Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 07:53 PM JST

PDB ID	:	7EWR
EMDB ID	:	EMD-31363
Title	:	Cryo-EM structure of human GPR158 in complex with RGS7-Gbeta5 in a 2:2:2 ratio
Authors	:	Kim, Y.; Jeong, E.; Jeong, J.; Cho, Y.
Deposited on	:	2021-05-26
Resolution	:	4.70 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:

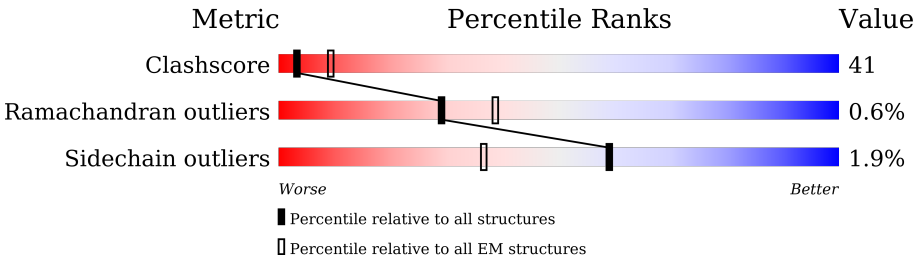
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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 <=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	C	530	27% 24% 49% · 25%
1	E	530	61% 22% 48% · 28%
2	D	395	19% 19% 63% · 14%
2	F	395	77% 17% 62% · 19%
3	A	1138	21% 40% 11% · 49%
3	B	1138	21% 35% 9% · 56%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25779 atoms, of which 6804 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 Regulator of G-protein signaling 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	381	Total	C	N	O	S	0	0
			3151	2018	534	587	12		
1	C	396	Total	C	N	O	S	0	0
			3288	2106	556	614	12		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	496	ARG	-	expression tag	UNP P49802
E	497	GLY	-	expression tag	UNP P49802
E	498	ARG	-	expression tag	UNP P49802
E	499	GLY	-	expression tag	UNP P49802
E	500	GLY	-	expression tag	UNP P49802
E	501	SER	-	expression tag	UNP P49802
E	502	GLU	-	expression tag	UNP P49802
E	503	ASN	-	expression tag	UNP P49802
E	504	LEU	-	expression tag	UNP P49802
E	505	TYR	-	expression tag	UNP P49802
E	506	PHE	-	expression tag	UNP P49802
E	507	GLN	-	expression tag	UNP P49802
E	508	GLY	-	expression tag	UNP P49802
E	509	GLY	-	expression tag	UNP P49802
E	510	SER	-	expression tag	UNP P49802
E	511	GLY	-	expression tag	UNP P49802
E	512	SER	-	expression tag	UNP P49802
E	513	GLY	-	expression tag	UNP P49802
E	514	GLY	-	expression tag	UNP P49802
E	515	ASP	-	expression tag	UNP P49802
E	516	TYR	-	expression tag	UNP P49802
E	517	LYS	-	expression tag	UNP P49802
E	518	ASP	-	expression tag	UNP P49802
E	519	ASP	-	expression tag	UNP P49802
E	520	ASP	-	expression tag	UNP P49802
E	521	ASP	-	expression tag	UNP P49802

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Chain	Residue	Modelled	Actual	Comment	Reference
E	522	LYS	-	expression tag	UNP P49802
E	523	ASP	-	expression tag	UNP P49802
E	524	TYR	-	expression tag	UNP P49802
E	525	LYS	-	expression tag	UNP P49802
E	526	ASP	-	expression tag	UNP P49802
E	527	ASP	-	expression tag	UNP P49802
E	528	ASP	-	expression tag	UNP P49802
E	529	ASP	-	expression tag	UNP P49802
E	530	LYS	-	expression tag	UNP P49802
C	496	ARG	-	expression tag	UNP P49802
C	497	GLY	-	expression tag	UNP P49802
C	498	ARG	-	expression tag	UNP P49802
C	499	GLY	-	expression tag	UNP P49802
C	500	GLY	-	expression tag	UNP P49802
C	501	SER	-	expression tag	UNP P49802
C	502	GLU	-	expression tag	UNP P49802
C	503	ASN	-	expression tag	UNP P49802
C	504	LEU	-	expression tag	UNP P49802
C	505	TYR	-	expression tag	UNP P49802
C	506	PHE	-	expression tag	UNP P49802
C	507	GLN	-	expression tag	UNP P49802
C	508	GLY	-	expression tag	UNP P49802
C	509	GLY	-	expression tag	UNP P49802
C	510	SER	-	expression tag	UNP P49802
C	511	GLY	-	expression tag	UNP P49802
C	512	SER	-	expression tag	UNP P49802
C	513	GLY	-	expression tag	UNP P49802
C	514	GLY	-	expression tag	UNP P49802
C	515	ASP	-	expression tag	UNP P49802
C	516	TYR	-	expression tag	UNP P49802
C	517	LYS	-	expression tag	UNP P49802
C	518	ASP	-	expression tag	UNP P49802
C	519	ASP	-	expression tag	UNP P49802
C	520	ASP	-	expression tag	UNP P49802
C	521	ASP	-	expression tag	UNP P49802
C	522	LYS	-	expression tag	UNP P49802
C	523	ASP	-	expression tag	UNP P49802
C	524	TYR	-	expression tag	UNP P49802
C	525	LYS	-	expression tag	UNP P49802
C	526	ASP	-	expression tag	UNP P49802
C	527	ASP	-	expression tag	UNP P49802
C	528	ASP	-	expression tag	UNP P49802

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Chain	Residue	Modelled	Actual	Comment	Reference
C	529	ASP	-	expression tag	UNP P49802
C	530	LYS	-	expression tag	UNP P49802

- Molecule 2 is a protein called Guanine nucleotide-binding protein subunit beta-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	319	Total	C	N	O	S	0	0
			2449	1525	426	475	23		
2	D	339	Total	C	N	O	S	0	0
			2609	1624	455	507	23		

- Molecule 3 is a protein called Probable G-protein coupled receptor 158.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	577	Total	C	H	N	O	S	0	0
			7323	2520	3393	690	693	27		
3	B	504	Total	C	H	N	O	S	0	0
			6959	2293	3411	612	617	26		

There are 550 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	864	ARG	-	expression tag	UNP Q5T848
A	865	GLY	-	expression tag	UNP Q5T848
A	866	ARG	-	expression tag	UNP Q5T848
A	867	LEU	-	expression tag	UNP Q5T848
A	868	GLU	-	expression tag	UNP Q5T848
A	869	VAL	-	expression tag	UNP Q5T848
A	870	LEU	-	expression tag	UNP Q5T848
A	871	PHE	-	expression tag	UNP Q5T848
A	872	GLN	-	expression tag	UNP Q5T848
A	873	GLY	-	expression tag	UNP Q5T848
A	874	PRO	-	expression tag	UNP Q5T848
A	875	GLY	-	expression tag	UNP Q5T848
A	876	GLY	-	expression tag	UNP Q5T848
A	877	SER	-	expression tag	UNP Q5T848
A	878	MET	-	expression tag	UNP Q5T848
A	879	SER	-	expression tag	UNP Q5T848
A	880	LYS	-	expression tag	UNP Q5T848
A	881	GLY	-	expression tag	UNP Q5T848
A	882	GLU	-	expression tag	UNP Q5T848
A	883	GLU	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
A	884	LEU	-	expression tag	UNP Q5T848
A	885	PHE	-	expression tag	UNP Q5T848
A	886	THR	-	expression tag	UNP Q5T848
A	887	GLY	-	expression tag	UNP Q5T848
A	888	VAL	-	expression tag	UNP Q5T848
A	889	VAL	-	expression tag	UNP Q5T848
A	890	PRO	-	expression tag	UNP Q5T848
A	891	ILE	-	expression tag	UNP Q5T848
A	892	LEU	-	expression tag	UNP Q5T848
A	893	VAL	-	expression tag	UNP Q5T848
A	894	GLU	-	expression tag	UNP Q5T848
A	895	LEU	-	expression tag	UNP Q5T848
A	896	ASP	-	expression tag	UNP Q5T848
A	897	GLY	-	expression tag	UNP Q5T848
A	898	ASP	-	expression tag	UNP Q5T848
A	899	VAL	-	expression tag	UNP Q5T848
A	900	ASN	-	expression tag	UNP Q5T848
A	901	GLY	-	expression tag	UNP Q5T848
A	902	HIS	-	expression tag	UNP Q5T848
A	903	LYS	-	expression tag	UNP Q5T848
A	904	PHE	-	expression tag	UNP Q5T848
A	905	SER	-	expression tag	UNP Q5T848
A	906	VAL	-	expression tag	UNP Q5T848
A	907	ARG	-	expression tag	UNP Q5T848
A	908	GLY	-	expression tag	UNP Q5T848
A	909	GLU	-	expression tag	UNP Q5T848
A	910	GLY	-	expression tag	UNP Q5T848
A	911	GLU	-	expression tag	UNP Q5T848
A	912	GLY	-	expression tag	UNP Q5T848
A	913	ASP	-	expression tag	UNP Q5T848
A	914	ALA	-	expression tag	UNP Q5T848
A	915	THR	-	expression tag	UNP Q5T848
A	916	ASN	-	expression tag	UNP Q5T848
A	917	GLY	-	expression tag	UNP Q5T848
A	918	LYS	-	expression tag	UNP Q5T848
A	919	LEU	-	expression tag	UNP Q5T848
A	920	THR	-	expression tag	UNP Q5T848
A	921	LEU	-	expression tag	UNP Q5T848
A	922	LYS	-	expression tag	UNP Q5T848
A	923	PHE	-	expression tag	UNP Q5T848
A	924	ILE	-	expression tag	UNP Q5T848
A	925	CYS	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
A	926	THR	-	expression tag	UNP Q5T848
A	927	THR	-	expression tag	UNP Q5T848
A	928	GLY	-	expression tag	UNP Q5T848
A	929	LYS	-	expression tag	UNP Q5T848
A	930	LEU	-	expression tag	UNP Q5T848
A	931	PRO	-	expression tag	UNP Q5T848
A	932	VAL	-	expression tag	UNP Q5T848
A	933	PRO	-	expression tag	UNP Q5T848
A	934	TRP	-	expression tag	UNP Q5T848
A	935	PRO	-	expression tag	UNP Q5T848
A	936	THR	-	expression tag	UNP Q5T848
A	937	LEU	-	expression tag	UNP Q5T848
A	938	VAL	-	expression tag	UNP Q5T848
A	939	THR	-	expression tag	UNP Q5T848
A	940	THR	-	expression tag	UNP Q5T848
A	941	LEU	-	expression tag	UNP Q5T848
A	942	THR	-	expression tag	UNP Q5T848
A	943	TYR	-	expression tag	UNP Q5T848
A	944	GLY	-	expression tag	UNP Q5T848
A	945	VAL	-	expression tag	UNP Q5T848
A	946	GLN	-	expression tag	UNP Q5T848
A	947	CYS	-	expression tag	UNP Q5T848
A	948	PHE	-	expression tag	UNP Q5T848
A	949	SER	-	expression tag	UNP Q5T848
A	950	ARG	-	expression tag	UNP Q5T848
A	951	TYR	-	expression tag	UNP Q5T848
A	952	PRO	-	expression tag	UNP Q5T848
A	953	ASP	-	expression tag	UNP Q5T848
A	954	HIS	-	expression tag	UNP Q5T848
A	955	MET	-	expression tag	UNP Q5T848
A	956	LYS	-	expression tag	UNP Q5T848
A	957	ARG	-	expression tag	UNP Q5T848
A	958	HIS	-	expression tag	UNP Q5T848
A	959	ASP	-	expression tag	UNP Q5T848
A	960	PHE	-	expression tag	UNP Q5T848
A	961	PHE	-	expression tag	UNP Q5T848
A	962	LYS	-	expression tag	UNP Q5T848
A	963	SER	-	expression tag	UNP Q5T848
A	964	ALA	-	expression tag	UNP Q5T848
A	965	MET	-	expression tag	UNP Q5T848
A	966	PRO	-	expression tag	UNP Q5T848
A	967	GLU	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
A	968	GLY	-	expression tag	UNP Q5T848
A	969	TYR	-	expression tag	UNP Q5T848
A	970	VAL	-	expression tag	UNP Q5T848
A	971	GLN	-	expression tag	UNP Q5T848
A	972	GLU	-	expression tag	UNP Q5T848
A	973	ARG	-	expression tag	UNP Q5T848
A	974	THR	-	expression tag	UNP Q5T848
A	975	ILE	-	expression tag	UNP Q5T848
A	976	SER	-	expression tag	UNP Q5T848
A	977	PHE	-	expression tag	UNP Q5T848
A	978	LYS	-	expression tag	UNP Q5T848
A	979	ASP	-	expression tag	UNP Q5T848
A	980	ASP	-	expression tag	UNP Q5T848
A	981	GLY	-	expression tag	UNP Q5T848
A	982	THR	-	expression tag	UNP Q5T848
A	983	TYR	-	expression tag	UNP Q5T848
A	984	LYS	-	expression tag	UNP Q5T848
A	985	THR	-	expression tag	UNP Q5T848
A	986	ARG	-	expression tag	UNP Q5T848
A	987	ALA	-	expression tag	UNP Q5T848
A	988	GLU	-	expression tag	UNP Q5T848
A	989	VAL	-	expression tag	UNP Q5T848
A	990	LYS	-	expression tag	UNP Q5T848
A	991	PHE	-	expression tag	UNP Q5T848
A	992	GLU	-	expression tag	UNP Q5T848
A	993	GLY	-	expression tag	UNP Q5T848
A	994	ASP	-	expression tag	UNP Q5T848
A	995	THR	-	expression tag	UNP Q5T848
A	996	LEU	-	expression tag	UNP Q5T848
A	997	VAL	-	expression tag	UNP Q5T848
A	998	ASN	-	expression tag	UNP Q5T848
A	999	ARG	-	expression tag	UNP Q5T848
A	1000	ILE	-	expression tag	UNP Q5T848
A	1001	GLU	-	expression tag	UNP Q5T848
A	1002	LEU	-	expression tag	UNP Q5T848
A	1003	LYS	-	expression tag	UNP Q5T848
A	1004	GLY	-	expression tag	UNP Q5T848
A	1005	ILE	-	expression tag	UNP Q5T848
A	1006	ASP	-	expression tag	UNP Q5T848
A	1007	PHE	-	expression tag	UNP Q5T848
A	1008	LYS	-	expression tag	UNP Q5T848
A	1009	GLU	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1010	ASP	-	expression tag	UNP Q5T848
A	1011	GLY	-	expression tag	UNP Q5T848
A	1012	ASN	-	expression tag	UNP Q5T848
A	1013	ILE	-	expression tag	UNP Q5T848
A	1014	LEU	-	expression tag	UNP Q5T848
A	1015	GLY	-	expression tag	UNP Q5T848
A	1016	HIS	-	expression tag	UNP Q5T848
A	1017	LYS	-	expression tag	UNP Q5T848
A	1018	LEU	-	expression tag	UNP Q5T848
A	1019	GLU	-	expression tag	UNP Q5T848
A	1020	TYR	-	expression tag	UNP Q5T848
A	1021	ASN	-	expression tag	UNP Q5T848
A	1022	PHE	-	expression tag	UNP Q5T848
A	1023	ASN	-	expression tag	UNP Q5T848
A	1024	SER	-	expression tag	UNP Q5T848
A	1025	HIS	-	expression tag	UNP Q5T848
A	1026	ASN	-	expression tag	UNP Q5T848
A	1027	VAL	-	expression tag	UNP Q5T848
A	1028	TYR	-	expression tag	UNP Q5T848
A	1029	ILE	-	expression tag	UNP Q5T848
A	1030	THR	-	expression tag	UNP Q5T848
A	1031	ALA	-	expression tag	UNP Q5T848
A	1032	ASP	-	expression tag	UNP Q5T848
A	1033	LYS	-	expression tag	UNP Q5T848
A	1034	GLN	-	expression tag	UNP Q5T848
A	1035	LYS	-	expression tag	UNP Q5T848
A	1036	ASN	-	expression tag	UNP Q5T848
A	1037	GLY	-	expression tag	UNP Q5T848
A	1038	ILE	-	expression tag	UNP Q5T848
A	1039	LYS	-	expression tag	UNP Q5T848
A	1040	ALA	-	expression tag	UNP Q5T848
A	1041	ASN	-	expression tag	UNP Q5T848
A	1042	PHE	-	expression tag	UNP Q5T848
A	1043	LYS	-	expression tag	UNP Q5T848
A	1044	ILE	-	expression tag	UNP Q5T848
A	1045	ARG	-	expression tag	UNP Q5T848
A	1046	HIS	-	expression tag	UNP Q5T848
A	1047	ASN	-	expression tag	UNP Q5T848
A	1048	VAL	-	expression tag	UNP Q5T848
A	1049	GLU	-	expression tag	UNP Q5T848
A	1050	ASP	-	expression tag	UNP Q5T848
A	1051	GLY	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1052	SER	-	expression tag	UNP Q5T848
A	1053	VAL	-	expression tag	UNP Q5T848
A	1054	GLN	-	expression tag	UNP Q5T848
A	1055	LEU	-	expression tag	UNP Q5T848
A	1056	ALA	-	expression tag	UNP Q5T848
A	1057	ASP	-	expression tag	UNP Q5T848
A	1058	HIS	-	expression tag	UNP Q5T848
A	1059	TYR	-	expression tag	UNP Q5T848
A	1060	GLN	-	expression tag	UNP Q5T848
A	1061	GLN	-	expression tag	UNP Q5T848
A	1062	ASN	-	expression tag	UNP Q5T848
A	1063	THR	-	expression tag	UNP Q5T848
A	1064	PRO	-	expression tag	UNP Q5T848
A	1065	ILE	-	expression tag	UNP Q5T848
A	1066	GLY	-	expression tag	UNP Q5T848
A	1067	ASP	-	expression tag	UNP Q5T848
A	1068	GLY	-	expression tag	UNP Q5T848
A	1069	PRO	-	expression tag	UNP Q5T848
A	1070	VAL	-	expression tag	UNP Q5T848
A	1071	LEU	-	expression tag	UNP Q5T848
A	1072	LEU	-	expression tag	UNP Q5T848
A	1073	PRO	-	expression tag	UNP Q5T848
A	1074	ASP	-	expression tag	UNP Q5T848
A	1075	ASN	-	expression tag	UNP Q5T848
A	1076	HIS	-	expression tag	UNP Q5T848
A	1077	TYR	-	expression tag	UNP Q5T848
A	1078	LEU	-	expression tag	UNP Q5T848
A	1079	SER	-	expression tag	UNP Q5T848
A	1080	THR	-	expression tag	UNP Q5T848
A	1081	GLN	-	expression tag	UNP Q5T848
A	1082	SER	-	expression tag	UNP Q5T848
A	1083	VAL	-	expression tag	UNP Q5T848
A	1084	LEU	-	expression tag	UNP Q5T848
A	1085	SER	-	expression tag	UNP Q5T848
A	1086	LYS	-	expression tag	UNP Q5T848
A	1087	ASP	-	expression tag	UNP Q5T848
A	1088	PRO	-	expression tag	UNP Q5T848
A	1089	ASN	-	expression tag	UNP Q5T848
A	1090	GLU	-	expression tag	UNP Q5T848
A	1091	LYS	-	expression tag	UNP Q5T848
A	1092	ARG	-	expression tag	UNP Q5T848
A	1093	ASP	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1094	HIS	-	expression tag	UNP Q5T848
A	1095	MET	-	expression tag	UNP Q5T848
A	1096	VAL	-	expression tag	UNP Q5T848
A	1097	LEU	-	expression tag	UNP Q5T848
A	1098	LEU	-	expression tag	UNP Q5T848
A	1099	GLU	-	expression tag	UNP Q5T848
A	1100	PHE	-	expression tag	UNP Q5T848
A	1101	VAL	-	expression tag	UNP Q5T848
A	1102	THR	-	expression tag	UNP Q5T848
A	1103	ALA	-	expression tag	UNP Q5T848
A	1104	ALA	-	expression tag	UNP Q5T848
A	1105	GLY	-	expression tag	UNP Q5T848
A	1106	ILE	-	expression tag	UNP Q5T848
A	1107	THR	-	expression tag	UNP Q5T848
A	1108	HIS	-	expression tag	UNP Q5T848
A	1109	GLY	-	expression tag	UNP Q5T848
A	1110	GLY	-	expression tag	UNP Q5T848
A	1111	SER	-	expression tag	UNP Q5T848
A	1112	TRP	-	expression tag	UNP Q5T848
A	1113	SER	-	expression tag	UNP Q5T848
A	1114	HIS	-	expression tag	UNP Q5T848
A	1115	PRO	-	expression tag	UNP Q5T848
A	1116	GLN	-	expression tag	UNP Q5T848
A	1117	PHE	-	expression tag	UNP Q5T848
A	1118	GLU	-	expression tag	UNP Q5T848
A	1119	LYS	-	expression tag	UNP Q5T848
A	1120	GLY	-	expression tag	UNP Q5T848
A	1121	GLY	-	expression tag	UNP Q5T848
A	1122	GLY	-	expression tag	UNP Q5T848
A	1123	SER	-	expression tag	UNP Q5T848
A	1124	GLY	-	expression tag	UNP Q5T848
A	1125	GLY	-	expression tag	UNP Q5T848
A	1126	GLY	-	expression tag	UNP Q5T848
A	1127	SER	-	expression tag	UNP Q5T848
A	1128	GLY	-	expression tag	UNP Q5T848
A	1129	GLY	-	expression tag	UNP Q5T848
A	1130	SER	-	expression tag	UNP Q5T848
A	1131	ALA	-	expression tag	UNP Q5T848
A	1132	TRP	-	expression tag	UNP Q5T848
A	1133	SER	-	expression tag	UNP Q5T848
A	1134	HIS	-	expression tag	UNP Q5T848
A	1135	PRO	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1136	GLN	-	expression tag	UNP Q5T848
A	1137	PHE	-	expression tag	UNP Q5T848
A	1138	GLU	-	expression tag	UNP Q5T848
B	864	ARG	-	expression tag	UNP Q5T848
B	865	GLY	-	expression tag	UNP Q5T848
B	866	ARG	-	expression tag	UNP Q5T848
B	867	LEU	-	expression tag	UNP Q5T848
B	868	GLU	-	expression tag	UNP Q5T848
B	869	VAL	-	expression tag	UNP Q5T848
B	870	LEU	-	expression tag	UNP Q5T848
B	871	PHE	-	expression tag	UNP Q5T848
B	872	GLN	-	expression tag	UNP Q5T848
B	873	GLY	-	expression tag	UNP Q5T848
B	874	PRO	-	expression tag	UNP Q5T848
B	875	GLY	-	expression tag	UNP Q5T848
B	876	GLY	-	expression tag	UNP Q5T848
B	877	SER	-	expression tag	UNP Q5T848
B	878	MET	-	expression tag	UNP Q5T848
B	879	SER	-	expression tag	UNP Q5T848
B	880	LYS	-	expression tag	UNP Q5T848
B	881	GLY	-	expression tag	UNP Q5T848
B	882	GLU	-	expression tag	UNP Q5T848
B	883	GLU	-	expression tag	UNP Q5T848
B	884	LEU	-	expression tag	UNP Q5T848
B	885	PHE	-	expression tag	UNP Q5T848
B	886	THR	-	expression tag	UNP Q5T848
B	887	GLY	-	expression tag	UNP Q5T848
B	888	VAL	-	expression tag	UNP Q5T848
B	889	VAL	-	expression tag	UNP Q5T848
B	890	PRO	-	expression tag	UNP Q5T848
B	891	ILE	-	expression tag	UNP Q5T848
B	892	LEU	-	expression tag	UNP Q5T848
B	893	VAL	-	expression tag	UNP Q5T848
B	894	GLU	-	expression tag	UNP Q5T848
B	895	LEU	-	expression tag	UNP Q5T848
B	896	ASP	-	expression tag	UNP Q5T848
B	897	GLY	-	expression tag	UNP Q5T848
B	898	ASP	-	expression tag	UNP Q5T848
B	899	VAL	-	expression tag	UNP Q5T848
B	900	ASN	-	expression tag	UNP Q5T848
B	901	GLY	-	expression tag	UNP Q5T848
B	902	HIS	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
B	903	LYS	-	expression tag	UNP Q5T848
B	904	PHE	-	expression tag	UNP Q5T848
B	905	SER	-	expression tag	UNP Q5T848
B	906	VAL	-	expression tag	UNP Q5T848
B	907	ARG	-	expression tag	UNP Q5T848
B	908	GLY	-	expression tag	UNP Q5T848
B	909	GLU	-	expression tag	UNP Q5T848
B	910	GLY	-	expression tag	UNP Q5T848
B	911	GLU	-	expression tag	UNP Q5T848
B	912	GLY	-	expression tag	UNP Q5T848
B	913	ASP	-	expression tag	UNP Q5T848
B	914	ALA	-	expression tag	UNP Q5T848
B	915	THR	-	expression tag	UNP Q5T848
B	916	ASN	-	expression tag	UNP Q5T848
B	917	GLY	-	expression tag	UNP Q5T848
B	918	LYS	-	expression tag	UNP Q5T848
B	919	LEU	-	expression tag	UNP Q5T848
B	920	THR	-	expression tag	UNP Q5T848
B	921	LEU	-	expression tag	UNP Q5T848
B	922	LYS	-	expression tag	UNP Q5T848
B	923	PHE	-	expression tag	UNP Q5T848
B	924	ILE	-	expression tag	UNP Q5T848
B	925	CYS	-	expression tag	UNP Q5T848
B	926	THR	-	expression tag	UNP Q5T848
B	927	THR	-	expression tag	UNP Q5T848
B	928	GLY	-	expression tag	UNP Q5T848
B	929	LYS	-	expression tag	UNP Q5T848
B	930	LEU	-	expression tag	UNP Q5T848
B	931	PRO	-	expression tag	UNP Q5T848
B	932	VAL	-	expression tag	UNP Q5T848
B	933	PRO	-	expression tag	UNP Q5T848
B	934	TRP	-	expression tag	UNP Q5T848
B	935	PRO	-	expression tag	UNP Q5T848
B	936	THR	-	expression tag	UNP Q5T848
B	937	LEU	-	expression tag	UNP Q5T848
B	938	VAL	-	expression tag	UNP Q5T848
B	939	THR	-	expression tag	UNP Q5T848
B	940	THR	-	expression tag	UNP Q5T848
B	941	LEU	-	expression tag	UNP Q5T848
B	942	THR	-	expression tag	UNP Q5T848
B	943	TYR	-	expression tag	UNP Q5T848
B	944	GLY	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
B	945	VAL	-	expression tag	UNP Q5T848
B	946	GLN	-	expression tag	UNP Q5T848
B	947	CYS	-	expression tag	UNP Q5T848
B	948	PHE	-	expression tag	UNP Q5T848
B	949	SER	-	expression tag	UNP Q5T848
B	950	ARG	-	expression tag	UNP Q5T848
B	951	TYR	-	expression tag	UNP Q5T848
B	952	PRO	-	expression tag	UNP Q5T848
B	953	ASP	-	expression tag	UNP Q5T848
B	954	HIS	-	expression tag	UNP Q5T848
B	955	MET	-	expression tag	UNP Q5T848
B	956	LYS	-	expression tag	UNP Q5T848
B	957	ARG	-	expression tag	UNP Q5T848
B	958	HIS	-	expression tag	UNP Q5T848
B	959	ASP	-	expression tag	UNP Q5T848
B	960	PHE	-	expression tag	UNP Q5T848
B	961	PHE	-	expression tag	UNP Q5T848
B	962	LYS	-	expression tag	UNP Q5T848
B	963	SER	-	expression tag	UNP Q5T848
B	964	ALA	-	expression tag	UNP Q5T848
B	965	MET	-	expression tag	UNP Q5T848
B	966	PRO	-	expression tag	UNP Q5T848
B	967	GLU	-	expression tag	UNP Q5T848
B	968	GLY	-	expression tag	UNP Q5T848
B	969	TYR	-	expression tag	UNP Q5T848
B	970	VAL	-	expression tag	UNP Q5T848
B	971	GLN	-	expression tag	UNP Q5T848
B	972	GLU	-	expression tag	UNP Q5T848
B	973	ARG	-	expression tag	UNP Q5T848
B	974	THR	-	expression tag	UNP Q5T848
B	975	ILE	-	expression tag	UNP Q5T848
B	976	SER	-	expression tag	UNP Q5T848
B	977	PHE	-	expression tag	UNP Q5T848
B	978	LYS	-	expression tag	UNP Q5T848
B	979	ASP	-	expression tag	UNP Q5T848
B	980	ASP	-	expression tag	UNP Q5T848
B	981	GLY	-	expression tag	UNP Q5T848
B	982	THR	-	expression tag	UNP Q5T848
B	983	TYR	-	expression tag	UNP Q5T848
B	984	LYS	-	expression tag	UNP Q5T848
B	985	THR	-	expression tag	UNP Q5T848
B	986	ARG	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
B	987	ALA	-	expression tag	UNP Q5T848
B	988	GLU	-	expression tag	UNP Q5T848
B	989	VAL	-	expression tag	UNP Q5T848
B	990	LYS	-	expression tag	UNP Q5T848
B	991	PHE	-	expression tag	UNP Q5T848
B	992	GLU	-	expression tag	UNP Q5T848
B	993	GLY	-	expression tag	UNP Q5T848
B	994	ASP	-	expression tag	UNP Q5T848
B	995	THR	-	expression tag	UNP Q5T848
B	996	LEU	-	expression tag	UNP Q5T848
B	997	VAL	-	expression tag	UNP Q5T848
B	998	ASN	-	expression tag	UNP Q5T848
B	999	ARG	-	expression tag	UNP Q5T848
B	1000	ILE	-	expression tag	UNP Q5T848
B	1001	GLU	-	expression tag	UNP Q5T848
B	1002	LEU	-	expression tag	UNP Q5T848
B	1003	LYS	-	expression tag	UNP Q5T848
B	1004	GLY	-	expression tag	UNP Q5T848
B	1005	ILE	-	expression tag	UNP Q5T848
B	1006	ASP	-	expression tag	UNP Q5T848
B	1007	PHE	-	expression tag	UNP Q5T848
B	1008	LYS	-	expression tag	UNP Q5T848
B	1009	GLU	-	expression tag	UNP Q5T848
B	1010	ASP	-	expression tag	UNP Q5T848
B	1011	GLY	-	expression tag	UNP Q5T848
B	1012	ASN	-	expression tag	UNP Q5T848
B	1013	ILE	-	expression tag	UNP Q5T848
B	1014	LEU	-	expression tag	UNP Q5T848
B	1015	GLY	-	expression tag	UNP Q5T848
B	1016	HIS	-	expression tag	UNP Q5T848
B	1017	LYS	-	expression tag	UNP Q5T848
B	1018	LEU	-	expression tag	UNP Q5T848
B	1019	GLU	-	expression tag	UNP Q5T848
B	1020	TYR	-	expression tag	UNP Q5T848
B	1021	ASN	-	expression tag	UNP Q5T848
B	1022	PHE	-	expression tag	UNP Q5T848
B	1023	ASN	-	expression tag	UNP Q5T848
B	1024	SER	-	expression tag	UNP Q5T848
B	1025	HIS	-	expression tag	UNP Q5T848
B	1026	ASN	-	expression tag	UNP Q5T848
B	1027	VAL	-	expression tag	UNP Q5T848
B	1028	TYR	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1029	ILE	-	expression tag	UNP Q5T848
B	1030	THR	-	expression tag	UNP Q5T848
B	1031	ALA	-	expression tag	UNP Q5T848
B	1032	ASP	-	expression tag	UNP Q5T848
B	1033	LYS	-	expression tag	UNP Q5T848
B	1034	GLN	-	expression tag	UNP Q5T848
B	1035	LYS	-	expression tag	UNP Q5T848
B	1036	ASN	-	expression tag	UNP Q5T848
B	1037	GLY	-	expression tag	UNP Q5T848
B	1038	ILE	-	expression tag	UNP Q5T848
B	1039	LYS	-	expression tag	UNP Q5T848
B	1040	ALA	-	expression tag	UNP Q5T848
B	1041	ASN	-	expression tag	UNP Q5T848
B	1042	PHE	-	expression tag	UNP Q5T848
B	1043	LYS	-	expression tag	UNP Q5T848
B	1044	ILE	-	expression tag	UNP Q5T848
B	1045	ARG	-	expression tag	UNP Q5T848
B	1046	HIS	-	expression tag	UNP Q5T848
B	1047	ASN	-	expression tag	UNP Q5T848
B	1048	VAL	-	expression tag	UNP Q5T848
B	1049	GLU	-	expression tag	UNP Q5T848
B	1050	ASP	-	expression tag	UNP Q5T848
B	1051	GLY	-	expression tag	UNP Q5T848
B	1052	SER	-	expression tag	UNP Q5T848
B	1053	VAL	-	expression tag	UNP Q5T848
B	1054	GLN	-	expression tag	UNP Q5T848
B	1055	LEU	-	expression tag	UNP Q5T848
B	1056	ALA	-	expression tag	UNP Q5T848
B	1057	ASP	-	expression tag	UNP Q5T848
B	1058	HIS	-	expression tag	UNP Q5T848
B	1059	TYR	-	expression tag	UNP Q5T848
B	1060	GLN	-	expression tag	UNP Q5T848
B	1061	GLN	-	expression tag	UNP Q5T848
B	1062	ASN	-	expression tag	UNP Q5T848
B	1063	THR	-	expression tag	UNP Q5T848
B	1064	PRO	-	expression tag	UNP Q5T848
B	1065	ILE	-	expression tag	UNP Q5T848
B	1066	GLY	-	expression tag	UNP Q5T848
B	1067	ASP	-	expression tag	UNP Q5T848
B	1068	GLY	-	expression tag	UNP Q5T848
B	1069	PRO	-	expression tag	UNP Q5T848
B	1070	VAL	-	expression tag	UNP Q5T848

