ILE:O	2.42	0.53
3:B:433:SER:HB2	3:B:482:ARG:HA	1.90	0.53
2:C:496:THR:O	2:C:499:GLN:NE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:578:LEU:HD13	3:A:636:LEU:HD11	1.91	0.53
3:A:861:GLU:O	3:A:878:ARG:N	2.41	0.53
2:C:203:ARG:NH2	2:C:272:ASP:O	2.34	0.53
2:C:359:ARG:HH21	2:C:362:PRO:HA	1.73	0.53
3:A:548:ARG:HE	3:A:582:ASN:HA	1.72	0.53
3:A:576:LEU:HD11	3:A:611:CYS:HB3	1.89	0.53
3:A:857:PRO:HB3	3:A:881:ASN:HB2	1.90	0.53
3:B:578:LEU:HD13	3:B:636:LEU:HD11	1.91	0.53
3:B:861:GLU:O	3:B:878:ARG:N	2.41	0.53
2:C:601:UNK:HA	2:C:641:UNK:O	2.09	0.53
2:D:601:UNK:HA	2:D:641:UNK:O	2.09	0.53
3:B:854:CYS:HB2	3:B:933:VAL:HG11	1.91	0.53
3:B:857:PRO:HB3	3:B:881:ASN:HB2	1.90	0.53
3:B:160:SER:HB2	3:B:186:THR:HG21	1.90	0.53
3:B:115:LYS:HE2	3:B:160:SER:HB3	1.90	0.53
3:B:1067:ILE:HG21	3:B:1121:LEU:HD22	1.91	0.53
3:B:1167:LEU:HB2	3:B:1195:ASP:HA	1.91	0.53
2:D:438:ARG:HB3	2:D:445:GLN:HE21	1.72	0.53
3:B:703:LEU:HD13	3:B:723:ALA:HB2	1.89	0.53
2:D:543:SER:OG	2:D:544:ARG:N	2.42	0.52
3:B:88:ASP:OD1	3:B:89:GLU:N	2.43	0.52
2:C:543:SER:OG	2:C:544:ARG:N	2.41	0.52
3:A:97:PRO:HB3	3:A:133:TYR:HD1	1.75	0.52
3:B:295:VAL:HA	3:B:414:VAL:HG22	1.90	0.52
1:E:216:GLY:HA2	1:E:242:VAL:HB	1.90	0.52
3:A:427:ASP:OD1	3:A:427:ASP:N	2.43	0.52
3:B:1039:PRO:HB3	3:B:1063:HIS:HB2	1.90	0.52
1:F:194:LEU:HD12	1:F:228:CYS:HA	1.92	0.52
1:F:216:GLY:HA2	1:F:242:VAL:HB	1.90	0.52
3:A:188:VAL:HG13	3:A:190:GLY:H	1.74	0.52
3:A:996:HIS:N	3:A:1004:ILE:O	2.42	0.52
3:B:592:CYS:HB3	3:B:634:LEU:HD11	1.92	0.52
1:E:238:SER:HB3	1:E:243:LEU:HG	1.92	0.52
2:D:37:LYS:NZ	2:D:38:GLU:OE2	2.37	0.52
3:A:783:VAL:HG22	3:A:789:ASN:HA	1.92	0.52
1:E:90:ILE:HA	1:E:99:LEU:HA	1.90	0.52
3:A:236:ILE:HG23	3:A:239:PHE:HB2	1.92	0.52
3:A:1167:LEU:HB2	3:A:1195:ASP:HA	1.91	0.52
3:B:188:VAL:HG13	3:B:190:GLY:H	1.74	0.52
3:B:675:LYS:HE3	3:B:676:TYR:HE2	1.74	0.52
1:E:484:TRP:HA	1:E:564:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:456:GLY:HA2	2:C:489:ILE:HG13	1.92	0.52
3:A:295:VAL:HA	3:A:414:VAL:HG22	1.90	0.52
1:E:137:ARG:HD2	2:C:385:THR:O	2.09	0.52
2:C:443:ASP:OD1	2:C:443:ASP:N	2.43	0.52
1:F:484:TRP:HA	1:F:564:ILE:O	2.10	0.52
3:A:675:LYS:HE3	3:A:676:TYR:HE2	1.74	0.52
1:F:238:SER:HB3	1:F:243:LEU:HG	1.92	0.51
3:A:592:CYS:HB3	3:A:634:LEU:HD11	1.91	0.51
3:A:931:ILE:HG12	3:A:942:ALA:HB3	1.92	0.51
3:A:1067:ILE:HG21	3:A:1121:LEU:HD22	1.91	0.51
3:A:701:PRO:HB3	3:A:727:PRO:HD3	1.91	0.51
3:B:988:PHE:HB2	3:B:1008:THR:HG22	1.92	0.51
2:D:456:GLY:HA2	2:D:489:ILE:HG13	1.92	0.51
3:A:988:PHE:HB2	3:A:1008:THR:HG22	1.92	0.51
1:E:80:ARG:O	1:E:83:LYS:NZ	2.35	0.51
2:D:276:HIS:ND1	2:D:393:LYS:O	2.44	0.51
3:B:308:LEU:HD11	3:B:345:LYS:HB3	1.92	0.51
3:B:701:PRO:HB3	3:B:727:PRO:HD3	1.91	0.51
3:B:931:ILE:HG12	3:B:942:ALA:HB3	1.92	0.51
1:E:188:GLU:N	1:E:261:ASN:O	2.41	0.51
2:C:382:PRO:HG3	2:C:392:THR:HG23	1.92	0.51
2:D:382:PRO:HG3	2:D:392:THR:HG23	1.92	0.51
3:A:88:ASP:OD1	3:A:89:GLU:N	2.43	0.51
2:C:276:HIS:ND1	2:C:393:LYS:O	2.44	0.51
3:A:737:GLU:HA	3:A:750:PRO:HA	1.91	0.51
3:B:97:PRO:HB3	3:B:133:TYR:HD1	1.75	0.51
3:B:236:ILE:HG23	3:B:239:PHE:HB2	1.92	0.51
2:D:443:ASP:N	2:D:443:ASP:OD1	2.43	0.51
3:A:854:CYS:HB2	3:A:933:VAL:HG11	1.91	0.51
3:B:1194:SER:N	3:B:1198:LEU:HD21	2.25	0.51
3:A:308:LEU:HD11	3:A:345:LYS:HB3	1.91	0.51
3:A:752:LEU:N	3:A:760:GLN:O	2.44	0.51
3:B:737:GLU:HA	3:B:750:PRO:HA	1.91	0.51
3:B:709:ILE:HG12	3:B:719:ILE:HG23	1.93	0.51
1:E:163:PHE:CG	1:E:164:PRO:HA	2.47	0.50
3:A:141:ARG:HD3	3:A:146:PHE:CE1	2.46	0.50
3:A:775:ASN:HA	3:A:800:LEU:O	2.11	0.50
2:D:76:HIS:CE1	2:D:92:VAL:HG13	2.46	0.50
1:E:194:LEU:HD12	1:E:228:CYS:HA	1.92	0.50
1:F:85:ASP:OD1	1:F:126:ASP:N	2.33	0.50
3:A:986:VAL:HA	3:A:1020:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:275:TYR:CE1	3:B:346:MET:HB2	2.47	0.50
3:B:626:ASN:ND2	3:B:630:HIS:HA	2.26	0.50
3:B:783:VAL:HG22	3:B:789:ASN:HA	1.92	0.50
3:B:1130:LEU:O	3:B:1133:THR:OG1	2.22	0.50
2:C:76:HIS:CE1	2:C:92:VAL:HG13	2.46	0.50
3:A:310:GLN:HB2	3:A:337:VAL:HG12	1.92	0.50
3:B:893:VAL:HG13	3:B:931:ILE:HG22	1.94	0.50
3:B:986:VAL:HA	3:B:1020:VAL:HA	1.93	0.50
2:C:634:UNK:O	2:C:638:UNK:CB	2.60	0.50
3:A:275:TYR:CE1	3:A:346:MET:HB2	2.47	0.50
3:B:713:VAL:HG13	3:B:767:SER:HA	1.94	0.50
3:A:626:ASN:ND2	3:A:630:HIS:HA	2.26	0.50
3:B:455:LYS:HG2	3:B:471:THR:HB	1.94	0.50
3:B:752:LEU:N	3:B:760:GLN:O	2.44	0.50
2:C:299:ASN:OD1	2:C:299:ASN:N	2.45	0.50
3:B:306:TYR:HA	3:B:340:LYS:HA	1.94	0.50
1:F:163:PHE:CG	1:F:164:PRO:HA	2.47	0.50
2:D:368:PRO:HD3	2:D:410:TYR:CZ	2.47	0.50
3:A:112:ASN:HB2	3:A:132:LEU:HD13	1.93	0.50
3:A:455:LYS:HG2	3:A:471:THR:HB	1.94	0.50
3:B:775:ASN:HA	3:B:800:LEU:O	2.11	0.50
3:A:713:VAL:HG11	3:A:802:LYS:HE2	1.94	0.49
3:B:310:GLN:HB2	3:B:337:VAL:HG12	1.92	0.49
3:A:306:TYR:HA	3:A:340:LYS:HA	1.94	0.49
3:A:453:LYS:HG2	3:A:473:GLN:HG2	1.94	0.49
2:D:634:UNK:O	2:D:638:UNK:CB	2.60	0.49
3:A:893:VAL:HG13	3:A:931:ILE:HG22	1.94	0.49
3:B:141:ARG:HD3	3:B:146:PHE:CE1	2.46	0.49
1:F:163:PHE:CE1	1:F:259:SER:HB2	2.47	0.49
1:F:188:GLU:N	1:F:261:ASN:O	2.41	0.49
1:F:340:GLY:O	1:F:420:GLU:N	2.45	0.49
3:B:877:ILE:HD13	3:B:929:VAL:HG11	1.93	0.49
3:B:1098:PRO:HD2	3:B:1137:TYR:OH	2.13	0.49
1:E:340:GLY:O	1:E:420:GLU:N	2.45	0.49
3:A:1049:SER:HG	3:A:1135:PHE:HE2	1.60	0.49
1:E:43:GLY:HA3	1:E:47:SER:O	2.13	0.49
1:E:163:PHE:CE1	1:E:259:SER:HB2	2.48	0.49
3:A:437:TYR:HB3	3:A:486:PHE:HE2	1.78	0.49
3:A:709:ILE:HG12	3:A:719:ILE:HG23	1.93	0.49
2:C:368:PRO:HD3	2:C:410:TYR:CZ	2.47	0.49
3:A:877:ILE:HD13	3:A:929:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:900:CYS:HA	3:A:917:MET:HA	1.94	0.49
3:A:1194:SER:N	3:A:1198:LEU:HD21	2.25	0.49
3:B:85:THR:OG1	3:B:112:ASN:ND2	2.31	0.49
3:A:54:VAL:HG12	3:A:63:TYR:HB2	1.95	0.49
3:B:437:TYR:HB3	3:B:486:PHE:HE2	1.78	0.49
3:B:569:VAL:HG22	3:B:652:PHE:HB3	1.94	0.49
2:C:237:ASN:HD22	2:C:385:THR:HG1	1.57	0.49
3:A:857:PRO:HA	3:A:881:ASN:ND2	2.28	0.49
3:B:857:PRO:HA	3:B:881:ASN:ND2	2.28	0.49
1:E:177:ILE:O	1:E:242:VAL:HA	2.13	0.49
1:F:128:GLU:HG2	3:A:343:LYS:HD2	1.95	0.49
2:D:210:PRO:HG2	3:B:220:GLU:HG2	1.95	0.49
2:D:237:ASN:HD22	2:D:385:THR:HG1	1.58	0.49
3:A:569:VAL:HG22	3:A:652:PHE:HB3	1.94	0.49
2:D:359:ARG:NH2	2:D:362:PRO:HA	2.28	0.48
3:A:39:PHE:HZ	3:A:472:VAL:HG11	1.78	0.48
3:B:1070:PRO:HB2	3:B:1085:CYS:HB2	1.95	0.48
2:C:443:ASP:OD2	2:C:446:TYR:OH	2.22	0.48
3:A:664:CYS:O	3:A:671:CYS:HB2	2.14	0.48
3:B:54:VAL:HG12	3:B:63:TYR:HB2	1.95	0.48
3:B:569:VAL:HG13	3:B:619:VAL:HG12	1.95	0.48
3:B:900:CYS:HA	3:B:917:MET:HA	1.94	0.48
3:A:68:ASN:OD1	3:A:112:ASN:N	2.35	0.48
3:A:475:VAL:HG11	3:A:497:SER:HB3	1.95	0.48
3:A:486:PHE:CE1	3:A:493:LEU:HD13	2.49	0.48
3:B:39:PHE:HZ	3:B:472:VAL:HG11	1.78	0.48
3:B:988:PHE:N	3:B:991:GLN:O	2.45	0.48
2:C:256:HIS:CE1	2:D:365:GLN:HG2	2.41	0.48
2:D:439:VAL:HG11	2:D:534:TYR:CZ	2.48	0.48
3:A:713:VAL:HG13	3:A:767:SER:HA	1.94	0.48
3:A:877:ILE:HG21	3:A:929:VAL:HG11	1.96	0.48
3:A:988:PHE:N	3:A:991:GLN:O	2.45	0.48
3:B:475:VAL:HG11	3:B:497:SER:HB3	1.95	0.48
3:B:713:VAL:HG11	3:B:802:LYS:HE2	1.94	0.48
2:C:439:VAL:HG11	2:C:534:TYR:CZ	2.48	0.48
3:A:902:PRO:HA	3:A:915:CYS:HA	1.95	0.48
3:A:1098:PRO:HD2	3:A:1137:TYR:OH	2.13	0.48
3:B:902:PRO:HA	3:B:915:CYS:HA	1.95	0.48
2:C:365:GLN:HG2	2:D:256:HIS:HE1	1.78	0.48
3:A:1044:ILE:HD11	3:A:1133:THR:HG22	1.96	0.48
3:B:112:ASN:HB2	3:B:132:LEU:HD13	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:VAL:HG23	2:C:482:VAL:HG21	1.95	0.48
3:A:536:THR:OG1	3:A:541:CYS:SG	2.72	0.48
3:B:486:PHE:CE1	3:B:493:LEU:HD13	2.49	0.48
3:B:536:THR:OG1	3:B:541:CYS:SG	2.72	0.48
2:C:378:PRO:HG3	2:C:399:VAL:HG13	1.96	0.48
1:F:340:GLY:N	1:F:420:GLU:O	2.46	0.48
3:A:1046:PRO:HG2	3:A:1057:ILE:HA	1.96	0.48
3:B:453:LYS:HG2	3:B:473:GLN:HG2	1.94	0.48
3:B:507:GLU:HB2	3:B:525:HIS:CE1	2.49	0.48
3:B:736:TYR:CE2	3:B:753:ARG:HB3	2.49	0.48
1:F:177:ILE:O	1:F:242:VAL:HA	2.13	0.48
3:A:882:LEU:HB2	3:A:910:ALA:N	2.20	0.48
3:B:250:GLY:O	3:B:284:LYS:NZ	2.46	0.48
3:B:664:CYS:O	3:B:671:CYS:HB2	2.14	0.48
3:B:1114:PRO:HG3	3:B:1137:TYR:CD2	2.49	0.48
3:B:1121:LEU:HD12	3:B:1127:LEU:HG	1.95	0.48
1:F:43:GLY:HA3	1:F:47:SER:O	2.13	0.48
1:F:149:GLN:NE2	1:F:151:TYR:OH	2.47	0.48
2:D:458:VAL:HG23	2:D:482:VAL:HG21	1.95	0.48
3:B:1044:ILE:HD11	3:B:1133:THR:HG22	1.96	0.48
1:F:227:TYR:CG	1:F:233:PRO:HG3	2.49	0.47
1:E:340:GLY:N	1:E:420:GLU:O	2.46	0.47
3:A:507:GLU:HB2	3:A:525:HIS:CE1	2.49	0.47
3:A:626:ASN:HD22	3:A:630:HIS:HA	1.79	0.47
3:A:1070:PRO:HB2	3:A:1085:CYS:HB2	1.95	0.47
3:A:1114:PRO:HG3	3:A:1137:TYR:CD2	2.49	0.47
3:B:614:PRO:HD2	3:B:652:PHE:CZ	2.48	0.47
3:B:626:ASN:HD22	3:B:630:HIS:HA	1.78	0.47
3:B:845:LEU:HD11	3:B:855:THR:H	1.80	0.47
3:B:877:ILE:HG21	3:B:929:VAL:HG11	1.96	0.47
2:C:48:PHE:CZ	2:C:50:GLY:HA2	2.49	0.47
2:C:464:VAL:O	2:C:472:LEU:CA	2.58	0.47
2:D:48:PHE:CZ	2:D:50:GLY:HA2	2.49	0.47
2:D:228:SER:OG	2:D:229:ALA:N	2.48	0.47
3:A:569:VAL:HG13	3:A:619:VAL:HG12	1.95	0.47
3:B:569:VAL:HG21	3:B:654:ASN:HB2	1.96	0.47
1:E:91:ASP:HA	1:E:119:LEU:HD23	1.96	0.47
1:E:149:GLN:NE2	1:E:151:TYR:OH	2.47	0.47
1:E:227:TYR:CG	1:E:233:PRO:HG3	2.49	0.47
3:A:614:PRO:HD2	3:A:652:PHE:CZ	2.48	0.47
3:A:1041:ILE:HG13	3:A:1119:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:ARG:NH2	2:C:362:PRO:HA	2.28	0.47
3:A:439:TYR:CE2	3:A:525:HIS:HA	2.50	0.47
3:B:204:THR:N	3:B:212:MET:SD	2.88	0.47
3:A:569:VAL:HG21	3:A:654:ASN:HB2	1.96	0.47
3:B:963:GLY:O	3:B:1036:VAL:N	2.47	0.47
3:B:1022:VAL:HG12	3:B:1023:ASP:H	1.80	0.47
3:A:845:LEU:HD11	3:A:855:THR:H	1.80	0.47
3:B:832:THR:HG23	3:B:837:CYS:HB2	1.96	0.47
2:D:378:PRO:HG3	2:D:399:VAL:HG13	1.96	0.47
3:A:1121:LEU:HD12	3:A:1127:LEU:HG	1.95	0.47
3:B:272:GLU:HG3	3:B:344:ARG:NH1	2.30	0.47
3:B:739:ILE:O	3:B:780:LEU:HA	2.15	0.47
3:B:929:VAL:N	3:B:944:SER:OG	2.48	0.47
1:F:91:ASP:HA	1:F:119:LEU:HD23	1.96	0.46
