



Full wwPDB EM Validation Report ⓘ

Mar 22, 2025 – 06:28 PM EDT

PDB ID : 6U5U
EMDB ID : EMD-20656
Title : Electron cryomicroscopy Structure of *S. cerevisiae* FAS in the KS-stalled state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 2.80 Å (reported)
Based on initial model : 2UV8

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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

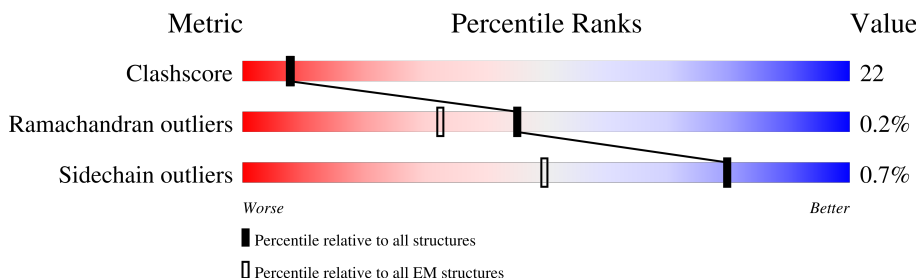
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	<div> <div>25%</div> <div>54%</div> <div>30%</div> <div>15%</div> </div>
2	G	2073	<div> <div>47%</div> <div>52%</div> <div>45%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	G	2102	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28298 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1611	Total	C	N	O	S	0	0
			12171	7684	2081	2362	44		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0
			15995	10253	2660	3026	56		

There are 22 discrepancies between the modelled and reference sequences:

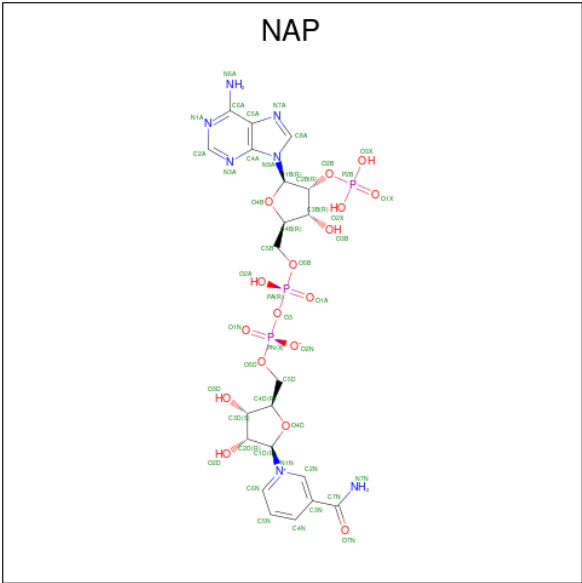
Chain	Residue	Modelled	Actual	Comment	Reference
G	2052	ASP	-	expression tag	UNP P07149
G	2053	TYR	-	expression tag	UNP P07149
G	2054	LYS	-	expression tag	UNP P07149
G	2055	ASP	-	expression tag	UNP P07149
G	2056	HIS	-	expression tag	UNP P07149
G	2057	ASP	-	expression tag	UNP P07149
G	2058	GLY	-	expression tag	UNP P07149
G	2059	ASP	-	expression tag	UNP P07149
G	2060	TYR	-	expression tag	UNP P07149
G	2061	LYS	-	expression tag	UNP P07149
G	2062	ASP	-	expression tag	UNP P07149
G	2063	HIS	-	expression tag	UNP P07149
G	2064	ASP	-	expression tag	UNP P07149
G	2065	ILE	-	expression tag	UNP P07149
G	2066	ASP	-	expression tag	UNP P07149
G	2067	TYR	-	expression tag	UNP P07149
G	2068	LYS	-	expression tag	UNP P07149
G	2069	ASP	-	expression tag	UNP P07149
G	2070	ASP	-	expression tag	UNP P07149
G	2071	ASP	-	expression tag	UNP P07149
G	2072	ASP	-	expression tag	UNP P07149

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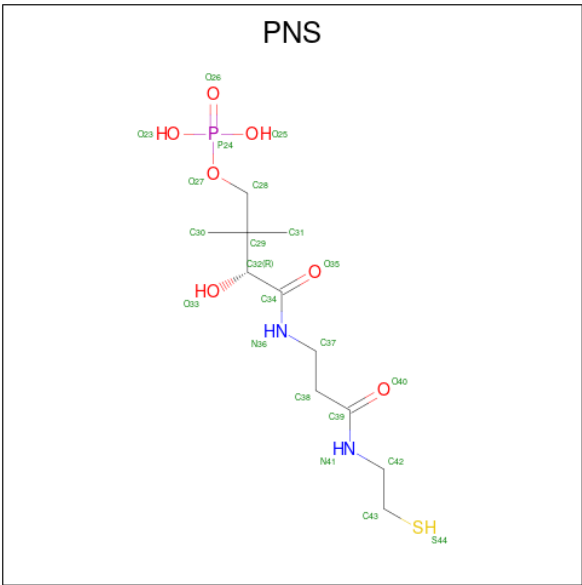
Chain	Residue	Modelled	Actual	Comment	Reference
G	2073	LYS	-	expression tag	UNP P07149

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



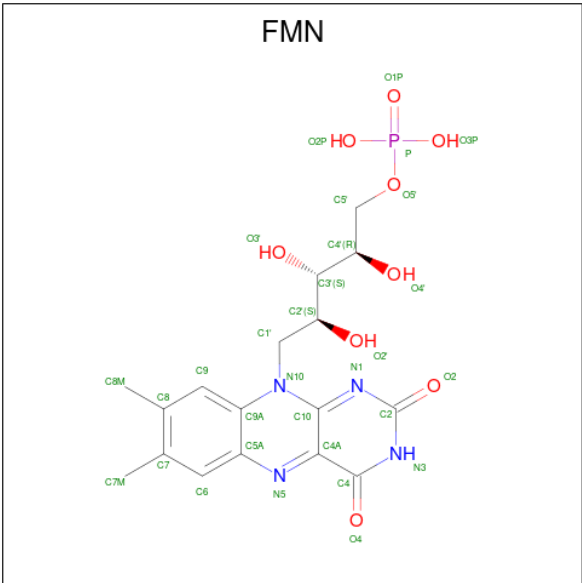
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	G	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			5	1	3	1	

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).