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1071	LEU	-	expression tag	UNP Q5T848
B	1072	LEU	-	expression tag	UNP Q5T848
B	1073	PRO	-	expression tag	UNP Q5T848
B	1074	ASP	-	expression tag	UNP Q5T848
B	1075	ASN	-	expression tag	UNP Q5T848
B	1076	HIS	-	expression tag	UNP Q5T848
B	1077	TYR	-	expression tag	UNP Q5T848
B	1078	LEU	-	expression tag	UNP Q5T848
B	1079	SER	-	expression tag	UNP Q5T848
B	1080	THR	-	expression tag	UNP Q5T848
B	1081	GLN	-	expression tag	UNP Q5T848
B	1082	SER	-	expression tag	UNP Q5T848
B	1083	VAL	-	expression tag	UNP Q5T848
B	1084	LEU	-	expression tag	UNP Q5T848
B	1085	SER	-	expression tag	UNP Q5T848
B	1086	LYS	-	expression tag	UNP Q5T848
B	1087	ASP	-	expression tag	UNP Q5T848
B	1088	PRO	-	expression tag	UNP Q5T848
B	1089	ASN	-	expression tag	UNP Q5T848
B	1090	GLU	-	expression tag	UNP Q5T848
B	1091	LYS	-	expression tag	UNP Q5T848
B	1092	ARG	-	expression tag	UNP Q5T848
B	1093	ASP	-	expression tag	UNP Q5T848
B	1094	HIS	-	expression tag	UNP Q5T848
B	1095	MET	-	expression tag	UNP Q5T848
B	1096	VAL	-	expression tag	UNP Q5T848
B	1097	LEU	-	expression tag	UNP Q5T848
B	1098	LEU	-	expression tag	UNP Q5T848
B	1099	GLU	-	expression tag	UNP Q5T848
B	1100	PHE	-	expression tag	UNP Q5T848
B	1101	VAL	-	expression tag	UNP Q5T848
B	1102	THR	-	expression tag	UNP Q5T848
B	1103	ALA	-	expression tag	UNP Q5T848
B	1104	ALA	-	expression tag	UNP Q5T848
B	1105	GLY	-	expression tag	UNP Q5T848
B	1106	ILE	-	expression tag	UNP Q5T848
B	1107	THR	-	expression tag	UNP Q5T848
B	1108	HIS	-	expression tag	UNP Q5T848
B	1109	GLY	-	expression tag	UNP Q5T848
B	1110	GLY	-	expression tag	UNP Q5T848
B	1111	SER	-	expression tag	UNP Q5T848
B	1112	TRP	-	expression tag	UNP Q5T848

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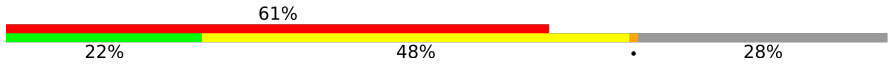
Chain	Residue	Modelled	Actual	Comment	Reference
B	1113	SER	-	expression tag	UNP Q5T848
B	1114	HIS	-	expression tag	UNP Q5T848
B	1115	PRO	-	expression tag	UNP Q5T848
B	1116	GLN	-	expression tag	UNP Q5T848
B	1117	PHE	-	expression tag	UNP Q5T848
B	1118	GLU	-	expression tag	UNP Q5T848
B	1119	LYS	-	expression tag	UNP Q5T848
B	1120	GLY	-	expression tag	UNP Q5T848
B	1121	GLY	-	expression tag	UNP Q5T848
B	1122	GLY	-	expression tag	UNP Q5T848
B	1123	SER	-	expression tag	UNP Q5T848
B	1124	GLY	-	expression tag	UNP Q5T848
B	1125	GLY	-	expression tag	UNP Q5T848
B	1126	GLY	-	expression tag	UNP Q5T848
B	1127	SER	-	expression tag	UNP Q5T848
B	1128	GLY	-	expression tag	UNP Q5T848
B	1129	GLY	-	expression tag	UNP Q5T848
B	1130	SER	-	expression tag	UNP Q5T848
B	1131	ALA	-	expression tag	UNP Q5T848
B	1132	TRP	-	expression tag	UNP Q5T848
B	1133	SER	-	expression tag	UNP Q5T848
B	1134	HIS	-	expression tag	UNP Q5T848
B	1135	PRO	-	expression tag	UNP Q5T848
B	1136	GLN	-	expression tag	UNP Q5T848
B	1137	PHE	-	expression tag	UNP Q5T848
B	1138	GLU	-	expression tag	UNP Q5T848

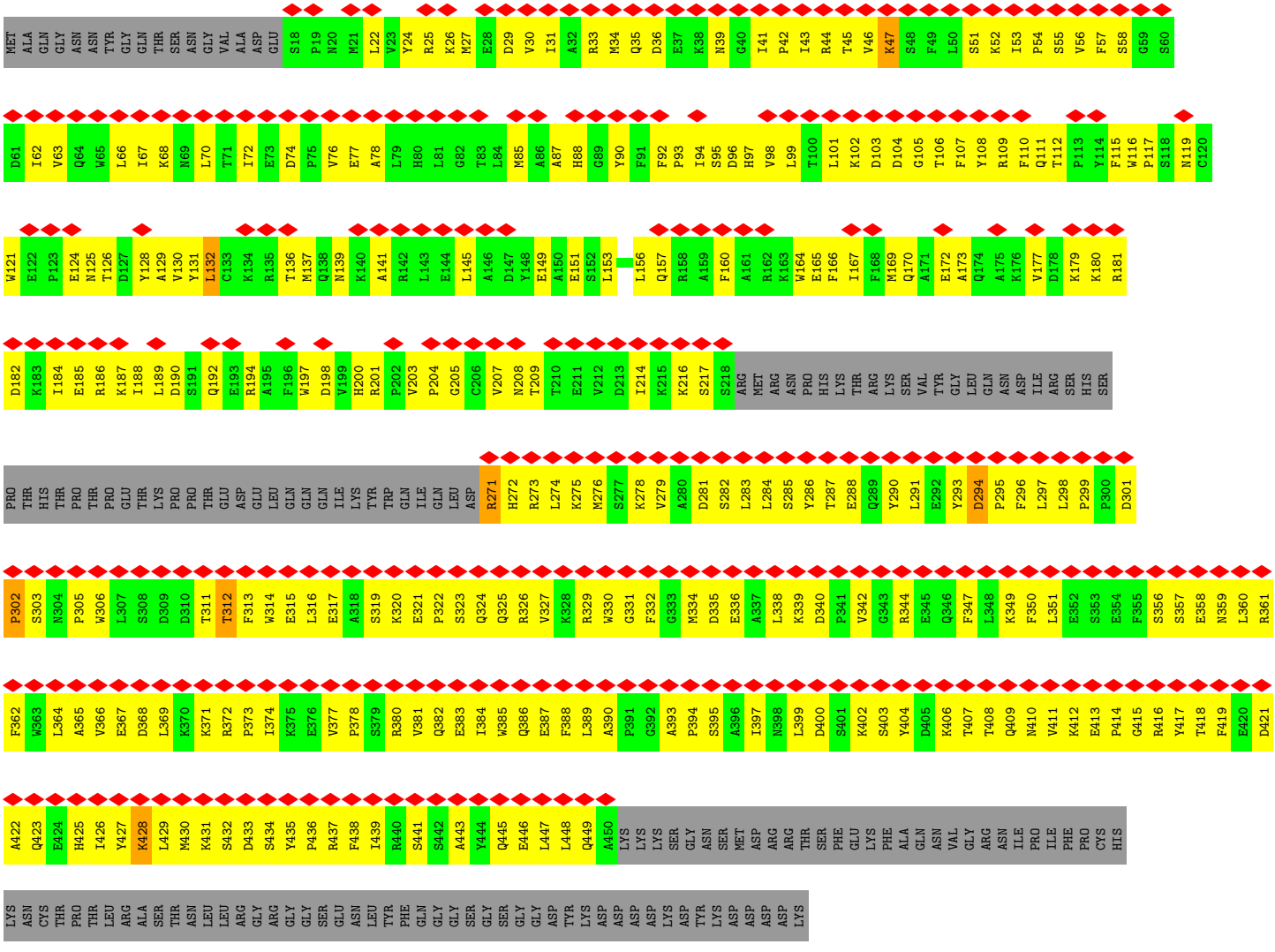
3 Residue-property plots (i)

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: Regulator of G-protein signaling 7

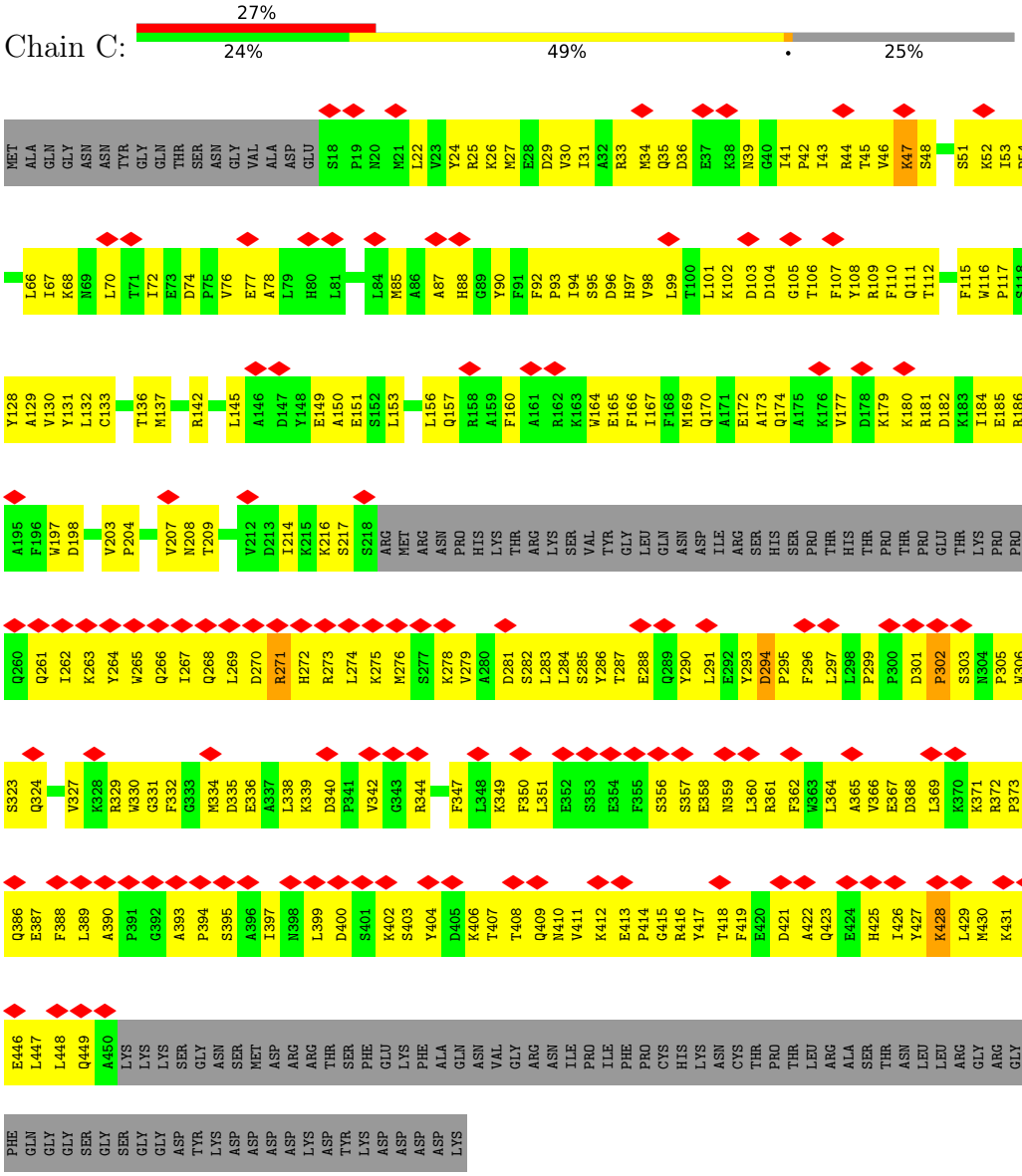
Chain E:





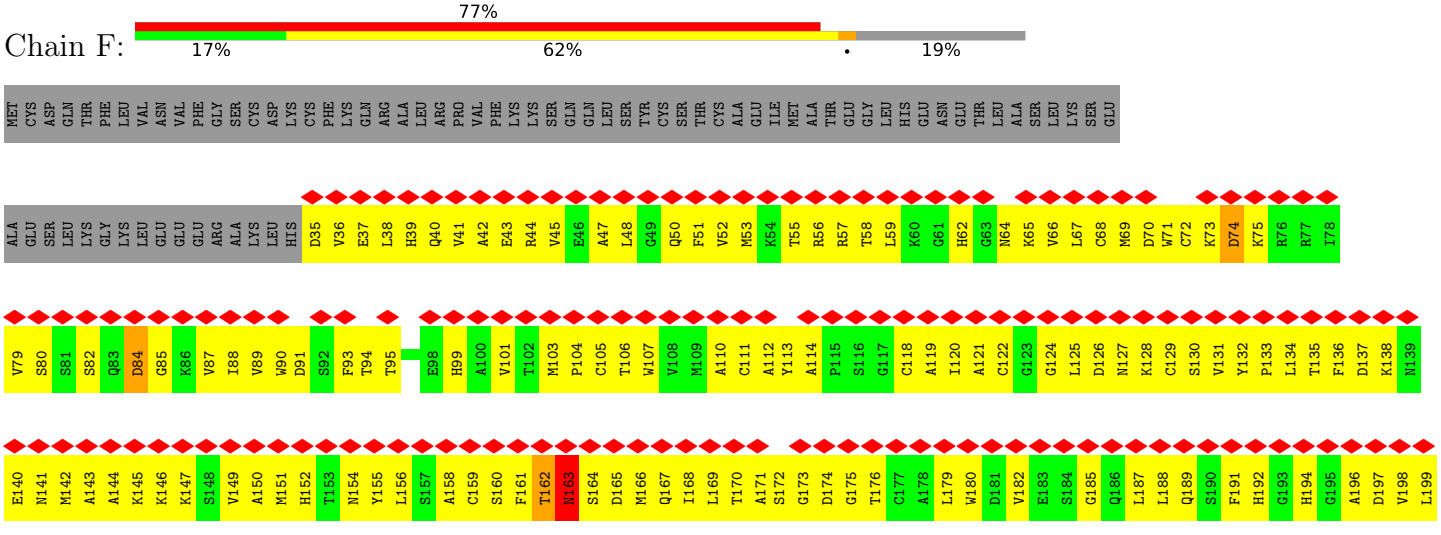
• Molecule 1: Regulator of G-protein signaling 7

Chain C:

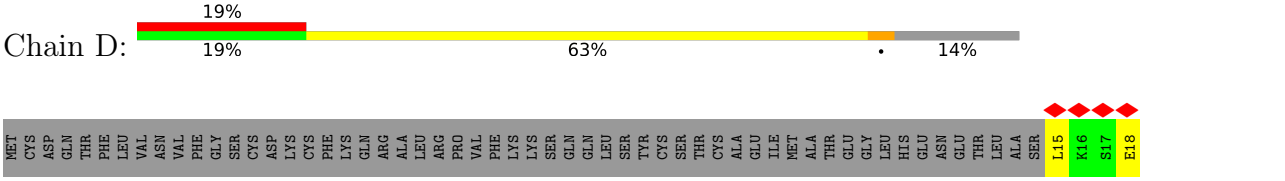


• Molecule 2: Guanine nucleotide-binding protein subunit beta-5

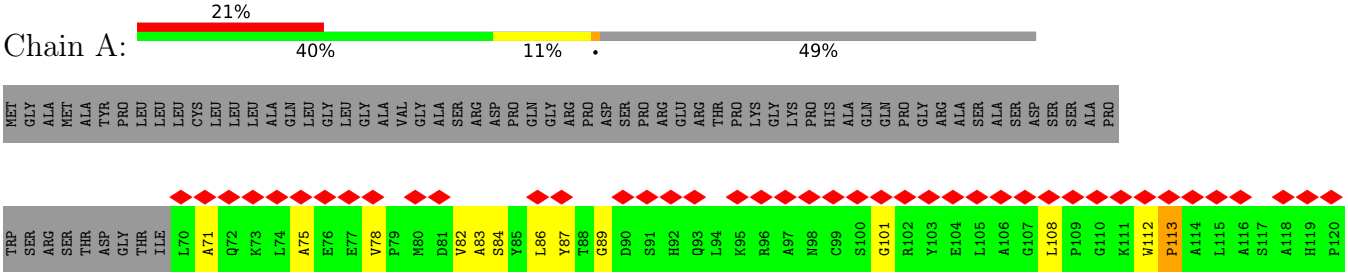
Chain F:

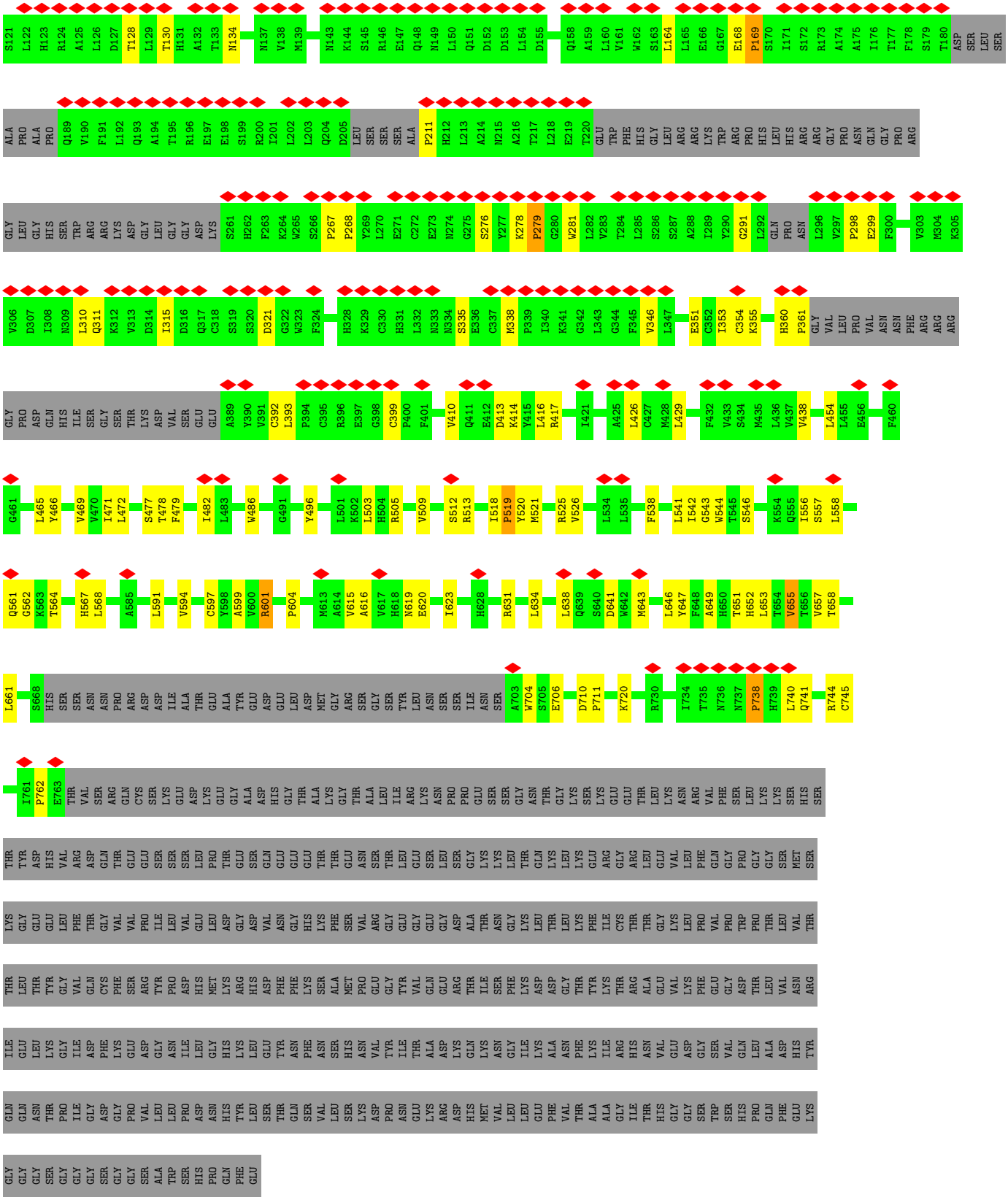


• Molecule 2: Guanine nucleotide-binding protein subunit beta-5



• Molecule 3: Probable G-protein coupled receptor 158





• Molecule 3: Probable G-protein coupled receptor 158

Chain B:


GLY ASN ILE LEU GLY HIS LYS LEU GLU TYR ASN PHE ASN SER HIS ASN VAL TYR ILE THR ALA ASP LYS GLN LYS ASN GLY ILE LYS ALA ASN PHE LYS ILE ARG HIS ASN VAL GLU ASP GLY SER VAL GLN LEU ALA ASP HIS TYR GLN GLN ASN THR PRO ILE GLY ASP GLY PRO VAL


LEU LEU PRO ASP ASN HIS TYR LEU SER THR GLN SER VAL LEU SER LYS ASP PRO ASN GLU LYS ARG ASP HIS MET VAL LEU LEU GLU PHE VAL THR ALA ALA GLY ILE THR HIS GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER


ALA TRP SER HIS PRO GLN PHE GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	236504	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.805	Depositor
Minimum map value	-0.923	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	374.48248, 374.48248, 374.48248	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06995, 1.06995, 1.06995	Depositor

5 Model quality

5.1 Standard geometry

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	C	0.44	0/3374	0.57	3/4564 (0.1%)
1	E	0.45	0/3234	0.58	3/4374 (0.1%)
2	D	0.52	0/2662	0.87	14/3596 (0.4%)
2	F	0.53	0/2501	0.86	9/3384 (0.3%)
3	A	0.69	2/4000 (0.1%)	0.80	15/5460 (0.3%)
3	B	0.76	5/3618 (0.1%)	0.96	23/4934 (0.5%)
All	All	0.59	7/19389 (0.0%)	0.78	67/26312 (0.3%)

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
3	A	0	3
3	B	0	3
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	544	TRP	CB-CG	-6.92	1.37	1.50
3	A	655	VAL	CB-CG2	-5.73	1.40	1.52
3	B	592	TRP	CB-CG	-5.66	1.40	1.50
3	B	600	VAL	CB-CG1	-5.54	1.41	1.52
3	B	492	PHE	CD2-CE2	-5.40	1.28	1.39
3	B	492	PHE	CB-CG	-5.39	1.42	1.51
3	B	492	PHE	CD1-CE1	-5.21	1.28	1.39

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	164	SER	CB-CA-C	-14.90	81.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	161	PHE	N-CA-CB	-14.19	85.05	110.60
3	B	113	PRO	N-CA-CB	13.71	119.75	103.30
2	F	164	SER	N-CA-C	13.65	147.86	111.00
2	D	161	PHE	N-CA-C	-12.30	77.79	111.00
2	D	160	SER	CB-CA-C	-11.33	88.57	110.10
2	F	84	ASP	CB-CA-C	-10.89	88.61	110.40
2	D	84	ASP	CB-CA-C	-10.88	88.64	110.40
2	F	164	SER	N-CA-CB	-10.68	94.47	110.50
3	B	562	GLY	N-CA-C	-9.71	88.83	113.10
3	B	112	TRP	N-CA-C	-9.69	84.83	111.00
3	B	560	GLY	N-CA-C	-9.60	89.10	113.10
3	B	567	HIS	N-CA-CB	9.43	127.56	110.60
3	B	112	TRP	CB-CA-C	9.19	128.79	110.40
3	A	615	VAL	CG1-CB-CG2	9.04	125.36	110.90
2	D	160	SER	N-CA-CB	-8.99	97.01	110.50
2	D	214	SER	CB-CA-C	8.85	126.91	110.10
1	E	302	PRO	CA-N-CD	-8.53	99.56	111.50
1	C	302	PRO	CA-N-CD	-8.53	99.56	111.50
2	F	163	ASN	CB-CA-C	8.42	127.24	110.40
2	D	159	CYS	CB-CA-C	-7.69	95.02	110.40
3	B	567	HIS	CB-CA-C	7.58	125.57	110.40
2	D	163	ASN	N-CA-C	7.55	131.39	111.00
3	A	279	PRO	N-CA-CB	7.53	112.33	103.30
3	A	438	VAL	CG1-CB-CG2	7.51	122.92	110.90
3	A	399	CYS	N-CA-C	-7.43	90.94	111.00
3	B	542	ILE	CG1-CB-CG2	7.41	127.69	111.40
2	D	85	GLY	N-CA-C	7.40	131.59	113.10
2	D	160	SER	N-CA-C	-7.09	91.86	111.00
3	B	113	PRO	N-CA-C	-6.99	93.92	112.10
3	B	567	HIS	N-CA-C	-6.72	92.86	111.00
3	B	268	PRO	N-CA-CB	6.56	111.17	103.30
3	A	738	PRO	N-CA-CB	6.49	111.09	103.30
2	F	162	THR	CB-CA-C	6.43	128.96	111.60
3	B	211	PRO	N-CA-CB	6.32	110.88	103.30
2	F	85	GLY	N-CA-C	6.30	128.86	113.10
3	A	298	PRO	N-CA-CB	6.17	110.70	103.30
2	D	214	SER	N-CA-C	-6.16	94.37	111.00
3	A	267	PRO	N-CA-CB	6.10	110.62	103.30
3	A	762	PRO	N-CA-CB	6.04	110.54	103.30
3	B	279	PRO	N-CA-CB	6.02	110.52	103.30
3	B	489	LEU	CB-CG-CD1	6.01	121.22	111.00
3	A	211	PRO	N-CA-CB	6.01	110.51	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	215	GLY	N-CA-C	-6.00	98.09	113.10
3	B	298	PRO	N-CA-CB	5.98	110.48	103.30
3	A	113	PRO	N-CA-CB	5.95	110.43	103.30
3	B	79	PRO	N-CA-CB	5.92	110.40	103.30
1	E	294	ASP	CB-CG-OD1	5.75	123.48	118.30
2	F	161	PHE	N-CA-C	5.75	126.53	111.00
1	C	294	ASP	CB-CG-OD1	5.73	123.46	118.30
3	A	169	PRO	N-CA-CB	5.70	110.14	103.30
3	B	486	TRP	CA-CB-CG	5.69	124.51	113.70
3	B	609	GLU	N-CA-CB	-5.61	100.51	110.60
3	A	519	PRO	N-CA-CB	5.59	110.00	103.30
3	B	169	PRO	N-CA-CB	5.55	109.96	103.30
3	A	268	PRO	N-CA-CB	5.53	109.94	103.30
3	A	711	PRO	N-CA-CB	5.40	109.78	103.30
3	B	489	LEU	CB-CG-CD2	5.34	120.08	111.00
3	B	568	LEU	N-CA-CB	-5.23	99.94	110.40
1	C	301	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	301	ASP	CB-CG-OD2	5.19	122.97	118.30
3	A	361	PRO	N-CA-CB	5.16	109.50	103.30
2	D	161	PHE	CB-CA-C	-5.14	100.11	110.40
3	B	489	LEU	CA-CB-CG	-5.14	103.48	115.30
2	D	290	ASP	CB-CG-OD1	5.11	122.90	118.30
2	F	290	ASP	CB-CG-OD1	5.06	122.85	118.30
3	B	560	GLY	O-C-N	-5.04	114.63	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	469	VAL	Peptide
3	A	601	ARG	Sidechain
3	A	658	THR	Peptide
3	B	408	CYS	Mainchain
3	B	476	PRO	Peptide
3	B	600	VAL	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	C	3288	0	3220	377	0
1	E	3151	0	3090	351	0
2	D	2609	0	2518	380	0
2	F	2449	0	2349	342	0
3	A	3930	3393	3366	85	0
3	B	3548	3411	3157	68	0
All	All	18975	6804	17700	1519	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 41.