3:A:832:THR:HG23	3:A:837:CYS:HB2	1.96	0.46
3:A:963:GLY:O	3:A:1036:VAL:N	2.47	0.46
3:A:1086:GLU:N	3:A:1094:THR:O	2.48	0.46
3:B:683:ASP:OD1	3:B:684:PRO:HD2	2.15	0.46
3:B:1070:PRO:HG2	3:B:1087:VAL:HG23	1.97	0.46
1:E:214:TRP:CZ3	1:E:223:HIS:HB2	2.50	0.46
2:C:292:ILE:O	2:C:415:PRO:HD3	2.15	0.46
3:A:600:MET:SD	3:A:600:MET:N	2.88	0.46
3:A:718:PRO:HA	3:A:761:CYS:O	2.16	0.46
3:A:736:TYR:CE2	3:A:753:ARG:HB3	2.49	0.46
3:B:439:TYR:CE2	3:B:525:HIS:HA	2.50	0.46
3:B:889:ILE:O	3:B:892:HIS:HD2	1.98	0.46
1:E:159:LYS:HE2	1:E:163:PHE:HB3	1.98	0.46
1:E:187:LEU:HA	1:E:262:TYR:HA	1.97	0.46
3:A:674:CYS:HB2	3:A:687:CYS:HB2	1.75	0.46
3:A:965:MET:N	3:A:1036:VAL:O	2.48	0.46
3:A:929:VAL:N	3:A:944:SER:OG	2.49	0.46
3:B:560:LEU:HB3	3:B:648:THR:OG1	2.15	0.46
3:A:1022:VAL:HG12	3:A:1023:ASP:H	1.80	0.46
3:B:567:ILE:HD11	3:B:652:PHE:CE1	2.51	0.46
3:B:811:GLY:H	3:B:881:ASN:CG	2.19	0.46
3:B:1041:ILE:HG13	3:B:1119:PHE:HB2	1.97	0.46
1:F:159:LYS:HE2	1:F:163:PHE:HB3	1.98	0.46
3:A:272:GLU:HG3	3:A:344:ARG:NH1	2.30	0.46
3:A:683:ASP:OD1	3:A:684:PRO:HD2	2.15	0.46
3:A:1070:PRO:HG2	3:A:1087:VAL:HG23	1.97	0.46
3:B:988:PHE:HA	3:B:1016:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:LEU:HG	1:E:189:PHE:HE1	1.81	0.46
2:C:228:SER:OG	2:C:229:ALA:N	2.48	0.46
3:A:891:SER:O	3:A:891:SER:OG	2.34	0.46
3:B:867:GLY:HA3	3:B:948:TYR:CZ	2.51	0.46
1:F:187:LEU:HA	1:F:262:TYR:HA	1.97	0.46
3:A:867:GLY:HA3	3:A:948:TYR:OH	2.16	0.46
3:A:1016:MET:SD	3:A:1017:LYS:N	2.89	0.46
3:B:1046:PRO:HG2	3:B:1057:ILE:HA	1.96	0.46
3:B:1086:GLU:N	3:B:1094:THR:O	2.48	0.46
3:A:85:THR:OG1	3:A:112:ASN:ND2	2.31	0.46
3:A:264:SER:HB2	3:A:265:PRO:HD3	1.97	0.46
1:F:187:LEU:HG	1:F:189:PHE:HE1	1.81	0.46
2:D:308:LEU:O	2:D:309:GLN:NE2	2.49	0.46
3:A:1050:ILE:HG13	3:A:1053:GLY:H	1.81	0.46
2:C:77:ILE:HD11	2:C:118:ILE:HG12	1.99	0.45
3:A:494:TYR:CE2	3:A:503:ARG:HD3	2.51	0.45
3:A:560:LEU:HB3	3:A:648:THR:OG1	2.15	0.45
3:A:739:ILE:O	3:A:780:LEU:HA	2.16	0.45
3:B:264:SER:HB2	3:B:265:PRO:HD3	1.97	0.45
3:B:494:TYR:CE2	3:B:503:ARG:HD3	2.51	0.45
3:B:867:GLY:HA3	3:B:948:TYR:OH	2.16	0.45
3:B:1016:MET:SD	3:B:1017:LYS:N	2.89	0.45
3:B:1066:LEU:HD12	3:B:1067:ILE:N	2.32	0.45
2:D:130:TYR:CZ	2:D:205:LEU:HD21	2.51	0.45
3:A:176:SER:OG	3:A:177:ASN:N	2.49	0.45
3:A:204:THR:N	3:A:212:MET:SD	2.88	0.45
3:A:567:ILE:HD11	3:A:652:PHE:CE1	2.51	0.45
3:B:882:LEU:HB2	3:B:910:ALA:N	2.20	0.45
1:F:149:GLN:H	1:F:175:TYR:HD1	1.65	0.45
3:B:600:MET:SD	3:B:600:MET:N	2.89	0.45
3:B:893:VAL:HB	3:B:900:CYS:HB3	1.98	0.45
1:E:126:ASP:OD2	3:B:343:LYS:NZ	2.49	0.45
2:C:45:VAL:HA	2:C:511:GLN:O	2.17	0.45
2:D:77:ILE:HD11	2:D:118:ILE:HG12	1.98	0.45
3:A:461:GLY:HA3	3:A:465:ASN:HB2	1.97	0.45
3:A:867:GLY:HA3	3:A:948:TYR:CZ	2.51	0.45
3:A:988:PHE:HA	3:A:1016:MET:SD	2.56	0.45
3:B:718:PRO:HA	3:B:761:CYS:O	2.16	0.45
3:B:873:THR:HG23	3:B:1023:ASP:HB3	1.98	0.45
3:B:965:MET:N	3:B:1036:VAL:O	2.48	0.45
3:B:1050:ILE:HG13	3:B:1053:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:SER:HB3	1:E:119:LEU:HD11	1.98	0.45
2:C:37:LYS:O	2:C:41:GLU:HG2	2.17	0.45
1:F:214:TRP:CZ3	1:F:223:HIS:HB2	2.50	0.45
3:A:281:ARG:NH1	3:A:366:ILE:HG21	2.32	0.45
3:A:860:THR:H	3:A:879:GLY:HA2	1.82	0.45
3:B:176:SER:OG	3:B:177:ASN:N	2.49	0.45
3:B:281:ARG:NH1	3:B:366:ILE:HG21	2.32	0.45
3:B:723:ALA:N	3:B:757:SER:O	2.50	0.45
3:A:250:GLY:O	3:A:284:LYS:NZ	2.46	0.45
3:A:569:VAL:HG22	3:A:623:ILE:HG21	1.99	0.45
1:F:114:SER:HB3	1:F:119:LEU:HD11	1.98	0.45
2:D:292:ILE:O	2:D:415:PRO:HD3	2.16	0.45
3:A:62:ILE:HG23	3:A:73:LEU:HB2	1.98	0.45
1:E:41:SER:OG	1:E:44:TYR:HB2	2.17	0.45
2:D:45:VAL:HA	2:D:511:GLN:O	2.17	0.45
3:A:1066:LEU:HD12	3:A:1067:ILE:N	2.32	0.45
3:B:891:SER:O	3:B:891:SER:OG	2.34	0.45
2:D:115:ALA:HB3	2:D:117:PHE:CE1	2.52	0.45
2:D:159:ASP:OD2	2:D:159:ASP:N	2.50	0.45
3:A:873:THR:HG23	3:A:1023:ASP:HB3	1.98	0.45
3:A:889:ILE:O	3:A:892:HIS:HD2	1.98	0.45
3:B:742:ILE:HG13	3:B:778:VAL:HG11	1.99	0.45
1:E:128:GLU:CG	1:E:129:THR:H	2.30	0.45
3:B:74:SER:HB3	3:B:80:LEU:HD21	1.99	0.45
3:B:860:THR:H	3:B:879:GLY:HA2	1.82	0.45
2:C:115:ALA:HB3	2:C:117:PHE:CE1	2.52	0.44
2:C:130:TYR:CZ	2:C:205:LEU:HD21	2.51	0.44
1:F:227:TYR:CD2	1:F:233:PRO:HG3	2.52	0.44
3:A:74:SER:HB3	3:A:80:LEU:HD21	1.99	0.44
3:A:810:CYS:SG	3:A:811:GLY:N	2.90	0.44
3:A:811:GLY:H	3:A:881:ASN:CG	2.19	0.44
3:A:827:SER:OG	3:A:828:PRO:HD3	2.16	0.44
3:B:283:CYS:HB2	3:B:404:CYS:HB2	1.25	0.44
3:B:569:VAL:HG22	3:B:623:ILE:HG21	1.99	0.44
3:B:753:ARG:HB2	3:B:759:VAL:HG13	1.99	0.44
3:B:810:CYS:SG	3:B:811:GLY:N	2.90	0.44
1:E:227:TYR:CD2	1:E:233:PRO:HG3	2.52	0.44
2:D:221:LEU:HD22	2:D:224:PRO:HG3	1.99	0.44
2:D:405:SER:HG	2:D:406:HIS:CE1	2.36	0.44
3:A:781:THR:HG23	3:A:792:ASN:HD22	1.82	0.44
3:A:790:ILE:H	3:A:790:ILE:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1039:PRO:HG2	3:A:1124:VAL:HG21	1.99	0.44
3:B:461:GLY:HA3	3:B:465:ASN:HB2	1.97	0.44
3:B:672:HIS:CE1	3:B:684:PRO:HD3	2.52	0.44
2:C:308:LEU:O	2:C:309:GLN:NE2	2.49	0.44
1:F:36:PRO:HB3	1:F:139:GLU:HB2	2.00	0.44
3:B:814:LEU:HD21	3:B:845:LEU:HD23	2.00	0.44
3:B:1039:PRO:HG2	3:B:1124:VAL:HG21	1.99	0.44
2:C:438:ARG:HG2	2:C:447:ASP:OD1	2.17	0.44
3:A:723:ALA:N	3:A:757:SER:O	2.50	0.44
3:A:988:PHE:CE2	3:A:1007:THR:HG22	2.53	0.44
3:B:781:THR:HG23	3:B:792:ASN:HD22	1.82	0.44
3:B:988:PHE:CE2	3:B:1007:THR:HG22	2.53	0.44
2:C:317:LYS:HA	2:C:317:LYS:HD3	1.76	0.44
2:D:82:LEU:HD23	2:D:82:LEU:HA	1.76	0.44
3:B:406:LEU:HD12	3:B:406:LEU:HA	1.86	0.44
3:B:727:PRO:HG2	3:B:784:TRP:HE1	1.83	0.44
1:F:41:SER:OG	1:F:44:TYR:HB2	2.17	0.44
3:A:672:HIS:CE1	3:A:684:PRO:HD3	2.52	0.44
3:A:727:PRO:HG2	3:A:784:TRP:HE1	1.83	0.44
3:A:893:VAL:HB	3:A:900:CYS:HB3	1.98	0.44
3:B:827:SER:OG	3:B:828:PRO:HD3	2.16	0.44
2:C:236:ASP:OD1	2:C:236:ASP:N	2.49	0.44
3:A:98:ARG:NH2	3:A:133:TYR:OH	2.51	0.44
3:B:137:CYS:HB2	3:B:213:PHE:HE2	1.82	0.44
1:E:149:GLN:H	1:E:175:TYR:HD1	1.64	0.44
3:A:186:THR:HG22	3:A:187:ALA:O	2.18	0.44
3:A:742:ILE:HG13	3:A:778:VAL:HG11	1.99	0.44
3:A:751:ALA:HA	3:A:761:CYS:HA	2.00	0.44
3:A:969:THR:HG22	3:A:1067:ILE:HD12	2.00	0.44
3:A:979:ASN:HA	3:A:998:ARG:HG2	2.00	0.44
3:B:53:LEU:HD13	3:B:501:LEU:HD11	2.00	0.44
3:B:98:ARG:NH2	3:B:133:TYR:OH	2.51	0.44
3:B:1051:VAL:H	3:B:1140:ASN:HB2	1.83	0.44
2:C:405:SER:HG	2:C:406:HIS:CE1	2.36	0.44
1:F:212:GLU:HB2	1:F:246:VAL:HG23	2.00	0.44
2:D:178:ALA:O	2:D:188:SER:HA	2.18	0.44
3:A:137:CYS:HB2	3:A:213:PHE:HE2	1.82	0.44
3:A:345:LYS:HD3	3:A:345:LYS:HA	1.76	0.44
2:D:32:LEU:O	2:D:478:GLU:HA	2.18	0.43
2:D:37:LYS:O	2:D:41:GLU:HG2	2.17	0.43
3:A:89:GLU:O	3:A:133:TYR:OH	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:519:LEU:HB3	3:A:554:MET:HG2	2.00	0.43
3:A:814:LEU:HD21	3:A:845:LEU:HD23	2.00	0.43
3:B:790:ILE:HD12	3:B:790:ILE:H	1.82	0.43
2:C:221:LEU:HD22	2:C:224:PRO:HG3	1.99	0.43
2:C:378:PRO:HG2	2:C:402:PHE:CD2	2.53	0.43
1:F:76:ASP:HB3	1:F:132:ALA:HB3	2.00	0.43
2:D:236:ASP:N	2:D:236:ASP:OD1	2.49	0.43
3:A:344:ARG:HH11	3:A:344:ARG:HG2	1.83	0.43
3:A:475:VAL:HG12	3:A:477:SER:N	2.27	0.43
3:B:475:VAL:HG12	3:B:477:SER:N	2.27	0.43
3:B:803:CYS:HB3	3:B:832:THR:HA	1.99	0.43
3:B:1087:VAL:HA	3:B:1093:MET:CB	2.48	0.43
3:B:1114:PRO:HG2	3:B:1117:PHE:HB2	2.01	0.43
3:A:569:VAL:HG11	3:A:623:ILE:HD13	2.00	0.43
3:A:1051:VAL:H	3:A:1140:ASN:HB2	1.83	0.43
3:B:979:ASN:HA	3:B:998:ARG:HG2	2.00	0.43
1:E:210:ARG:HG2	1:E:248:TYR:HB2	2.00	0.43
2:C:32:LEU:O	2:C:478:GLU:HA	2.18	0.43
2:C:116:ASN:HA	2:C:134:THR:O	2.18	0.43
1:F:212:GLU:HB2	1:F:246:VAL:CG2	2.49	0.43
2:D:116:ASN:HA	2:D:134:THR:O	2.18	0.43
2:D:378:PRO:HG2	2:D:402:PHE:CD2	2.53	0.43
3:B:62:ILE:HG23	3:B:73:LEU:HB2	1.98	0.43
3:B:453:LYS:HE2	3:B:473:GLN:HE21	1.83	0.43
3:A:753:ARG:HB2	3:A:759:VAL:HG13	1.99	0.43
3:A:803:CYS:HB3	3:A:832:THR:HA	1.99	0.43
3:B:519:LEU:HB3	3:B:554:MET:HG2	2.00	0.43
1:E:89:VAL:HG13	1:E:100:TRP:HB2	2.00	0.43
1:F:502:GLY:HA3	1:F:546:TYR:HA	2.01	0.43
2:D:244:TYR:HA	2:D:266:GLY:O	2.19	0.43
2:D:358:HIS:HD2	2:D:406:HIS:CE1	2.37	0.43
2:D:518:ASP:OD1	2:D:518:ASP:N	2.52	0.43
3:A:433:SER:O	3:A:447:VAL:HA	2.18	0.43
3:A:1015:ASP:HA	3:A:1034:GLN:HA	2.00	0.43
3:A:1141:PRO:HA	3:A:1165:LYS:O	2.19	0.43
3:B:127:ILE:HD12	3:B:172:ILE:HD11	2.01	0.43
3:B:428:ARG:CZ	3:B:428:ARG:HA	2.49	0.43
3:B:433:SER:O	3:B:447:VAL:HA	2.18	0.43
3:B:971:VAL:O	3:B:1004:ILE:HD12	2.19	0.43
2:C:82:LEU:O	2:C:502:TYR:OH	2.36	0.43
2:D:317:LYS:HA	2:D:317:LYS:HD3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:438:ARG:HG2	2:D:447:ASP:OD1	2.17	0.43
3:A:712:PRO:HB3	3:A:833:LEU:HD11	2.01	0.43
3:A:937:ARG:O	3:A:941:MET:N	2.52	0.43
3:A:971:VAL:O	3:A:1004:ILE:HD12	2.19	0.43
3:A:53:LEU:HD13	3:A:501:LEU:HD11	2.00	0.43
3:A:127:ILE:HD12	3:A:172:ILE:HD11	2.01	0.43
3:A:558:VAL:HG11	3:A:646:ALA:HB2	2.00	0.43
3:A:1087:VAL:HA	3:A:1093:MET:CB	2.48	0.43
3:A:1114:PRO:HG2	3:A:1117:PHE:HB2	2.01	0.43
3:B:186:THR:HG22	3:B:187:ALA:O	2.18	0.43
3:B:998:ARG:HA	3:B:1003:ILE:HG12	2.01	0.43
2:C:32:LEU:HD12	2:C:32:LEU:HA	1.83	0.43
2:C:82:LEU:HD23	2:C:82:LEU:HA	1.76	0.43
1:F:80:ARG:HD3	1:F:80:ARG:HA	1.86	0.43
2:D:299:ASN:N	2:D:299:ASN:OD1	2.45	0.43
3:A:638:SER:O	3:A:642:GLY:N	2.34	0.43
3:B:345:LYS:HD3	3:B:345:LYS:HA	1.76	0.43
3:B:488:LYS:HD2	3:B:488:LYS:HA	1.70	0.43
3:B:713:VAL:N	3:B:836:HIS:HE2	2.16	0.43
1:E:36:PRO:HB3	1:E:139:GLU:HB2	2.00	0.43
2:C:244:TYR:HA	2:C:266:GLY:O	2.19	0.43
2:C:358:HIS:HD2	2:C:406:HIS:CE1	2.37	0.43
1:F:128:GLU:CG	1:F:129:THR:H	2.30	0.43
3:B:344:ARG:HG2	3:B:344:ARG:HH11	1.83	0.43
3:B:751:ALA:HA	3:B:761:CYS:HA	2.00	0.43
3:B:937:ARG:O	3:B:941:MET:N	2.52	0.43
3:B:1191:VAL:HG12	3:B:1200:CYS:HB3	2.01	0.43
1:E:128:GLU:HG2	3:B:343:LYS:HD2	2.00	0.42
1:E:189:PHE:HA	1:E:260:ALA:HA	2.01	0.42
2:C:178:ALA:O	2:C:188:SER:HA	2.18	0.42
2:C:513:PRO:O	2:C:516:ARG:NH2	2.52	0.42
3:A:100:VAL:HG23	3:A:101:GLN:H	1.84	0.42