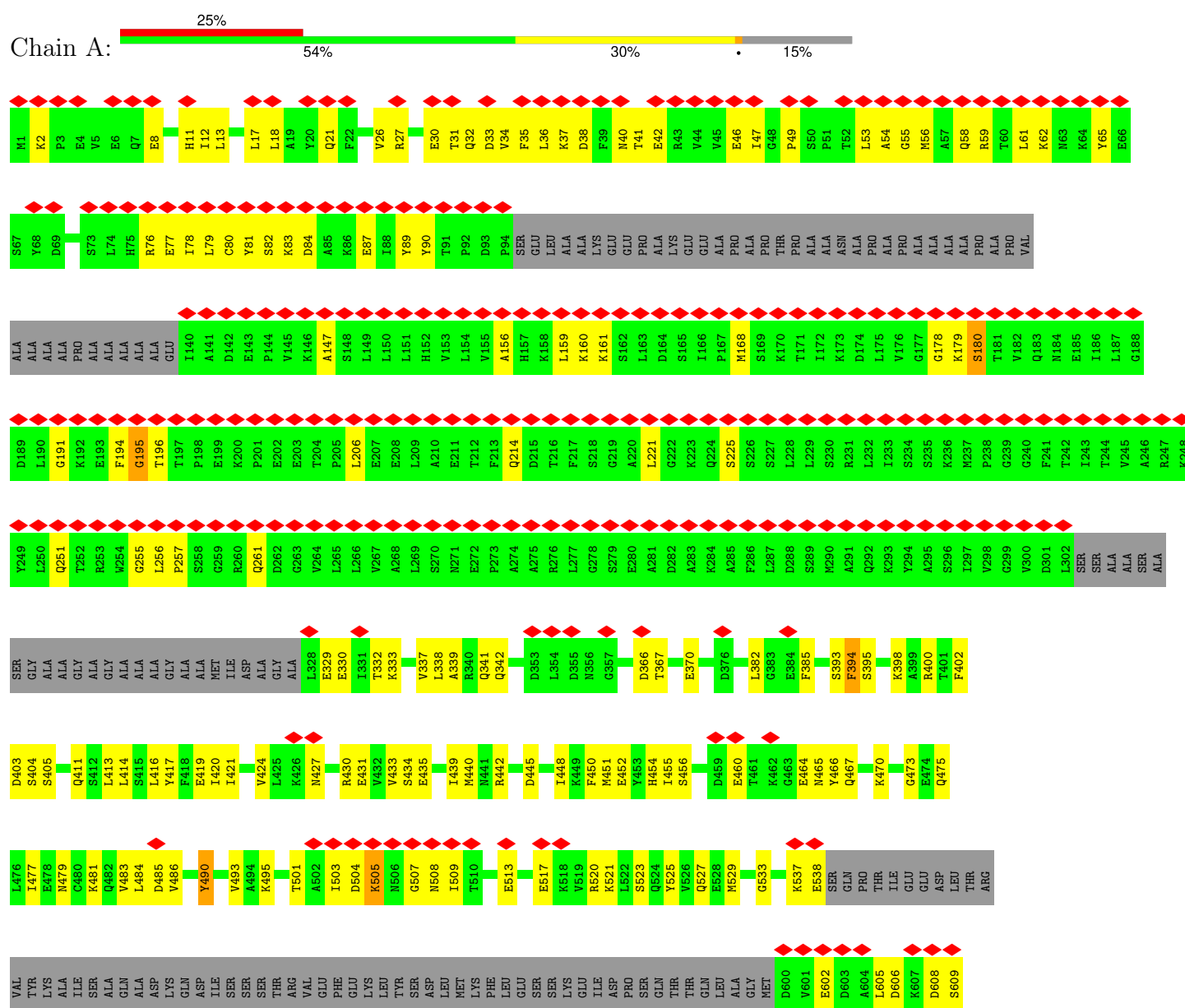


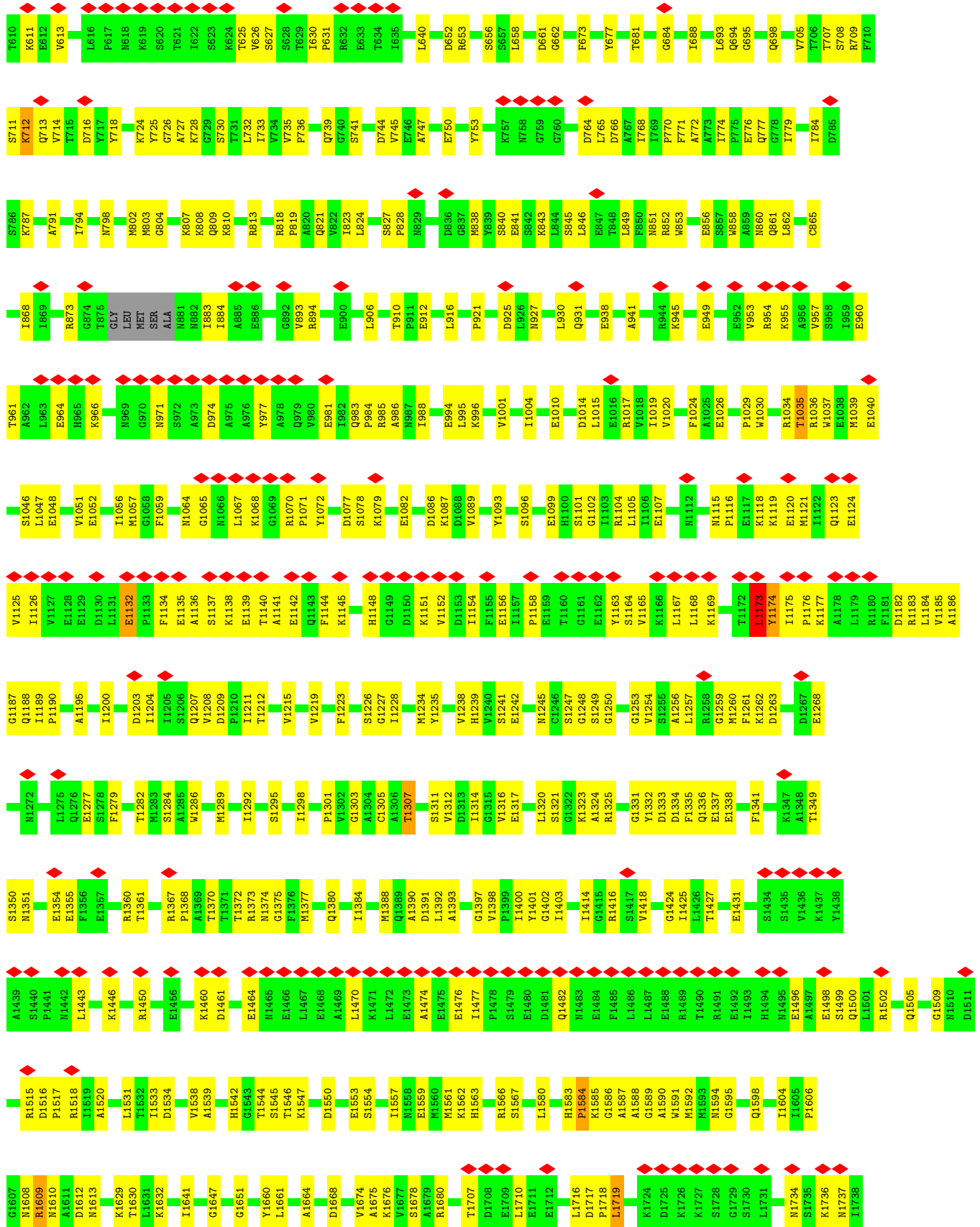
Mol	Chain	Residues	Atoms				AltConf
5	G	1	Total	C	N	O	P
			31	17	4	9	1

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fatty acid synthase subunit alpha







L1464	P1536	L1465	I1537	F1466	P1538	E1467	T1468	E1469	A1540	V1541	L1542	D1543	S1544	A1477	N1478	S1481	K1484	C1485	E1551	G1487	P1488	Y1491	K1496	E1500	I1501	G1502	I1503	V1504	D1505	Y1506	E1507	A1510	S1511	H1512	G1513	N1514	P1515	V1516	G1577	T1578	I1579	T1580	H1581	G1582	M1583	S1584	S1585	S1586	V1589	A1590	A1591	L1592	I1593	E1594	N1595	W1596	A1597	A1598	D1599	S1600
I1338	K1401	P1402	V1403	V1406	S1409	F1410	F1411	Y1412	R1413	G1414	N1415	Y1416	T1417	D1418	F1419	E1420	N1421	T1422	F1423	Q1424	T1425	T1426	V1427	E1428	F1429	V1430	V1431	Q1432	M1433	H1434	I1435	K1436	T1437	S1438	K1439	D1440	I1441	V1442	V1443	L1444	R1445	S1446	K1447	W1449	L1452	D1453	D1454	E1455	D1456	F1457	D1458	L1459	L1460	L1461	K1462	L1463				
F1275	N1276	L1277	D1278	F1279	D1280	P1281	R1282	D1283	V1284	I1285	K1286	G1287	K1288	D1289	F1290	E1291	T1292	T1293	A1294	V1297	D1298	F1299	F1300	T1301	H1302	A1303	V1304	G1305	N1306	N1307	C1308	T1309	E1310	F1311	S1312	S1313	R1314	P1315	D1316	R1317	T1318	M1319	L1320	A1321	P1322	M1323	D1324	F1325	A1326	V1327	V1328	G1330	R1332	I1335						
E1199	P1200	V1201	Q1202	G1203	E1204	L1205	K1206	I1210	K1215	E1216	N1217	I1218	I1219	E1222	M1223	I1224	E1225	N1226	R1227	T1228	M1229	D1230	G1231	K1232	P1233	V1234	S1235	L1236	L1239	Y1240	N1241	F1242	N1243	P1250	I1251	M1255	E1256	D1257	Q1260	R1261	I1262	K1263	E1264	M1265	Y1266	W1267	K1268	L1269	D1272	F1274										
SER	GLU	D1123	S1124	A1125	V1126	F1127	K1128	A1129	T1130	S1131	S1132	T1133	D1134	E1135	E1136	S1137	W1138	L1142	A1143	E1146	I1147	N1148	W1149	R1150	H1151	L1155	F1158	D1162	K1163	M1164	N1168	K1172	K1175	P1176	S1177	Q1178	G1179	M1180	V1181	E1182	E1183	I1184	G1187	N1188	T1189	T1193	L1197	S1198												
T1051	C1052	L1053	H1054	G1056	V1058	Q1061	F1062	T1063	K1064	V1065	I1066	D1067	E1068	P1069	T1070	K1071	M1074	H1078	D1079	G1080	H1081	I1082	L1085	L1086	H1087	Y1090	G1091	D1092	D1093	E1094	S1095	I1096	I1097	P1098	A1099	V1100	E1101	S1107	P1108	V1109	ASP	GLN	SER	GLN	SER	SER	SER	VAL												
P882	E885	A886	K887	R888	D889	Y890	I891	R894	L895	N896	A897	D898	F899	Q900	K901	P902	T906	V907	N908	G909	T945	V846	R947	S948	E949	M917	T918	Y919	R925	L926	I932	R933	S934	T935	W938	F939	D940	R944	R952	R953	Y954	E955	F956	R957	F958	T959	D1044	Q1046	D1047	V1048	Q1049	R1050								
I967	D974	K975	P976	D977	E978	A979	I980	E981	K982	V983	F984	Y987	R991	E992	Q993	F994	D999	I1000	D1001	N1009	P1010	M1011	Q1012	K1013	V1018	D1022	R1023	R1024	E1025	E1026	F1029	K1030	K1031	D1032	S1033	L1034	S1037	E1038	H1039	L1040	E1041	V1044	D1045	Q1046	D1047	V1048	Q1049	R1050												
W811	K812	T813	S814	P815	D816	A817	K818	I821	A822	D829	D830	K831	W832	E833	Q834	H747	T748	V749	M750	L751	I757	R758	R759	I763	M764	L765	I766	F767	G768	S769	G770	F771	G772	S773	A774	D775	D776	W785	K788	F789	M794	D797	S803	R804	V805	M806	I807	A808	K809	E810										
L728	A729	L730	T733	G734	G735	R736	G737	G738	H740	H741	S742	F743	E744	D745	E833	H747	T748	V749	M750	L751	I757	R758	R759	I763	M764	L765	I766	F767	G768	S769	G770	F771	G772	S773	A774	D775	D776	W785	K788	F789	M794	D797	S803	R804	V805	M806	I807	A808	K809	E810										
L665	I666	K667	E668	L669	R670	S671	K672	G673	Y674	Q677	F678	L679	T680	I681	G682	A683	G684	V685	P686	S687	L688	E689	V690	A691	S692	E693	Y694	I695	E696	T697	L698	G699	L700	L703	G704	K706	P707	I710	D711	A712	I713	S714	Q715	V716	I717	N718	I719	A720	K721	A722	H723	P724	N725	F726	P727					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	594818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTFFIND4 within cryoSPARC2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.727	Depositor
Minimum map value	-1.412	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.706	Depositor
Map size (\AA)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PNS, NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	3/12392 (0.0%)	0.60	3/16775 (0.0%)
2	G	0.44	0/16360	0.51	0/22198
All	All	0.52	3/28752 (0.0%)	0.55	3/38973 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1174	TYR	CD1-CE1	-6.37	1.29	1.39
1	A	1174	TYR	CE1-CZ	-6.33	1.30	1.38
1	A	490	TYR	CD1-CE1	-5.27	1.31	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1173	LEU	CA-CB-CG	5.66	128.33	115.30
1	A	1719	LEU	CA-CB-CG	-5.06	103.67	115.30
1	A	1174	TYR	CB-CG-CD2	5.05	124.03	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1132	GLU	Peptide
1	A	1173	LEU	Peptide
1	A	1584	PRO	Peptide
1	A	1716	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12171	0	11679	490	0
2	G	15995	0	15978	772	0
3	A	48	0	22	19	0
3	G	48	0	25	27	0
4	A	5	0	0	0	0
5	G	31	0	19	3	0
All	All	28298	0	27723	1241	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 22.