All (1519) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:242:ILE:HD12	2:F:258:SER:HB3	1.37	1.06
2:F:284:PHE:HB3	2:F:303:ASN:HB2	1.40	1.03
3:A:521:MET:CE	3:A:525:ARG:HG2	1.90	1.01
2:D:84:ASP:CG	2:D:84:ASP:O	1.92	1.00
2:D:225:ASP:OD2	2:D:232:VAL:HG21	1.61	0.99
2:D:220:LYS:HG2	2:D:236:GLU:HB3	1.44	0.94
1:C:45:THR:HA	1:C:54:PRO:HA	1.50	0.94
1:E:45:THR:HA	1:E:54:PRO:HA	1.50	0.93
1:E:132:LEU:HB3	1:E:153:LEU:HD12	1.50	0.93
1:E:41:ILE:HD13	1:E:62:ILE:HD11	1.49	0.92
3:A:521:MET:HE1	3:A:525:ARG:HG2	1.49	0.92
1:E:130:VAL:HG22	1:E:167:ILE:HG23	1.51	0.91
2:F:156:LEU:HD11	2:F:170:THR:HB	1.52	0.90
1:C:130:VAL:HG22	1:C:167:ILE:HG23	1.51	0.90
2:F:162:THR:HA	2:F:203:LEU:HD11	1.53	0.90
2:D:84:ASP:O	2:D:84:ASP:OD2	1.90	0.90
2:D:156:LEU:HD11	2:D:170:THR:HB	1.52	0.90
2:D:176:THR:HG22	2:D:192:HIS:HA	1.53	0.90
2:D:167:GLN:HB3	2:D:179:LEU:HD21	1.54	0.90
2:F:176:THR:HG22	2:F:192:HIS:HA	1.53	0.89
2:F:75:LYS:HD2	2:F:336:ASP:HB3	1.53	0.89
1:C:359:ASN:HB3	1:C:426:ILE:HD11	1.54	0.89
2:F:167:GLN:HB3	2:F:179:LEU:HD21	1.54	0.88
3:A:591:LEU:O	3:A:594:VAL:HG12	1.73	0.88
2:D:75:LYS:HD2	2:D:336:ASP:HB3	1.53	0.88
2:F:210:ASN:H	2:F:210:ASN:ND2	1.58	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ASN:HB3	1:E:426:ILE:HD11	1.54	0.88
1:E:66:LEU:HA	1:E:70:LEU:HD13	1.56	0.87
1:C:275:LYS:HE3	1:C:278:LYS:HE3	1.55	0.87
2:D:249:PRO:HD3	2:D:291:PHE:HD2	1.39	0.86
2:F:249:PRO:HD3	2:F:291:PHE:HD2	1.39	0.86
1:C:66:LEU:HA	1:C:70:LEU:HD13	1.56	0.85
2:D:204:ALA:HA	2:D:247:TYR:CD2	2.12	0.85
1:E:275:LYS:HE3	1:E:278:LYS:HE3	1.55	0.85
1:C:132:LEU:HB3	1:C:153:LEU:HD12	1.59	0.85
2:D:284:PHE:HB3	2:D:303:ASN:HB2	1.57	0.85
1:C:258:LEU:HD13	2:D:15:LEU:HD13	1.56	0.84
1:C:287:THR:HG22	1:C:291:LEU:HG	1.59	0.84
1:C:327:VAL:HG21	1:C:448:LEU:HA	1.59	0.84
2:D:301:GLY:HA3	2:D:328:VAL:HG11	1.60	0.83
1:E:287:THR:HG22	1:E:291:LEU:HG	1.59	0.83
2:F:301:GLY:HA3	2:F:328:VAL:HG11	1.60	0.82
1:E:327:VAL:HG21	1:E:448:LEU:HA	1.59	0.82
2:F:124:GLY:HA2	2:F:156:LEU:H	1.44	0.82
2:D:39:HIS:HA	2:D:42:ALA:HB3	1.62	0.82
1:E:338:LEU:HD13	1:E:344:ARG:HG2	1.62	0.82
3:A:704:TRP:HA	1:C:109:ARG:HH21	1.45	0.82
1:C:265:TRP:HB3	2:D:22:LEU:HD12	1.62	0.82
2:D:69:MET:HE1	2:D:341:CYS:HB3	1.62	0.82
2:D:220:LYS:HG2	2:D:236:GLU:CB	2.09	0.81
2:D:124:GLY:HA2	2:D:156:LEU:H	1.45	0.81
1:C:275:LYS:HA	2:D:33:LEU:HB3	1.61	0.81
2:F:39:HIS:HA	2:F:42:ALA:HB3	1.62	0.81
2:F:291:PHE:HE1	2:F:298:LEU:HD13	1.46	0.81
1:C:338:LEU:HD13	1:C:344:ARG:HG2	1.62	0.81
1:C:369:LEU:HD13	1:C:380:ARG:HG2	1.63	0.81
2:F:125:LEU:H	2:F:155:TYR:HA	1.46	0.81
2:D:291:PHE:HE1	2:D:298:LEU:HD13	1.46	0.81
1:E:369:LEU:HD13	1:E:380:ARG:HG2	1.63	0.81
1:C:294:ASP:HB2	2:D:294:SER:HB3	1.63	0.81
2:D:120:ILE:HG23	2:D:134:LEU:HD21	1.64	0.80
1:E:294:ASP:HB2	2:F:294:SER:HB3	1.63	0.80
2:D:125:LEU:H	2:D:155:TYR:HA	1.46	0.80
1:E:31:ILE:HD12	1:E:90:TYR:HB3	1.63	0.80
2:F:120:ILE:HG23	2:F:134:LEU:HD21	1.64	0.79
1:C:129:ALA:HB2	1:C:156:LEU:HD13	1.64	0.79
2:F:82:SER:OG	2:F:84:ASP:OD1	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:THR:HG1	2:F:266:TYR:HH	1.31	0.79
1:C:31:ILE:HD12	1:C:90:TYR:HB3	1.63	0.79
1:E:129:ALA:HB2	1:E:156:LEU:HD13	1.64	0.78
1:E:378:PRO:HG3	1:E:414:PRO:HG2	1.65	0.78
2:F:69:MET:HE1	2:F:341:CYS:HB3	1.65	0.77
1:C:378:PRO:HG3	1:C:414:PRO:HG2	1.66	0.77
3:A:354:CYS:SG	3:A:392:CYS:N	2.58	0.77
3:B:417:ARG:NH2	3:B:641:ASP:OD1	2.18	0.76
1:E:43:ILE:HG12	1:E:55:SER:HA	1.67	0.76
2:D:206:SER:HB2	2:D:208:THR:HG23	1.67	0.76
1:E:288:GLU:HA	1:E:291:LEU:HD12	1.68	0.76
2:F:189:GLN:NE2	2:F:228:SER:O	2.19	0.76
2:D:347:HIS:O	2:D:348:THR:HG23	1.85	0.76
1:E:41:ILE:HG21	1:E:62:ILE:HD13	1.66	0.76
2:D:179:LEU:HB2	2:D:226:MET:HE3	1.66	0.76
2:F:221:ALA:N	2:F:235:PHE:O	2.17	0.76
2:D:72:CYS:HB3	2:D:74:ASP:OD1	1.85	0.76
2:D:219:LYS:HZ3	2:D:236:GLU:C	1.89	0.76
2:F:214:SER:O	2:F:222:MET:N	2.17	0.76
2:F:245:VAL:HG12	2:F:256:SER:HB2	1.66	0.75
2:D:245:VAL:HG12	2:D:256:SER:HB2	1.66	0.75
2:F:118:CYS:O	2:F:134:LEU:N	2.19	0.75
1:C:288:GLU:HA	1:C:291:LEU:HD12	1.68	0.75
1:E:302:PRO:HD2	1:E:303:SER:H	1.52	0.75
2:D:23:LYS:HZ2	2:D:26:LEU:HD13	1.49	0.75
2:F:260:ASP:OD2	2:F:262:THR:OG1	2.04	0.75
2:F:347:HIS:O	2:F:348:THR:HG23	1.85	0.75
1:C:330:TRP:O	1:C:435:TYR:OH	2.04	0.75
2:F:206:SER:HB2	2:F:208:THR:HG23	1.67	0.75
3:B:319:SER:OG	3:B:325:SER:OG	2.03	0.75
1:C:43:ILE:HG12	1:C:55:SER:HA	1.67	0.75
2:D:244:SER:O	2:D:256:SER:OG	2.05	0.74
1:C:271:ARG:HH21	2:D:271:ASP:HB2	1.51	0.74
2:D:118:CYS:O	2:D:134:LEU:N	2.19	0.74
2:D:91:ASP:O	2:D:95:THR:N	2.20	0.74
2:D:260:ASP:OD2	2:D:262:THR:OG1	2.04	0.74
1:E:330:TRP:O	1:E:435:TYR:OH	2.04	0.74
2:D:43:GLU:HA	2:D:314:LYS:HE2	1.70	0.74
2:F:179:LEU:HB2	2:F:226:MET:HE1	1.69	0.74
3:B:496:TYR:OH	3:B:620:GLU:OE1	2.04	0.74
2:D:37:GLU:HB3	2:D:40:GLN:CG	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:THR:HG22	2:D:203:LEU:HD21	1.70	0.74
2:D:237:THR:HG22	2:D:264:ARG:CZ	2.18	0.74
1:E:271:ARG:HH21	2:F:271:ASP:HB2	1.51	0.73
1:C:258:LEU:HD22	2:D:15:LEU:HD22	1.68	0.73
1:C:302:PRO:HD2	1:C:303:SER:H	1.51	0.73
3:A:130:THR:O	3:A:134:ASN:ND2	2.21	0.73
3:B:333:ASN:ND2	3:B:392:CYS:O	2.22	0.73
2:D:160:SER:OG	2:D:203:LEU:CD2	2.37	0.73
2:D:334:SER:OG	2:D:336:ASP:OD1	2.04	0.73
1:E:287:THR:HG21	2:F:296:ARG:HD3	1.71	0.73
2:F:244:SER:O	2:F:256:SER:OG	2.05	0.73
3:B:596:LEU:O	3:B:600:VAL:HG12	1.89	0.73
2:D:233:GLN:HG3	2:D:235:PHE:CZ	2.22	0.73
1:E:130:VAL:CG2	1:E:167:ILE:HG23	2.19	0.72
1:C:41:ILE:HG21	1:C:62:ILE:HD13	1.71	0.72
3:B:281:TRP:O	3:B:310:LEU:N	2.20	0.72
2:F:70:ASP:O	2:F:79:VAL:HG12	1.89	0.72
3:A:83:ALA:O	3:A:87:TYR:N	2.21	0.72
1:C:287:THR:HG21	2:D:296:ARG:HD3	1.71	0.72
2:F:200:CYS:SG	2:F:215:GLY:N	2.63	0.72
2:F:204:ALA:HA	2:F:247:TYR:HD2	1.54	0.72
1:C:112:THR:HG23	1:C:115:PHE:H	1.54	0.72
2:F:91:ASP:O	2:F:95:THR:N	2.20	0.72
2:F:210:ASN:H	2:F:210:ASN:HD22	1.34	0.72
1:C:181:ARG:NE	1:C:185:GLU:OE2	2.18	0.72
1:C:265:TRP:O	1:C:268:GLN:HG2	1.90	0.72
2:F:43:GLU:HA	2:F:314:LYS:HE2	1.70	0.72
1:C:439:ILE:O	1:C:445:GLN:NE2	2.22	0.72
1:E:357:SER:O	1:E:361:ARG:NE	2.24	0.71
2:F:155:TYR:OH	2:F:197:ASP:OD2	2.06	0.71
1:E:112:THR:HG23	1:E:115:PHE:H	1.55	0.71
1:E:302:PRO:HD2	1:E:303:SER:N	2.05	0.71
1:E:415:GLY:O	1:E:418:THR:OG1	2.08	0.71
2:D:70:ASP:O	2:D:79:VAL:HG12	1.89	0.71
2:D:158:ALA:HB3	2:D:201:LEU:HD21	1.73	0.71
2:F:204:ALA:HA	2:F:247:TYR:CD2	2.25	0.71
1:C:63:VAL:O	1:C:67:ILE:HG12	1.90	0.71
1:C:302:PRO:HD2	1:C:303:SER:N	2.05	0.71
2:D:111:CYS:SG	2:D:112:ALA:N	2.64	0.71
1:E:63:VAL:O	1:E:67:ILE:HG12	1.90	0.71
1:E:322:PRO:HB2	1:E:326:ARG:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:111:CYS:SG	2:F:112:ALA:N	2.64	0.71
3:B:475:GLU:O	3:B:480:ARG:NE	2.23	0.71
1:E:139:ASN:OD1	1:E:141:ALA:N	2.18	0.71
1:E:385:TRP:O	1:E:390:ALA:N	2.24	0.71
3:A:740:LEU:O	3:A:744:ARG:N	2.24	0.70
1:E:92:PHE:HB3	1:E:99:LEU:HD11	1.73	0.70
1:E:426:ILE:HD12	1:E:429:LEU:HD22	1.73	0.70
2:F:67:LEU:HD12	2:F:329:SER:HB3	1.73	0.70
3:A:486:TRP:CD1	3:A:541:LEU:HD13	2.25	0.70
1:E:439:ILE:O	1:E:445:GLN:NE2	2.22	0.70
1:C:92:PHE:HB3	1:C:99:LEU:HD11	1.73	0.70
1:C:130:VAL:CG2	1:C:167:ILE:HG23	2.19	0.70
2:D:200:CYS:HB2	2:D:245:VAL:HG22	1.73	0.70
2:F:255:ALA:HB2	2:F:265:LEU:HD13	1.72	0.70
2:F:267:ASP:OD1	2:F:269:ARG:N	2.22	0.70
3:A:631:ARG:NE	3:A:647:TYR:OH	2.24	0.70
1:C:385:TRP:O	1:C:390:ALA:N	2.24	0.70
1:C:415:GLY:O	1:C:418:THR:OG1	2.08	0.70
2:D:204:ALA:HA	2:D:247:TYR:HD2	1.50	0.70
1:C:357:SER:O	1:C:361:ARG:NE	2.23	0.70
2:D:255:ALA:HB2	2:D:265:LEU:HD13	1.73	0.70
2:F:334:SER:OG	2:F:336:ASP:OD1	2.04	0.70
1:C:274:LEU:HD12	1:C:278:LYS:HD3	1.74	0.70
2:F:158:ALA:HB3	2:F:201:LEU:HD21	1.73	0.70
1:C:268:GLN:O	1:C:273:ARG:NH2	2.19	0.70
2:D:67:LEU:HD12	2:D:329:SER:HB3	1.73	0.70
2:D:87:VAL:HB	2:D:101:VAL:CG1	2.22	0.70
1:E:31:ILE:HA	1:E:34:MET:HB2	1.74	0.69
1:C:426:ILE:HD12	1:C:429:LEU:HD22	1.73	0.69
1:C:433:ASP:HB3	1:C:437:ARG:HH12	1.57	0.69
2:D:38:LEU:HD12	2:D:274:VAL:HB	1.75	0.69
2:D:155:TYR:OH	2:D:197:ASP:OD2	2.06	0.69
2:D:37:GLU:HB3	2:D:40:GLN:HG2	1.72	0.69
3:A:561:GLN:NE2	3:A:562:GLY:O	2.26	0.69
3:A:706:GLU:O	3:A:710:ASP:CB	2.40	0.69
2:F:200:CYS:HB2	2:F:245:VAL:HG22	1.73	0.69
2:F:210:ASN:ND2	2:F:210:ASN:N	2.32	0.69
1:E:433:ASP:HB3	1:E:437:ARG:HH12	1.57	0.69
2:F:240:SER:OG	2:F:241:ASP:OD1	2.10	0.69
1:E:274:LEU:HD12	1:E:278:LYS:HD3	1.74	0.68
2:F:87:VAL:HB	2:F:101:VAL:CG1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:336:ASP:OD1	2:F:336:ASP:N	2.25	0.68
3:B:130:THR:O	3:B:134:ASN:ND2	2.25	0.68
2:F:38:LEU:HD12	2:F:274:VAL:HB	1.75	0.68
2:F:174:ASP:OD1	2:F:176:THR:N	2.25	0.68
2:D:242:ILE:HA	2:D:258:SER:HB3	1.76	0.68
2:D:267:ASP:OD1	2:D:269:ARG:N	2.22	0.68
1:E:334:MET:HE2	1:E:435:TYR:HB2	1.76	0.68
2:D:115:PRO:HD2	2:D:165:ASP:OD1	1.94	0.68
2:D:341:CYS:SG	2:D:342:SER:N	2.67	0.68
1:C:265:TRP:HZ3	2:D:23:LYS:HE2	1.58	0.68
2:D:240:SER:OG	2:D:241:ASP:OD1	2.10	0.68
3:A:496:TYR:OH	3:A:620:GLU:OE1	2.09	0.68
2:D:255:ALA:HA	2:D:265:LEU:HA	1.76	0.68
2:D:336:ASP:OD1	2:D:336:ASP:N	2.25	0.68
1:C:31:ILE:HA	1:C:34:MET:HB2	1.74	0.67
1:E:166:PHE:HD1	1:E:169:MET:HE3	1.58	0.67
2:F:341:CYS:SG	2:F:342:SER:N	2.67	0.67
2:F:237:THR:OG1	2:F:266:TYR:OH	2.05	0.67
2:D:59:LEU:HG	2:D:90:TRP:CE3	2.30	0.67
1:E:119:ASN:HB3	1:E:121:TRP:CD1	2.30	0.67
2:D:89:VAL:HB	2:D:99:HIS:HB2	1.75	0.67
2:F:245:VAL:HG12	2:F:256:SER:CB	2.24	0.67
2:F:189:GLN:HE22	2:F:229:GLY:HA3	1.60	0.67
1:C:166:PHE:HD1	1:C:169:MET:HE3	1.59	0.67
2:F:255:ALA:HA	2:F:265:LEU:HA	1.77	0.67
3:A:521:MET:HE1	3:A:525:ARG:CG	2.23	0.67
1:C:389:LEU:HB2	1:C:397:ILE:HD11	1.77	0.67
1:C:165:GLU:OE1	1:C:165:GLU:N	2.28	0.66
1:C:426:ILE:HG13	1:C:430:MET:HE2	1.77	0.66
2:D:106:THR:O	2:D:125:LEU:HD23	1.95	0.66
1:C:119:ASN:HB3	1:C:121:TRP:CD1	2.30	0.66
1:C:128:TYR:HA	1:C:197:TRP:HZ3	1.60	0.66
2:D:245:VAL:HG12	2:D:256:SER:CB	2.24	0.66
1:E:165:GLU:N	1:E:165:GLU:OE1	2.28	0.66
2:F:89:VAL:HB	2:F:99:HIS:HB2	1.75	0.66
2:F:303:ASN:CG	2:F:327:ARG:HD2	2.15	0.66
1:E:173:ALA:O	1:E:177:VAL:HG23	1.95	0.66
1:E:181:ARG:NE	1:E:185:GLU:OE2	2.19	0.66
2:F:221:ALA:O	2:F:235:PHE:N	2.25	0.66
1:C:275:LYS:N	2:D:33:LEU:HD22	2.11	0.66
1:E:347:PHE:HA	1:E:438:PHE:CE2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:LEU:HB2	1:E:397:ILE:HD11	1.77	0.66
2:F:106:THR:O	2:F:125:LEU:HD23	1.95	0.66
1:C:437:ARG:O	1:C:441:SER:OG	2.14	0.66
2:F:303:ASN:HA	2:F:327:ARG:HG3	1.78	0.66
2:F:37:GLU:HB3	2:F:40:GLN:HB2	1.77	0.66
1:C:36:ASP:OD2	1:C:39:ASN:N	2.24	0.66
2:D:128:LYS:HB3	2:D:151:MET:HG3	1.78	0.66
1:E:128:TYR:HA	1:E:197:TRP:HZ3	1.60	0.66
2:F:59:LEU:HG	2:F:90:TRP:CE3	2.30	0.66
2:D:18:GLU:O	2:D:22:LEU:HG	1.96	0.66
2:D:214:SER:O	2:D:222:MET:O	2.14	0.66
1:E:36:ASP:OD2	1:E:39:ASN:N	2.24	0.66
2:F:101:VAL:HB	2:F:142:MET:HB2	1.78	0.66
2:F:210:ASN:HD22	2:F:210:ASN:N	1.91	0.66
1:C:173:ALA:O	1:C:177:VAL:HG23	1.95	0.66
1:C:347:PHE:HA	1:C:438:PHE:CE2	2.30	0.66
2:F:110:ALA:HB1	2:F:158:ALA:HA	1.78	0.65
2:F:119:ALA:CA	2:F:134:LEU:HG	2.25	0.65
2:D:174:ASP:OD1	2:D:176:THR:N	2.25	0.65
3:B:84:SER:O	3:B:89:GLY:N	2.30	0.65
2:D:119:ALA:CA	2:D:134:LEU:HG	2.25	0.65
2:F:128:LYS:HB3	2:F:151:MET:HG3	1.78	0.65
2:F:196:ALA:HB1	2:F:217:CYS:HB2	1.78	0.65
3:A:128:THR:HG23	3:A:164:LEU:HD11	1.78	0.65
2:F:62:HIS:CE1	2:F:82:SER:HB3	2.32	0.65
1:C:203:VAL:HG13	1:C:204:PRO:HD2	1.79	0.65
1:C:387:GLU:O	1:C:395:SER:OG	2.14	0.65
2:F:42:ALA:O	2:F:45:VAL:HG12	1.96	0.65
2:D:119:ALA:N	2:D:134:LEU:HG	2.12	0.65
3:A:643:MET:O	3:A:646:LEU:N	2.30	0.65
2:D:103:MET:HG3	2:D:104:PRO:HD2	1.79	0.65
2:D:248:TYR:N	2:D:253:ALA:O	2.24	0.64
2:F:129:CYS:HB2	2:F:156:LEU:CD2	2.27	0.64
1:C:275:LYS:HG2	1:C:278:LYS:HD2	1.78	0.64
2:D:129:CYS:HB2	2:D:156:LEU:CD2	2.27	0.64
3:A:338:MET:N	3:A:351:GLU:O	2.30	0.64
3:B:82:VAL:O	3:B:86:LEU:N	2.30	0.64
2:D:101:VAL:HB	2:D:142:MET:HB2	1.78	0.64
1:E:46:VAL:N	1:E:53:ILE:O	2.30	0.64
1:E:329:ARG:HA	1:E:332:PHE:CE2	2.32	0.64
3:A:477:SER:OG	3:A:478:THR:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:N	1:C:53:ILE:O	2.30	0.64
1:C:288:GLU:HA	1:C:291:LEU:HB2	1.80	0.64
2:D:42:ALA:O	2:D:45:VAL:HG12	1.96	0.64
2:D:303:ASN:CG	2:D:327:ARG:HD2	2.17	0.64
1:C:358:GLU:N	1:C:358:GLU:OE2	2.31	0.64
2:D:62:HIS:CE1	2:D:82:SER:HB3	2.32	0.64
2:D:110:ALA:HB1	2:D:158:ALA:HA	1.78	0.64
1:E:387:GLU:O	1:E:395:SER:OG	2.14	0.64
1:E:426:ILE:HG13	1:E:430:MET:HE2	1.79	0.64
1:C:334:MET:CE	1:C:435:TYR:HB2	2.28	0.64
2:D:196:ALA:HB1	2:D:217:CYS:HB2	1.78	0.64
1:E:275:LYS:HG2	1:E:278:LYS:HD2	1.78	0.64
2:D:265:LEU:O	2:D:274:VAL:HG22	1.98	0.64
2:F:220:LYS:HG2	2:F:236:GLU:HB3	1.80	0.64
2:F:265:LEU:O	2:F:274:VAL:HG22	1.98	0.64
1:E:276:MET:CE	2:F:38:LEU:HB2	2.28	0.64
1:C:261:GLN:OE1	1:C:262:ILE:HG13	1.97	0.64
1:C:329:ARG:HA	1:C:332:PHE:CE2	2.32	0.64
1:C:312:THR:O	1:C:316:LEU:HG	1.98	0.64
1:E:203:VAL:HG13	1:E:204:PRO:HD2	1.79	0.63
2:F:329:SER:N	2:F:343:GLY:O	2.30	0.63
2:D:114:ALA:HB1	2:D:165:ASP:OD1	1.98	0.63
2:D:329:SER:N	2:D:343:GLY:O	2.30	0.63
1:E:334:MET:CE	1:E:435:TYR:HB2	2.28	0.63
2:F:284:PHE:HB3	2:F:303:ASN:CB	2.21	0.63
1:C:72:ILE:HB	1:C:78:ALA:HB2	1.80	0.63
1:E:312:THR:O	1:E:316:LEU:HG	1.98	0.63
2:F:291:PHE:O	2:F:333:VAL:HG21	1.98	0.63
3:B:130:THR:HG22	3:B:134:ASN:HD21	1.63	0.63
2:D:246:ARG:O	2:D:254:PHE:HB2	1.99	0.63
1:E:41:ILE:HG21	1:E:62:ILE:CD1	2.28	0.63
1:E:72:ILE:HB	1:E:78:ALA:HB2	1.80	0.63
1:E:287:THR:HG22	1:E:291:LEU:CG	2.29	0.63
1:E:403:SER:O	1:E:407:THR:HG23	1.98	0.63
2:F:119:ALA:N	2:F:134:LEU:HG	2.12	0.63
2:D:303:ASN:HA	2:D:327:ARG:HG3	1.81	0.63
1:E:112:THR:CG2	1:E:115:PHE:HB2	2.29	0.63
1:C:112:THR:CG2	1:C:115:PHE:HB2	2.29	0.63
1:C:403:SER:O	1:C:407:THR:HG23	1.98	0.63
2:F:145:LYS:O	2:F:147:LYS:HG3	1.99	0.63
1:C:378:PRO:HA	1:C:381:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:PRO:HA	1:E:381:VAL:HG22	1.80	0.63
2:F:68:CYS:SG	2:F:111:CYS:N	2.68	0.63
1:C:145:LEU:HD21	1:C:149:GLU:HB3	1.81	0.63
1:C:276:MET:CE	2:D:38:LEU:HB2	2.28	0.63
1:C:297:LEU:HD11	2:D:48:LEU:HD13	1.81	0.63
2:F:246:ARG:O	2:F:254:PHE:HB2	1.99	0.63
2:F:290:ASP:OD2	2:F:333:VAL:N	2.31	0.63
1:E:145:LEU:HD21	1:E:149:GLU:HB3	1.81	0.62
1:E:358:GLU:OE2	1:E:358:GLU:N	2.30	0.62
2:D:191:PHE:CE2	2:D:229:GLY:HA2	2.34	0.62
2:D:204:ALA:HA	2:D:247:TYR:CE2	2.34	0.62
1:C:263:LYS:O	1:C:267:ILE:HG12	1.99	0.62
2:F:103:MET:HG3	2:F:104:PRO:HD2	1.79	0.62
2:F:172:SER:HB3	2:F:174:ASP:OD2	1.99	0.62
3:A:478:THR:O	3:A:482:ILE:HD12	1.99	0.62
1:C:377:VAL:HB	1:C:378:PRO:HD3	1.80	0.62
1:E:288:GLU:HA	1:E:291:LEU:HB2	1.80	0.62
1:E:297:LEU:HD11	2:F:48:LEU:HD13	1.81	0.62
2:F:191:PHE:CE2	2:F:229:GLY:HA2	2.34	0.62
1:C:389:LEU:HD21	1:C:407:THR:HB	1.81	0.62
1:C:72:ILE:CG2	1:C:77:GLU:HG2	2.29	0.62
1:C:305:PRO:HG2	1:C:314:TRP:CE2	2.35	0.62
2:D:290:ASP:OD2	2:D:333:VAL:N	2.31	0.62
2:D:291:PHE:O	2:D:333:VAL:HG21	1.98	0.62
1:E:311:THR:O	1:E:315:GLU:HG2	2.00	0.62
2:F:114:ALA:HB2	2:F:119:ALA:H	1.65	0.62
2:D:127:ASN:O	2:D:151:MET:HG2	2.00	0.62
1:E:45:THR:CA	1:E:54:PRO:HA	2.29	0.62
1:E:389:LEU:HD21	1:E:407:THR:HB	1.81	0.62
3:A:101:GLY:O	3:A:276:SER:N	2.32	0.62
3:A:556:ILE:HG21	3:B:556:ILE:HD12	1.82	0.62
2:D:145:LYS:O	2:D:147:LYS:HG3	1.99	0.62
2:D:237:THR:HG22	2:D:264:ARG:NH1	2.15	0.62
2:F:222:MET:HG2	2:F:234:ALA:CB	2.29	0.62
2:F:242:ILE:HD12	2:F:258:SER:CB	2.21	0.62
2:D:50:GLN:OE1	2:D:51:PHE:N	2.31	0.62
2:D:114:ALA:HB2	2:D:119:ALA:H	1.65	0.62
2:D:172:SER:HB3	2:D:174:ASP:OD2	1.99	0.62
1:E:377:VAL:HB	1:E:378:PRO:HD3	1.80	0.61
1:E:72:ILE:CG2	1:E:77:GLU:HG2	2.29	0.61
1:E:305:PRO:HG2	1:E:314:TRP:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:512:SER:CB	3:A:520:TYR:CB	2.78	0.61
3:A:521:MET:CE	3:A:525:ARG:CG	2.74	0.61
1:C:207:VAL:HG22	1:C:208:ASN:O	2.00	0.61
1:C:311:THR:O	1:C:315:GLU:HG2	2.00	0.61
2:D:71:TRP:CD1	2:D:334:SER:HA	2.35	0.61
2:F:197:ASP:HB2	2:F:217:CYS:SG	2.41	0.61
1:C:362:PHE:CE2	1:C:426:ILE:HG21	2.36	0.61
1:E:207:VAL:HG22	1:E:208:ASN:O	2.00	0.61
2:F:127:ASN:O	2:F:151:MET:HG2	2.00	0.61
2:D:154:ASN:HB3	2:D:172:SER:OG	2.00	0.61
2:D:197:ASP:HB2	2:D:217:CYS:SG	2.41	0.61
1:E:362:PHE:CE2	1:E:426:ILE:HG21	2.35	0.61
1:E:381:VAL:HA	1:E:384:ILE:HD11	1.83	0.61
2:F:120:ILE:HG12	2:F:134:LEU:HD21	1.83	0.61
3:A:355:LYS:N	3:A:392:CYS:SG	2.74	0.61
1:C:387:GLU:OE1	1:C:395:SER:OG	2.12	0.61
2:D:209:GLY:O	2:D:211:THR:HG23	2.01	0.61
1:E:271:ARG:NH2	2:F:271:ASP:HB2	2.16	0.61
1:E:435:TYR:CE1	1:E:439:ILE:HD11	2.36	0.61
2:F:154:ASN:HB3	2:F:172:SER:OG	2.00	0.61
2:F:209:GLY:O	2:F:211:THR:HG23	2.01	0.61
2:F:220:LYS:HG2	2:F:236:GLU:CB	2.29	0.61
1:E:112:THR:HG22	1:E:115:PHE:HB2	1.83	0.61
1:C:112:THR:HG22	1:C:115:PHE:HB2	1.83	0.61
1:C:381:VAL:HA	1:C:384:ILE:CD1	2.31	0.61
1:E:387:GLU:OE1	1:E:395:SER:OG	2.12	0.60
1:E:435:TYR:O	1:E:439:ILE:HG12	2.01	0.60
3:B:586:GLU:OE2	3:B:628:HIS:NE2	2.32	0.60
1:C:275:LYS:HA	2:D:33:LEU:CB	2.29	0.60
1:C:435:TYR:CE1	1:C:439:ILE:HD11	2.36	0.60
1:E:214:ILE:HA	1:E:217:SER:OG	2.01	0.60
1:E:281:ASP:HA	1:E:284:LEU:HD21	1.83	0.60
1:E:399:LEU:HD21	1:E:407:THR:HG21	1.82	0.60
1:E:406:LYS:O	1:E:409:GLN:HG2	2.01	0.60
1:E:437:ARG:O	1:E:441:SER:OG	2.14	0.60
1:C:22:LEU:HD12	1:C:25:ARG:HE	1.66	0.60
2:D:75:LYS:CD	2:D:336:ASP:HB3	2.30	0.60
3:B:489:LEU:HD21	3:B:582:THR:CG2	2.30	0.60
3:B:629:THR:O	3:B:633:VAL:HG23	2.02	0.60
1:C:271:ARG:NH1	1:C:272:HIS:O	2.34	0.60
2:D:85:GLY:O	2:D:103:MET:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:PRO:HG3	1:E:184:ILE:HD11	1.83	0.60
1:E:381:VAL:HA	1:E:384:ILE:CD1	2.31	0.60
1:C:256:ASP:HA	1:C:259:GLN:HB2	1.84	0.60
1:C:287:THR:HG22	1:C:291:LEU:CG	2.29	0.60
1:C:381:VAL:HA	1:C:384:ILE:HD11	1.83	0.60
1:C:435:TYR:O	1:C:439:ILE:HG12	2.01	0.60
2:D:87:VAL:O	2:D:88:ILE:HD13	2.01	0.60
1:E:42:PRO:HB2	1:E:44:ARG:NE	2.17	0.60
1:E:410:ASN:HA	1:E:413:GLU:OE1	2.02	0.60
2:F:71:TRP:CD1	2:F:334:SER:HA	2.35	0.60
3:A:360:HIS:HA	3:A:393:LEU:HD11	1.83	0.60
1:C:42:PRO:HB2	1:C:44:ARG:NE	2.17	0.60
1:C:399:LEU:HD21	1:C:407:THR:HG21	1.82	0.60
1:C:406:LYS:O	1:C:409:GLN:HG2	2.01	0.60
2:D:120:ILE:HG12	2:D:134:LEU:HD21	1.82	0.60
2:D:149:VAL:O	2:D:185:GLY:HA2	2.02	0.60
1:E:22:LEU:HD12	1:E:25:ARG:HE	1.66	0.60
3:A:542:ILE:O	3:A:546:SER:OG	2.13	0.60
1:C:271:ARG:NH2	2:D:271:ASP:HB2	2.16	0.60
1:E:311:THR:HG22	1:E:315:GLU:HG2	1.84	0.60
2:F:72:CYS:SG	2:F:73:LYS:N	2.75	0.60
2:F:267:ASP:OD1	2:F:268:LEU:N	2.34	0.60
1:C:311:THR:HG22	1:C:315:GLU:HG2	1.84	0.60
1:C:446:GLU:OE1	1:C:447:LEU:HG	2.02	0.60
2:D:120:ILE:CG2	2:D:134:LEU:HD21	2.32	0.60
2:D:267:ASP:OD1	2:D:268:LEU:N	2.34	0.60
2:F:87:VAL:O	2:F:88:ILE:HD13	2.01	0.60
2:F:110:ALA:CB	2:F:158:ALA:HA	2.32	0.60
2:D:72:CYS:SG	2:D:73:LYS:N	2.75	0.60
1:E:271:ARG:NH1	1:E:272:HIS:O	2.34	0.59
2:F:149:VAL:O	2:F:185:GLY:HA2	2.02	0.59
2:F:156:LEU:HD12	2:F:171:ALA:O	2.02	0.59
2:F:248:TYR:N	2:F:253:ALA:O	2.24	0.59
2:D:255:ALA:HB2	2:D:265:LEU:CD1	2.32	0.59
1:E:137:MET:HB3	1:E:172:GLU:OE2	2.03	0.59
3:A:128:THR:CG2	3:A:164:LEU:HD11	2.33	0.59
3:A:649:ALA:O	3:A:653:LEU:HD12	2.02	0.59
1:C:54:PRO:HG3	1:C:184:ILE:HD11	1.83	0.59
1:C:214:ILE:HA	1:C:217:SER:OG	2.01	0.59
2:D:240:SER:OG	2:D:241:ASP:N	2.35	0.59
1:E:445:GLN:O	1:E:448:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ASP:HA	1:C:284:LEU:HD21	1.83	0.59
2:F:48:LEU:HD11	2:F:296:ARG:CZ	2.33	0.59
2:F:240:SER:OG	2:F:241:ASP:N	2.35	0.59
2:D:176:THR:HG21	2:D:192:HIS:ND1	2.18	0.59
1:E:446:GLU:OE1	1:E:447:LEU:HG	2.02	0.59
2:F:293:LEU:HD23	2:F:293:LEU:O	2.02	0.59
1:C:410:ASN:HA	1:C:413:GLU:OE1	2.02	0.59
1:C:445:GLN:O	1:C:448:LEU:HG	2.02	0.59
2:D:147:LYS:O	2:D:149:VAL:HG13	2.02	0.59
2:D:156:LEU:HD12	2:D:171:ALA:O	2.02	0.59
1:E:275:LYS:HZ2	1:E:278:LYS:HG3	1.67	0.59
1:C:381:VAL:HG21	1:C:414:PRO:HB3	1.85	0.59
2:D:293:LEU:HD23	2:D:293:LEU:O	2.02	0.59
1:C:265:TRP:CZ3	2:D:23:LYS:HE2	2.38	0.59
2:D:107:TRP:HB2	2:D:125:LEU:CD2	2.32	0.59
2:D:162:THR:CB	2:D:203:LEU:HD11	2.33	0.59
2:F:50:GLN:OE1	2:F:51:PHE:N	2.32	0.59
2:F:330:THR:O	2:F:343:GLY:N	2.36	0.59
1:E:334:MET:HE3	1:E:431:LYS:HA	1.84	0.58
2:F:147:LYS:O	2:F:149:VAL:HG13	2.02	0.58
1:C:45:THR:CA	1:C:54:PRO:HA	2.29	0.58
1:E:336:GLU:OE2	1:E:339:LYS:HD2	2.03	0.58
1:C:334:MET:HB3	1:C:435:TYR:CD1	2.39	0.58
2:D:18:GLU:OE1	2:D:22:LEU:HD11	2.03	0.58
2:D:104:PRO:HG2	2:D:105:CYS:SG	2.43	0.58
2:F:75:LYS:CD	2:F:336:ASP:HB3	2.30	0.58
1:C:137:MET:HB3	1:C:172:GLU:OE2	2.03	0.58
2:D:162:THR:HG22	2:D:203:LEU:CD2	2.32	0.58
2:F:255:ALA:HB2	2:F:265:LEU:CD1	2.32	0.58
2:D:138:LYS:NZ	2:D:141:ASN:O	2.37	0.58
1:E:381:VAL:HG21	1:E:414:PRO:HB3	1.84	0.58
2:F:107:TRP:HB2	2:F:125:LEU:CD2	2.32	0.58
3:B:417:ARG:NH2	3:B:640:SER:O	2.35	0.58
2:D:48:LEU:HD11	2:D:296:ARG:CZ	2.33	0.58
2:D:121:ALA:HB1	2:D:129:CYS:SG	2.44	0.58
2:D:162:THR:HB	2:D:203:LEU:HD11	1.85	0.58
2:D:237:THR:CG2	2:D:264:ARG:NH1	2.67	0.58
2:D:308:ASN:HB3	2:D:310:TRP:HE1	1.68	0.58
2:D:330:THR:O	2:D:343:GLY:N	2.36	0.58
1:E:88:HIS:CE1	1:E:209:THR:HB	2.39	0.58
3:B:410:VAL:HG12	3:B:411:GLN:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG11	1:C:107:PHE:CE1	2.38	0.58
2:D:68:CYS:SG	2:D:111:CYS:N	2.68	0.58
2:F:138:LYS:NZ	2:F:141:ASN:O	2.37	0.58
1:C:88:HIS:CE1	1:C:209:THR:HB	2.39	0.58
2:D:114:ALA:HB3	2:D:118:CYS:H	1.68	0.58
1:C:446:GLU:O	1:C:449:GLN:HG3	2.03	0.58
1:E:286:TYR:CE2	2:F:250:SER:HB2	2.39	0.58
1:E:446:GLU:O	1:E:449:GLN:HG3	2.03	0.58
1:C:334:MET:HE3	1:C:435:TYR:HB2	1.85	0.58
2:D:172:SER:OG	2:D:173:GLY:N	2.37	0.58
2:F:43:GLU:OE1	2:F:43:GLU:N	2.37	0.57
2:F:172:SER:OG	2:F:173:GLY:N	2.37	0.57
2:F:298:LEU:HD12	2:F:299:PHE:N	2.19	0.57
3:B:472:LEU:HD23	3:B:472:LEU:O	2.03	0.57
1:C:265:TRP:CE2	2:D:19:ALA:HB1	2.38	0.57
1:C:336:GLU:OE2	1:C:339:LYS:HD2	2.03	0.57
2:D:23:LYS:NZ	2:D:26:LEU:HD13	2.18	0.57
2:D:110:ALA:CB	2:D:158:ALA:HA	2.32	0.57
2:F:121:ALA:HB1	2:F:129:CYS:SG	2.44	0.57
2:F:176:THR:HG21	2:F:192:HIS:ND1	2.18	0.57
1:C:31:ILE:CD1	1:C:90:TYR:HB3	2.34	0.57
1:C:58:SER:OG	1:C:105:GLY:HA2	2.05	0.57
1:C:399:LEU:HD22	1:C:404:TYR:HD1	1.70	0.57
2:F:104:PRO:HG2	2:F:105:CYS:SG	2.43	0.57
2:F:308:ASN:HB3	2:F:310:TRP:HE1	1.68	0.57
3:B:444:ALA:O	3:B:447:ILE:HG22	2.04	0.57
1:C:132:LEU:CB	1:C:153:LEU:HD12	2.33	0.57
2:D:30:ARG:HD2	2:D:272:ARG:CD	2.34	0.57
2:D:298:LEU:HD12	2:D:299:PHE:N	2.18	0.57
2:D:319:SER:HB2	2:D:321:LEU:HD21	1.86	0.57
2:F:72:CYS:SG	2:F:74:ASP:N	2.68	0.57