3:A:998:ARG:HA	3:A:1003:ILE:HG12	2.01	0.42
3:A:1191:VAL:HG12	3:A:1200:CYS:HB3	2.01	0.42
3:B:307:ARG:HA	3:B:307:ARG:HD3	1.83	0.42
3:B:1015:ASP:HA	3:B:1034:GLN:HA	2.00	0.42
3:B:1042:VAL:H	3:B:1061:GLY:HA2	1.84	0.42
2:C:515:HIS:CD2	2:C:515:HIS:N	2.88	0.42
3:A:453:LYS:HE2	3:A:473:GLN:HE21	1.83	0.42
3:A:512:TYR:HB3	3:A:517:GLU:HB2	2.01	0.42
1:E:293:ALA:HA	1:E:326:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:272:GLU:HG3	3:A:344:ARG:HH11	1.85	0.42
3:A:428:ARG:HA	3:A:428:ARG:CZ	2.49	0.42
3:A:523:ASP:HB3	3:A:525:HIS:NE2	2.34	0.42
3:A:775:ASN:HD21	3:A:799:TYR:HB3	1.84	0.42
3:A:1143:PHE:HD2	3:A:1220:TYR:CD2	2.37	0.42
3:B:553:GLU:HG2	3:B:554:MET:N	2.34	0.42
3:B:558:VAL:HG11	3:B:646:ALA:HB2	2.00	0.42
3:B:969:THR:HG22	3:B:1067:ILE:HD12	2.00	0.42
1:E:502:GLY:HA3	1:E:546:TYR:HA	2.01	0.42
1:F:89:VAL:HG13	1:F:100:TRP:HB2	2.00	0.42
3:A:553:GLU:HG2	3:A:554:MET:N	2.34	0.42
3:A:1044:ILE:HG12	3:A:1059:VAL:HG23	2.01	0.42
1:E:212:GLU:HB2	1:E:246:VAL:CG2	2.49	0.42
3:A:67:VAL:HG22	3:A:113:VAL:HG22	2.02	0.42
3:A:1181:THR:HA	3:A:1191:VAL:HG21	2.02	0.42
1:E:76:ASP:HB3	1:E:132:ALA:HB3	2.00	0.42
1:E:212:GLU:HB2	1:E:246:VAL:HG23	2.00	0.42
2:C:262:HIS:HB3	2:C:264:ARG:HD3	2.02	0.42
1:F:86:TYR:HA	1:F:104:CYS:HB3	2.01	0.42
1:F:179:ALA:HB1	1:F:264:VAL:HG11	2.01	0.42
3:B:117:LEU:HG	3:B:126:LEU:HD11	2.01	0.42
3:B:206:ASN:HB3	3:B:208:GLU:OE2	2.20	0.42
3:B:385:LEU:HD23	3:B:385:LEU:HA	1.90	0.42
3:B:569:VAL:HG11	3:B:623:ILE:HD13	2.00	0.42
3:B:1181:THR:HA	3:B:1191:VAL:HG21	2.02	0.42
2:C:109:ASP:OD1	2:C:111:LEU:N	2.47	0.42
1:F:28:GLY:CA	1:F:55:GLU:O	2.65	0.42
1:F:210:ARG:HG2	1:F:248:TYR:HB2	2.00	0.42
2:D:32:LEU:HD12	2:D:32:LEU:HA	1.83	0.42
2:D:443:ASP:OD2	2:D:446:TYR:OH	2.22	0.42
2:D:513:PRO:O	2:D:516:ARG:NH2	2.52	0.42
3:A:179:ASP:HB2	3:A:203:LEU:O	2.20	0.42
3:B:93:LYS:HE2	3:B:93:LYS:HB3	1.94	0.42
3:B:117:LEU:HD11	3:B:126:LEU:HD21	2.01	0.42
3:B:702:GLN:HA	3:B:791:ASP:O	2.20	0.42
3:B:847:LEU:HG	3:B:850:ALA:HA	2.02	0.42
1:F:215:ASP:HB3	1:F:222:PRO:HD2	2.02	0.42
2:D:66:ARG:O	2:D:68:ARG:HG2	2.20	0.42
2:D:493:GLU:O	2:D:501:LEU:HD12	2.20	0.42
3:A:117:LEU:HD11	3:A:126:LEU:HD21	2.02	0.42
3:A:619:VAL:O	3:A:623:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:774:ASN:HA	3:A:805:ALA:HB3	2.02	0.42
3:B:512:TYR:HB3	3:B:517:GLU:HB2	2.01	0.42
3:B:1044:ILE:HG12	3:B:1059:VAL:HG23	2.01	0.42
3:B:1143:PHE:HD2	3:B:1220:TYR:CD2	2.37	0.42
3:B:1180:TYR:CE2	3:B:1198:LEU:HD13	2.55	0.42
2:C:518:ASP:OD1	2:C:518:ASP:N	2.52	0.42
2:D:110:ILE:HA	2:D:114:CYS:HB2	2.02	0.42
3:A:53:LEU:HA	3:A:63:TYR:O	2.19	0.42
3:A:206:ASN:HB3	3:A:208:GLU:OE2	2.20	0.42
3:A:729:PRO:HA	3:A:784:TRP:CZ3	2.55	0.42
3:A:824:TRP:CE3	3:A:831:CYS:HB3	2.55	0.42
3:B:39:PHE:CG	3:B:504:VAL:HG12	2.55	0.42
3:B:67:VAL:HG22	3:B:113:VAL:HG22	2.02	0.42
3:B:100:VAL:HG23	3:B:101:GLN:H	1.84	0.42
3:B:1141:PRO:HA	3:B:1165:LYS:O	2.19	0.42
2:C:110:ILE:HA	2:C:114:CYS:HB2	2.02	0.42
1:F:218:PRO:HG3	1:F:244:SER:HB3	2.02	0.42
2:D:194:PHE:CE1	3:B:408:MET:HB3	2.55	0.42
3:B:53:LEU:HA	3:B:63:TYR:O	2.19	0.42
3:B:492:GLN:HG2	3:B:503:ARG:HD2	2.02	0.42
3:B:674:CYS:HB2	3:B:687:CYS:HB2	1.75	0.42
3:B:964:PRO:HB2	3:B:967:GLY:H	1.85	0.42
1:E:179:ALA:HB1	1:E:264:VAL:HG11	2.01	0.41
1:E:186:ILE:O	1:E:186:ILE:HG13	2.20	0.41
2:C:145:GLU:N	2:C:156:LYS:O	2.50	0.41
3:A:492:GLN:HG2	3:A:503:ARG:HD2	2.02	0.41
3:A:702:GLN:HA	3:A:791:ASP:O	2.20	0.41
3:A:964:PRO:HB2	3:A:967:GLY:H	1.85	0.41
3:B:712:PRO:HB3	3:B:833:LEU:HD11	2.01	0.41
3:B:775:ASN:HD21	3:B:799:TYR:HB3	1.84	0.41
1:E:86:TYR:HA	1:E:104:CYS:HB3	2.01	0.41
1:E:172:GLU:HA	1:E:247:PHE:O	2.20	0.41
2:D:216:HIS:HB3	3:B:229:PRO:HB3	2.02	0.41
2:D:515:HIS:CD2	2:D:515:HIS:N	2.88	0.41
3:A:81:VAL:HG13	3:A:145:LEU:HD12	2.02	0.41
3:A:448:GLY:HA3	3:A:480:VAL:HG21	2.01	0.41
3:A:753:ARG:HB3	3:A:753:ARG:HE	1.69	0.41
3:A:892:HIS:ND1	3:A:931:ILE:HB	2.35	0.41
3:B:523:ASP:HB3	3:B:525:HIS:NE2	2.34	0.41
3:B:619:VAL:O	3:B:623:ILE:HG23	2.20	0.41
2:C:125:ASN:HB3	2:C:127:THR:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:493:GLU:O	2:C:501:LEU:HD12	2.20	0.41
1:F:41:SER:HB3	1:F:134:PHE:CD1	2.56	0.41
3:A:333:LEU:HD22	3:A:358:ILE:HG22	2.02	0.41
3:A:397:LEU:HD21	3:A:403:PHE:CE1	2.56	0.41
3:B:81:VAL:HG13	3:B:145:LEU:HD12	2.02	0.41
3:B:729:PRO:HA	3:B:784:TRP:CZ3	2.55	0.41
3:B:892:HIS:ND1	3:B:931:ILE:HB	2.35	0.41
1:E:28:GLY:CA	1:E:55:GLU:O	2.65	0.41
1:E:215:ASP:HB3	1:E:222:PRO:HD2	2.02	0.41
1:E:218:PRO:HG3	1:E:244:SER:HB3	2.02	0.41
2:C:66:ARG:O	2:C:68:ARG:HG2	2.20	0.41
3:A:39:PHE:CG	3:A:504:VAL:HG12	2.55	0.41
3:A:488:LYS:HD2	3:A:488:LYS:HA	1.70	0.41
3:A:492:GLN:HB3	3:A:503:ARG:HG3	2.02	0.41
3:A:1042:VAL:H	3:A:1061:GLY:HA2	1.84	0.41
3:B:179:ASP:HB2	3:B:203:LEU:O	2.20	0.41
2:C:198:ASP:OD1	2:C:215:GLN:NE2	2.54	0.41
2:D:125:ASN:HB3	2:D:127:THR:H	1.85	0.41
2:D:411:ASN:HD22	2:D:411:ASN:HA	1.72	0.41
3:A:117:LEU:HG	3:A:126:LEU:HD11	2.02	0.41
3:A:1167:LEU:HD12	3:A:1195:ASP:C	2.41	0.41
3:B:448:GLY:HA3	3:B:480:VAL:HG21	2.01	0.41
3:B:1167:LEU:HD12	3:B:1195:ASP:C	2.41	0.41
1:F:293:ALA:HA	1:F:326:ILE:HA	2.02	0.41
2:D:58:HIS:CE1	2:D:506:THR:HG22	2.56	0.41
2:D:198:ASP:OD1	2:D:215:GLN:NE2	2.54	0.41
3:A:468:GLN:NE2	3:A:471:THR:HB	2.36	0.41
3:A:810:CYS:O	3:A:814:LEU:HG	2.20	0.41
3:A:814:LEU:HD13	3:A:847:LEU:HD13	2.03	0.41
3:A:845:LEU:HD12	3:A:855:THR:HG23	2.02	0.41
3:B:774:ASN:HA	3:B:805:ALA:HB3	2.02	0.41
1:E:36:PRO:HA	1:E:138:TYR:O	2.21	0.41
2:D:262:HIS:HB3	2:D:264:ARG:HD3	2.02	0.41
3:A:320:VAL:HB	3:A:441:ASN:O	2.21	0.41
3:A:637:LYS:HA	3:A:644:THR:HA	2.03	0.41
3:A:1180:TYR:CE2	3:A:1198:LEU:HD13	2.55	0.41
3:B:272:GLU:HG3	3:B:344:ARG:HH11	1.85	0.41
3:B:468:GLN:NE2	3:B:471:THR:HB	2.36	0.41
3:B:810:CYS:O	3:B:814:LEU:HG	2.20	0.41
1:E:356:LYS:O	1:E:383:GLY:N	2.53	0.41
2:C:426:ASP:OD1	2:C:426:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:PHE:HA	1:F:260:ALA:HA	2.01	0.41
2:D:464:VAL:O	2:D:472:LEU:CA	2.58	0.41
3:A:100:VAL:CG1	3:A:153:HIS:HA	2.51	0.41
3:B:397:LEU:HD21	3:B:403:PHE:CE1	2.56	0.41
3:B:594:PHE:CE1	3:B:614:PRO:HD3	2.56	0.41
1:E:486:GLN:HA	1:E:562:ILE:O	2.21	0.41
2:C:33:LYS:HG3	2:C:479:GLU:OE1	2.21	0.41
2:C:58:HIS:CE1	2:C:506:THR:HG22	2.56	0.41
2:C:77:ILE:HD12	2:C:144:ILE:HD11	2.03	0.41
1:F:67:ILE:N	1:F:114:SER:OG	2.44	0.41
1:F:75:PHE:CG	1:F:109:PRO:HD3	2.56	0.41
1:F:126:ASP:OD2	3:A:343:LYS:NZ	2.54	0.41
2:D:212:ARG:O	2:D:282:LYS:HA	2.21	0.41
2:D:274:GLY:HA2	2:D:282:LYS:O	2.21	0.41
2:D:426:ASP:OD1	2:D:426:ASP:N	2.54	0.41
3:A:93:LYS:HE2	3:A:93:LYS:HB3	1.94	0.41
3:A:562:VAL:HG12	3:A:564:PRO:HD2	2.03	0.41
3:A:676:TYR:O	3:A:733:GLN:NE2	2.54	0.41
3:B:546:GLU:OE1	3:B:549:ARG:NE	2.54	0.41
3:B:676:TYR:O	3:B:733:GLN:NE2	2.54	0.41
2:C:274:GLY:HA2	2:C:282:LYS:O	2.21	0.41
2:D:145:GLU:N	2:D:156:LYS:O	2.50	0.41
3:A:314:LEU:HD12	3:A:333:LEU:O	2.21	0.41
3:A:432:THR:OG1	3:A:480:VAL:O	2.30	0.41
3:B:532:HIS:HB2	3:B:534:THR:HG22	2.03	0.41
2:C:123:ALA:O	2:C:181:LEU:HD22	2.22	0.40
2:C:212:ARG:O	2:C:282:LYS:HA	2.21	0.40
2:C:312:PHE:CE1	2:C:435:VAL:HG12	2.56	0.40
2:C:492:MET:HG2	2:C:503:ILE:HG13	2.03	0.40
1:F:172:GLU:HA	1:F:247:PHE:O	2.20	0.40
2:D:312:PHE:CE1	2:D:435:VAL:HG12	2.56	0.40
3:A:40:VAL:HG11	3:A:503:ARG:NH2	2.36	0.40
3:A:594:PHE:O	3:A:632:VAL:HG22	2.21	0.40
3:A:594:PHE:CE1	3:A:614:PRO:HD3	2.56	0.40
3:A:694:VAL:HG13	3:A:699:ASP:HB2	2.02	0.40
3:A:875:VAL:HG22	3:A:877:ILE:HG13	2.03	0.40
3:B:273:GLN:O	3:B:344:ARG:NH1	2.54	0.40
3:B:694:VAL:HG13	3:B:699:ASP:HB2	2.02	0.40
3:B:845:LEU:HD12	3:B:855:THR:HG23	2.02	0.40
3:B:894:LYS:N	3:B:930:GLU:O	2.54	0.40
3:B:1052:SER:HB3	3:B:1218:MET:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:SER:HB3	1:E:134:PHE:CD1	2.56	0.40
1:E:75:PHE:CG	1:E:109:PRO:HD3	2.56	0.40
2:D:35:SER:OG	2:D:36:TYR:N	2.54	0.40
2:D:70:TYR:HA	2:D:78:PHE:O	2.21	0.40
3:A:202:LYS:HB3	3:A:202:LYS:HE2	1.85	0.40
3:A:847:LEU:HG	3:A:850:ALA:HA	2.02	0.40
3:A:1052:SER:HB3	3:A:1218:MET:HB2	2.02	0.40
3:B:824:TRP:CE3	3:B:831:CYS:HB3	2.55	0.40
3:B:1049:SER:HG	3:B:1135:PHE:HE2	1.65	0.40
3:B:1072:ILE:O	3:B:1098:PRO:HG3	2.21	0.40
1:F:358:TYR:O	1:F:381:PHE:N	2.55	0.40
3:A:380:LEU:HD13	3:A:411:PRO:O	2.22	0.40
3:A:638:SER:HB3	3:A:645:PHE:CD1	2.57	0.40
3:A:658:HIS:HB2	3:A:680:CYS:SG	2.61	0.40
3:A:833:LEU:HD12	3:A:836:HIS:H	1.87	0.40
3:B:40:VAL:HG11	3:B:503:ARG:NH2	2.36	0.40
3:B:314:LEU:HD12	3:B:333:LEU:O	2.21	0.40
3:B:316:LYS:HD2	3:B:316:LYS:HA	1.92	0.40
3:B:833:LEU:HD12	3:B:836:HIS:H	1.87	0.40
1:F:91:ASP:OD2	1:F:115:SER:OG	2.33	0.40
1:F:356:LYS:O	1:F:383:GLY:N	2.53	0.40
2:D:33:LYS:HG3	2:D:479:GLU:OE1	2.21	0.40
3:A:369:ARG:NH2	3:A:379:THR:O	2.51	0.40
3:B:320:VAL:HB	3:B:441:ASN:O	2.21	0.40
3:B:878:ARG:HA	3:B:912:GLN:HA	2.04	0.40
1:F:36:PRO:HA	1:F:138:TYR:O	2.21	0.40
3:A:439:TYR:HE2	3:A:525:HIS:HA	1.86	0.40
3:A:894:LYS:N	3:A:930:GLU:O	2.54	0.40
3:B:333:LEU:HD22	3:B:358:ILE:HG22	2.02	0.40
3:B:638:SER:HB3	3:B:645:PHE:CD1	2.57	0.40
3:B:875:VAL:HG22	3:B:877:ILE:HG13	2.03	0.40
3:B:1042:VAL:N	3:B:1060:TRP:O	2.51	0.40
3:B:1198:LEU:HD23	3:B:1198:LEU:HA	1.91	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	E	432/567 (76%)	418 (97%)	14 (3%)	0	100	100
1	F	432/567 (76%)	418 (97%)	14 (3%)	0	100	100
2	C	517/614 (84%)	497 (96%)	20 (4%)	0	100	100
2	D	517/614 (84%)	498 (96%)	19 (4%)	0	100	100
3	A	1117/1194 (94%)	1059 (95%)	58 (5%)	0	100	100
3	B	1117/1194 (94%)	1060 (95%)	57 (5%)	0	100	100
All	All	4132/4750 (87%)	3950 (96%)	182 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	E	193/496 (39%)	193 (100%)	0	100	100
1	F	193/496 (39%)	193 (100%)	0	100	100
2	C	458/482 (95%)	451 (98%)	7 (2%)	65	81
2	D	458/482 (95%)	451 (98%)	7 (2%)	65	81
3	A	793/1056 (75%)	782 (99%)	11 (1%)	67	82
3	B	793/1056 (75%)	782 (99%)	11 (1%)	67	82
All	All	2888/4068 (71%)	2852 (99%)	36 (1%)	72	84