All (1241) 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:G:740:HIS:HB2	3:G:2102:NAP:C7N	1.22	1.59
1:A:147:ALA:CB	1:A:214:GLN:HA	1.50	1.41
2:G:740:HIS:HD2	3:G:2102:NAP:C2N	1.33	1.39
2:G:740:HIS:HD2	3:G:2102:NAP:C3N	1.40	1.34
2:G:740:HIS:CB	3:G:2102:NAP:C7N	2.06	1.32
1:A:147:ALA:HB2	1:A:214:GLN:CA	1.63	1.29
2:G:1034:LEU:HD13	3:G:2102:NAP:O1N	1.29	1.25
2:G:740:HIS:CD2	3:G:2102:NAP:C2N	2.19	1.24
1:A:147:ALA:CB	1:A:214:GLN:CA	2.14	1.23
2:G:740:HIS:HB2	3:G:2102:NAP:O7N	1.07	1.22
2:G:740:HIS:CD2	3:G:2102:NAP:C3N	2.22	1.20
2:G:1032:ASP:N	3:G:2102:NAP:O1A	1.74	1.20
1:A:688:ILE:CD1	3:A:1901:NAP:O4D	1.89	1.19
2:G:740:HIS:CB	3:G:2102:NAP:O7N	1.91	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:HB3	1:A:214:GLN:CB	1.78	1.12
1:A:688:ILE:HB	3:A:1901:NAP:H51N	1.30	1.10
2:G:740:HIS:HB2	3:G:2102:NAP:N7N	1.75	0.99
2:G:1034:LEU:CD1	3:G:2102:NAP:O1N	2.10	0.99
2:G:740:HIS:CG	3:G:2102:NAP:C7N	2.48	0.96
1:A:688:ILE:CB	3:A:1901:NAP:H51N	1.91	0.93
2:G:740:HIS:CD2	3:G:2102:NAP:C7N	2.52	0.92
1:A:1019:ILE:HG13	1:A:1316:VAL:HG23	1.52	0.92
1:A:688:ILE:HD13	3:A:1901:NAP:O4D	1.06	0.90
1:A:147:ALA:CB	1:A:214:GLN:CB	2.46	0.89
1:A:739:GLN:O	1:A:798:ASN:ND2	2.05	0.88
2:G:740:HIS:CB	3:G:2102:NAP:N7N	2.36	0.87
1:A:1125:VAL:HG12	1:A:1126:ILE:H	1.37	0.87
1:A:753:TYR:O	1:A:813:ARG:NH2	2.10	0.85
2:G:740:HIS:N	3:G:2102:NAP:O7N	2.10	0.84
1:A:771:PHE:HB3	3:A:1901:NAP:H52N	1.57	0.84
1:A:178:GLY:O	1:A:180:SER:N	2.12	0.83
1:A:971:ASN:HA	1:A:974:ASP:HB2	1.60	0.83
2:G:706:LYS:NZ	5:G:2101:FMN:O2'	2.11	0.83
2:G:1888:ILE:HD13	2:G:1900:ALA:HB2	1.60	0.82
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.44	0.82
1:A:709:ARG:NH2	3:A:1901:NAP:O2X	2.06	0.81
1:A:843:LYS:HE3	3:A:1901:NAP:O2D	1.80	0.81
2:G:1313:SER:N	2:G:1319:MET:SD	2.54	0.80
1:A:1123:GLN:HG2	1:A:1124:GLU:H	1.46	0.80
2:G:821:ILE:HG13	2:G:857:ILE:HD11	1.63	0.80
2:G:394:ARG:HA	2:G:397:LYS:HG3	1.64	0.80
2:G:1839:GLN:O	2:G:1844:ARG:NH1	2.15	0.79
1:A:194:PHE:O	1:A:196:THR:N	2.15	0.79
2:G:610:THR:HB	2:G:617:ILE:HD11	1.65	0.79
2:G:1430:VAL:HG13	2:G:1527:LEU:HB3	1.64	0.78
2:G:736:ARG:HD2	2:G:1058:VAL:HG11	1.65	0.78
1:A:395:SER:HB3	1:A:398:LYS:HB2	1.66	0.77
1:A:1219:VAL:HG22	1:A:1384:ILE:HD13	1.67	0.77
1:A:490:TYR:OH	1:A:906:LEU:HB3	1.85	0.77
2:G:739:GLY:HA2	2:G:1054:LEU:HD13	1.67	0.77
2:G:881:VAL:HG13	2:G:882:PRO:HD3	1.67	0.77
2:G:1855:ILE:HD13	2:G:1960:LEU:HD21	1.64	0.77
1:A:1584:PRO:HB2	1:A:1587:ALA:HB3	1.65	0.76
1:A:41:THR:O	1:A:76:ARG:NH1	2.18	0.76
1:A:1183:ARG:NH1	1:A:1350:SER:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:456:GLN:O	2:G:469:ARG:NH2	2.18	0.76
2:G:688:LEU:HD22	2:G:715:GLN:HE22	1.50	0.76
2:G:1881:ARG:HH12	2:G:1949:LYS:HE3	1.50	0.76
1:A:1241:SER:HA	1:A:1295:SER:HB2	1.68	0.76
3:A:1901:NAP:O2X	3:A:1901:NAP:O3B	2.04	0.75
1:A:1067:LEU:HD23	1:A:1068:LYS:HG2	1.69	0.75
2:G:688:LEU:HD13	2:G:719:ILE:HD13	1.69	0.75
2:G:1842:VAL:O	2:G:1844:ARG:NH1	2.20	0.75
2:G:1890:ASN:HB2	2:G:1899:VAL:HG22	1.67	0.75
2:G:524:GLY:O	2:G:526:ARG:NH1	2.20	0.74
2:G:1319:MET:HB3	2:G:1368:VAL:HG21	1.68	0.74
2:G:1704:PHE:CE1	2:G:1709:ILE:HD11	2.22	0.74
2:G:914:LEU:HD23	2:G:1000:ILE:HG23	1.68	0.74
2:G:1623:LYS:HB2	2:G:1643:ARG:HB2	1.69	0.74
2:G:1636:LYS:HB2	2:G:1657:ILE:HG23	1.69	0.74
2:G:1037:SER:HB2	2:G:1053:ILE:HG22	1.69	0.74
1:A:1533:ILE:O	1:A:1566:ARG:NH1	2.19	0.74
2:G:952:ARG:NH2	2:G:967:ILE:O	2.21	0.74
2:G:1621:ALA:N	2:G:1645:GLU:OE1	2.19	0.73
2:G:1210:ILE:HB	2:G:1222:GLU:HB2	1.68	0.73
2:G:128:THR:O	2:G:132:MET:HB2	1.89	0.73
1:A:768:ILE:HG22	1:A:770:PRO:HD3	1.71	0.73
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.22	0.73
2:G:183:LEU:HD11	2:G:254:LYS:HG2	1.69	0.73
2:G:1022:ASP:OD2	2:G:1024:ARG:NH2	2.19	0.72
2:G:1704:PHE:HE1	2:G:1709:ILE:HD11	1.54	0.72
1:A:40:ASN:HA	1:A:76:ARG:HH22	1.53	0.72
1:A:1249:SER:OG	1:A:1250:GLY:N	2.21	0.72
2:G:896:ASN:O	2:G:1050:ARG:NH2	2.22	0.72
2:G:1034:LEU:HD13	3:G:2102:NAP:PN	2.29	0.72
2:G:2047:LYS:O	2:G:2050:GLN:NE2	2.22	0.72
2:G:716:VAL:HG21	2:G:730:LEU:HD21	1.71	0.72
2:G:1739:GLU:HB2	2:G:1987:PRO:HB3	1.70	0.72
2:G:1701:THR:O	2:G:1732:ASN:ND2	2.23	0.72
1:A:1182:ASP:OD2	1:A:1183:ARG:N	2.21	0.72
2:G:1904:LEU:HB3	2:G:1958:LEU:HD22	1.72	0.71
2:G:1031:LYS:HD2	3:G:2102:NAP:O5B	1.90	0.71
1:A:827:SER:OG	3:A:1901:NAP:C5N	2.38	0.71
2:G:1201:VAL:HG11	2:G:1226:ASN:HD21	1.54	0.71
2:G:175:ASP:O	2:G:179:THR:N	2.16	0.71
2:G:596:GLY:N	2:G:618:GLU:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1279:PHE:HB3	2:G:1340:PRO:HB3	1.73	0.71
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.71	0.71
2:G:11:LEU:HB3	2:G:13:HIS:HE1	1.56	0.70
1:A:411:GLN:HE21	1:A:1629:LYS:HE2	1.56	0.70
2:G:56:THR:OG1	2:G:59:GLU:OE1	2.09	0.70
1:A:1077:ASP:OD2	1:A:1078:SER:N	2.24	0.70
2:G:1284:VAL:HG23	2:G:1377:VAL:HB	1.72	0.70
1:A:26:VAL:HG13	2:G:2013:ASN:HB3	1.74	0.70
2:G:326:ASP:O	2:G:330:ASN:ND2	2.22	0.70
2:G:907:VAL:HG23	2:G:917:MET:HE2	1.73	0.70
2:G:1013:LYS:NZ	2:G:1032:ASP:OD2	2.24	0.70
1:A:507:GLY:O	1:A:955:LYS:NZ	2.19	0.70
2:G:1549:THR:HG23	2:G:1552:PRO:HD3	1.74	0.70
2:G:1180:MET:HG2	2:G:1199:GLU:HG2	1.74	0.69
1:A:430:ARG:NH2	1:A:520:ARG:O	2.21	0.69
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	1.74	0.69
1:A:727:ALA:O	1:A:730:SER:OG	2.07	0.69
1:A:843:LYS:CE	3:A:1901:NAP:O2D	2.40	0.69
2:G:174:ARG:NH2	2:G:218:TRP:O	2.25	0.69
2:G:686:PRO:HB2	2:G:691:ALA:HB2	1.72	0.69
1:A:1545:SER:OG	1:A:1545:SER:O	2.10	0.69
2:G:596:GLY:HA3	2:G:650:ASN:HD22	1.57	0.69
2:G:2023:LYS:HD2	2:G:2045:TRP:CE2	2.28	0.69
1:A:1470:LEU:O	1:A:1474:ALA:N	2.26	0.69
2:G:1738:PHE:HB2	2:G:1751:ILE:HD13	1.73	0.69
2:G:1199:GLU:OE2	2:G:1567:ARG:NH2	2.24	0.69
1:A:1123:GLN:HB3	1:A:1177:LYS:HD3	1.75	0.69
2:G:218:TRP:HB3	2:G:225:THR:HG22	1.75	0.68
2:G:626:SER:OG	2:G:627:ALA:N	2.26	0.68
2:G:740:HIS:CA	3:G:2102:NAP:O7N	2.40	0.68
1:A:1414:ILE:O	1:A:1416:ARG:HG2	1.93	0.68
1:A:1186:ALA:O	1:A:1188:GLN:NE2	2.27	0.68
1:A:1373:ARG:HH11	1:A:1547:LYS:HA	1.57	0.68
2:G:1893:VAL:HG23	2:G:1896:GLN:HB3	1.74	0.68