2:F:222:MET:HB3	2:F:231:CYS:SG	2.44	0.57
2:F:303:ASN:HA	2:F:327:ARG:CG	2.34	0.57
2:D:222:MET:HB3	2:D:231:CYS:SG	2.44	0.57
1:E:34:MET:CE	1:E:62:ILE:HD12	2.34	0.57
1:E:46:VAL:HG11	1:E:107:PHE:CE1	2.39	0.57
1:E:334:MET:HB3	1:E:435:TYR:CD1	2.39	0.57
2:F:187:LEU:HD23	2:F:188:LEU:N	2.19	0.57
3:A:417:ARG:NH2	3:A:641:ASP:OD1	2.37	0.57
1:E:285:SER:HA	1:E:288:GLU:OE1	2.05	0.57
2:F:120:ILE:CG2	2:F:134:LEU:HD21	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:SER:HA	1:C:288:GLU:OE1	2.05	0.57
2:D:175:GLY:O	2:D:194:HIS:HB2	2.05	0.57
1:E:302:PRO:CD	1:E:303:SER:N	2.68	0.57
1:E:399:LEU:HD22	1:E:404:TYR:HD1	1.70	0.57
1:E:58:SER:HA	1:E:106:THR:O	2.05	0.57
2:F:189:GLN:NE2	2:F:229:GLY:HA3	2.18	0.57
2:F:262:THR:OG1	2:F:262:THR:O	2.22	0.57
1:C:258:LEU:HA	1:C:261:GLN:HB3	1.87	0.57
1:C:286:TYR:CE2	2:D:250:SER:HB2	2.39	0.57
2:D:220:LYS:CG	2:D:236:GLU:HB3	2.28	0.57
1:E:166:PHE:HA	1:E:169:MET:HB3	1.87	0.57
1:E:274:LEU:HD12	1:E:278:LYS:CD	2.35	0.57
2:F:130:SER:HB2	2:F:146:LYS:NZ	2.20	0.57
1:C:389:LEU:CB	1:C:397:ILE:HD11	2.35	0.57
2:D:43:GLU:OE1	2:D:43:GLU:N	2.37	0.57
2:D:266:TYR:CD1	2:D:273:GLU:HA	2.40	0.57
1:E:22:LEU:HD12	1:E:25:ARG:HH11	1.69	0.56
1:E:58:SER:OG	1:E:105:GLY:HA2	2.05	0.56
1:C:274:LEU:HD12	1:C:278:LYS:CD	2.35	0.56
1:E:445:GLN:HA	1:E:448:LEU:HD21	1.87	0.56
2:F:317:ARG:HD2	2:F:320:ILE:HG13	1.86	0.56
1:C:265:TRP:HB3	2:D:22:LEU:CD1	2.33	0.56
1:C:275:LYS:HZ2	1:C:278:LYS:HG3	1.69	0.56
2:D:130:SER:HB2	2:D:146:LYS:NZ	2.20	0.56
2:D:187:LEU:HD23	2:D:188:LEU:N	2.19	0.56
2:F:114:ALA:HB3	2:F:118:CYS:H	1.68	0.56
2:F:175:GLY:O	2:F:194:HIS:HB2	2.05	0.56
2:F:261:ALA:HB2	2:F:284:PHE:O	2.05	0.56
3:A:71:ALA:O	3:A:75:ALA:N	2.35	0.56
3:B:613:MET:O	3:B:617:VAL:HG23	2.05	0.56
1:C:166:PHE:HA	1:C:169:MET:HB3	1.87	0.56
1:C:166:PHE:HA	1:C:169:MET:HE3	1.86	0.56
1:C:286:TYR:CD2	2:D:250:SER:HB2	2.41	0.56
1:C:290:TYR:O	1:C:293:TYR:N	2.34	0.56
1:C:445:GLN:HA	1:C:448:LEU:HD21	1.87	0.56
2:D:91:ASP:OD1	2:D:94:THR:HG23	2.06	0.56
2:D:317:ARG:HD2	2:D:320:ILE:HG13	1.86	0.56
1:E:36:ASP:O	1:E:39:ASN:O	2.23	0.56
1:E:426:ILE:HG13	1:E:430:MET:CE	2.36	0.56
1:E:445:GLN:HA	1:E:448:LEU:CD2	2.35	0.56
2:F:74:ASP:OD1	2:F:74:ASP:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:317:ARG:NE	2:F:320:ILE:HD11	2.20	0.56
2:F:319:SER:HB2	2:F:321:LEU:HD21	1.86	0.56
2:D:331:LEU:O	2:D:332:ARG:HD2	2.06	0.56
1:E:130:VAL:HG11	1:E:170:GLN:HE21	1.71	0.56
1:E:286:TYR:CD2	2:F:250:SER:HB2	2.41	0.56
2:F:91:ASP:OD1	2:F:94:THR:HG23	2.05	0.56
1:C:22:LEU:HD12	1:C:25:ARG:HH11	1.69	0.56
2:D:39:HIS:HA	2:D:42:ALA:CB	2.33	0.56
2:F:331:LEU:O	2:F:332:ARG:HD2	2.06	0.56
1:C:24:TYR:HA	1:C:27:MET:HG2	1.88	0.56
2:D:317:ARG:NE	2:D:320:ILE:HD11	2.20	0.56
1:E:389:LEU:CB	1:E:397:ILE:HD11	2.35	0.56
1:C:130:VAL:HG11	1:C:170:GLN:HE21	1.71	0.56
1:E:380:ARG:HD2	1:E:383:GLU:OE2	2.06	0.56
1:E:389:LEU:CA	1:E:397:ILE:HD11	2.36	0.56
2:F:201:LEU:HD12	2:F:201:LEU:O	2.06	0.56
2:F:255:ALA:HB2	2:F:265:LEU:HB2	1.87	0.56
3:B:410:VAL:HG22	3:B:568:LEU:HD13	1.88	0.56
1:E:179:LYS:HD3	1:E:186:ARG:HD3	1.88	0.56
2:F:103:MET:CG	2:F:104:PRO:HD2	2.36	0.56
1:C:389:LEU:CA	1:C:397:ILE:HD11	2.36	0.56
1:E:31:ILE:CD1	1:E:90:TYR:HB3	2.34	0.56
1:E:302:PRO:CD	1:E:303:SER:H	2.18	0.56
3:A:465:LEU:HD23	3:A:465:LEU:O	2.06	0.56
3:B:653:LEU:O	3:B:657:VAL:HG23	2.05	0.56
1:C:377:VAL:HG12	1:C:414:PRO:CB	2.36	0.56
1:C:445:GLN:HA	1:C:448:LEU:CD2	2.35	0.56
2:D:255:ALA:HB2	2:D:265:LEU:HB2	1.87	0.56
2:F:347:HIS:O	2:F:348:THR:CG2	2.53	0.55
1:C:166:PHE:CD1	1:C:169:MET:HE3	2.41	0.55
1:C:265:TRP:O	1:C:269:LEU:HG	2.06	0.55
1:E:157:GLN:OE1	1:E:164:TRP:NE1	2.39	0.55
3:B:408:CYS:O	3:B:569:ILE:HG22	2.07	0.55
1:C:58:SER:HA	1:C:106:THR:O	2.05	0.55
1:C:425:HIS:O	1:C:428:LYS:HG3	2.07	0.55
2:D:291:PHE:CE1	2:D:298:LEU:HD13	2.34	0.55
1:E:54:PRO:CG	1:E:184:ILE:HD11	2.36	0.55
1:E:132:LEU:HD12	1:E:153:LEU:HB2	1.87	0.55
1:E:378:PRO:HA	1:E:381:VAL:CG2	2.36	0.55
2:F:264:ARG:HD3	2:F:266:TYR:OH	2.07	0.55
1:E:46:VAL:CG2	1:E:53:ILE:HB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:HIS:HA	2:F:42:ALA:CB	2.33	0.55
2:F:266:TYR:CD1	2:F:273:GLU:HA	2.40	0.55
1:E:51:SER:O	1:E:52:LYS:HD3	2.07	0.55
1:E:417:TYR:CZ	2:F:227:ARG:HA	2.42	0.55
1:C:54:PRO:CG	1:C:184:ILE:HD11	2.36	0.55
1:C:378:PRO:HA	1:C:381:VAL:CG2	2.36	0.55
2:D:67:LEU:CD1	2:D:329:SER:HB3	2.36	0.55
1:C:157:GLN:OE1	1:C:164:TRP:NE1	2.39	0.55
1:C:417:TYR:CZ	2:D:227:ARG:HA	2.42	0.55
2:D:207:GLU:N	2:D:207:GLU:OE1	2.40	0.55
1:E:377:VAL:HG12	1:E:414:PRO:CB	2.36	0.55
2:F:67:LEU:CD1	2:F:329:SER:HB3	2.36	0.55
3:A:521:MET:HE3	3:A:525:ARG:HG2	1.84	0.55
3:B:600:VAL:HG13	3:B:600:VAL:O	2.06	0.55
1:C:179:LYS:HD3	1:C:186:ARG:HD3	1.88	0.55
1:C:380:ARG:HD2	1:C:383:GLU:OE2	2.06	0.55
1:C:426:ILE:HG13	1:C:430:MET:CE	2.36	0.55
2:D:72:CYS:CB	2:D:74:ASP:OD1	2.55	0.55
1:E:182:ASP:N	1:E:182:ASP:OD1	2.40	0.55
2:F:38:LEU:CD1	2:F:274:VAL:HB	2.37	0.55
2:F:59:LEU:O	2:F:348:THR:HB	2.07	0.55
1:C:29:ASP:O	1:C:33:ARG:HG3	2.07	0.55
1:C:36:ASP:O	1:C:39:ASN:O	2.23	0.55
2:D:241:ASP:OD1	2:D:241:ASP:N	2.39	0.55
2:D:262:THR:OG1	2:D:262:THR:O	2.22	0.55
2:F:291:PHE:CE1	2:F:298:LEU:HD13	2.34	0.55
3:A:604:PRO:HD3	1:C:150:ALA:HB1	1.88	0.55
3:B:420:ILE:HG21	3:B:644:LEU:HD21	1.89	0.55
1:C:46:VAL:CG2	1:C:53:ILE:HB	2.37	0.55
1:C:377:VAL:O	1:C:381:VAL:HG22	2.06	0.55
2:D:266:TYR:HD1	2:D:273:GLU:HA	1.72	0.55
2:D:303:ASN:CB	2:D:327:ARG:HD2	2.37	0.55
1:E:24:TYR:HA	1:E:27:MET:HG2	1.88	0.55
2:F:207:GLU:N	2:F:207:GLU:OE1	2.40	0.55
2:D:72:CYS:SG	2:D:74:ASP:N	2.68	0.55
2:D:132:TYR:CE1	2:D:143:ALA:HA	2.42	0.55
1:E:377:VAL:O	1:E:381:VAL:HG22	2.06	0.54
2:D:103:MET:CG	2:D:104:PRO:HD2	2.36	0.54
1:C:271:ARG:O	1:C:273:ARG:NH1	2.41	0.54
2:D:59:LEU:HG	2:D:90:TRP:CD2	2.41	0.54
1:C:338:LEU:CD1	1:C:344:ARG:HG2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ILE:CD1	1:C:429:LEU:HD22	2.38	0.54
1:E:166:PHE:CD1	1:E:169:MET:HE3	2.39	0.54
1:E:271:ARG:O	1:E:273:ARG:NH1	2.41	0.54
2:F:59:LEU:HG	2:F:90:TRP:CD2	2.41	0.54
2:F:306:THR:HB	2:F:320:ILE:CG2	2.37	0.54
1:C:56:VAL:HB	1:C:107:PHE:HB3	1.89	0.54
1:C:302:PRO:CD	1:C:303:SER:H	2.18	0.54
2:D:201:LEU:O	2:D:201:LEU:HD12	2.06	0.54
1:E:26:LYS:O	1:E:30:VAL:HG23	2.08	0.54
1:E:29:ASP:O	1:E:33:ARG:HG3	2.07	0.54
3:A:512:SER:HB2	3:A:520:TYR:CB	2.38	0.54
1:C:382:GLN:O	1:C:386:GLN:HG2	2.07	0.54
2:D:264:ARG:HD3	2:D:266:TYR:OH	2.07	0.54
1:E:425:HIS:O	1:E:428:LYS:HG3	2.07	0.54
2:F:132:TYR:CE1	2:F:143:ALA:HA	2.42	0.54
2:F:160:SER:OG	2:F:203:LEU:HD23	2.07	0.54
1:C:51:SER:O	1:C:52:LYS:HD3	2.07	0.54
2:D:303:ASN:HA	2:D:327:ARG:CG	2.37	0.54
1:E:426:ILE:CD1	1:E:429:LEU:HD22	2.38	0.54
2:D:56:ARG:HG3	2:D:353:ALA:HB3	1.90	0.54
1:E:338:LEU:CD1	1:E:344:ARG:HG2	2.35	0.54
2:F:327:ARG:O	2:F:345:TRP:N	2.39	0.54
1:C:74:ASP:HB3	1:C:77:GLU:HB3	1.90	0.54
1:C:287:THR:O	1:C:291:LEU:N	2.41	0.54
2:D:59:LEU:O	2:D:348:THR:HB	2.07	0.54
2:D:306:THR:HB	2:D:320:ILE:CG2	2.37	0.54
1:C:359:ASN:CB	1:C:426:ILE:HD11	2.33	0.54
1:E:56:VAL:HB	1:E:107:PHE:HB3	1.89	0.54
1:E:112:THR:HG23	1:E:115:PHE:N	2.23	0.54
2:F:319:SER:CB	2:F:321:LEU:HD21	2.38	0.54
3:A:426:LEU:HA	3:A:429:LEU:HD12	1.89	0.54
3:A:471:ILE:HG22	3:A:472:LEU:HD12	1.90	0.54
1:C:287:THR:CG2	2:D:296:ARG:HD3	2.38	0.54
2:D:179:LEU:CB	2:D:226:MET:HE3	2.37	0.54
1:E:287:THR:O	1:E:291:LEU:N	2.41	0.53
3:A:413:ASP:OD2	3:A:416:LEU:N	2.41	0.53
1:C:88:HIS:O	1:C:117:PRO:HG3	2.08	0.53
2:D:38:LEU:CD1	2:D:274:VAL:HB	2.37	0.53
2:D:166:MET:HA	2:D:182:VAL:CG2	2.37	0.53
1:E:359:ASN:CB	1:E:426:ILE:HD11	2.33	0.53
1:E:382:GLN:O	1:E:386:GLN:HG2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:ILE:O	1:E:430:MET:HE2	2.07	0.53
1:C:96:ASP:OD1	1:C:97:HIS:N	2.41	0.53
1:C:335:ASP:N	1:C:335:ASP:OD1	2.40	0.53
2:D:319:SER:CB	2:D:321:LEU:HD21	2.38	0.53
2:D:347:HIS:O	2:D:348:THR:CG2	2.53	0.53
3:A:466:TYR:CE1	3:A:655:VAL:HG11	2.43	0.53
1:E:93:PRO:HG2	1:E:96:ASP:HB3	1.91	0.53
1:E:166:PHE:HA	1:E:169:MET:HE3	1.90	0.53
2:F:132:TYR:OH	2:F:146:LYS:HG3	2.09	0.53
1:C:262:ILE:O	1:C:266:GLN:HG2	2.09	0.53
2:D:114:ALA:CB	2:D:118:CYS:H	2.21	0.53
3:A:564:THR:HG22	3:A:568:LEU:O	2.08	0.53
1:C:164:TRP:O	1:C:167:ILE:HB	2.09	0.53
1:E:96:ASP:OD1	1:E:97:HIS:N	2.41	0.53
1:E:132:LEU:HD12	1:E:153:LEU:CD1	2.39	0.53
1:E:164:TRP:O	1:E:167:ILE:HB	2.09	0.53
3:B:572:MET:CE	3:B:573:CYS:O	2.57	0.53
1:E:287:THR:CG2	2:F:296:ARG:HD3	2.38	0.53
1:C:26:LYS:O	1:C:30:VAL:HG23	2.08	0.53
1:C:288:GLU:HA	1:C:291:LEU:CD1	2.38	0.53
2:D:132:TYR:OH	2:D:146:LYS:HG3	2.09	0.53
2:F:56:ARG:HG3	2:F:353:ALA:HB3	1.90	0.53
2:F:114:ALA:CB	2:F:118:CYS:H	2.21	0.53
2:F:323:GLY:O	2:F:350:ARG:NH2	2.42	0.53
3:B:417:ARG:HA	3:B:420:ILE:HD12	1.89	0.53
1:C:30:VAL:HG11	1:C:85:MET:CE	2.39	0.53
2:F:266:TYR:HD1	2:F:273:GLU:HA	1.72	0.53
3:A:591:LEU:O	3:A:594:VAL:CG1	2.54	0.53
1:C:365:ALA:HA	1:C:368:ASP:OD2	2.09	0.53
1:E:365:ALA:HA	1:E:368:ASP:OD2	2.09	0.53
2:F:107:TRP:HB2	2:F:125:LEU:HD22	1.91	0.53
2:F:298:LEU:HD12	2:F:299:PHE:H	1.73	0.53
3:B:572:MET:HE2	3:B:573:CYS:O	2.09	0.53
2:D:70:ASP:HB3	2:D:79:VAL:CG1	2.39	0.53
2:D:162:THR:O	2:D:163:ASN:CG	2.47	0.53
2:D:166:MET:HA	2:D:182:VAL:HG21	1.90	0.53
2:D:323:GLY:O	2:D:350:ARG:NH2	2.42	0.53
1:E:26:LYS:O	1:E:29:ASP:HB3	2.09	0.52
1:E:74:ASP:HB3	1:E:77:GLU:HB3	1.90	0.52
1:E:422:ALA:O	1:E:426:ILE:HG22	2.10	0.52
2:F:121:ALA:HB3	2:F:159:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LYS:O	1:C:29:ASP:HB3	2.09	0.52
1:C:266:GLN:HA	1:C:269:LEU:HG	1.90	0.52
1:C:422:ALA:O	1:C:426:ILE:HG22	2.10	0.52
2:D:298:LEU:HD12	2:D:299:PHE:H	1.73	0.52
1:E:30:VAL:HG11	1:E:85:MET:CE	2.39	0.52
2:F:70:ASP:HB3	2:F:79:VAL:CG1	2.39	0.52
1:C:57:PHE:O	1:C:107:PHE:HA	2.09	0.52
1:C:145:LEU:HD11	1:C:149:GLU:HB3	1.91	0.52
1:C:302:PRO:CD	1:C:303:SER:N	2.68	0.52
1:E:88:HIS:O	1:E:117:PRO:HG3	2.08	0.52
2:F:66:VAL:HG21	2:F:349:LEU:CD2	2.40	0.52
1:C:426:ILE:O	1:C:430:MET:HE2	2.09	0.52
2:D:66:VAL:HG21	2:D:349:LEU:CD2	2.40	0.52
2:D:219:LYS:HE2	2:D:237:THR:C	2.29	0.52
1:E:44:ARG:O	1:E:55:SER:N	2.43	0.52
1:E:57:PHE:O	1:E:107:PHE:HA	2.09	0.52
2:F:179:LEU:CB	2:F:226:MET:HE1	2.38	0.52
3:B:631:ARG:NE	3:B:647:TYR:OH	2.42	0.52
2:D:30:ARG:HD2	2:D:272:ARG:HD2	1.91	0.52
2:D:213:VAL:HG13	2:D:223:VAL:HB	1.92	0.52
1:E:34:MET:HE1	1:E:62:ILE:HD12	1.92	0.52
2:F:66:VAL:HG21	2:F:349:LEU:HD21	1.92	0.52
2:F:303:ASN:CB	2:F:327:ARG:HD2	2.38	0.52
3:A:638:LEU:HD22	3:A:643:MET:CG	2.40	0.52
3:B:179:SER:N	3:B:301:ARG:O	2.38	0.52
1:C:111:GLN:HG3	1:C:112:THR:H	1.74	0.52
1:C:334:MET:HB3	1:C:435:TYR:CG	2.45	0.52
1:E:288:GLU:HA	1:E:291:LEU:CD1	2.38	0.52
1:E:335:ASP:OD1	1:E:335:ASP:N	2.40	0.52
2:F:218:ASP:HB2	2:F:220:LYS:NZ	2.25	0.52
3:A:512:SER:OG	3:A:520:TYR:CB	2.57	0.52
3:A:638:LEU:HD22	3:A:643:MET:HG2	1.92	0.52
1:C:93:PRO:HG2	1:C:96:ASP:HB3	1.91	0.52
2:D:218:ASP:HB2	2:D:220:LYS:NZ	2.25	0.52
1:E:271:ARG:HE	2:F:271:ASP:HB2	1.75	0.52
2:F:119:ALA:HA	2:F:134:LEU:HG	1.92	0.52
2:F:241:ASP:OD1	2:F:241:ASP:N	2.40	0.52
1:C:112:THR:HG23	1:C:115:PHE:N	2.23	0.52
1:E:284:LEU:HD12	1:E:285:SER:N	2.25	0.51
2:F:292:SER:O	2:F:295:GLY:N	2.24	0.51
1:C:182:ASP:N	1:C:182:ASP:OD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:GLN:HG3	1:E:112:THR:H	1.74	0.51
1:E:214:ILE:HG12	2:F:107:TRP:CE3	2.46	0.51
1:E:281:ASP:HA	1:E:284:LEU:CD2	2.40	0.51
3:A:556:ILE:HG21	3:B:556:ILE:HG23	1.93	0.51
1:C:283:LEU:HD22	2:D:248:TYR:CZ	2.46	0.51
3:A:704:TRP:CA	1:C:109:ARG:HH21	2.19	0.51
1:C:44:ARG:O	1:C:55:SER:N	2.43	0.51
1:C:372:ARG:HB3	1:C:373:PRO:HD2	1.93	0.51
2:D:119:ALA:HA	2:D:134:LEU:HG	1.92	0.51
2:D:149:VAL:HG23	2:D:150:ALA:H	1.75	0.51
2:D:160:SER:OG	2:D:203:LEU:HD22	2.09	0.51
1:E:145:LEU:HD11	1:E:149:GLU:HB3	1.91	0.51
1:C:406:LYS:HA	1:C:409:GLN:OE1	2.11	0.51
1:E:283:LEU:HD22	2:F:248:TYR:CZ	2.46	0.51
1:E:372:ARG:HB3	1:E:373:PRO:HD2	1.93	0.51
2:F:127:ASN:HA	2:F:154:ASN:O	2.11	0.51
2:F:305:TYR:CZ	2:F:326:ASN:HA	2.45	0.51
3:A:281:TRP:O	3:A:310:LEU:N	2.43	0.51
3:A:503:LEU:HD13	3:A:597:CYS:SG	2.50	0.51
1:C:284:LEU:HD12	1:C:285:SER:N	2.25	0.51
2:D:107:TRP:HB2	2:D:125:LEU:HD22	1.91	0.51
1:E:334:MET:HB3	1:E:435:TYR:CG	2.45	0.51
1:E:406:LYS:HA	1:E:409:GLN:OE1	2.11	0.51
2:F:169:LEU:O	2:F:170:THR:HG23	2.11	0.51
2:F:265:LEU:HD23	2:F:274:VAL:HG21	1.93	0.51
1:C:109:ARG:NH1	1:C:192:GLN:HE21	2.09	0.51
1:C:281:ASP:HA	1:C:284:LEU:CD2	2.40	0.51
1:C:294:ASP:OD1	1:C:296:PHE:N	2.36	0.51
2:D:127:ASN:HA	2:D:154:ASN:O	2.11	0.51
2:D:253:ALA:HB1	2:D:266:TYR:O	2.11	0.51
2:D:305:TYR:CZ	2:D:326:ASN:HA	2.45	0.51
2:F:285:GLY:H	2:F:303:ASN:HB2	1.75	0.51
3:A:84:SER:O	3:A:89:GLY:N	2.42	0.51
1:C:214:ILE:HG12	2:D:107:TRP:CE3	2.46	0.51
2:D:66:VAL:HG21	2:D:349:LEU:HD21	1.92	0.51
2:D:179:LEU:HD12	2:D:180:TRP:H	1.76	0.51
1:E:27:MET:HA	1:E:30:VAL:CG2	2.41	0.51
2:F:62:HIS:ND1	2:F:82:SER:HB3	2.26	0.51
2:F:222:MET:HG2	2:F:234:ALA:HB2	1.92	0.51
2:F:331:LEU:HD23	2:F:332:ARG:N	2.26	0.51
3:B:442:ARG:O	3:B:447:ILE:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ASP:OD2	1:C:76:VAL:HB	2.11	0.51
1:C:378:PRO:CG	1:C:414:PRO:HG2	2.39	0.51
2:D:124:GLY:HA2	2:D:156:LEU:N	2.20	0.51
2:D:331:LEU:HD23	2:D:332:ARG:N	2.26	0.51
1:E:132:LEU:HB3	1:E:153:LEU:CD1	2.33	0.50
2:F:253:ALA:HB1	2:F:266:TYR:O	2.11	0.50
3:A:601:ARG:O	3:A:601:ARG:HG2	2.10	0.50
1:C:27:MET:HA	1:C:30:VAL:CG2	2.41	0.50
1:C:271:ARG:HE	2:D:271:ASP:HB2	1.75	0.50
1:C:350:PHE:HB3	1:C:438:PHE:HE2	1.76	0.50
1:E:350:PHE:HB3	1:E:438:PHE:HE2	1.76	0.50
1:C:381:VAL:O	1:C:384:ILE:HG12	2.12	0.50
1:E:74:ASP:OD2	1:E:76:VAL:HB	2.11	0.50
1:E:271:ARG:NH2	2:F:268:LEU:O	2.45	0.50
2:F:149:VAL:HG23	2:F:150:ALA:H	1.75	0.50
1:C:30:VAL:HG11	1:C:85:MET:HE2	1.93	0.50
1:C:271:ARG:NH2	2:D:268:LEU:O	2.45	0.50
2:D:87:VAL:HB	2:D:101:VAL:HG13	1.94	0.50
1:E:381:VAL:O	1:E:384:ILE:HG12	2.12	0.50
3:A:557:SER:OG	3:A:558:LEU:N	2.45	0.50
1:E:42:PRO:HB2	1:E:44:ARG:HE	1.76	0.50
1:E:400:ASP:N	1:E:403:SER:OG	2.45	0.50
2:D:327:ARG:O	2:D:345:TRP:N	2.39	0.50
2:F:135:THR:HG23	2:F:137:ASP:HB3	1.94	0.50
3:B:653:LEU:O	3:B:657:VAL:CG2	2.59	0.50
2:D:265:LEU:HD23	2:D:274:VAL:HG21	1.93	0.50
1:E:109:ARG:NH1	1:E:192:GLN:HE21	2.09	0.50
1:E:275:LYS:CE	1:E:278:LYS:HE3	2.34	0.50
1:E:290:TYR:O	1:E:293:TYR:N	2.34	0.50
1:C:63:VAL:HG21	1:C:103:ASP:OD2	2.12	0.50
1:C:275:LYS:CE	1:C:278:LYS:HE3	2.34	0.50
1:E:294:ASP:OD1	1:E:296:PHE:N	2.36	0.50
1:C:262:ILE:HD11	2:D:15:LEU:HD11	1.93	0.50
2:D:169:LEU:O	2:D:170:THR:HG23	2.11	0.50
1:C:269:LEU:HD21	2:D:22:LEU:HB3	1.94	0.50
1:C:294:ASP:CB	2:D:294:SER:HB3	2.40	0.50
1:C:385:TRP:CD1	1:C:390:ALA:HB2	2.47	0.50
1:C:425:HIS:O	1:C:428:LYS:HE3	2.12	0.50
2:F:168:ILE:O	2:F:179:LEU:HD12	2.12	0.49
2:F:300:ALA:HB3	2:F:302:TYR:HE1	1.76	0.49
1:C:70:LEU:HB3	1:C:72:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:PHE:O	1:C:397:ILE:HG12	2.12	0.49
1:E:399:LEU:HB3	1:E:403:SER:OG	2.12	0.49
3:B:548:VAL:HG11	3:B:559:ILE:HD11	1.94	0.49
2:D:218:ASP:O	2:D:219:LYS:HB3	2.12	0.49
2:D:300:ALA:HB3	2:D:302:TYR:HE1	1.77	0.49
1:E:385:TRP:HZ3	1:E:407:THR:HB	1.76	0.49
2:F:179:LEU:HD12	2:F:180:TRP:H	1.76	0.49
3:A:164:LEU:O	3:A:168:GLU:N	2.42	0.49
1:C:42:PRO:HB2	1:C:44:ARG:HE	1.76	0.49
1:C:400:ASP:N	1:C:403:SER:OG	2.45	0.49
2:D:69:MET:HE1	2:D:341:CYS:CB	2.39	0.49
2:D:135:THR:HG23	2:D:137:ASP:HB3	1.94	0.49
1:E:27:MET:HA	1:E:30:VAL:HG23	1.95	0.49
1:E:418:THR:HB	1:E:419:PHE:CD2	2.47	0.49
1:C:385:TRP:HZ3	1:C:407:THR:HB	1.76	0.49
2:D:91:ASP:OD1	2:D:93:PHE:HB3	2.12	0.49
1:E:425:HIS:O	1:E:428:LYS:HE3	2.11	0.49
2:F:212:PHE:O	2:F:223:VAL:HG23	2.13	0.49
3:A:599:ALA:CB	1:C:142:ARG:HG2	2.42	0.49
1:C:427:TYR:HA	1:C:430:MET:CE	2.43	0.49
2:D:101:VAL:CG2	2:D:143:ALA:HB2	2.42	0.49
2:D:233:GLN:OE1	2:D:233:GLN:HA	2.09	0.49
1:E:63:VAL:HG21	1:E:103:ASP:OD2	2.12	0.49
1:E:427:TYR:HA	1:E:430:MET:CE	2.43	0.49
2:F:91:ASP:OD1	2:F:93:PHE:HB3	2.12	0.49
3:B:431:ASP:OD2	3:B:463:LEU:N	2.46	0.49
1:C:388:PHE:HA	1:C:395:SER:O	2.13	0.49
2:D:26:LEU:HA	2:D:29:GLU:CG	2.43	0.49
2:D:62:HIS:ND1	2:D:82:SER:HB3	2.26	0.49
2:D:168:ILE:O	2:D:179:LEU:HD12	2.12	0.49
1:E:377:VAL:HG12	1:E:414:PRO:HB2	1.94	0.49
1:C:418:THR:HB	1:C:419:PHE:CD2	2.47	0.49
2:D:125:LEU:H	2:D:155:TYR:CA	2.20	0.49
1:E:380:ARG:O	1:E:384:ILE:HG23	2.13	0.49
1:E:385:TRP:CD1	1:E:390:ALA:HB2	2.47	0.49
3:B:84:SER:O	3:B:90:ASP:N	2.42	0.49
1:C:399:LEU:HB3	1:C:403:SER:OG	2.12	0.49
2:F:47:ALA:C	2:F:48:LEU:HD23	2.33	0.49
2:F:101:VAL:CG2	2:F:143:ALA:HB2	2.43	0.49
2:F:264:ARG:NH1	2:F:273:GLU:OE2	2.46	0.49
3:B:611:ARG:O	3:B:615:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:647:TYR:O	3:B:651:THR:HG22	2.12	0.49
1:C:362:PHE:O	1:C:366:VAL:HG23	2.12	0.49
1:C:374:ILE:HD12	1:C:377:VAL:HG21	1.95	0.49
2:D:47:ALA:C	2:D:48:LEU:HD23	2.33	0.49
1:E:70:LEU:HB3	1:E:72:ILE:HD11	1.94	0.49
1:E:386:GLN:HA	1:E:390:ALA:CB	2.43	0.49
2:F:222:MET:HA	2:F:234:ALA:HA	1.95	0.49
3:B:464:LEU:HD21	3:B:490:LEU:HB3	1.94	0.49
1:C:334:MET:HE2	1:C:435:TYR:HB2	1.95	0.49
2:D:119:ALA:HB1	2:D:131:VAL:CG2	2.43	0.49
1:E:388:PHE:O	1:E:397:ILE:HG12	2.12	0.48
3:A:651:THR:HG23	3:A:652:HIS:N	2.29	0.48
1:C:380:ARG:O	1:C:384:ILE:HG23	2.13	0.48
2:D:166:MET:C	2:D:167:GLN:HG3	2.33	0.48
2:D:212:PHE:O	2:D:223:VAL:HG23	2.12	0.48
2:D:236:GLU:N	2:D:236:GLU:CD	2.66	0.48
2:D:263:CYS:N	2:D:277:TYR:O	2.46	0.48
2:F:218:ASP:O	2:F:219:LYS:HB3	2.12	0.48
1:C:92:PHE:CE1	1:C:109:ARG:HB3	2.48	0.48
2:D:72:CYS:HB2	2:D:113:TYR:CE2	2.48	0.48
2:D:120:ILE:HG23	2:D:134:LEU:HD11	1.95	0.48
2:D:264:ARG:NH1	2:D:273:GLU:OE2	2.46	0.48
2:D:284:PHE:HB3	2:D:303:ASN:CB	2.36	0.48
2:D:67:LEU:HD12	2:D:67:LEU:HA	1.58	0.48
1:E:279:VAL:O	1:E:283:LEU:HG	2.13	0.48
2:F:70:ASP:OD1	2:F:71:TRP:N	2.46	0.48
2:F:72:CYS:HB2	2:F:113:TYR:CE2	2.48	0.48
1:C:386:GLN:HA	1:C:390:ALA:CB	2.43	0.48
2:D:162:THR:HG22	2:D:203:LEU:HD11	1.94	0.48
1:E:362:PHE:O	1:E:366:VAL:HG23	2.12	0.48
1:E:388:PHE:HA	1:E:395:SER:O	2.13	0.48
2:F:107:TRP:HB2	2:F:125:LEU:HD23	1.95	0.48
2:F:119:ALA:HB1	2:F:131:VAL:CG2	2.43	0.48
2:F:263:CYS:N	2:F:277:TYR:O	2.46	0.48
3:A:315:ILE:HD11	3:A:346:VAL:C	2.33	0.48
3:A:616:ALA:HB2	3:A:661:LEU:HD12	1.95	0.48
2:D:57:ARG:NH2	2:D:93:PHE:HA	2.29	0.48
1:E:92:PHE:CE1	1:E:109:ARG:HB3	2.48	0.48
1:E:364:LEU:HA	1:E:367:GLU:HG3	1.96	0.48
1:E:389:LEU:HD21	1:E:407:THR:CB	2.44	0.48
2:F:198:VAL:C	2:F:199:LEU:HD22	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG22	1:C:53:ILE:HB	1.96	0.48
1:C:66:LEU:HA	1:C:70:LEU:CD1	2.36	0.48
1:C:323:SER:O	1:C:327:VAL:HG13	2.13	0.48
2:D:138:LYS:HZ1	2:D:144:ALA:HB3	1.78	0.48
2:F:120:ILE:HG23	2:F:134:LEU:HD11	1.95	0.48
1:C:27:MET:HA	1:C:30:VAL:HG23	1.95	0.48
1:C:279:VAL:O	1:C:283:LEU:HG	2.13	0.48
2:D:107:TRP:HB2	2:D:125:LEU:HD23	1.95	0.48
1:E:373:PRO:HD3	2:F:166:MET:SD	2.53	0.48
1:C:389:LEU:HD21	1:C:407:THR:CB	2.44	0.48
2:D:260:ASP:OD1	2:D:260:ASP:N	2.47	0.48
2:D:292:SER:O	2:D:295:GLY:N	2.24	0.48
1:E:279:VAL:HG11	2:F:267:ASP:OD2	2.14	0.48
1:E:287:THR:C	1:E:291:LEU:HG	2.34	0.48
1:E:374:ILE:HD12	1:E:377:VAL:HG21	1.95	0.48
2:F:160:SER:OG	2:F:160:SER:O	2.24	0.48
1:C:287:THR:C	1:C:291:LEU:HG	2.34	0.48
2:D:18:GLU:HA	2:D:21:SER:OG	2.14	0.48
2:D:198:VAL:C	2:D:199:LEU:HD22	2.33	0.48
1:E:132:LEU:CB	1:E:153:LEU:HD12	2.33	0.48
2:F:57:ARG:NH2	2:F:93:PHE:HA	2.29	0.48
3:B:291:GLY:N	3:B:299:GLU:O	2.43	0.48
1:C:364:LEU:HA	1:C:367:GLU:HG3	1.96	0.48
1:C:377:VAL:HG12	1:C:414:PRO:HB2	1.94	0.48
2:D:287:SER:O	2:D:287:SER:OG	2.26	0.48
1:C:97:HIS:HA	1:C:198:ASP:OD2	2.14	0.47
1:C:358:GLU:HA	1:C:361:ARG:CZ	2.44	0.47
1:C:435:TYR:HB3	1:C:436:PRO:HD3	1.96	0.47
2:D:48:LEU:HD11	2:D:296:ARG:NH2	2.29	0.47
2:D:70:ASP:OD1	2:D:71:TRP:N	2.46	0.47
2:D:202:ASP:OD1	2:D:203:LEU:N	2.47	0.47
1:E:364:LEU:HA	1:E:367:GLU:CG	2.45	0.47
2:F:48:LEU:HD11	2:F:296:ARG:NH2	2.29	0.47
2:F:219:LYS:HD3	2:F:219:LYS:O	2.14	0.47
2:D:120:ILE:CG1	2:D:134:LEU:HD21	2.44	0.47
1:E:216:LYS:NZ	2:F:241:ASP:OD2	2.48	0.47
1:E:358:GLU:HA	1:E:361:ARG:CZ	2.44	0.47
3:B:194:ALA:HA	3:B:202:LEU:O	2.13	0.47
1:C:111:GLN:HG3	1:C:112:THR:N	2.29	0.47
1:C:181:ARG:HB3	1:C:185:GLU:OE1	2.14	0.47
1:C:334:MET:CE	1:C:431:LYS:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:ASP:OD1	2:D:36:VAL:N	2.47	0.47
2:D:158:ALA:HB3	2:D:201:LEU:CD2	2.44	0.47
1:E:131:TYR:OH	1:E:194:ARG:HA	2.15	0.47
1:E:378:PRO:CG	1:E:414:PRO:HG2	2.39	0.47
2:F:202:ASP:OD1	2:F:203:LEU:N	2.47	0.47
2:F:327:ARG:H	2:F:345:TRP:HB2	1.79	0.47
1:C:279:VAL:HG11	2:D:267:ASP:OD2	2.14	0.47
1:E:63:VAL:HG11	1:E:103:ASP:OD2	2.14	0.47
1:E:97:HIS:HA	1:E:198:ASP:OD2	2.15	0.47
1:E:330:TRP:NE1	1:E:340:ASP:OD2	2.46	0.47
2:F:65:LYS:HE3	2:F:345:TRP:CD1	2.49	0.47
2:D:65:LYS:HE3	2:D:345:TRP:CD1	2.49	0.47
2:D:160:SER:HB2	2:D:169:LEU:HB2	1.97	0.47
2:D:319:SER:OG	2:D:321:LEU:HD21	2.15	0.47
1:E:156:LEU:O	1:E:160:PHE:HB2	2.15	0.47
1:C:267:ILE:HA	1:C:270:ASP:OD1	2.14	0.47
1:C:364:LEU:HA	1:C:367:GLU:CG	2.45	0.47
2:D:319:SER:O	2:D:320:ILE:HG13	2.15	0.47
1:E:187:LYS:HA	1:E:187:LYS:HD2	1.61	0.47
1:E:381:VAL:HG21	1:E:414:PRO:CB	2.44	0.47
1:E:404:TYR:O	1:E:408:THR:HG23	2.14	0.47
2:F:124:GLY:HA2	2:F:156:LEU:N	2.20	0.47
2:F:124:GLY:O	2:F:125:LEU:HB3	2.14	0.47
3:A:599:ALA:HB2	1:C:142:ARG:HG2	1.97	0.47
1:C:433:ASP:HB3	1:C:437:ARG:NH1	2.27	0.47
2:D:26:LEU:HA	2:D:29:GLU:HG2	1.97	0.47
2:D:124:GLY:O	2:D:125:LEU:HB3	2.14	0.47
2:D:257:GLY:HA3	2:D:263:CYS:SG	2.55	0.47
1:E:435:TYR:HB3	1:E:436:PRO:HD3	1.97	0.47
2:F:158:ALA:CB	2:F:201:LEU:HD21	2.45	0.47
2:F:321:LEU:HB3	2:F:352:TRP:HZ3	1.80	0.47
1:C:63:VAL:HG11	1:C:103:ASP:OD2	2.14	0.47
1:C:216:LYS:HA	1:C:216:LYS:HD3	1.75	0.47
1:C:311:THR:HG22	1:C:315:GLU:CG	2.44	0.47
2:D:110:ALA:O	2:D:122:CYS:HA	2.15	0.47
2:D:149:VAL:HG23	2:D:150:ALA:N	2.30	0.47
1:E:58:SER:OG	1:E:104:ASP:O	2.33	0.47
1:E:177:VAL:O	1:E:180:LYS:HE3	2.14	0.47
1:E:275:LYS:HG3	1:E:278:LYS:H	1.80	0.47
1:E:351:LEU:HB3	1:E:357:SER:HA	1.97	0.47
2:F:132:TYR:CZ	2:F:146:LYS:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:230:GLN:O	2:F:232:VAL:HG23	2.15	0.47
2:F:257:GLY:HA3	2:F:263:CYS:SG	2.55	0.47
3:A:335:SER:OG	3:A:353:ILE:O	2.23	0.47
3:A:556:ILE:CG2	3:B:556:ILE:HD12	2.43	0.47
1:C:156:LEU:O	1:C:160:PHE:HB2	2.15	0.47
1:C:262:ILE:HD11	2:D:15:LEU:CD1	2.45	0.47
1:C:264:TYR:HA	1:C:267:ILE:HD11	1.97	0.47
1:C:441:SER:O	1:C:445:GLN:HG2	2.15	0.47