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	45	VAL
2	C	62	LEU
2	C	391	SER
2	C	455	VAL
2	C	488	THR
2	C	541	SER
2	C	543	SER
2	D	45	VAL
2	D	62	LEU
2	D	391	SER
2	D	455	VAL
2	D	488	THR
2	D	541	SER
2	D	543	SER
3	A	58	ARG
3	A	204	THR
3	A	347	LYS
3	A	558	VAL
3	A	568	SER
3	A	624	THR
3	A	660	SER
3	A	854	CYS
3	A	891	SER
3	A	1005	CYS
3	A	1124	VAL
3	B	58	ARG
3	B	204	THR
3	B	347	LYS
3	B	558	VAL
3	B	568	SER
3	B	624	THR
3	B	660	SER
3	B	854	CYS
3	B	891	SER
3	B	1005	CYS
3	B	1124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	72	ASN

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Mol	Chain	Res	Type
1	E	74	HIS
1	E	130	HIS
1	E	149	GLN
1	E	150	ASN
2	C	44	ASN
2	C	76	HIS
2	C	209	HIS
2	C	215	GLN
2	C	216	HIS
2	C	256	HIS
2	C	309	GLN
2	C	358	HIS
2	C	411	ASN
2	C	433	GLN
2	C	445	GLN
2	C	566	HIS
1	F	72	ASN
1	F	130	HIS
1	F	149	GLN
1	F	150	ASN
2	D	44	ASN
2	D	76	HIS
2	D	209	HIS
2	D	215	GLN
2	D	216	HIS
2	D	256	HIS
2	D	309	GLN
2	D	358	HIS
2	D	365	GLN
2	D	411	ASN
2	D	433	GLN
2	D	445	GLN
2	D	566	HIS
3	A	51	ASN
3	A	114	ASN
3	A	206	ASN
3	A	218	HIS
3	A	273	GLN
3	A	775	ASN
3	A	979	ASN
3	B	51	ASN
3	B	114	ASN