2:G:1800:ALA:O	2:G:2009:LYS:NZ	2.26	0.67
1:A:479:ASN:ND2	1:A:613:VAL:O	2.26	0.67
2:G:517:HIS:HB2	2:G:527:VAL:HG11	1.74	0.67
1:A:332:THR:OG1	1:A:333:LYS:NZ	2.27	0.67
2:G:56:THR:N	2:G:59:GLU:OE2	2.20	0.67
1:A:1259:GLY:HA2	1:A:1263:ASP:HB2	1.75	0.67
2:G:1319:MET:H	2:G:1368:VAL:HB	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:409:PHE:HA	2:G:412:ARG:HD2	1.77	0.67
1:A:985:ARG:N	2:G:956:GLU:O	2.27	0.67
2:G:245:GLN:HG2	2:G:505:GLY:HA2	1.75	0.67
1:A:147:ALA:HB2	1:A:214:GLN:HA	0.71	0.66
2:G:1878:VAL:HG22	2:G:1944:ILE:HD11	1.77	0.66
1:A:1138:LYS:NZ	1:A:1163:TYR:O	2.25	0.66
2:G:1135:GLU:HA	2:G:1176:PRO:HG2	1.77	0.66
1:A:21:GLN:NE2	2:G:1811:GLU:OE2	2.29	0.66
2:G:297:ARG:NH2	2:G:447:ASN:OD1	2.29	0.66
2:G:1126:VAL:HG12	2:G:1183:GLU:HG2	1.77	0.66
2:G:1629:VAL:HB	2:G:1639:LYS:HZ3	1.60	0.66
1:A:46:GLU:OE1	1:A:54:ALA:N	2.25	0.66
2:G:174:ARG:HA	2:G:177:TYR:CE1	2.31	0.66
2:G:362:ALA:HA	2:G:365:GLN:HG3	1.77	0.66
2:G:1863:ALA:HB3	2:G:1866:PHE:HB2	1.76	0.66
3:G:2102:NAP:O2N	3:G:2102:NAP:H3D	1.94	0.66
1:A:1034:ARG:NH2	1:A:1052:GLU:OE2	2.29	0.66
2:G:1424:GLN:HE22	2:G:1426:THR:HB	1.60	0.66
2:G:1767:GLU:HG2	2:G:1768:LYS:HG3	1.78	0.66
2:G:1550:ASN:ND2	2:G:1564:HIS:O	2.26	0.66
2:G:1742:VAL:HG23	2:G:1745:LYS:HB3	1.76	0.66
1:A:688:ILE:HB	3:A:1901:NAP:C5D	2.18	0.66
2:G:1877:ARG:HD3	2:G:1940:LEU:HD13	1.78	0.66
2:G:130:ARG:NH2	2:G:136:PRO:O	2.27	0.65
2:G:1032:ASP:CA	3:G:2102:NAP:O1A	2.44	0.65
1:A:776:GLU:HB2	1:A:779:ILE:HD13	1.78	0.65
1:A:1203:ASP:OD2	1:A:1204:ILE:N	2.28	0.65
1:A:490:TYR:HB3	1:A:698:GLN:HB2	1.79	0.65
1:A:517:GLU:N	1:A:517:GLU:OE1	2.29	0.65
1:A:1403:ILE:HD11	1:A:1661:LEU:HB2	1.77	0.65
2:G:56:THR:HG21	2:G:108:LEU:HD11	1.79	0.65
2:G:818:LYS:HB3	2:G:1066:ILE:HD11	1.78	0.65
2:G:590:PRO:HB3	2:G:1078:HIS:CD2	2.31	0.65
1:A:852:ARG:NH1	1:A:856:GLU:OE2	2.29	0.65
2:G:1775:GLN:HE22	2:G:1836:MET:HB2	1.62	0.65
2:G:23:PRO:HD2	2:G:86:LEU:HD11	1.77	0.65
2:G:740:HIS:CD2	3:G:2102:NAP:H2N	2.27	0.64
2:G:1695:ASP:OD1	2:G:1707:LEU:N	2.21	0.64
1:A:36:LEU:O	1:A:76:ARG:NH2	2.31	0.64
1:A:1144:PHE:HZ	1:A:1174:TYR:CZ	2.15	0.64
1:A:513:GLU:OE2	1:A:873:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:343:ASN:HB2	2:G:416:PHE:HB3	1.80	0.64
2:G:1716:ASN:HD22	2:G:1765:ARG:HA	1.63	0.64
1:A:1584:PRO:O	1:A:1587:ALA:N	2.29	0.64
2:G:720:ALA:HB2	2:G:728:ILE:HD11	1.80	0.64
1:A:394:PHE:HB3	1:A:744:ASP:OD1	1.98	0.64
2:G:213:LEU:HD12	2:G:236:ILE:HG13	1.80	0.64
2:G:1041:GLU:HA	2:G:1046:GLN:HE22	1.62	0.64
2:G:1674:GLN:HE22	2:G:1713:ASN:HB2	1.63	0.64
2:G:707:PRO:HG3	2:G:730:LEU:HD22	1.79	0.63
1:A:464:GLU:OE2	1:A:465:ASN:ND2	2.32	0.63
2:G:993:GLN:NE2	2:G:994:PHE:O	2.32	0.63
1:A:445:ASP:OD1	1:A:445:ASP:N	2.31	0.63
2:G:161:GLY:O	2:G:245:GLN:NE2	2.31	0.63
2:G:2036:GLU:HA	2:G:2039:LYS:HG2	1.80	0.63
1:A:32:GLN:HA	1:A:35:PHE:HE2	1.64	0.63
1:A:413:LEU:HB2	1:A:439:ILE:HD12	1.80	0.63
1:A:1102:GLY:O	1:A:1104:ARG:HG3	1.99	0.63
2:G:740:HIS:CG	3:G:2102:NAP:N7N	2.65	0.63
2:G:1885:LEU:O	2:G:1903:ASP:N	2.30	0.63
1:A:1121:MET:N	1:A:1177:LYS:O	2.23	0.63
2:G:1040:LEU:HD21	2:G:1048:VAL:HB	1.81	0.63
2:G:1491:VAL:HB	2:G:1501:ILE:HD11	1.79	0.63
2:G:37:PHE:CE1	2:G:64:PHE:HA	2.34	0.62
1:A:843:LYS:NZ	3:A:1901:NAP:O2D	2.31	0.62
1:A:1414:ILE:HD13	1:A:1416:ARG:HH21	1.64	0.62
1:A:1070:ARG:HE	1:A:1071:PRO:HD2	1.62	0.62
2:G:54:PRO:HB3	2:G:59:GLU:HG2	1.80	0.62
2:G:148:ALA:HB1	2:G:153:ASN:HB3	1.81	0.62
2:G:259:THR:HG22	2:G:262:GLU:HB2	1.80	0.62
1:A:433:VAL:HG23	1:A:493:VAL:HG11	1.82	0.62
1:A:442:ARG:HD3	1:A:726:GLY:O	2.00	0.62
2:G:199:ILE:HD11	2:G:213:LEU:HD22	1.80	0.62
1:A:400:ARG:NH1	1:A:1367:ARG:HH22	1.97	0.62
1:A:1139:GLU:N	1:A:1139:GLU:OE1	2.33	0.62
2:G:1737:ILE:HG21	2:G:1748:THR:HG23	1.81	0.62
2:G:1866:PHE:HE2	2:G:1871:LEU:HG	1.64	0.62
1:A:1089:VAL:HG23	1:A:1093:TYR:HD2	1.64	0.62
2:G:1366:LEU:HD23	2:G:1366:LEU:H	1.65	0.62
1:A:251:GLN:HA	1:A:256:LEU:H	1.65	0.62
1:A:1120:GLU:OE1	1:A:1120:GLU:N	2.32	0.62
2:G:1172:LYS:NZ	2:G:1574:ASN:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:GLN:O	1:A:1177:LYS:NZ	2.21	0.62
2:G:180:TYR:HB3	2:G:183:LEU:HB3	1.81	0.62
1:A:503:ILE:HG12	1:A:509:ILE:HG13	1.81	0.62
1:A:1134:PHE:HE1	1:A:1168:LEU:O	1.83	0.62
1:A:1334:ASP:OD1	1:A:1335:PHE:N	2.33	0.62
2:G:11:LEU:HD11	2:G:20:LEU:HB2	1.81	0.62
2:G:1550:ASN:ND2	2:G:1579:ILE:O	2.32	0.62
2:G:1685:LYS:NZ	2:G:1689:ASP:OD2	2.33	0.62
2:G:1546:THR:OG1	2:G:1620:THR:N	2.30	0.61
1:A:931:GLN:OE1	1:A:931:GLN:N	2.27	0.61
1:A:1268:GLU:N	1:A:1268:GLU:OE1	2.33	0.61
1:A:1367:ARG:NH1	1:A:1612:ASP:OD1	2.34	0.61
2:G:55:THR:HG23	2:G:56:THR:HG23	1.83	0.61
2:G:696:GLU:N	2:G:696:GLU:OE1	2.33	0.61
2:G:860:ARG:NH1	2:G:898:ASP:OD1	2.32	0.61
2:G:1189:THR:O	2:G:1193:THR:OG1	2.18	0.61
2:G:1468:THR:HA	2:G:1487:GLY:HA3	1.82	0.61
1:A:32:GLN:HA	1:A:35:PHE:CE2	2.34	0.61
2:G:1376:ALA:HA	2:G:1394:GLY:HA2	1.83	0.61
1:A:1474:ALA:O	1:A:1482:GLN:NE2	2.34	0.61
2:G:1963:GLY:N	2:G:1966:CYS:SG	2.72	0.61
1:A:764:ASP:OD2	1:A:818:ARG:NH1	2.33	0.61
1:A:1604:ILE:HG12	1:A:1632:LYS:HG3	1.83	0.61
2:G:96:LEU:HD23	2:G:98:GLY:H	1.66	0.61
2:G:875:LEU:HG	2:G:876:PRO:HD2	1.82	0.61
2:G:723:HIS:HB3	2:G:726:PHE:CD2	2.36	0.61
2:G:1475:LYS:HB3	2:G:1481:SER:HB2	1.82	0.61
1:A:631:PRO:O	1:A:653:ARG:NH2	2.31	0.61
1:A:1176:PRO:C	1:A:1177:LYS:HD2	2.21	0.61
2:G:1667:THR:OG1	2:G:1785:GLU:OE2	2.16	0.61
1:A:191:GLY:O	1:A:195:GLY:N	2.33	0.61
1:A:856:GLU:OE1	1:A:858:TRP:NE1	2.34	0.61
1:A:1544:THR:HG23	1:A:1546:THR:H	1.65	0.61
2:G:953:ARG:HA	2:G:956:GLU:HB2	1.83	0.61
2:G:1828:VAL:HA	2:G:1831:VAL:HG12	1.83	0.60
1:A:1584:PRO:O	1:A:1586:GLY:N	2.35	0.60
2:G:569:LEU:HD21	2:G:1085:LEU:HB3	1.82	0.60
2:G:703:LEU:HB3	2:G:728:ILE:HG22	1.84	0.60
2:G:1877:ARG:HD2	2:G:1944:ILE:HB	1.82	0.60
1:A:1505:GLN:O	1:A:1509:GLY:N	2.34	0.60
2:G:11:LEU:HB3	2:G:13:HIS:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1277:LEU:HB3	2:G:1341:ASN:HB2	1.83	0.60
1:A:1183:ARG:NE	1:A:1349:THR:OG1	2.35	0.60
1:A:1337:GLU:OE1	1:A:1337:GLU:N	2.26	0.60
2:G:305:PHE:CD2	2:G:442:ASP:HB3	2.35	0.60