1:E:111:GLN:HG3	1:E:112:THR:N	2.29	0.47
3:A:649:ALA:C	3:A:653:LEU:HD12	2.36	0.47
1:C:334:MET:CG	1:C:431:LYS:HD2	2.45	0.47
1:C:340:ASP:OD1	1:C:342:VAL:N	2.47	0.47
2:D:132:TYR:CZ	2:D:146:LYS:HG3	2.50	0.47
2:D:219:LYS:O	2:D:219:LYS:HD3	2.14	0.47
2:D:327:ARG:H	2:D:345:TRP:HB2	1.79	0.47
1:E:311:THR:HG22	1:E:315:GLU:CG	2.44	0.46
1:E:433:ASP:HB3	1:E:437:ARG:NH1	2.27	0.46
1:E:441:SER:O	1:E:445:GLN:HG2	2.15	0.46
2:F:319:SER:O	2:F:320:ILE:HG13	2.15	0.46
1:C:404:TYR:O	1:C:408:THR:HG23	2.15	0.46
2:D:30:ARG:HD2	2:D:272:ARG:HD3	1.96	0.46
1:E:46:VAL:HG22	1:E:53:ILE:HB	1.96	0.46
2:F:36:VAL:CG2	2:F:41:VAL:HG13	2.45	0.46
2:F:87:VAL:HB	2:F:101:VAL:HG13	1.94	0.46
2:F:119:ALA:HA	2:F:132:TYR:O	2.16	0.46
2:F:125:LEU:H	2:F:155:TYR:CA	2.20	0.46
3:A:619:ASN:OD1	3:A:623:ILE:HD12	2.15	0.46
3:B:408:CYS:C	3:B:569:ILE:HG22	2.36	0.46
1:C:47:LYS:CB	1:C:52:LYS:HD2	2.46	0.46
1:C:131:TYR:OH	1:C:194:ARG:HA	2.15	0.46
1:C:264:TYR:HA	1:C:267:ILE:CG1	2.44	0.46
1:C:275:LYS:HG3	1:C:278:LYS:H	1.80	0.46
1:C:330:TRP:NE1	1:C:340:ASP:OD2	2.46	0.46
2:D:317:ARG:HD2	2:D:320:ILE:CG1	2.45	0.46
2:D:344:SER:OG	2:D:346:ASP:OD1	2.30	0.46
1:E:428:LYS:HD2	1:E:429:LEU:N	2.31	0.46
2:F:258:SER:OG	2:F:260:ASP:OD1	2.16	0.46
2:F:319:SER:OG	2:F:321:LEU:HD21	2.15	0.46
2:D:321:LEU:HB3	2:D:352:TRP:HZ3	1.80	0.46
1:E:330:TRP:HZ2	1:E:342:VAL:HB	1.81	0.46
2:F:120:ILE:CG1	2:F:134:LEU:HD21	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:350:ARG:HB2	2:F:352:TRP:HE1	1.80	0.46
1:C:177:VAL:O	1:C:180:LYS:HE3	2.14	0.46
1:C:265:TRP:CZ2	2:D:19:ALA:HB1	2.50	0.46
1:C:330:TRP:HZ2	1:C:342:VAL:HB	1.81	0.46
1:C:351:LEU:HB3	1:C:357:SER:HA	1.97	0.46
2:D:26:LEU:HA	2:D:29:GLU:OE1	2.16	0.46
1:E:47:LYS:CB	1:E:52:LYS:HD2	2.46	0.46
2:F:84:ASP:OD1	2:F:84:ASP:C	2.53	0.46
2:F:138:LYS:HZ1	2:F:144:ALA:HB3	1.81	0.46
2:F:187:LEU:HD23	2:F:189:GLN:H	1.81	0.46
2:F:219:LYS:HE2	2:F:237:THR:C	2.36	0.46
3:A:410:VAL:HG13	3:A:410:VAL:O	2.15	0.46
3:A:653:LEU:O	3:A:657:VAL:HG23	2.15	0.46
3:A:741:GLN:O	3:A:745:CYS:N	2.38	0.46
1:C:27:MET:O	1:C:30:VAL:HB	2.16	0.46
1:C:46:VAL:HG22	1:C:53:ILE:O	2.16	0.46
2:D:171:ALA:HB1	2:D:198:VAL:HG23	1.97	0.46
1:E:27:MET:O	1:E:30:VAL:HB	2.16	0.46
1:E:98:VAL:HG22	1:E:203:VAL:HB	1.98	0.46
1:E:287:THR:HG22	1:E:291:LEU:CD2	2.46	0.46
1:E:294:ASP:CB	2:F:294:SER:HB3	2.40	0.46
2:F:110:ALA:O	2:F:122:CYS:HA	2.15	0.46
3:B:410:VAL:HG12	3:B:411:GLN:N	2.30	0.46
1:C:381:VAL:HG21	1:C:414:PRO:CB	2.44	0.46
1:E:340:ASP:OD1	1:E:342:VAL:N	2.47	0.46
1:E:386:GLN:HA	1:E:390:ALA:HB2	1.98	0.46
3:A:82:VAL:O	3:A:86:LEU:N	2.49	0.46
3:A:591:LEU:HA	3:A:594:VAL:HG12	1.97	0.46
1:C:288:GLU:HA	1:C:291:LEU:CG	2.46	0.46
1:E:334:MET:CG	1:E:431:LYS:HD2	2.45	0.46
2:F:56:ARG:CG	2:F:353:ALA:HB3	2.46	0.46
2:F:263:CYS:O	2:F:277:TYR:HB2	2.16	0.46
3:A:281:TRP:O	3:A:311:GLN:N	2.48	0.46
1:C:35:GLN:HG3	1:C:35:GLN:O	2.15	0.46
2:D:36:VAL:CG2	2:D:41:VAL:HG13	2.45	0.46
1:E:181:ARG:HB3	1:E:185:GLU:OE1	2.14	0.46
2:F:119:ALA:HB1	2:F:131:VAL:HG22	1.98	0.46
2:F:138:LYS:NZ	2:F:140:GLU:OE2	2.42	0.46
2:F:149:VAL:HG23	2:F:150:ALA:N	2.30	0.46
2:F:259:ASP:OD1	2:F:285:GLY:HA3	2.16	0.46
3:A:704:TRP:HA	1:C:109:ARG:NH2	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:392:CYS:C	3:B:393:LEU:HD12	2.36	0.46
3:B:569:ILE:HG12	3:B:570:PHE:N	2.31	0.46
1:C:156:LEU:HA	1:C:156:LEU:HD23	1.55	0.46
2:D:56:ARG:CG	2:D:353:ALA:HB3	2.46	0.46
2:D:223:VAL:HG12	2:D:233:GLN:HB3	1.97	0.46
2:D:285:GLY:N	2:D:303:ASN:HB2	2.30	0.46
1:E:30:VAL:HG11	1:E:85:MET:HE2	1.97	0.46
1:E:334:MET:CE	1:E:431:LYS:HA	2.45	0.46
2:F:243:ASN:O	2:F:244:SER:HB2	2.16	0.46
3:B:442:ARG:O	3:B:447:ILE:CD1	2.63	0.46
1:C:279:VAL:HA	1:C:282:SER:OG	2.16	0.46
1:C:334:MET:HE3	1:C:431:LYS:HA	1.97	0.46
2:D:235:PHE:CD1	2:D:235:PHE:N	2.83	0.46
1:E:35:GLN:HG3	1:E:35:GLN:O	2.15	0.45
1:E:281:ASP:O	1:E:284:LEU:HG	2.16	0.45
2:F:331:LEU:HG	2:F:341:CYS:O	2.17	0.45
1:C:98:VAL:HG22	1:C:203:VAL:HB	1.98	0.45
1:C:393:ALA:HB1	1:C:394:PRO:HD2	1.98	0.45
2:D:37:GLU:HG2	2:D:39:HIS:CE1	2.52	0.45
2:D:138:LYS:NZ	2:D:144:ALA:HB3	2.31	0.45
2:D:162:THR:CG2	2:D:203:LEU:HD11	2.45	0.45
2:D:263:CYS:O	2:D:277:TYR:HB2	2.16	0.45
1:E:41:ILE:HD13	1:E:62:ILE:CD1	2.35	0.45
2:F:171:ALA:HB1	2:F:198:VAL:HG23	1.97	0.45
1:C:428:LYS:HD2	1:C:429:LEU:N	2.31	0.45
2:D:141:ASN:OD1	2:D:142:MET:N	2.49	0.45
2:D:187:LEU:HD23	2:D:189:GLN:H	1.81	0.45
2:D:259:ASP:OD1	2:D:285:GLY:HA3	2.16	0.45
2:F:35:ASP:OD1	2:F:36:VAL:N	2.47	0.45
2:F:141:ASN:OD1	2:F:142:MET:N	2.50	0.45
1:C:58:SER:OG	1:C:104:ASP:O	2.33	0.45
1:C:351:LEU:HB3	1:C:356:SER:O	2.16	0.45
1:C:416:ARG:NH2	2:D:167:GLN:OE1	2.40	0.45
2:D:119:ALA:HB1	2:D:131:VAL:HG22	1.98	0.45
2:D:247:TYR:HD1	2:D:254:PHE:HB3	1.81	0.45
2:D:255:ALA:HB2	2:D:265:LEU:CB	2.46	0.45
1:E:132:LEU:HA	1:E:132:LEU:HD22	1.59	0.45
1:C:287:THR:O	1:C:291:LEU:HG	2.17	0.45
2:D:158:ALA:CB	2:D:201:LEU:HD21	2.45	0.45
2:F:238:HIS:CD2	2:F:242:ILE:HD13	2.52	0.45
2:F:252:ASP:HB3	2:F:269:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:567:HIS:C	3:A:568:LEU:HD12	2.36	0.45
3:B:604:PRO:O	3:B:605:SER:OG	2.24	0.45
1:C:66:LEU:CA	1:C:70:LEU:HD13	2.39	0.45
1:C:177:VAL:HG13	1:C:180:LYS:HE3	1.98	0.45
2:D:305:TYR:CE2	2:D:326:ASN:HA	2.52	0.45
2:D:331:LEU:HG	2:D:341:CYS:O	2.17	0.45
1:E:46:VAL:HG22	1:E:53:ILE:O	2.16	0.45
1:E:188:ILE:HG13	1:E:189:LEU:N	2.32	0.45
1:E:288:GLU:HA	1:E:291:LEU:CG	2.46	0.45
2:F:236:GLU:OE1	2:F:236:GLU:N	2.49	0.45
2:F:241:ASP:O	2:F:258:SER:HB2	2.17	0.45
3:B:503:LEU:HD21	3:B:613:MET:SD	2.57	0.45
3:B:582:THR:O	3:B:585:ALA:HB3	2.16	0.45
1:C:216:LYS:NZ	2:D:241:ASP:OD2	2.48	0.45
2:D:119:ALA:HA	2:D:132:TYR:O	2.16	0.45
2:D:252:ASP:HB3	2:D:269:ARG:NH1	2.32	0.45
2:D:266:TYR:HE1	2:D:273:GLU:HG3	1.82	0.45
1:E:27:MET:HG3	1:E:90:TYR:OH	2.17	0.45
1:E:47:LYS:HB2	1:E:52:LYS:HD2	1.98	0.45
2:F:166:MET:HA	2:F:182:VAL:CG2	2.46	0.45
2:F:247:TYR:HD1	2:F:254:PHE:HB3	1.81	0.45
2:F:305:TYR:CE2	2:F:326:ASN:HA	2.52	0.45
1:C:287:THR:HG22	1:C:291:LEU:CD2	2.46	0.45
1:E:34:MET:HE2	1:E:62:ILE:HD12	1.99	0.45
1:E:177:VAL:HG13	1:E:180:LYS:HE3	1.98	0.45
1:E:331:GLY:HA2	1:E:439:ILE:HD12	1.99	0.45
1:E:393:ALA:HB1	1:E:394:PRO:HD2	1.97	0.45
1:E:408:THR:O	1:E:411:VAL:HG12	2.17	0.45
1:E:416:ARG:NH2	2:F:167:GLN:OE1	2.40	0.45
2:F:288:SER:HB2	2:F:330:THR:HA	1.99	0.45
2:F:317:ARG:HD2	2:F:320:ILE:CG1	2.45	0.45
1:C:408:THR:O	1:C:411:VAL:HG12	2.17	0.45
2:D:225:ASP:OD2	2:D:232:VAL:CG2	2.49	0.45
2:D:243:ASN:O	2:D:244:SER:HB2	2.16	0.45
1:E:399:LEU:CD2	1:E:407:THR:HG21	2.46	0.45
2:F:138:LYS:NZ	2:F:144:ALA:HB3	2.31	0.45
2:F:279:LYS:HA	2:F:279:LYS:HD3	1.80	0.45
3:A:321:ASP:OD1	3:A:321:ASP:N	2.50	0.45
3:A:741:GLN:HA	3:A:744:ARG:CB	2.46	0.45
1:C:101:LEU:HA	1:C:108:TYR:OH	2.17	0.45
1:C:188:ILE:HG13	1:C:189:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:CD1	2:D:15:LEU:HD13	2.39	0.45
1:C:281:ASP:O	1:C:284:LEU:HG	2.16	0.45
1:E:95:SER:O	1:E:95:SER:OG	2.32	0.45
1:E:101:LEU:HA	1:E:108:TYR:OH	2.17	0.45
1:E:287:THR:O	1:E:291:LEU:HG	2.17	0.45
1:E:303:SER:OG	1:E:313:PHE:HB2	2.17	0.45
2:F:158:ALA:C	2:F:201:LEU:HD21	2.37	0.45
2:F:166:MET:C	2:F:182:VAL:HG23	2.37	0.45
2:F:166:MET:O	2:F:182:VAL:HG23	2.17	0.45
1:C:47:LYS:HB2	1:C:52:LYS:HD2	1.98	0.45
1:C:331:GLY:HA2	1:C:439:ILE:HD12	1.99	0.45
2:D:288:SER:HB2	2:D:330:THR:HA	1.99	0.45
2:D:350:ARG:HB2	2:D:352:TRP:HE1	1.80	0.45
1:E:271:ARG:O	1:E:273:ARG:HG3	2.17	0.44
1:E:279:VAL:HA	1:E:282:SER:OG	2.16	0.44
1:E:295:PRO:HA	1:E:299:PRO:HB3	1.99	0.44
1:E:380:ARG:HG3	1:E:384:ILE:CG2	2.47	0.44
1:C:264:TYR:HA	1:C:267:ILE:HG12	1.99	0.44
1:E:104:ASP:OD1	1:E:106:THR:OG1	2.30	0.44
1:E:276:MET:HE2	2:F:38:LEU:HB2	1.98	0.44
1:E:283:LEU:HD22	2:F:248:TYR:CE2	2.52	0.44
1:E:369:LEU:HD22	1:E:384:ILE:HD13	2.00	0.44
2:F:55:THR:O	2:F:56:ARG:HD3	2.18	0.44
2:F:69:MET:HE1	2:F:341:CYS:CB	2.42	0.44
2:F:260:ASP:OD1	2:F:260:ASP:N	2.47	0.44
2:F:326:ASN:OD1	2:F:327:ARG:N	2.49	0.44
1:C:95:SER:O	1:C:95:SER:OG	2.32	0.44
1:C:380:ARG:HG3	1:C:384:ILE:CG2	2.47	0.44
2:D:218:ASP:HB2	2:D:220:LYS:HZ3	1.81	0.44
1:E:31:ILE:HD12	1:E:90:TYR:HD2	1.83	0.44
1:E:323:SER:OG	1:E:325:GLN:HB2	2.17	0.44
2:F:266:TYR:HE1	2:F:273:GLU:HG3	1.82	0.44
1:C:31:ILE:HD12	1:C:90:TYR:HD2	1.83	0.44
1:C:276:MET:SD	2:D:38:LEU:N	2.91	0.44
1:E:276:MET:SD	2:F:38:LEU:N	2.91	0.44
1:E:351:LEU:HB3	1:E:356:SER:O	2.16	0.44
1:E:445:GLN:OE1	1:E:448:LEU:HD21	2.17	0.44
2:F:238:HIS:CG	2:F:242:ILE:HD13	2.53	0.44
1:C:271:ARG:O	1:C:273:ARG:HG3	2.17	0.44
1:C:295:PRO:HA	1:C:299:PRO:HB3	1.99	0.44
1:C:386:GLN:HA	1:C:390:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:TYR:CE1	2:D:146:LYS:HG3	2.53	0.44
2:D:135:THR:HG23	2:D:137:ASP:OD1	2.18	0.44
2:D:249:PRO:HD3	2:D:291:PHE:CD2	2.32	0.44
2:D:255:ALA:CA	2:D:265:LEU:HA	2.44	0.44
2:D:255:ALA:CB	2:D:265:LEU:HA	2.48	0.44
2:F:37:GLU:HG2	2:F:39:HIS:CE1	2.52	0.44
1:C:72:ILE:CB	1:C:78:ALA:HB2	2.48	0.44
1:C:283:LEU:HD22	2:D:248:TYR:CE2	2.51	0.44
1:C:297:LEU:CD1	2:D:48:LEU:HD13	2.47	0.44
1:C:303:SER:OG	1:C:313:PHE:HB2	2.17	0.44
1:C:399:LEU:CD2	1:C:407:THR:HG21	2.45	0.44
2:D:158:ALA:C	2:D:201:LEU:HD21	2.37	0.44
2:F:285:GLY:N	2:F:303:ASN:HB2	2.32	0.44
3:A:556:ILE:HG21	3:B:556:ILE:CG2	2.48	0.44
3:B:619:ASN:ND2	3:B:657:VAL:HG11	2.33	0.44
1:E:350:PHE:CD2	1:E:351:LEU:HD23	2.53	0.44
2:F:132:TYR:CE1	2:F:146:LYS:HG3	2.53	0.44
2:F:255:ALA:HB2	2:F:265:LEU:CB	2.46	0.44
2:F:255:ALA:CA	2:F:265:LEU:HA	2.44	0.44
3:A:128:THR:HG23	3:B:131:HIS:CE1	2.52	0.44
1:C:27:MET:HG3	1:C:90:TYR:OH	2.17	0.44
1:C:274:LEU:O	2:D:33:LEU:HD13	2.18	0.44
1:C:350:PHE:CD2	1:C:351:LEU:HD23	2.53	0.44
2:D:26:LEU:HA	2:D:29:GLU:CD	2.38	0.44
2:D:281:SER:O	2:D:283:ILE:HG13	2.18	0.44
1:E:102:LYS:HB2	1:E:102:LYS:HE3	1.66	0.44
1:E:347:PHE:HZ	1:E:434:SER:HB2	1.83	0.44
2:F:91:ASP:HB3	2:F:94:THR:OG1	2.18	0.44
2:F:218:ASP:HB2	2:F:220:LYS:HZ3	1.81	0.44
3:A:720:LYS:CB	1:C:174:GLN:HG2	2.48	0.44
1:C:334:MET:SD	1:C:431:LYS:HD2	2.58	0.44
1:C:385:TRP:CZ3	1:C:407:THR:HB	2.53	0.44
2:D:47:ALA:O	2:D:48:LEU:HD23	2.17	0.44
1:E:297:LEU:CD1	2:F:48:LEU:HD13	2.47	0.44
1:E:334:MET:SD	1:E:431:LYS:HD2	2.58	0.44
1:E:427:TYR:HA	1:E:430:MET:HG2	2.00	0.44
1:E:443:ALA:HA	1:E:446:GLU:HG3	2.00	0.44
2:F:47:ALA:O	2:F:48:LEU:HD23	2.17	0.44
2:F:255:ALA:CB	2:F:265:LEU:HA	2.48	0.44
2:F:306:THR:HB	2:F:320:ILE:HG22	1.99	0.44
2:D:138:LYS:HE3	2:D:145:LYS:HZ2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:GLN:HG3	2:D:235:PHE:HZ	1.77	0.44
1:E:323:SER:HB2	1:E:325:GLN:OE1	2.18	0.43
2:F:281:SER:O	2:F:283:ILE:HG13	2.18	0.43
2:F:317:ARG:CD	2:F:320:ILE:HD11	2.48	0.43
3:A:291:GLY:N	3:A:299:GLU:O	2.51	0.43
1:C:48:SER:O	1:C:52:LYS:NZ	2.42	0.43
1:C:369:LEU:HD22	1:C:384:ILE:HD13	2.00	0.43
1:E:179:LYS:CD	1:E:186:ARG:HD3	2.49	0.43
1:C:87:ALA:O	1:C:209:THR:HG21	2.19	0.43
1:C:288:GLU:HA	1:C:291:LEU:CB	2.48	0.43
1:C:445:GLN:OE1	1:C:448:LEU:HD21	2.17	0.43
2:D:306:THR:HB	2:D:320:ILE:HG22	1.99	0.43
1:E:87:ALA:O	1:E:209:THR:HG21	2.19	0.43
1:E:109:ARG:HG3	1:E:110:PHE:N	2.33	0.43
1:E:288:GLU:HA	1:E:291:LEU:CB	2.48	0.43
2:F:52:VAL:HG22	2:F:52:VAL:O	2.18	0.43
2:F:126:ASP:OD1	2:F:128:LYS:HG2	2.18	0.43
1:C:109:ARG:HG3	1:C:110:PHE:N	2.33	0.43
1:C:427:TYR:HA	1:C:430:MET:HG2	2.00	0.43
1:C:443:ALA:HA	1:C:446:GLU:HG3	2.00	0.43
2:D:57:ARG:O	2:D:58:THR:HG23	2.18	0.43
1:E:36:ASP:HB3	1:E:39:ASN:O	2.19	0.43
1:E:273:ARG:C	1:E:274:LEU:HD22	2.39	0.43
1:E:324:GLN:HA	1:E:327:VAL:HG22	2.01	0.43
2:F:225:ASP:OD2	2:F:232:VAL:HG21	2.17	0.43
2:F:296:ARG:O	2:F:312:VAL:HB	2.18	0.43
2:D:55:THR:O	2:D:56:ARG:HD3	2.18	0.43
2:F:57:ARG:O	2:F:58:THR:HG23	2.18	0.43
3:B:471:ILE:HG22	3:B:472:LEU:N	2.33	0.43
1:C:276:MET:HE2	2:D:38:LEU:HB2	1.98	0.43
1:C:429:LEU:HD23	1:C:430:MET:N	2.34	0.43
2:D:53:MET:HB3	2:D:353:ALA:O	2.19	0.43
2:D:326:ASN:OD1	2:D:327:ARG:N	2.49	0.43
1:E:43:ILE:HG23	1:E:43:ILE:O	2.19	0.43
1:E:385:TRP:CZ3	1:E:407:THR:HB	2.53	0.43
2:F:64:ASN:O	2:F:347:HIS:HA	2.18	0.43
2:F:214:SER:N	2:F:222:MET:O	2.52	0.43
2:F:344:SER:OG	2:F:346:ASP:OD1	2.30	0.43
1:C:360:LEU:HD11	1:C:364:LEU:HD11	2.00	0.43
2:D:23:LYS:O	2:D:27:GLU:HG2	2.18	0.43
2:D:334:SER:OG	2:D:335:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:CYS:O	2:F:133:PRO:HA	2.19	0.43
2:F:158:ALA:HB3	2:F:201:LEU:CD2	2.43	0.43
1:C:36:ASP:HB3	1:C:39:ASN:O	2.19	0.43
1:C:314:TRP:O	1:C:317:GLU:HB3	2.19	0.43
2:D:91:ASP:HB3	2:D:94:THR:OG1	2.18	0.43
2:D:167:GLN:CB	2:D:179:LEU:HD21	2.38	0.43
1:E:364:LEU:O	1:E:367:GLU:HG3	2.19	0.43
1:E:366:VAL:HB	1:E:423:GLN:NE2	2.34	0.43
2:F:127:ASN:O	2:F:152:HIS:N	2.52	0.43
2:F:128:LYS:HA	2:F:151:MET:HA	2.00	0.43
2:F:290:ASP:O	2:F:299:PHE:HB2	2.19	0.43
3:B:410:VAL:CG2	3:B:568:LEU:HD13	2.48	0.43
1:C:366:VAL:HG11	1:C:423:GLN:OE1	2.19	0.43
1:E:429:LEU:HD23	1:E:430:MET:N	2.34	0.43
3:A:543:GLY:HA3	3:B:578:TRP:CZ3	2.54	0.43
3:B:396:ARG:NE	3:B:405:ASP:O	2.50	0.43
1:C:102:LYS:HE3	1:C:102:LYS:HB2	1.66	0.43
1:C:273:ARG:C	1:C:274:LEU:HD22	2.39	0.43
2:D:128:LYS:HA	2:D:151:MET:HA	2.00	0.43
2:D:220:LYS:HG2	2:D:236:GLU:HB2	1.97	0.43
2:D:279:LYS:O	2:D:282:ILE:HG13	2.19	0.43
2:D:296:ARG:O	2:D:312:VAL:HB	2.18	0.43
1:E:360:LEU:HD11	1:E:364:LEU:HD11	2.00	0.43
2:F:334:SER:OG	2:F:335:PRO:HD2	2.18	0.43
3:A:478:THR:OG1	3:A:479:PHE:N	2.52	0.43
1:C:34:MET:CE	1:C:62:ILE:HG23	2.49	0.43
1:C:45:THR:HG23	1:C:45:THR:O	2.19	0.43
1:C:116:TRP:HB3	1:C:117:PRO:HD2	2.00	0.43
1:C:358:GLU:O	1:C:361:ARG:HB2	2.19	0.43
1:C:364:LEU:O	1:C:367:GLU:HG3	2.19	0.43
1:C:366:VAL:HB	1:C:423:GLN:NE2	2.34	0.43
2:D:200:CYS:SG	2:D:215:GLY:N	2.92	0.43
2:D:246:ARG:HH22	2:D:332:ARG:NH1	2.17	0.43
2:F:242:ILE:HA	2:F:258:SER:HB3	2.00	0.42
2:F:301:GLY:CA	2:F:328:VAL:HG11	2.39	0.42
3:A:466:TYR:CZ	3:A:655:VAL:HG11	2.54	0.42
3:B:133:THR:HG22	3:B:137:ASN:ND2	2.34	0.42
1:C:43:ILE:HG23	1:C:43:ILE:O	2.19	0.42
2:D:118:CYS:O	2:D:133:PRO:HA	2.19	0.42
2:D:127:ASN:O	2:D:152:HIS:N	2.51	0.42
2:D:285:GLY:H	2:D:303:ASN:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:THR:HG23	1:E:45:THR:O	2.19	0.42
1:E:275:LYS:HG2	1:E:278:LYS:CD	2.49	0.42
1:E:324:GLN:O	1:E:327:VAL:HG22	2.19	0.42
1:E:417:TYR:CE2	2:F:227:ARG:HA	2.54	0.42
2:F:135:THR:HG23	2:F:137:ASP:OD1	2.18	0.42
2:F:166:MET:HA	2:F:182:VAL:HG21	2.00	0.42
2:F:279:LYS:O	2:F:282:ILE:HG13	2.19	0.42
3:A:591:LEU:C	3:A:594:VAL:HG12	2.37	0.42
3:B:485:ARG:NE	3:B:579:ASP:OD2	2.53	0.42
1:C:106:THR:HG22	1:C:107:PHE:H	1.84	0.42
1:C:179:LYS:CD	1:C:186:ARG:HD3	2.48	0.42
1:C:261:GLN:OE1	2:D:15:LEU:HD21	2.18	0.42
1:C:306:TRP:HA	1:C:306:TRP:CE3	2.54	0.42
2:D:30:ARG:CD	2:D:272:ARG:HD3	2.49	0.42
2:D:52:VAL:HG22	2:D:52:VAL:O	2.18	0.42
2:D:64:ASN:O	2:D:347:HIS:HA	2.18	0.42
2:D:138:LYS:NZ	2:D:140:GLU:OE2	2.42	0.42
2:D:160:SER:OG	2:D:203:LEU:HD23	2.16	0.42
1:E:314:TRP:O	1:E:317:GLU:HB3	2.19	0.42
3:A:454:LEU:CD2	3:A:526:VAL:HG11	2.49	0.42
1:C:102:LYS:HG2	1:C:104:ASP:OD2	2.19	0.42
2:D:120:ILE:HG12	2:D:134:LEU:CD2	2.49	0.42
2:D:126:ASP:OD1	2:D:128:LYS:HG2	2.18	0.42
2:D:282:ILE:HD12	2:D:302:TYR:HE2	1.85	0.42
2:D:302:TYR:CE1	2:D:308:ASN:HB2	2.54	0.42
3:A:505:ARG:O	3:A:509:VAL:HG23	2.19	0.42
3:B:654:THR:OG1	3:B:655:VAL:HG23	2.19	0.42
1:C:324:GLN:O	1:C:327:VAL:HG22	2.19	0.42
1:C:433:ASP:C	1:C:436:PRO:HD2	2.40	0.42
1:E:106:THR:HG22	1:E:107:PHE:H	1.84	0.42
1:E:362:PHE:O	1:E:365:ALA:HB3	2.20	0.42
2:F:163:ASN:OD1	2:F:163:ASN:N	2.52	0.42
2:F:317:ARG:NH1	2:F:320:ILE:HG12	2.34	0.42
1:C:271:ARG:NE	2:D:271:ASP:HB2	2.35	0.42
1:C:417:TYR:CE2	2:D:227:ARG:HA	2.54	0.42
2:D:317:ARG:CD	2:D:320:ILE:HD11	2.48	0.42
2:D:317:ARG:NH1	2:D:320:ILE:HG12	2.34	0.42
1:E:42:PRO:C	1:E:44:ARG:HE	2.23	0.42
1:E:72:ILE:CB	1:E:78:ALA:HB2	2.48	0.42
1:E:358:GLU:O	1:E:361:ARG:HB2	2.19	0.42
1:E:366:VAL:HG11	1:E:423:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:LYS:HE3	2:F:145:LYS:HZ2	1.84	0.42
2:F:302:TYR:CE1	2:F:308:ASN:HB2	2.54	0.42
2:F:307:ILE:HG22	2:F:308:ASN:H	1.83	0.42
3:A:619:ASN:ND2	3:A:657:VAL:HG11	2.35	0.42
3:B:492:PHE:HZ	3:B:586:GLU:HA	1.85	0.42
1:C:275:LYS:O	1:C:278:LYS:HB2	2.20	0.42
2:D:154:ASN:OD1	2:D:173:GLY:HA3	2.20	0.42
2:D:307:ILE:HG22	2:D:308:ASN:H	1.83	0.42
1:E:66:LEU:HA	1:E:70:LEU:CD1	2.36	0.42
1:E:351:LEU:HD23	1:E:351:LEU:HA	1.80	0.42
2:F:53:MET:HB3	2:F:353:ALA:O	2.19	0.42
2:F:208:THR:OG1	2:F:209:GLY:N	2.53	0.42
1:E:45:THR:CB	1:E:54:PRO:HA	2.50	0.42
1:E:68:LYS:HE2	1:E:68:LYS:HA	2.02	0.42
1:E:374:ILE:HD12	1:E:374:ILE:HA	1.87	0.42
2:F:112:ALA:O	2:F:120:ILE:HG22	2.20	0.42
2:F:282:ILE:HD12	2:F:302:TYR:HE2	1.85	0.42
1:C:187:LYS:HD2	1:C:187:LYS:HA	1.61	0.42
1:C:324:GLN:HA	1:C:327:VAL:HG22	2.01	0.42
1:E:177:VAL:CG1	1:E:180:LYS:HE3	2.50	0.42
2:F:255:ALA:HB1	2:F:264:ARG:O	2.20	0.42
2:F:282:ILE:CD1	2:F:302:TYR:HE2	2.33	0.42
1:C:347:PHE:HZ	1:C:434:SER:HB2	1.83	0.42
1:E:330:TRP:HH2	1:E:342:VAL:HG12	1.84	0.42
1:E:362:PHE:HE2	1:E:426:ILE:HG21	1.82	0.42
1:E:387:GLU:HB3	1:E:388:PHE:CD1	2.55	0.42
2:F:67:LEU:HD12	2:F:67:LEU:HA	1.58	0.42
1:C:72:ILE:HG23	1:C:77:GLU:HG2	2.02	0.42
1:C:362:PHE:O	1:C:365:ALA:HB3	2.20	0.42
2:D:59:LEU:HG	2:D:90:TRP:CZ3	2.55	0.42
2:D:72:CYS:SG	2:D:74:ASP:OD1	2.78	0.42
2:D:163:ASN:OD1	2:D:163:ASN:C	2.58	0.42
2:D:282:ILE:CD1	2:D:302:TYR:HE2	2.33	0.42
1:E:132:LEU:HD12	1:E:153:LEU:HD13	2.01	0.41
1:E:432:SER:OG	1:E:433:ASP:OD1	2.34	0.41
2:F:59:LEU:HG	2:F:90:TRP:CZ3	2.55	0.41
2:F:246:ARG:HH22	2:F:332:ARG:NH1	2.17	0.41
1:C:68:LYS:HA	1:C:68:LYS:HE2	2.02	0.41
1:C:124:GLU:OE2	1:C:124:GLU:N	2.53	0.41
1:C:177:VAL:CG1	1:C:180:LYS:HE3	2.49	0.41
1:C:371:LYS:HE2	2:D:166:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:219:LYS:HG2	2:D:238:HIS:O	2.20	0.41
2:D:255:ALA:HB1	2:D:264:ARG:O	2.20	0.41
2:D:290:ASP:O	2:D:299:PHE:HB2	2.19	0.41
1:E:102:LYS:HG2	1:E:104:ASP:OD2	2.19	0.41
1:E:124:GLU:N	1:E:124:GLU:OE2	2.53	0.41
1:E:306:TRP:HA	1:E:306:TRP:CE3	2.54	0.41
3:A:704:TRP:CB	1:C:109:ARG:HE	2.34	0.41
1:C:45:THR:CB	1:C:54:PRO:HA	2.50	0.41
1:E:116:TRP:HB3	1:E:117:PRO:HD2	2.01	0.41
2:D:112:ALA:O	2:D:120:ILE:HG22	2.20	0.41
2:D:208:THR:OG1	2:D:209:GLY:N	2.53	0.41
2:D:236:GLU:O	2:D:236:GLU:HG2	2.20	0.41
1:E:369:LEU:HA	1:E:369:LEU:HD12	1.66	0.41
2:F:128:LYS:O	2:F:128:LYS:HG3	2.20	0.41
2:F:135:THR:OG1	2:F:136:PHE:N	2.53	0.41
3:B:568:LEU:C	3:B:568:LEU:HD12	2.40	0.41
1:C:357:SER:HG	1:C:361:ARG:HE	1.69	0.41
1:C:377:VAL:HG12	1:C:414:PRO:HB3	2.02	0.41
2:D:135:THR:OG1	2:D:136:PHE:N	2.53	0.41
2:F:154:ASN:OD1	2:F:173:GLY:HA3	2.20	0.41
3:B:467:PHE:O	3:B:470:VAL:HG22	2.21	0.41
3:B:569:ILE:CG1	3:B:570:PHE:N	2.84	0.41
1:C:42:PRO:C	1:C:44:ARG:HE	2.23	0.41
1:C:104:ASP:OD1	1:C:106:THR:OG1	2.30	0.41
1:C:432:SER:OG	1:C:433:ASP:OD1	2.34	0.41
1:E:166:PHE:HA	1:E:169:MET:CE	2.50	0.41
1:E:297:LEU:HD11	2:F:48:LEU:CD1	2.50	0.41
1:C:297:LEU:HD11	2:D:48:LEU:CD1	2.50	0.41
1:E:94:ILE:HG22	1:E:107:PHE:O	2.21	0.41
1:E:97:HIS:CE1	1:E:194:ARG:HH21	2.38	0.41
1:E:125:ASN:OD1	1:E:126:THR:N	2.53	0.41
1:E:271:ARG:NE	2:F:271:ASP:HB2	2.35	0.41
1:E:275:LYS:O	1:E:278:LYS:HB2	2.20	0.41
3:A:634:LEU:HD23	3:A:638:LEU:HD21	2.03	0.41
1:C:330:TRP:HH2	1:C:342:VAL:HG12	1.84	0.41
1:C:387:GLU:HB3	1:C:388:PHE:CD1	2.55	0.41
1:C:402:LYS:NZ	1:C:406:LYS:HG2	2.36	0.41
1:E:151:GLU:OE1	1:E:151:GLU:HA	2.21	0.41
3:A:647:TYR:O	3:A:651:THR:HG22	2.20	0.41
1:C:94:ILE:HG22	1:C:107:PHE:O	2.21	0.41
1:C:133:CYS:O	1:C:136:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLU:HA	1:C:151:GLU:OE1	2.21	0.41
1:C:166:PHE:HA	1:C:169:MET:CE	2.50	0.41
2:D:112:ALA:O	2:D:120:ILE:HA	2.21	0.41
1:E:336:GLU:OE2	1:E:339:LYS:HB3	2.21	0.41
1:E:421:ASP:OD1	1:E:422:ALA:N	2.54	0.41
1:E:433:ASP:C	1:E:436:PRO:HD2	2.40	0.41
2:F:112:ALA:O	2:F:120:ILE:HA	2.21	0.41
2:F:130:SER:HB2	2:F:146:LYS:HZ3	1.85	0.41
2:F:150:ALA:HB2	2:F:180:TRP:CG	2.56	0.41
2:F:287:SER:O	2:F:287:SER:OG	2.26	0.41
3:A:413:ASP:OD1	3:A:414:LYS:N	2.54	0.41
3:B:442:ARG:HB3	3:B:447:ILE:HD12	2.02	0.41
3:B:496:TYR:CD2	3:B:590:LEU:HD21	2.56	0.41
1:C:97:HIS:CE1	1:C:194:ARG:HH21	2.38	0.41
1:C:132:LEU:HD13	1:C:153:LEU:HB2	2.03	0.41
1:C:258:LEU:HB3	2:D:15:LEU:HD11	2.02	0.41
1:C:271:ARG:O	1:C:271:ARG:HD3	2.21	0.41
2:D:227:ARG:NH2	2:D:228:SER:HB3	2.36	0.41
2:D:301:GLY:CA	2:D:328:VAL:HG11	2.39	0.41
1:E:216:LYS:HD3	1:E:216:LYS:HA	1.75	0.41
1:E:271:ARG:O	1:E:271:ARG:HD3	2.21	0.41
2:F:43:GLU:CA	2:F:314:LYS:HE2	2.46	0.41
3:B:310:LEU:HA	3:B:313:VAL:HG21	2.02	0.41
2:D:128:LYS:O	2:D:128:LYS:HG3	2.20	0.41
1:E:132:LEU:O	1:E:136:THR:HG22	2.21	0.40
1:E:409:GLN:HA	1:E:412:LYS:NZ	2.36	0.40
2:F:68:CYS:O	2:F:80:SER:HA	2.21	0.40
2:F:167:GLN:HB3	2:F:179:LEU:HD11	2.03	0.40
3:B:609:GLU:N	3:B:610:PRO:HD2	2.36	0.40
1:C:336:GLU:OE2	1:C:339:LYS:HB3	2.21	0.40
1:C:421:ASP:OD1	1:C:422:ALA:N	2.54	0.40
2:D:36:VAL:HG22	2:D:41:VAL:HG13	2.03	0.40
2:D:260:ASP:O	2:D:262:THR:HG23	2.21	0.40
2:D:325:GLU:HG2	2:D:346:ASP:HB3	2.04	0.40
1:E:200:HIS:O	1:E:201:ARG:HG2	2.21	0.40
1:E:402:LYS:NZ	1:E:406:LYS:HG2	2.36	0.40
1:E:413:GLU:HG2	1:E:413:GLU:O	2.21	0.40
2:F:260:ASP:O	2:F:262:THR:HG23	2.21	0.40
1:C:125:ASN:OD1	1:C:126:THR:N	2.53	0.40
1:C:374:ILE:HD12	1:C:374:ILE:HA	1.87	0.40
1:C:409:GLN:HA	1:C:412:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:GLY:HA3	2:D:224:TRP:HH2	1.86	0.40
1:E:399:LEU:HD22	1:E:404:TYR:CD1	2.54	0.40
2:F:224:TRP:CZ3	2:F:231:CYS:HB2	2.56	0.40
1:C:362:PHE:HE2	1:C:426:ILE:HG21	1.82	0.40
1:C:385:TRP:CZ3	1:C:389:LEU:HG	2.57	0.40
1:E:203:VAL:HG12	1:E:205:GLY:H	1.87	0.40
1:E:350:PHE:HB3	1:E:438:PHE:CE2	2.56	0.40
1:E:371:LYS:O	1:E:371:LYS:HG2	2.21	0.40
2:F:36:VAL:HG22	2:F:41:VAL:HG13	2.03	0.40
2:F:325:GLU:HG2	2:F:346:ASP:HB3	2.04	0.40
1:E:377:VAL:HG12	1:E:414:PRO:HB3	2.02	0.40
2:F:89:VAL:HG11	2:F:99:HIS:HD2	1.87	0.40
1:C:350:PHE:HB3	1:C:438:PHE:CE2	2.56	0.40
2:D:68:CYS:O	2:D:80:SER:HA	2.21	0.40
2:D:128:LYS:HB3	2:D:151:MET:CG	2.47	0.40
2:D:162:THR:HG22	2:D:203:LEU:CD1	2.51	0.40
2:D:219:LYS:CG	2:D:238:HIS:O	2.70	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	C	392/530 (74%)	358 (91%)	34 (9%)	0	100 100
1	E	377/530 (71%)	345 (92%)	32 (8%)	0	100 100
2	D	337/395 (85%)	279 (83%)	58 (17%)	0	100 100
2	F	317/395 (80%)	258 (81%)	59 (19%)	0	100 100
3	A	563/1138 (50%)	470 (84%)	83 (15%)	10 (2%)	8 41
3	B	492/1138 (43%)	418 (85%)	68 (14%)	6 (1%)	13 50
All	All	2478/4126 (60%)	2128 (86%)	334 (14%)	16 (1%)	29 65