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Mol	Chain	Res	Type
3	B	124	ASN
3	B	218	HIS
3	B	273	GLN
3	B	371	GLN
3	B	626	ASN
3	B	775	ASN
3	B	979	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	6
2	D	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	569:ASP	C	592:UNK	N	26.06
1	D	569:ASP	C	592:UNK	N	26.06
1	C	620:UNK	C	630:UNK	N	16.07
1	D	620:UNK	C	630:UNK	N	16.07
1	C	644:UNK	C	650:UNK	N	10.23
1	D	644:UNK	C	650:UNK	N	10.23
1	C	659:UNK	C	663:UNK	N	5.94
1	D	659:UNK	C	663:UNK	N	5.94
1	C	597:UNK	C	600:UNK	N	3.87
1	D	597:UNK	C	600:UNK	N	3.87
1	C	635:UNK	C	637:UNK	N	3.55
1	D	635:UNK	C	637:UNK	N	3.55

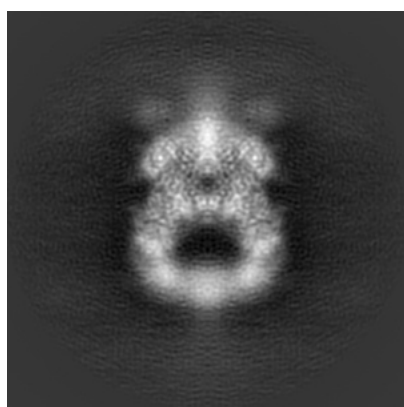
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23613. These allow visual inspection of the internal detail of the map and identification of artifacts.