2:G:919:TYR:OH	2:G:999:ASP:OD2	2.13	0.60
1:A:56:MET:HG2	1:A:59:ARG:HH21	1.66	0.60
1:A:983:GLN:HB3	1:A:1087:LYS:HG3	1.82	0.60
1:A:1719:LEU:HD12	1:A:1744:TYR:HA	1.84	0.60
1:A:807:LYS:HD2	1:A:858:TRP:HB3	1.83	0.60
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.37	0.60
2:G:1227:ARG:HD3	2:G:1555:ARG:HH12	1.65	0.60
2:G:1844:ARG:HB3	2:G:1848:GLY:HA2	1.84	0.60
1:A:1718:PRO:HD2	1:A:1744:TYR:CE1	2.37	0.60
2:G:1142:LEU:O	2:G:1150:ARG:NE	2.29	0.60
1:A:739:GLN:HB2	1:A:794:ILE:HG23	1.83	0.59
1:A:807:LYS:NZ	1:A:861:GLN:OE1	2.32	0.59
1:A:1550:ASP:O	1:A:1554:SER:OG	2.16	0.59
2:G:156:LEU:HD22	2:G:502:LEU:HD22	1.84	0.59
2:G:1925:ILE:H	2:G:1925:ILE:HD12	1.66	0.59
1:A:1035:THR:O	1:A:1035:THR:OG1	2.16	0.59
2:G:59:GLU:CB	2:G:122:LEU:HD21	2.32	0.59
2:G:121:GLU:OE2	2:G:125:ASN:ND2	2.35	0.59
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.85	0.59
1:A:1020:VAL:HG21	1:A:1400:ILE:HG12	1.84	0.59
1:A:1590:ALA:O	1:A:1594:ASN:HB2	2.02	0.59
2:G:37:PHE:CZ	2:G:67:TYR:HB3	2.37	0.59
2:G:459:VAL:HG23	2:G:468:LEU:HB2	1.85	0.59
2:G:515:LEU:O	2:G:519:ASN:ND2	2.35	0.59
1:A:1067:LEU:HB3	1:A:1072:TYR:CD2	2.38	0.59
2:G:408:PRO:HB2	2:G:411:GLU:HG2	1.85	0.59
2:G:1380:SER:HB2	2:G:1424:GLN:HA	1.85	0.59
2:G:1427:VAL:HG22	2:G:1469:GLU:HG2	1.85	0.59
2:G:241:ILE:HB	2:G:275:GLN:HE22	1.68	0.59
1:A:1185:VAL:HG23	1:A:1377:MET:HE1	1.84	0.59
2:G:666:ILE:HG22	2:G:698:LEU:HD22	1.84	0.59
2:G:1243:ASN:N	2:G:1250:PRO:O	2.36	0.59
1:A:1301:PRO:HG3	1:A:1314:ILE:HD13	1.84	0.59
1:A:1542:HIS:N	1:A:1553:GLU:OE2	2.32	0.59
2:G:1034:LEU:CD1	3:G:2102:NAP:PN	2.88	0.59
2:G:1905:ARG:NH1	2:G:1955:PRO:O	2.36	0.59
1:A:81:TYR:HH	1:A:89:TYR:HH	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:580:GLU:OE2	2:G:585:LYS:HE2	2.03	0.58
2:G:1037:SER:HA	2:G:1051:THR:HG21	1.84	0.58
1:A:1247:SER:HG	1:A:1332:TYR:HE1	1.51	0.58
1:A:1168:LEU:HG	1:A:1169:LYS:H	1.68	0.58
2:G:745:ASP:OD1	2:G:746:ALA:N	2.35	0.58
2:G:1936:VAL:O	2:G:1940:LEU:HG	2.03	0.58
1:A:938:GLU:HA	1:A:941:ALA:HB3	1.85	0.58
1:A:1256:ALA:O	1:A:1259:GLY:N	2.36	0.58
2:G:1432:GLN:HG2	2:G:1465:THR:HG22	1.86	0.58
1:A:404:SER:O	1:A:404:SER:OG	2.16	0.58
1:A:1037:TRP:HB2	1:A:1598:GLN:NE2	2.19	0.58
1:A:1377:MET:O	1:A:1583:HIS:N	2.34	0.57
2:G:329:GLU:OE1	2:G:329:GLU:N	2.37	0.57
1:A:1014:ASP:HB2	1:A:1505:GLN:HB2	1.86	0.57
1:A:1675:ALA:O	1:A:1678:SER:OG	2.22	0.57
2:G:1871:LEU:HA	2:G:1874:VAL:HG12	1.85	0.57
2:G:37:PHE:HD1	2:G:63:LYS:HZ2	1.51	0.57
1:A:147:ALA:CB	1:A:214:GLN:N	2.67	0.57
1:A:1589:GLY:HA2	1:A:1592:MET:HG2	1.87	0.57
2:G:1386:THR:HG23	2:G:1411:PHE:HZ	1.69	0.57
1:A:1360:ARG:HG2	1:A:1367:ARG:NH2	2.19	0.57
1:A:1499:SER:HA	1:A:1502:ARG:HG2	1.87	0.57
2:G:582:LYS:HE2	2:G:1108:PRO:HB3	1.86	0.57
2:G:860:ARG:NH2	2:G:1047:ASP:OD2	2.37	0.57
1:A:984:PRO:HG2	1:A:1087:LYS:HD3	1.87	0.57
1:A:1010:GLU:HA	1:A:1664:ALA:HA	1.86	0.57
1:A:1235:TYR:OH	1:A:1292:ILE:O	2.11	0.57
2:G:156:LEU:HD23	2:G:500:HIS:HB2	1.86	0.57
2:G:1101:GLU:HB3	2:G:1147:ILE:HG22	1.86	0.57
1:A:442:ARG:HG3	1:A:727:ALA:HA	1.87	0.57
1:A:708:SER:OG	3:A:1901:NAP:O3X	2.22	0.57
2:G:440:ASN:ND2	2:G:477:GLU:HG2	2.20	0.57
2:G:571:LYS:HB2	2:G:1097:ILE:HG12	1.86	0.57
1:A:1388:MET:HE1	1:A:1398:VAL:HG21	1.87	0.56
2:G:1859:PRO:HB3	2:G:1866:PHE:HD2	1.69	0.56
2:G:740:HIS:HA	2:G:854:ILE:HD13	1.87	0.56
1:A:1189:ILE:HG12	1:A:1380:GLN:HE21	1.71	0.56
2:G:130:ARG:NE	2:G:135:ARG:O	2.35	0.56
2:G:869:ASP:HA	2:G:873:PHE:HD2	1.70	0.56
1:A:986:ALA:HB1	1:A:1051:VAL:HG11	1.87	0.56
1:A:1139:GLU:HG2	1:A:1140:THR:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:161:GLY:H	2:G:505:GLY:HA3	1.70	0.56
1:A:984:PRO:HB3	2:G:959:THR:HG23	1.87	0.56
2:G:1138:TRP:O	2:G:1142:LEU:HG	2.06	0.56
1:A:681:THR:HG21	1:A:802:MET:HE3	1.87	0.56
2:G:260:PRO:HD3	2:G:289:TRP:CE2	2.41	0.56
2:G:1264:GLU:HA	2:G:1267:TRP:HD1	1.69	0.56
1:A:677:TYR:H	1:A:766:ASP:HB2	1.71	0.56
1:A:810:LYS:HB3	1:A:861:GLN:HG2	1.88	0.56
2:G:389:LEU:HA	2:G:392:THR:HG22	1.87	0.56
1:A:840:SER:OG	1:A:841:GLU:N	2.38	0.56
1:A:1239:HIS:CD2	1:A:1241:SER:H	2.23	0.56
2:G:662:GLY:O	2:G:666:ILE:N	2.23	0.56
2:G:688:LEU:HD22	2:G:715:GLN:NE2	2.21	0.56
1:A:442:ARG:HA	1:A:728:LYS:HG3	1.87	0.56
1:A:1360:ARG:NH2	1:A:1372:THR:O	2.38	0.56
2:G:1300:PHE:HA	2:G:1556:VAL:HG11	1.87	0.56
1:A:893:VAL:HG11	1:A:930:LEU:HD21	1.87	0.55
1:A:1239:HIS:CE1	1:A:1718:PRO:HA	2.41	0.55
1:A:1333:ASP:OD2	1:A:1334:ASP:N	2.37	0.55
2:G:220:GLU:HG2	2:G:221:ASN:N	2.21	0.55
2:G:404:GLN:NE2	2:G:413:LYS:H	2.05	0.55
2:G:581:THR:H	2:G:584:SER:HG	1.54	0.55
2:G:586:LEU:HD21	2:G:1107:SER:HA	1.88	0.55
2:G:1227:ARG:NE	2:G:1551:GLU:OE2	2.30	0.55
2:G:1924:ILE:HA	2:G:1927:LEU:HD12	1.87	0.55
1:A:520:ARG:HH12	1:A:521:LYS:NZ	2.04	0.55
2:G:475:ILE:O	2:G:479:ILE:HG13	2.05	0.55
1:A:1137:SER:O	1:A:1138:LYS:HE2	2.06	0.55
1:A:1515:ARG:HH12	1:A:1517:PRO:HD3	1.72	0.55
2:G:1706:ILE:O	2:G:1709:ILE:N	2.39	0.55
1:A:339:ALA:HA	1:A:342:GLN:HG3	1.89	0.55
1:A:804:GLY:O	1:A:808:LYS:NZ	2.24	0.55
2:G:1789:PHE:CD2	2:G:1817:SER:HB2	2.42	0.55
1:A:484:LEU:HD23	1:A:485:ASP:HB2	1.89	0.55
1:A:625:THR:HG22	1:A:627:SER:H	1.72	0.55
1:A:1096:SER:HA	1:A:1099:GLU:HB3	1.87	0.55
2:G:1543:ASP:HA	2:G:1622:LEU:O	2.07	0.55
2:G:1547:PRO:HD3	2:G:1584:PHE:CE2	2.42	0.55
2:G:1637:LEU:O	2:G:1639:LYS:NZ	2.39	0.55
2:G:1914:LEU:HA	2:G:1917:ILE:HG22	1.89	0.55
1:A:960:GLU:O	1:A:964:GLU:N	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:404:GLN:HB3	2:G:412:ARG:HG2	1.88	0.55
2:G:940:ASP:OD2	2:G:1013:LYS:HD2	2.07	0.55
2:G:2015:THR:HG22	2:G:2017:LYS:H	1.71	0.55
2:G:528:ILE:HD12	2:G:547:ILE:HG12	1.88	0.55
2:G:529:VAL:HB	2:G:543:PHE:HD1	1.72	0.55
2:G:881:VAL:CG1	2:G:882:PRO:HD3	2.35	0.55
2:G:1830:VAL:HG12	2:G:1991:PHE:HE2	1.72	0.55
2:G:2041:ILE:HG12	2:G:2047:LYS:NZ	2.22	0.55
1:A:1104:ARG:NH2	1:A:1107:GLU:OE1	2.34	0.55
1:A:1148:HIS:ND1	1:A:1151:LYS:HD3	2.22	0.55
1:A:1189:ILE:H	1:A:1380:GLN:HE21	1.53	0.55
1:A:1286:TRP:HA	1:A:1289:MET:HB2	1.88	0.55
2:G:9:LEU:N	2:G:20:LEU:O	2.32	0.55
2:G:37:PHE:CZ	2:G:64:PHE:HA	2.42	0.55