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	108	LEU
3	A	112	TRP
3	A	113	PRO
3	A	278	LYS
3	A	279	PRO
3	A	519	PRO
3	A	738	PRO
3	B	79	PRO
3	B	113	PRO
3	B	211	PRO
3	A	169	PRO
3	B	267	PRO
3	A	518	ILE
3	A	78	VAL
3	B	298	PRO
3	B	78	VAL

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	C	360/476 (76%)	356 (99%)	4 (1%)	73	85
1	E	345/476 (72%)	334 (97%)	11 (3%)	39	62
2	D	284/334 (85%)	276 (97%)	8 (3%)	43	65
2	F	267/334 (80%)	260 (97%)	7 (3%)	46	67
3	A	312/981 (32%)	310 (99%)	2 (1%)	86	92
3	B	304/981 (31%)	301 (99%)	3 (1%)	76	86
All	All	1872/3582 (52%)	1837 (98%)	35 (2%)	59	75

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	47	LYS

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Mol	Chain	Res	Type
1	E	132	LEU
1	E	190	ASP
1	E	271	ARG
1	E	298	LEU
1	E	312	THR
1	E	319	SER
1	E	320	LYS
1	E	321	GLU
1	E	349	LYS
1	E	428	LYS
2	F	44	ARG
2	F	74	ASP
2	F	163	ASN
2	F	165	ASP
2	F	210	ASN
2	F	247	TYR
2	F	269	ARG
3	A	513	ARG
3	A	538	PHE
3	B	557	SER
3	B	587	PHE
3	B	650	HIS
1	C	47	LYS
1	C	271	ARG
1	C	349	LYS
1	C	428	LYS
2	D	44	ARG
2	D	160	SER
2	D	161	PHE
2	D	213	VAL
2	D	233	GLN
2	D	235	PHE
2	D	236	GLU
2	D	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	88	HIS
1	E	170	GLN
1	E	346	GLN
2	F	64	ASN

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Mol	Chain	Res	Type
2	F	186	GLN
2	F	189	GLN
2	F	210	ASN
2	F	238	HIS
2	F	243	ASN
3	A	334	ASN
3	A	555	GLN
3	A	561	GLN
3	B	131	HIS
3	B	134	ASN
3	B	137	ASN
3	B	333	ASN
3	B	424	GLN
3	B	652	HIS
1	C	88	HIS
1	C	170	GLN
1	C	346	GLN
2	D	64	ASN
2	D	186	GLN
2	D	243	ASN
2	D	347	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

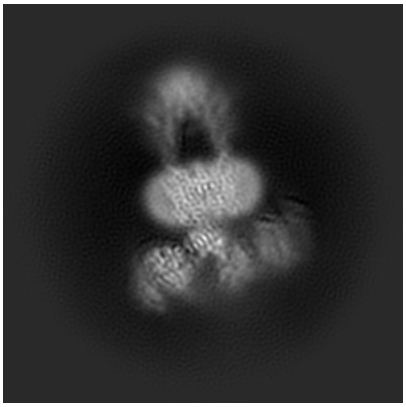
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31363. These allow visual inspection of the internal detail of the map and identification of artifacts.