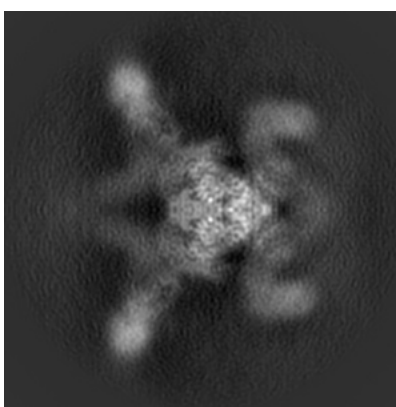
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

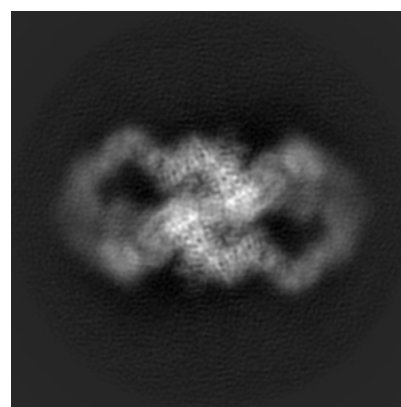
6.1.1 Primary map



X



Y

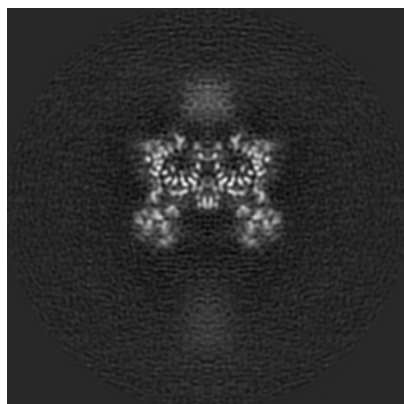


Z

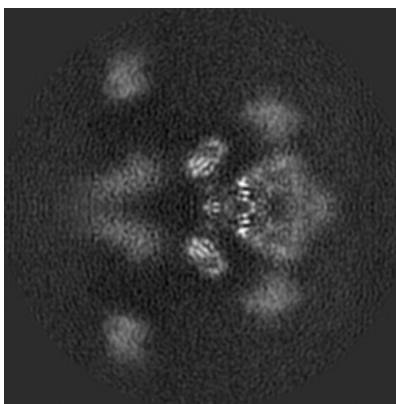
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

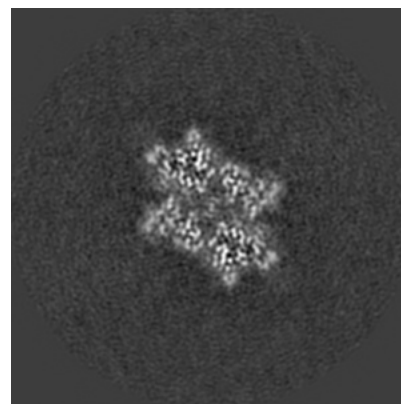
6.2.1 Primary map



X Index: 140



Y Index: 140

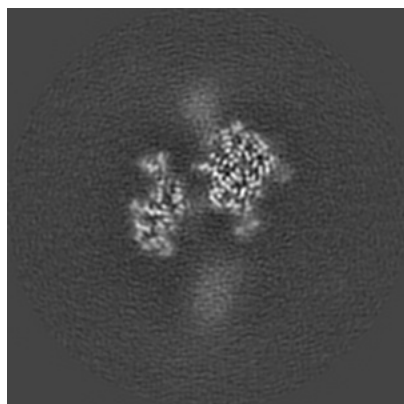


Z Index: 140

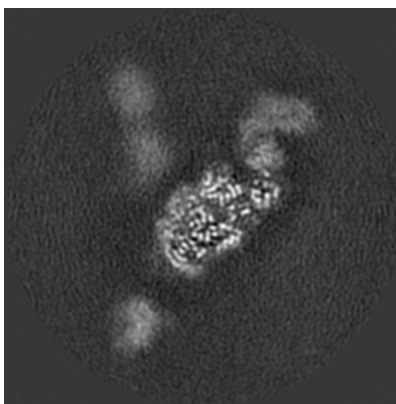
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