2:G:879:LYS:C	2:G:882:PRO:HD2	2.26	0.55
2:G:1321:ALA:HB3	2:G:1366:LEU:HG	1.88	0.55
1:A:684:GLY:HA3	1:A:709:ARG:HH22	1.72	0.54
2:G:668:GLU:N	2:G:668:GLU:OE1	2.40	0.54
2:G:695:ILE:HD11	2:G:723:HIS:CD2	2.42	0.54
2:G:582:LYS:HA	2:G:585:LYS:HE3	1.88	0.54
2:G:1339:PHE:N	2:G:1340:PRO:HD2	2.22	0.54
2:G:1433:MET:N	2:G:1464:LEU:O	2.39	0.54
2:G:1511:SER:OG	2:G:1512:HIS:N	2.40	0.54
2:G:573:LYS:HG2	2:G:1101:GLU:HA	1.89	0.54
2:G:669:LEU:HD22	2:G:674:TYR:CE2	2.42	0.54
2:G:1590:ARG:NH2	2:G:1594:GLU:OE2	2.40	0.54
1:A:1141:ALA:HB1	1:A:1145:LYS:HE2	1.90	0.54
1:A:1148:HIS:HB3	1:A:1151:LYS:HD3	1.90	0.54
2:G:1431:TYR:HE1	2:G:1526:THR:HG22	1.71	0.54
1:A:777:GLN:N	1:A:777:GLN:OE1	2.41	0.54
2:G:881:VAL:O	2:G:885:GLU:HG2	2.08	0.54
2:G:1130:THR:N	2:G:1133:THR:OG1	2.28	0.54
1:A:1173:LEU:HB2	1:A:1174:TYR:CD2	2.42	0.54
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.43	0.54
2:G:1738:PHE:O	2:G:1749:GLU:HG3	2.08	0.54
2:G:2024:GLU:O	2:G:2028:ASP:N	2.38	0.54
1:A:53:LEU:HD13	2:G:1665:VAL:HB	1.89	0.54
1:A:58:GLN:HB3	1:A:78:ILE:HD13	1.89	0.54
2:G:349:VAL:HG21	2:G:377:LEU:HD22	1.89	0.54
2:G:619:LEU:H	2:G:649:ILE:HA	1.73	0.54
2:G:1698:PHE:CZ	2:G:1828:VAL:HG22	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HD21	1:A:87:GLU:HB2	1.89	0.54
1:A:1245:ASN:ND2	1:A:1284:SER:OG	2.41	0.54
2:G:9:LEU:O	2:G:20:LEU:N	2.32	0.54
1:A:194:PHE:C	1:A:196:THR:H	2.07	0.53
2:G:404:GLN:HE22	2:G:413:LYS:H	1.56	0.53
1:A:403:ASP:OD1	1:A:1613:ASN:ND2	2.28	0.53
1:A:1544:THR:O	1:A:1545:SER:HB3	2.08	0.53
2:G:259:THR:HG23	2:G:262:GLU:H	1.73	0.53
2:G:264:ARG:NH2	2:G:456:GLN:OE1	2.42	0.53
2:G:1138:TRP:CD1	2:G:1176:PRO:HG3	2.43	0.53
2:G:2026:PHE:HB3	2:G:2038:ILE:HG23	1.89	0.53
1:A:652:ASP:OD1	1:A:653:ARG:N	2.41	0.53
1:A:753:TYR:CE1	1:A:764:ASP:HA	2.43	0.53
2:G:1123:ASP:OD2	2:G:1187:GLY:N	2.41	0.53
2:G:1539:ILE:HB	2:G:1626:ILE:HG22	1.89	0.53
2:G:1691:TRP:HB3	2:G:1707:LEU:HD21	1.91	0.53
1:A:1105:LEU:HA	1:A:1185:VAL:HG12	1.91	0.53
1:A:1137:SER:C	1:A:1138:LYS:HE2	2.29	0.53
1:A:1595:GLY:HA2	1:A:1598:GLN:HG3	1.90	0.53
2:G:1148:ASN:H	2:G:1151:HIS:HB2	1.72	0.53
2:G:1607:GLY:O	2:G:1656:GLU:N	2.29	0.53
1:A:1239:HIS:HD2	1:A:1241:SER:H	1.57	0.53
2:G:55:THR:N	2:G:59:GLU:OE2	2.42	0.53
2:G:220:GLU:HG2	2:G:221:ASN:H	1.74	0.53
2:G:382:PRO:HD3	2:G:431:LEU:HD11	1.89	0.53
2:G:526:ARG:CG	2:G:558:ASN:H	2.22	0.53
2:G:1533:LEU:HD23	2:G:1534:GLU:N	2.23	0.53
2:G:1895:ASN:H	2:G:1898:TYR:HE2	1.57	0.53
2:G:2023:LYS:HD2	2:G:2045:TRP:CZ2	2.44	0.53
2:G:160:PHE:CE2	2:G:504:PHE:HB2	2.43	0.53
2:G:728:ILE:HG13	2:G:763:ILE:HD13	1.91	0.53
2:G:1517:VAL:O	2:G:1521:LYS:N	2.42	0.53
2:G:1754:GLU:OE1	2:G:1754:GLU:N	2.42	0.53
2:G:803:SER:N	5:G:2101:FMN:O1P	2.38	0.53
2:G:1226:ASN:HA	2:G:1233:PRO:HA	1.90	0.53
2:G:1866:PHE:HA	2:G:1925:ILE:HD11	1.91	0.53
2:G:1997:ILE:HG22	2:G:1999:GLU:H	1.74	0.53
1:A:1077:ASP:HB3	1:A:1082:GLU:H	1.73	0.53
1:A:1136:ALA:O	1:A:1164:SER:OG	2.18	0.53
1:A:1174:TYR:O	1:A:1175:ILE:HG13	2.09	0.53
1:A:1397:GLY:O	1:A:1680:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:461:ASP:HB3	2:G:465:GLY:H	1.74	0.53
2:G:1281:PRO:HG2	2:G:1342:THR:OG1	2.09	0.53
2:G:1356:GLY:HA2	2:G:1609:THR:HA	1.89	0.53
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.23	0.53
1:A:483:VAL:O	1:A:486:VAL:HG12	2.08	0.53
1:A:490:TYR:CZ	1:A:906:LEU:HD13	2.43	0.53
1:A:533:GLY:O	1:A:537:LYS:HG2	2.09	0.53
1:A:707:THR:HG21	1:A:718:TYR:HE2	1.74	0.53
2:G:720:ALA:HB2	2:G:763:ILE:HD11	1.90	0.53
2:G:847:ARG:HB3	2:G:851:GLY:HA2	1.89	0.53
2:G:1146:GLU:HG2	2:G:1148:ASN:ND2	2.24	0.53
2:G:1698:PHE:CD2	2:G:1706:ILE:HD11	2.43	0.53
2:G:860:ARG:HB3	2:G:898:ASP:HB3	1.90	0.52
2:G:873:PHE:CD1	2:G:1026:GLU:HB3	2.44	0.52
2:G:1830:VAL:HG12	2:G:1991:PHE:CE2	2.44	0.52
1:A:661:ASP:OD2	1:A:662:GLY:N	2.42	0.52
2:G:145:LEU:HG	2:G:146:PHE:HD1	1.74	0.52
2:G:306:ILE:HD11	2:G:480:VAL:HG12	1.89	0.52
2:G:610:THR:HB	2:G:617:ILE:CD1	2.38	0.52
2:G:1323:MET:H	2:G:1590:ARG:NH2	2.06	0.52
1:A:42:GLU:N	1:A:42:GLU:OE2	2.42	0.52
1:A:87:GLU:OE2	1:A:87:GLU:N	2.33	0.52
1:A:774:ILE:CG2	3:A:1901:NAP:N7A	2.73	0.52
2:G:59:GLU:HB2	2:G:122:LEU:HD21	1.91	0.52
2:G:148:ALA:O	2:G:151:GLU:HG2	2.09	0.52
2:G:843:ILE:HG21	2:G:1057:PRO:HA	1.91	0.52
1:A:858:TRP:HE3	1:A:862:LEU:HB2	1.74	0.52
1:A:1247:SER:OG	1:A:1332:TYR:HE1	1.92	0.52
1:A:520:ARG:HH12	1:A:521:LYS:HZ3	1.55	0.52
1:A:966:LYS:HD3	1:A:971:ASN:HB3	1.91	0.52
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	1.91	0.52
2:G:1234:VAL:HG11	2:G:1269:LEU:HD21	1.92	0.52
2:G:1026:GLU:HA	2:G:1029:PHE:HB3	1.91	0.52
2:G:1709:ILE:HG22	2:G:1771:LEU:HD11	1.91	0.52
1:A:1360:ARG:NH1	1:A:1367:ARG:HG3	2.25	0.52
2:G:716:VAL:HG11	2:G:730:LEU:HD21	1.92	0.52
2:G:1614:ASP:OD1	2:G:1650:VAL:HG12	2.09	0.52
2:G:509:ALA:O	2:G:514:VAL:HG21	2.10	0.52
2:G:741:HIS:HB3	2:G:853:PRO:HG2	1.92	0.52
2:G:1338:ILE:HG22	2:G:1390:VAL:HG21	1.92	0.52
2:G:1359:MET:HE3	2:G:1365:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:ILE:HG21	1:A:1253:GLY:H	1.75	0.52
2:G:569:LEU:HB3	2:G:1097:ILE:CD1	2.40	0.52
2:G:1859:PRO:HG3	2:G:1871:LEU:HD21	1.91	0.52
1:A:490:TYR:HB3	1:A:698:GLN:CB	2.40	0.52
1:A:995:LEU:HD13	1:A:1674:VAL:HG22	1.90	0.52
1:A:1037:TRP:HB2	1:A:1598:GLN:HE21	1.75	0.52
1:A:1139:GLU:HG2	1:A:1140:THR:N	2.25	0.52
2:G:37:PHE:CE2	2:G:67:TYR:HD2	2.28	0.52
2:G:116:LEU:O	2:G:119:THR:HG22	2.10	0.52
1:A:501:THR:HG21	1:A:883:ILE:O	2.10	0.51
2:G:747:HIS:O	2:G:751:LEU:N	2.43	0.51
1:A:711:SER:OG	1:A:713:GLN:OE1	2.14	0.51
1:A:741:SER:OG	1:A:744:ASP:HB2	2.10	0.51
1:A:1104:ARG:HH22	1:A:1188:GLN:HB2	1.75	0.51
1:A:1132:GLU:O	1:A:1132:GLU:HG2	2.10	0.51
2:G:1311:PHE:HA	2:G:1320:LEU:HD21	1.92	0.51
2:G:1678:MET:HG3	2:G:1711:ILE:HG22	1.92	0.51
2:G:873:PHE:CE1	2:G:1026:GLU:HB3	2.45	0.51
1:A:77:GLU:HG3	1:A:79:LEU:CD1	2.40	0.51
1:A:953:VAL:HG12	2:G:1439:LYS:HB2	1.92	0.51
2:G:162:GLY:N	2:G:273:HIS:HB3	2.25	0.51
2:G:205:ALA:O	2:G:208:VAL:HG12	2.10	0.51
1:A:1115:ASN:HD22	1:A:1118:LYS:HB2	1.75	0.51
2:G:1911:THR:HG23	2:G:1966:CYS:SG	2.51	0.51