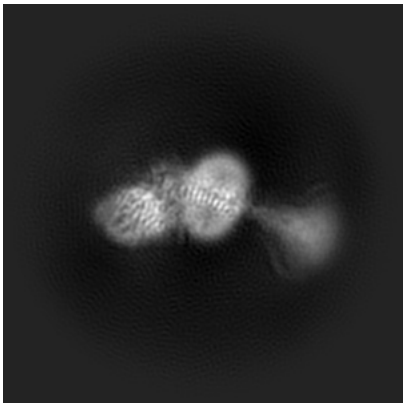
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

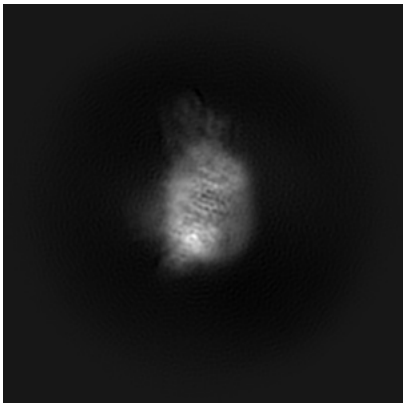
6.1.1 Primary map



X



Y

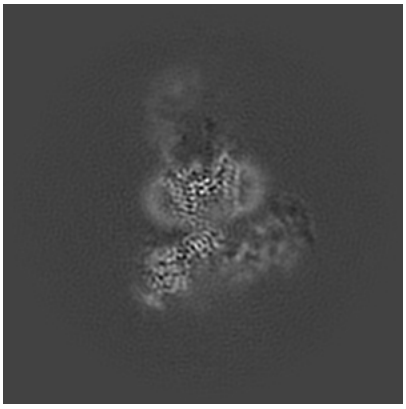


Z

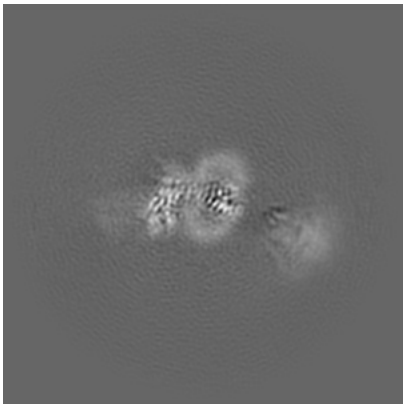
The images above show the map projected in three orthogonal directions.

6.2 Central slices

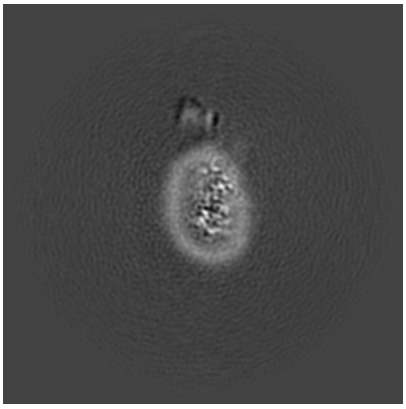
6.2.1 Primary map



X Index: 175



Y Index: 175

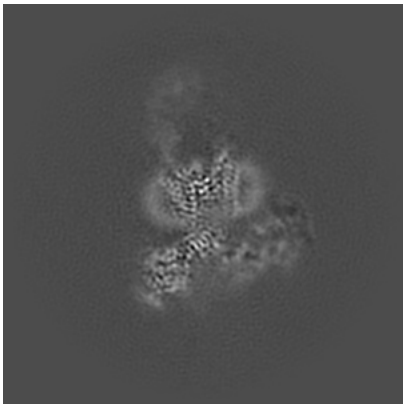


Z Index: 175

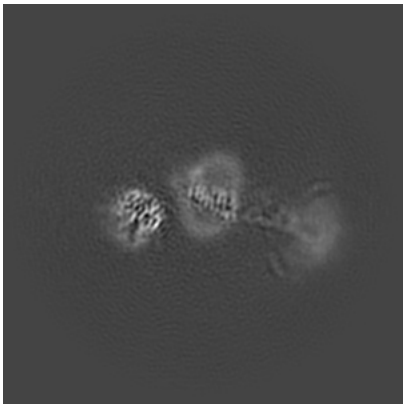
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

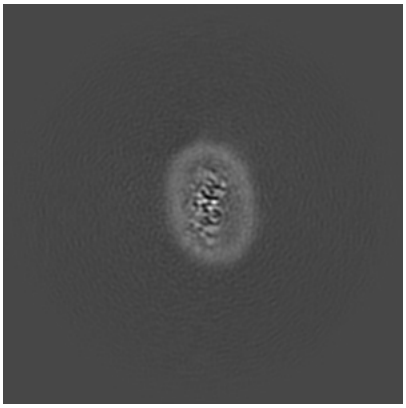
6.3.1 Primary map



X Index: 176



Y Index: 152



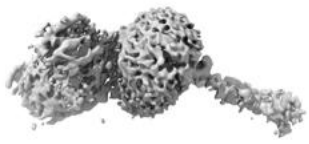
Z Index: 189

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

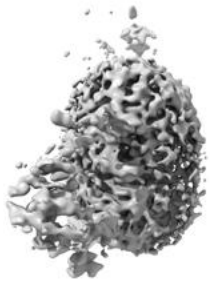
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

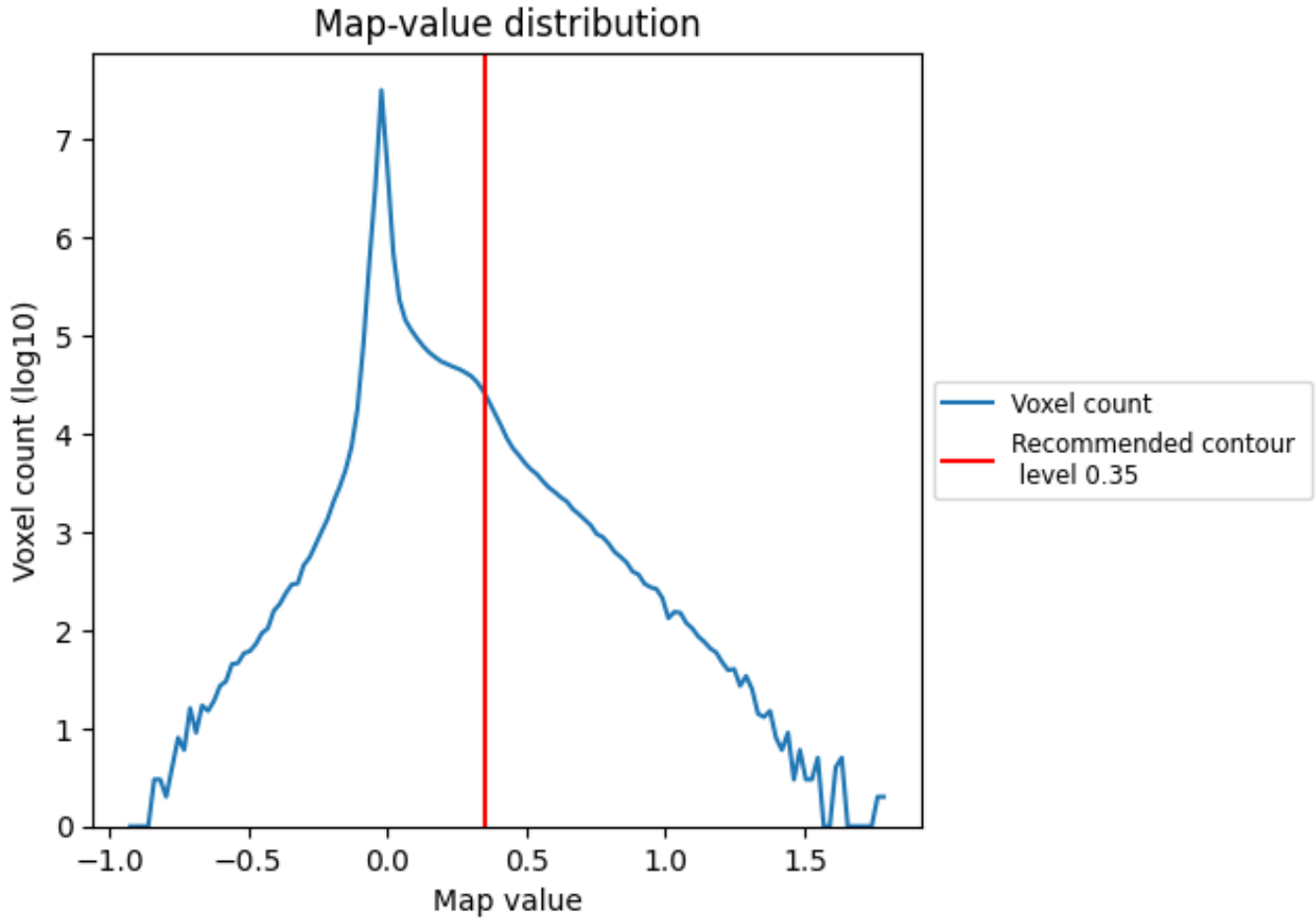
6.5 Mask visualisation (i)

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

7 Map analysis

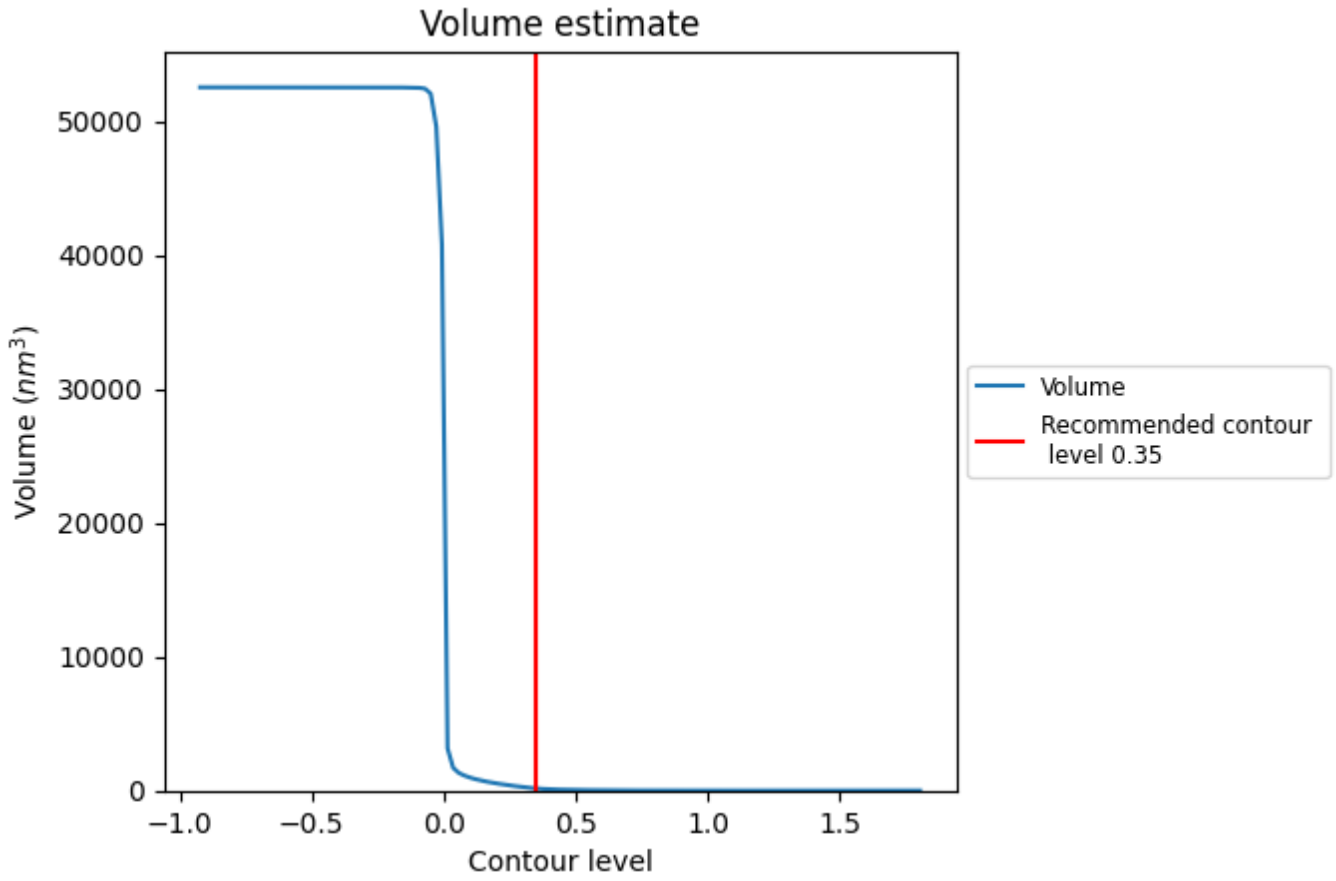
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

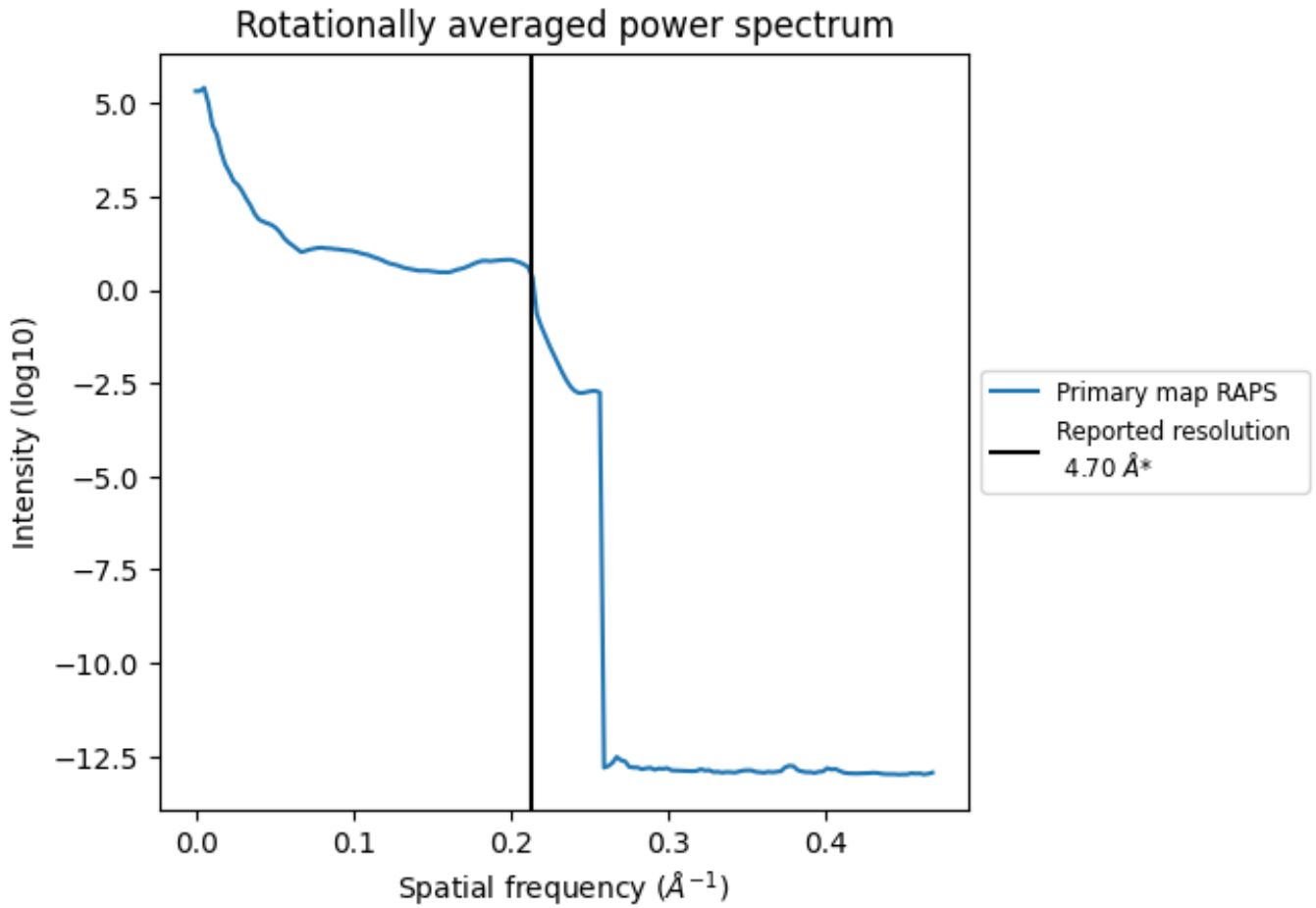
7.2 Volume estimate



The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 145 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 0.213 $Å^{-1}$

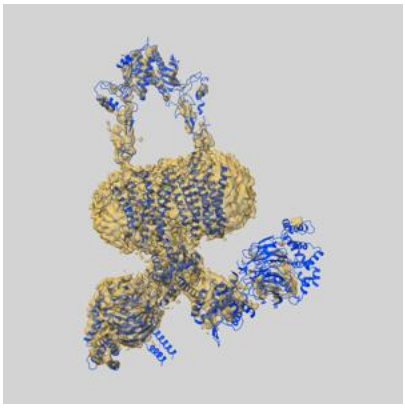
8 Fourier-Shell correlation (i)

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

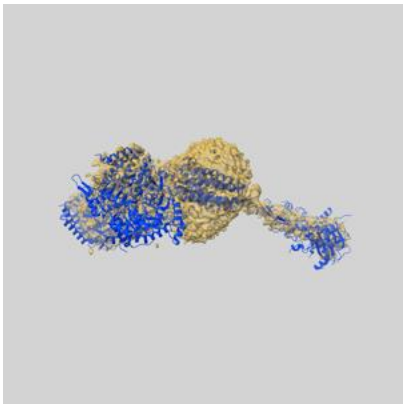
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31363 and PDB model 7EWR. Per-residue inclusion information can be found in section 3 on page 19.

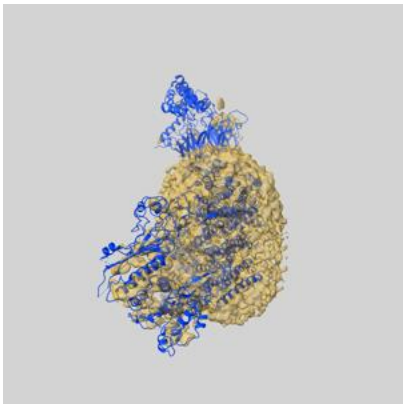
9.1 Map-model overlay



X



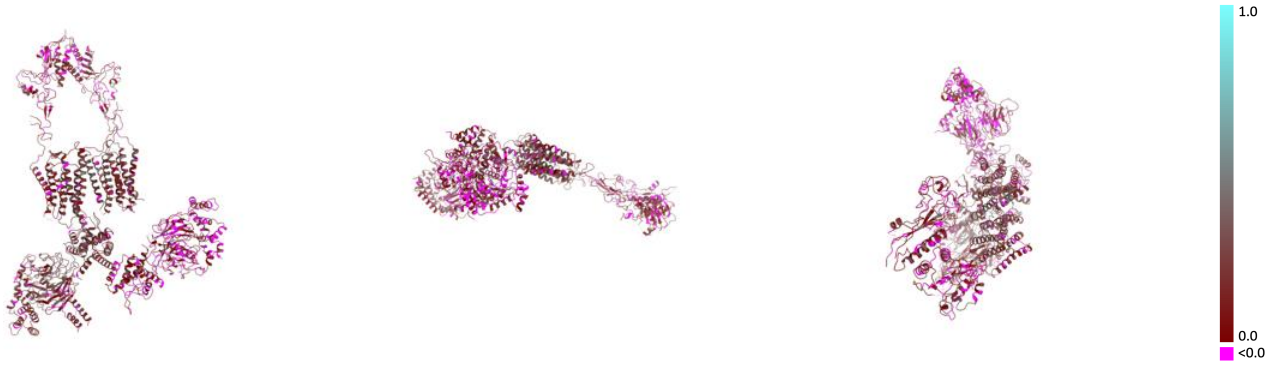
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

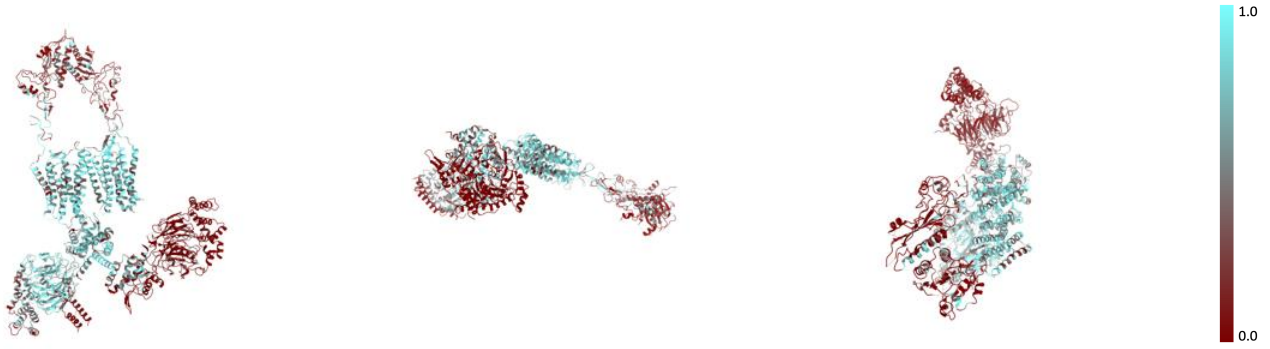
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

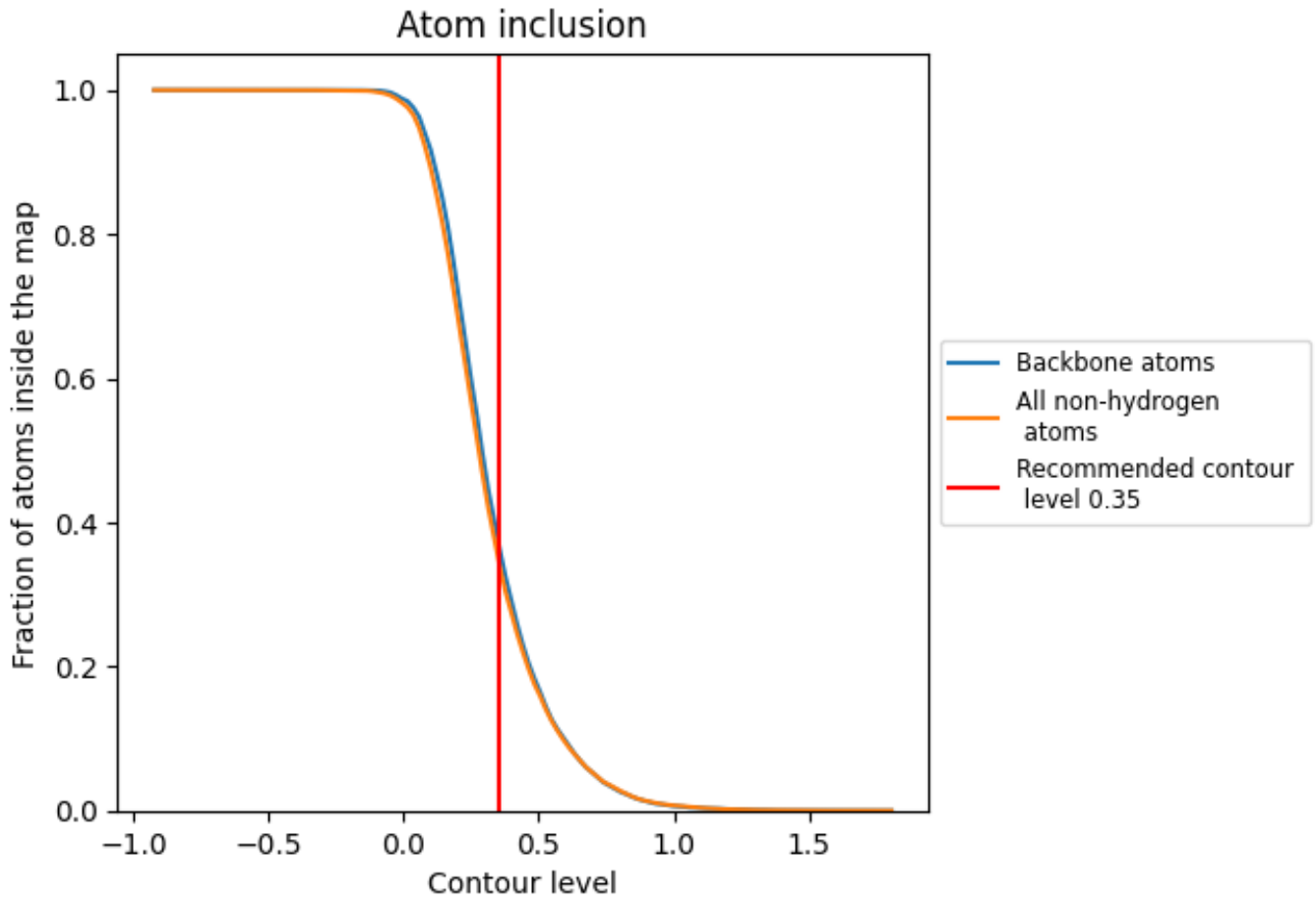
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 37% of all backbone atoms, 35% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3496	0.1600
A	0.5357	0.1830
B	0.4918	0.1960
C	0.5307	0.2120
D	0.6426	0.2190
E	0.1352	0.0670
F	0.0566	0.0600