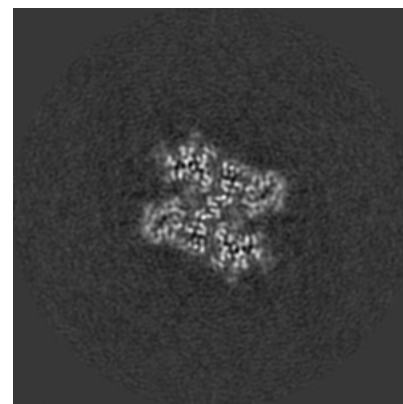
6.3.1 Primary map



X Index: 151



Y Index: 168



Z Index: 145

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

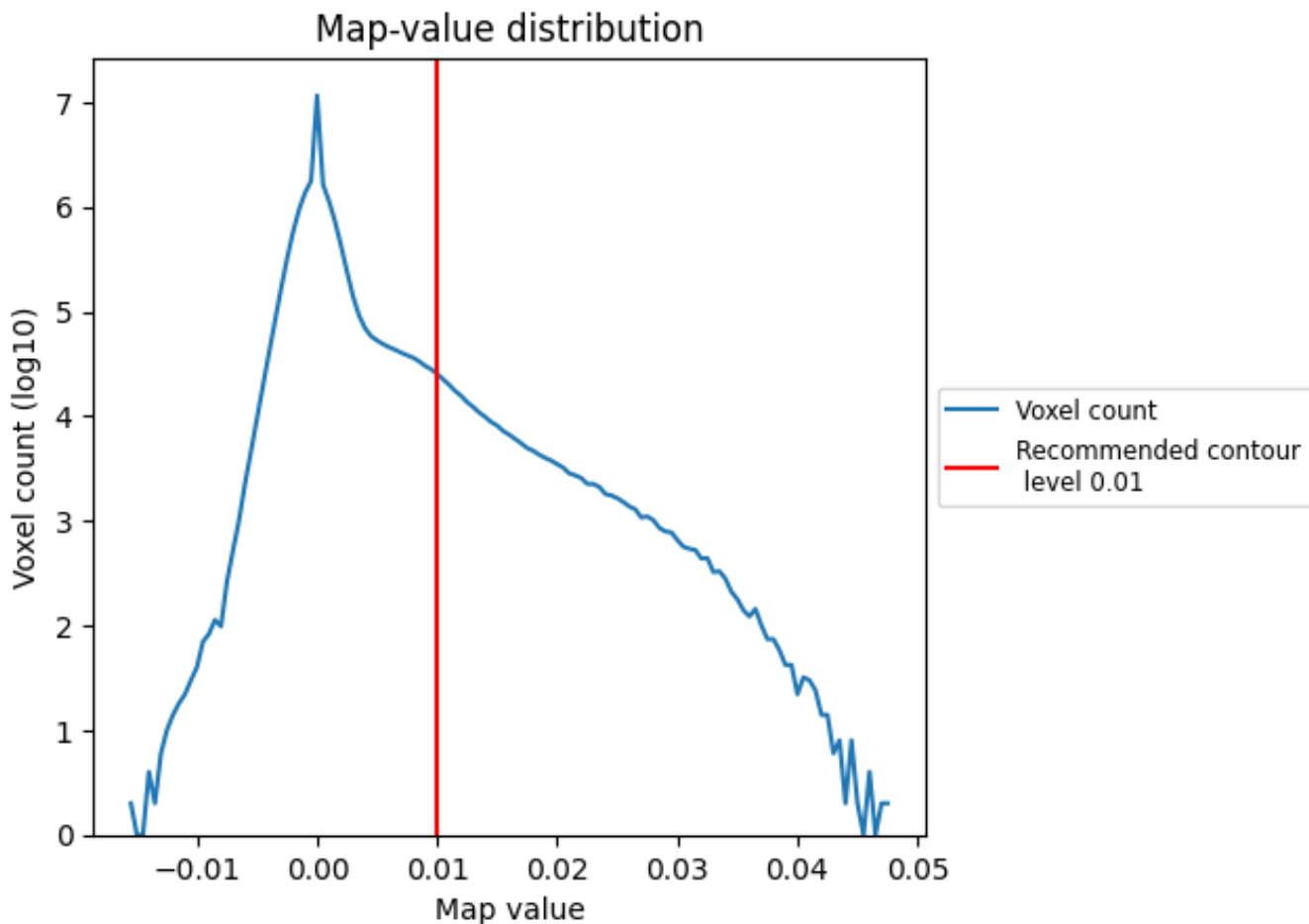
6.5 Mask visualisation

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

7 Map analysis [i](#)

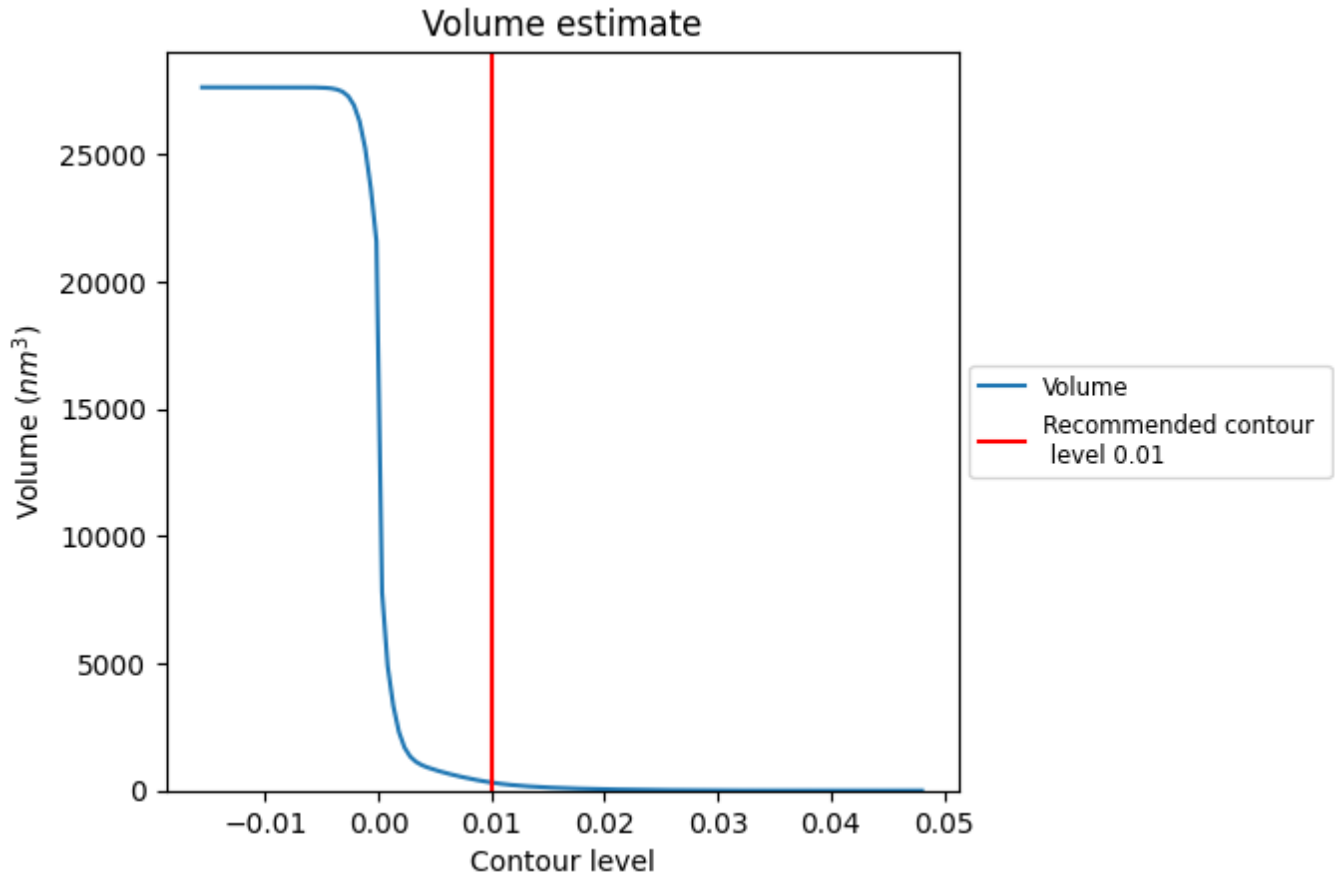
This section contains the results of statistical analysis of the map.

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.

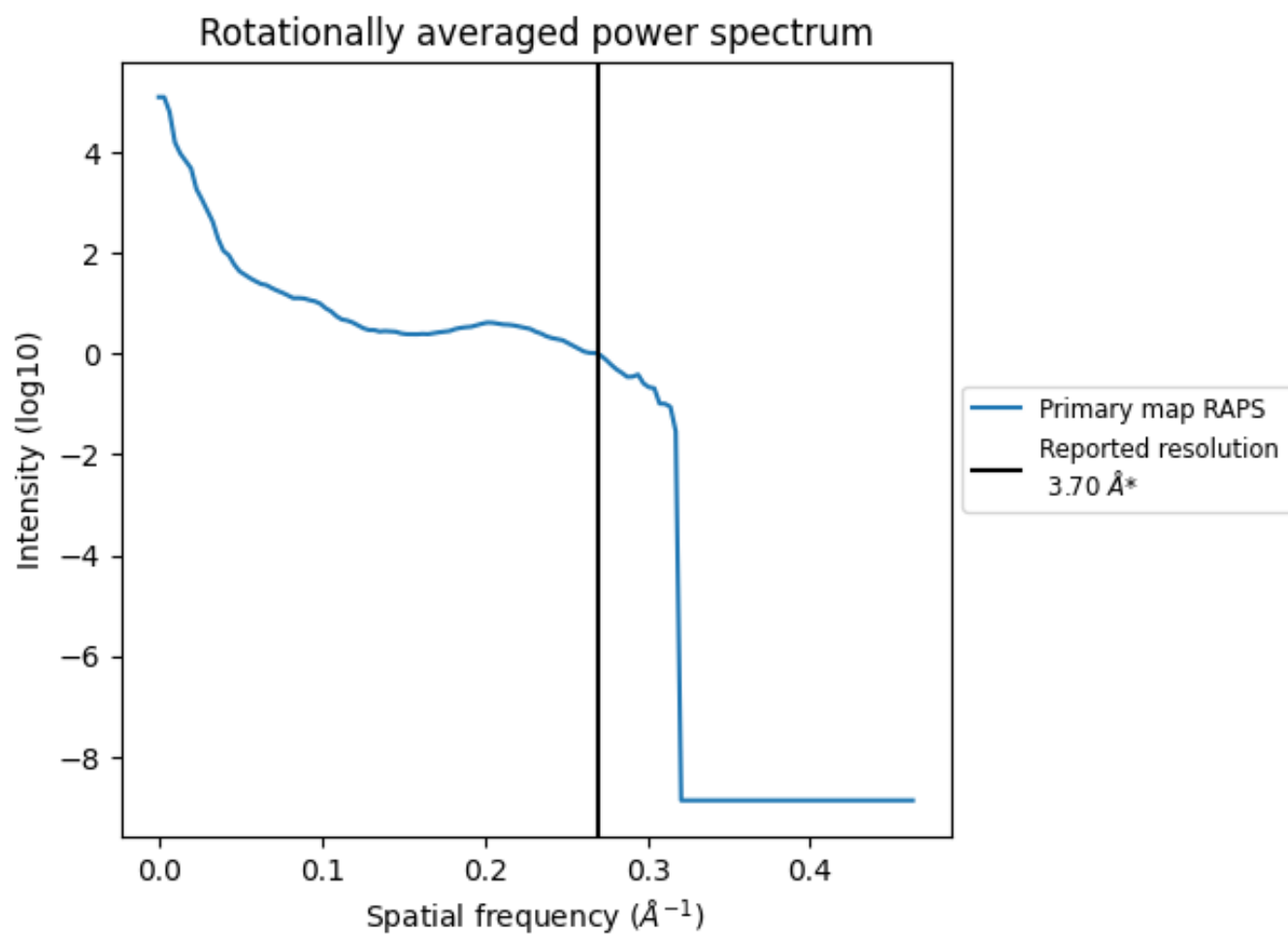
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 318 nm³; this corresponds to an approximate mass of 287 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 i