1:A:1718:PRO:HD2	1:A:1744:TYR:HE1	1.74	0.51
2:G:955:GLU:HG2	2:G:987:TYR:HE2	1.75	0.51
1:A:221:LEU:O	1:A:225:SER:CB	2.59	0.51
1:A:430:ARG:NH2	1:A:606:ASP:OD2	2.42	0.51
1:A:1215:VAL:O	1:A:1219:VAL:HG23	2.10	0.51
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	1.92	0.51
1:A:1370:THR:HG22	1:A:1372:THR:H	1.76	0.51
2:G:785:TRP:NE1	2:G:794:MET:O	2.35	0.51
2:G:1519:PHE:O	2:G:1523:ASN:ND2	2.44	0.51
1:A:684:GLY:CA	1:A:709:ARG:HH22	2.23	0.51
1:A:1262:LYS:NZ	1:A:1338:GLU:OE2	2.38	0.51
1:A:1668:ASP:OD2	1:A:1668:ASP:N	2.43	0.51
1:A:608:ASP:OD2	1:A:611:LYS:HG2	2.11	0.51
1:A:329:GLU:O	1:A:333:LYS:NZ	2.34	0.51
1:A:1017:ARG:HH11	1:A:1320:LEU:HD12	1.74	0.51
1:A:1148:HIS:CD2	1:A:1167:LEU:HD22	2.46	0.51
2:G:116:LEU:HA	2:G:119:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1804:PHE:CD1	2:G:1818:LEU:HG	2.46	0.51
2:G:695:ILE:HD11	2:G:723:HIS:CG	2.46	0.50
2:G:1458:ASP:OD1	2:G:1458:ASP:N	2.44	0.50
1:A:1425:ILE:CG1	1:A:1651:GLY:H	2.24	0.50
2:G:145:LEU:H	2:G:145:LEU:HD23	1.75	0.50
2:G:234:ILE:HG13	2:G:235:PRO:HD3	1.93	0.50
2:G:569:LEU:HD23	2:G:1090:TYR:HE1	1.75	0.50
2:G:1383:ASN:ND2	2:G:1416:TYR:HB2	2.25	0.50
2:G:1906:ALA:O	2:G:1910:VAL:HG23	2.12	0.50
1:A:416:LEU:HD22	1:A:420:ILE:HD11	1.93	0.50
2:G:619:LEU:N	2:G:648:GLY:O	2.44	0.50
2:G:694:TYR:O	2:G:698:LEU:HB2	2.12	0.50
2:G:737:GLY:O	2:G:855:HIS:ND1	2.32	0.50
2:G:740:HIS:CD2	3:G:2102:NAP:N7N	2.79	0.50
2:G:1452:LEU:HB3	2:G:1501:ILE:HG22	1.92	0.50
1:A:828:PRO:HG3	1:A:927:ASN:ND2	2.26	0.50
1:A:846:LEU:O	1:A:849:LEU:HB2	2.10	0.50
1:A:1226:SER:O	1:A:1226:SER:OG	2.23	0.50
2:G:480:VAL:O	2:G:484:ILE:HG12	2.11	0.50
2:G:625:PHE:HD2	3:G:2102:NAP:C6A	1.85	0.50
2:G:900:GLN:HE21	2:G:1052:CYS:H	1.60	0.50
2:G:1300:PHE:CZ	2:G:1304:VAL:HG21	2.46	0.50
2:G:1397:SER:HA	2:G:1403:VAL:HG23	1.93	0.50
2:G:1562:PRO:HB2	2:G:1569:PHE:CD2	2.46	0.50
1:A:609:SER:O	1:A:613:VAL:HG23	2.12	0.50
1:A:1360:ARG:HH21	1:A:1372:THR:HG23	1.77	0.50
2:G:9:LEU:HB3	2:G:20:LEU:HB3	1.94	0.50
2:G:1855:ILE:HB	2:G:1907:LEU:HD21	1.94	0.50
1:A:868:ILE:HG13	1:A:925:ASP:HA	1.94	0.50
1:A:1077:ASP:OD2	1:A:1079:LYS:N	2.39	0.50
1:A:1303:GLY:H	1:A:1307:THR:HB	1.77	0.50
2:G:72:VAL:HG21	2:G:84:LEU:HD22	1.93	0.50
2:G:1318:THR:OG1	2:G:1369:GLY:N	2.44	0.50
2:G:1668:GLY:HA2	2:G:1809:LEU:HB3	1.94	0.50
2:G:118:LYS:O	2:G:122:LEU:HD23	2.10	0.50
2:G:1206:LYS:HD3	2:G:1226:ASN:HD22	1.76	0.50
2:G:1595:ASN:OD1	2:G:1596:TRP:N	2.44	0.50
1:A:42:GLU:OE2	2:G:1661:VAL:HB	2.11	0.50
1:A:403:ASP:O	1:A:405:SER:N	2.44	0.50
1:A:753:TYR:CB	1:A:809:GLN:HG2	2.42	0.50
2:G:1440:ASP:OD1	2:G:1441:ILE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1878:VAL:HG21	2:G:1910:VAL:HG22	1.92	0.50
1:A:1136:ALA:H	1:A:1164:SER:HB3	1.75	0.49
2:G:1320:LEU:H	2:G:1320:LEU:HD23	1.77	0.49
1:A:1373:ARG:HD2	1:A:1547:LYS:HA	1.92	0.49
2:G:139:LYS:NZ	2:G:140:LYS:O	2.38	0.49
2:G:426:PRO:HG3	2:G:431:LEU:HD12	1.95	0.49
2:G:670:ARG:HH11	2:G:670:ARG:HA	1.77	0.49
2:G:1884:TRP:HB2	2:G:1906:ALA:HB2	1.93	0.49
2:G:2015:THR:OG1	2:G:2029:VAL:HG12	2.13	0.49
1:A:431:GLU:OE1	1:A:434:SER:OG	2.31	0.49
1:A:1476:GLU:OE2	1:A:1477:ILE:HG13	2.12	0.49
2:G:1294:ALA:HA	2:G:1368:VAL:HG11	1.94	0.49
1:A:47:ILE:HD13	1:A:81:TYR:HB2	1.93	0.49
1:A:168:MET:O	1:A:206:LEU:CB	2.60	0.49
1:A:460:GLU:OE1	1:A:470:LYS:NZ	2.41	0.49
1:A:475:GLN:O	1:A:479:ASN:N	2.40	0.49
1:A:1335:PHE:O	1:A:1336:GLN:HG2	2.12	0.49
2:G:368:ILE:HG22	2:G:379:VAL:HG12	1.93	0.49
2:G:1706:ILE:HA	2:G:1709:ILE:HD12	1.95	0.49
1:A:520:ARG:HH21	1:A:602:GLU:CD	2.15	0.49
1:A:1207:GLN:NE2	1:A:1277:GLU:OE2	2.45	0.49
2:G:615:TYR:CZ	2:G:1074:MET:HB3	2.47	0.49
2:G:844:VAL:HG12	2:G:845:THR:N	2.27	0.49
2:G:1635:ARG:HD2	2:G:1656:GLU:OE1	2.12	0.49
2:G:1874:VAL:HA	2:G:1877:ARG:CZ	2.42	0.49
2:G:1941:PHE:HA	2:G:1944:ILE:HG22	1.94	0.49
1:A:994:GLU:OE1	1:A:994:GLU:N	2.46	0.49
1:A:1135:GLU:OE1	1:A:1135:GLU:N	2.44	0.49
2:G:818:LYS:O	2:G:821:ILE:HG22	2.13	0.49
1:A:1026:GLU:HB2	1:A:1594:ASN:ND2	2.28	0.49
2:G:435:ALA:O	2:G:439:ILE:HG13	2.12	0.49
2:G:1485:CYS:SG	2:G:1514:ASN:ND2	2.77	0.49
1:A:784:ILE:HD13	1:A:838:MET:HG3	1.93	0.49
2:G:31:SER:HA	2:G:34:GLN:HE21	1.78	0.49
2:G:59:GLU:HB3	2:G:122:LEU:HD21	1.95	0.49
2:G:691:ALA:HA	2:G:694:TYR:CD2	2.47	0.49
2:G:736:ARG:NE	2:G:769:SER:O	2.33	0.49
1:A:521:LYS:HZ3	1:A:605:LEU:HD12	1.78	0.49
2:G:549:ASP:HB3	2:G:554:GLY:HA3	1.93	0.49
2:G:698:LEU:O	2:G:700:LEU:N	2.44	0.49
2:G:902:PRO:HG3	2:G:1044:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1447:LYS:HG2	2:G:1449:TRP:CE2	2.46	0.49
2:G:1452:LEU:HA	2:G:1502:GLY:HA3	1.94	0.49
1:A:1138:LYS:N	1:A:1139:GLU:OE1	2.46	0.49
2:G:202:THR:HG21	2:G:205:ALA:HB3	1.94	0.49
2:G:275:GLN:HE21	2:G:303:LEU:HD13	1.77	0.49
2:G:1215:LYS:O	2:G:1218:ILE:HG12	2.13	0.49
2:G:1695:ASP:OD1	2:G:1705:SER:OG	2.24	0.49
1:A:411:GLN:NE2	1:A:1629:LYS:HG2	2.27	0.48
1:A:727:ALA:N	1:A:730:SER:OG	2.46	0.48
1:A:1354:GLU:OE2	1:A:1374:ASN:ND2	2.28	0.48
2:G:59:GLU:HA	2:G:122:LEU:HD11	1.95	0.48
2:G:610:THR:OG1	2:G:1070:ILE:HG12	2.12	0.48
2:G:1604:ARG:O	2:G:1657:ILE:HD12	2.13	0.48
2:G:1917:ILE:O	2:G:1921:LYS:N	2.43	0.48
1:A:1141:ALA:O	1:A:1145:LYS:HD3	2.13	0.48
2:G:35:GLU:HA	2:G:38:ASN:HD21	1.78	0.48
1:A:1189:ILE:HG12	1:A:1380:GLN:NE2	2.27	0.48
1:A:750:GLU:OE1	1:A:750:GLU:N	2.37	0.48
1:A:827:SER:HG	3:A:1901:NAP:C5N	2.25	0.48
2:G:1738:PHE:HB2	2:G:1751:ILE:CD1	2.43	0.48
1:A:159:LEU:O	1:A:161:LYS:N	2.45	0.48
2:G:887:LYS:O	2:G:891:ILE:HG23	2.13	0.48
2:G:1359:MET:HG3	2:G:1606:ARG:HH21	1.79	0.48
2:G:1484:LYS:NZ	2:G:1507:GLU:HB2	2.28	0.48
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	1.95	0.48
1:A:30:GLU:HB2	2:G:2016:ALA:CB	2.43	0.48
1:A:974:ASP:HA	1:A:977:TYR:CD2	2.49	0.48
2:G:733:THR:OG1	2:G:769:SER:HB3	2.12	0.48
2:G:1224:ILE:O	2:G:1568:HIS:NE2	2.46	0.48
2:G:1373:SER:N	2:G:1397:SER:O	2.42	0.48
2:G:1454:ASP:OD1	2:G:1454:ASP:N	2.45	0.48
2:G:1822:MET:HG3	2:G:1827:LEU:HB2	1.94	0.48
1:A:27:ARG:HH21	2:G:2016:ALA:H	1.60	0.48
1:A:440:MET:CE	1:A:479:ASN:HB3	2.43	0.48
1:A:1317:GLU:O	1:A:1321:SER:HB3	2.13	0.48