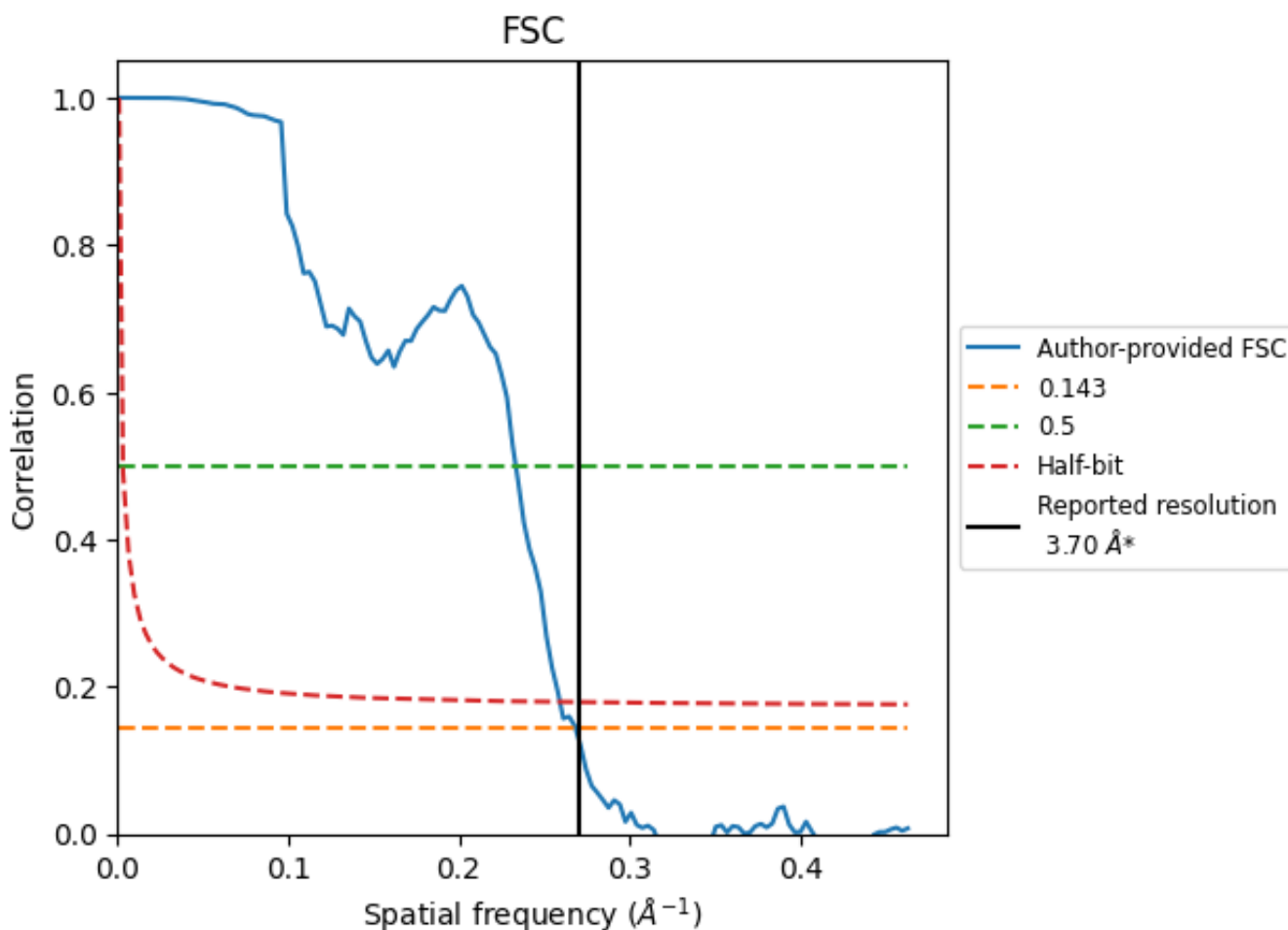


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

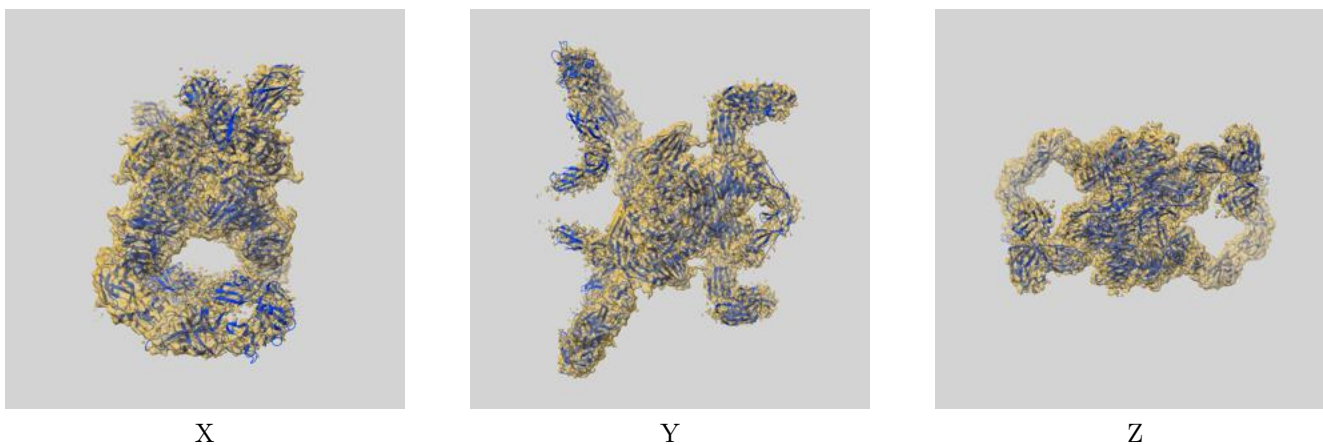
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.29	3.86
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23613 and PDB model 7M0R. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



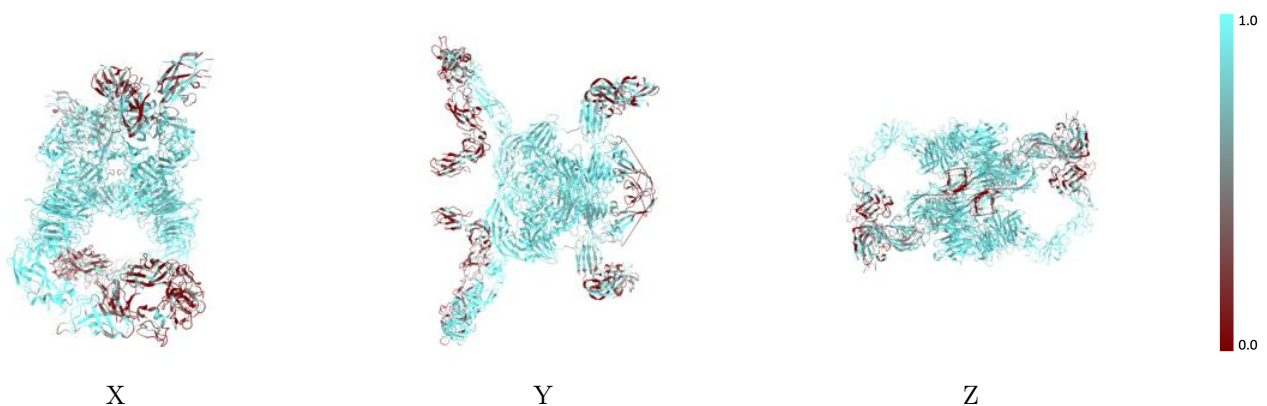
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



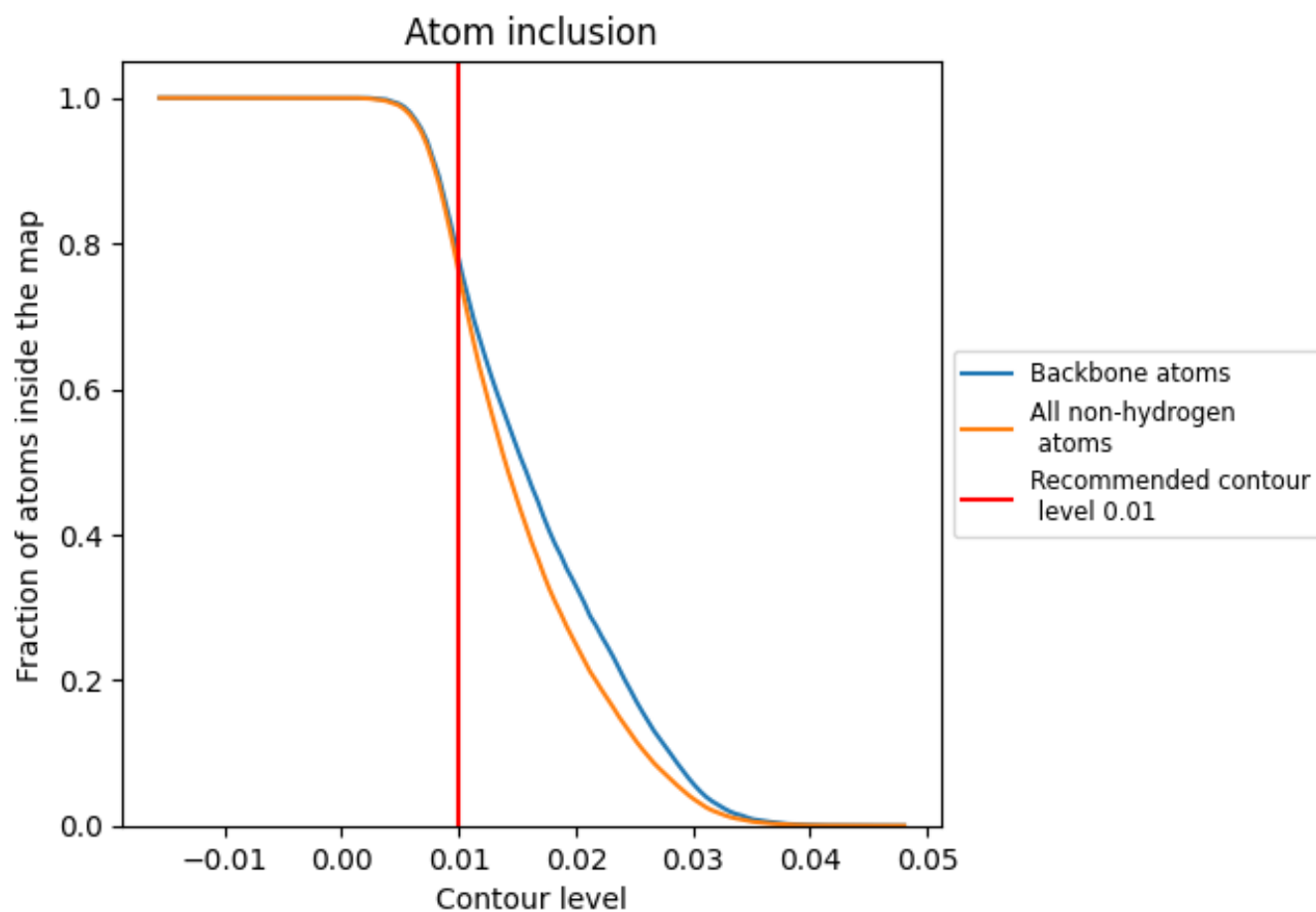
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).















9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7606	 0.3300
A	 0.7204	 0.2870
B	 0.7199	 0.2870
C	 0.8798	 0.4390
D	 0.8852	 0.4460
E	 0.6854	 0.2780
F	 0.6854	 0.2780