2:G:214:ASN:HB3	2:G:217:GLU:OE2	2.13	0.48
2:G:1924:ILE:HD12	2:G:1924:ILE:H	1.77	0.48
2:G:215:ILE:HD12	2:G:240:LEU:HD21	1.94	0.48
2:G:646:THR:HG21	2:G:677:GLN:HB2	1.95	0.48
2:G:1079:ASP:OD2	2:G:1080:GLY:N	2.46	0.48
2:G:1129:ALA:HB2	2:G:1138:TRP:CH2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1957:PRO:HB2	2:G:1959:LYS:HE2	1.95	0.48
1:A:1116:PRO:HB2	1:A:1184:LEU:HD13	1.96	0.48
1:A:1144:PHE:HZ	1:A:1174:TYR:HH	1.62	0.48
2:G:45:THR:O	2:G:48:PHE:N	2.47	0.48
2:G:246:LEU:O	2:G:250:VAL:HG13	2.13	0.48
2:G:809:LYS:HB3	2:G:1067:ASP:O	2.13	0.48
2:G:2046:GLU:N	2:G:2046:GLU:OE1	2.46	0.48
1:A:421:ILE:HA	1:A:465:ASN:HB3	1.96	0.48
1:A:1052:GLU:O	1:A:1056:ILE:HG23	2.14	0.48
2:G:543:PHE:HB2	2:G:545:GLN:HE22	1.79	0.48
2:G:725:ASN:HA	2:G:1109:VAL:HG11	1.96	0.48
2:G:1839:GLN:HE21	2:G:1844:ARG:HD2	1.79	0.48
1:A:985:ARG:HG3	2:G:956:GLU:HB3	1.95	0.47
1:A:1334:ASP:CG	1:A:1335:PHE:H	2.17	0.47
2:G:270:ALA:O	2:G:459:VAL:HA	2.13	0.47
1:A:1608:ASN:O	1:A:1610:ASN:N	2.47	0.47
2:G:16:LEU:HD23	2:G:48:PHE:CD2	2.50	0.47
2:G:155:GLN:HG2	2:G:499:THR:HG23	1.95	0.47
2:G:336:SER:OG	2:G:423:VAL:O	2.32	0.47
2:G:710:ILE:HD13	2:G:749:PRO:HB3	1.96	0.47
2:G:1889:VAL:HG23	2:G:1899:VAL:HG23	1.97	0.47
1:A:33:ASP:O	1:A:37:LYS:N	2.45	0.47
2:G:20:LEU:HD12	2:G:90:GLU:CD	2.35	0.47
2:G:900:GLN:NE2	2:G:1052:CYS:H	2.11	0.47
2:G:1491:VAL:CB	2:G:1501:ILE:HD11	2.44	0.47
2:G:1908:ASP:OD2	2:G:1954:LYS:HD3	2.14	0.47
2:G:1976:PHE:HD1	2:G:1977:HIS:HD1	1.59	0.47
1:A:1125:VAL:CG1	1:A:1126:ILE:H	2.16	0.47
2:G:109:LEU:HG	2:G:114:THR:HG23	1.95	0.47
2:G:864:LEU:HD11	2:G:868:PHE:CZ	2.49	0.47
2:G:1038:GLU:H	2:G:1038:GLU:HG2	1.53	0.47
2:G:1485:CYS:HB2	2:G:1506:TYR:HB3	1.95	0.47
2:G:1850:SER:HB3	2:G:1973:SER:OG	2.14	0.47
1:A:385:PHE:CD2	1:A:787:LYS:HA	2.50	0.47
1:A:810:LYS:CB	1:A:861:GLN:HG2	2.45	0.47
1:A:1040:GLU:HA	1:A:1580:LEU:HD11	1.97	0.47
1:A:1390:ALA:O	1:A:1393:ALA:N	2.48	0.47
2:G:1310:ASP:OD1	2:G:1602:SER:N	2.45	0.47
2:G:1730:ARG:NH2	2:G:1757:GLU:O	2.47	0.47
2:G:259:THR:HA	2:G:289:TRP:NE1	2.30	0.47
2:G:865:TRP:HE1	2:G:1030:LYS:HZ3	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1058:VAL:O	2:G:1061:GLN:HG2	2.15	0.47
2:G:1517:VAL:O	2:G:1521:LYS:HG2	2.13	0.47
1:A:413:LEU:HD23	1:A:450:PHE:CD2	2.49	0.47
1:A:433:VAL:HG13	1:A:609:SER:HB2	1.95	0.47
1:A:1584:PRO:HG2	1:A:1588:ALA:N	2.30	0.47
2:G:598:THR:OG1	2:G:599:PRO:HD3	2.14	0.47
2:G:633:ALA:O	2:G:637:VAL:HG13	2.14	0.47
2:G:895:LEU:HD13	2:G:1018:VAL:HG21	1.95	0.47
2:G:1201:VAL:HG11	2:G:1226:ASN:ND2	2.27	0.47
2:G:1287:GLY:HA3	2:G:1374:THR:HG23	1.97	0.47
2:G:1718:THR:HA	2:G:1763:THR:HA	1.96	0.47
2:G:1858:ASN:ND2	2:G:1861:ARG:HG3	2.30	0.47
2:G:1960:LEU:HD23	2:G:1968:PRO:HB3	1.96	0.47
1:A:13:LEU:HD22	2:G:2026:PHE:CE1	2.50	0.47
1:A:695:GLY:HA3	1:A:906:LEU:HD11	1.97	0.47
1:A:1120:GLU:H	1:A:1120:GLU:CD	2.18	0.47
2:G:66:GLY:O	2:G:69:SER:OG	2.22	0.47
2:G:530:ALA:HA	2:G:547:ILE:HD11	1.95	0.47
2:G:1263:LYS:HD3	2:G:1347:LEU:HD11	1.96	0.47
2:G:1323:MET:H	2:G:1590:ARG:HH22	1.60	0.47
2:G:1775:GLN:HE22	2:G:1836:MET:CB	2.26	0.47
2:G:1956:ARG:O	2:G:1956:ARG:NE	2.48	0.47
1:A:712:LYS:HB3	1:A:1361:THR:HG21	1.96	0.47
2:G:6:THR:HA	2:G:23:PRO:HA	1.96	0.47
2:G:421:LEU:O	2:G:423:VAL:N	2.48	0.47
2:G:589:ARG:HG2	2:G:590:PRO:HD2	1.96	0.47
2:G:1381:VAL:HG12	2:G:1390:VAL:HG12	1.97	0.47
2:G:1799:PRO:HD2	2:G:1802:ALA:HB2	1.96	0.47
1:A:640:LEU:N	1:A:656:SER:OG	2.48	0.47
1:A:1059:PHE:HA	1:A:1079:LYS:NZ	2.30	0.47
1:A:1298:ILE:HD13	1:A:1298:ILE:HA	1.65	0.47
2:G:67:TYR:CZ	2:G:71:LEU:HD11	2.50	0.47
2:G:831:LYS:HE2	2:G:834:GLN:HG3	1.97	0.47
2:G:857:ILE:O	2:G:862:VAL:HG11	2.15	0.47
1:A:257:PRO:O	1:A:261:GLN:N	2.41	0.46
1:A:338:LEU:O	1:A:342:GLN:N	2.28	0.46
1:A:1064:ASN:HA	1:A:1072:TYR:O	2.15	0.46
2:G:1324:ASP:O	2:G:1327:ILE:HG22	2.15	0.46
2:G:1342:THR:O	2:G:1421:ASN:ND2	2.48	0.46
2:G:1351:VAL:HG21	2:G:1413:ARG:NH2	2.30	0.46
1:A:49:PRO:HD3	2:G:1784:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:VAL:HG11	1:A:1154:ILE:HG23	1.96	0.46
2:G:138:ASP:OD1	2:G:138:ASP:N	2.48	0.46
2:G:264:ARG:HH21	2:G:456:GLN:HB2	1.80	0.46
1:A:1119:LYS:HE3	1:A:1341:PHE:CD1	2.49	0.46
1:A:1397:GLY:O	1:A:1680:ARG:HG3	2.15	0.46
1:A:1446:LYS:O	1:A:1450:ARG:HG3	2.14	0.46
2:G:748:THR:HA	2:G:751:LEU:HB3	1.98	0.46
2:G:932:ILE:HD11	2:G:939:PHE:HB2	1.97	0.46
2:G:1323:MET:HE1	2:G:1608:TYR:HB3	1.97	0.46
2:G:1550:ASN:HB3	2:G:1581:HIS:CE1	2.51	0.46
2:G:2030:TYR:HB2	2:G:2038:ILE:HG21	1.97	0.46
1:A:1360:ARG:NH2	1:A:1367:ARG:HD2	2.30	0.46
2:G:36:GLN:O	2:G:40:ILE:HG13	2.16	0.46
2:G:1737:ILE:O	2:G:1833:TYR:OH	2.34	0.46
1:A:46:GLU:HB3	1:A:80:CYS:HA	1.97	0.46
1:A:693:LEU:HD13	1:A:705:VAL:HG11	1.97	0.46
1:A:858:TRP:CE3	1:A:862:LEU:HB2	2.50	0.46
2:G:273:HIS:CG	2:G:274:SER:H	2.34	0.46
2:G:573:LYS:CG	2:G:1101:GLU:HA	2.45	0.46
2:G:804:ARG:NH2	2:G:1068:GLU:OE1	2.37	0.46
2:G:1643:ARG:HB3	2:G:1647:ASP:HA	1.96	0.46
2:G:1812:TYR:OH	2:G:1834:ARG:NE	2.48	0.46
2:G:1924:ILE:O	2:G:1928:GLN:NE2	2.48	0.46
2:G:239:PRO:O	2:G:243:VAL:HG13	2.16	0.46
2:G:1093:ASP:OD1	2:G:1096:LYS:HB2	2.16	0.46
2:G:1138:TRP:NE1	2:G:1142:LEU:HD11	2.30	0.46
2:G:1722:GLY:N	2:G:1726:GLY:HA3	2.31	0.46
1:A:467:GLN:O	1:A:467:GLN:NE2	2.49	0.46
2:G:490:TRP:CH2	2:G:512:LEU:HD21	2.51	0.46
2:G:649:ILE:HD13	2:G:666:ILE:HD11	1.98	0.46
1:A:803:MET:HE1	1:A:849:LEU:HD21	1.98	0.46
1:A:1029:PRO:HG3	1:A:1187:GLY:O	2.16	0.46
2:G:2036:GLU:CD	2:G:2037:PRO:HD3	2.36	0.46
1:A:55:GLY:O	1:A:59:ARG:HG2	2.16	0.46
1:A:1534:ASP:OD2	1:A:1567:SER:OG	2.32	0.46
2:G:978:GLU:OE1	2:G:978:GLU:N	2.49	0.46
2:G:1149:TRP:HB2	2:G:1219:ILE:HD11	1.98	0.46
1:A:395:SER:HB3	1:A:398:LYS:HD2	1.97	0.46
1:A:452:GLU:O	1:A:456:SER:OG	2.29	0.46
1:A:521:LYS:HD2	1:A:523:SER:OG	2.15	0.46
1:A:527:GLN:HG2	1:A:626:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:GLU:CD	1:A:1135:GLU:H	2.19	0.46
1:A:1461:ASP:O	1:A:1464:GLU:HG2	2.15	0.46
2:G:310:CYS:O	2:G:313:ALA:N	2.49	0.46
2:G:410:SER:OG	2:G:411:GLU:OE2	2.33	0.46
2:G:1741:ILE:HD11	2:G:1986:LYS:HG2	1.97	0.46
2:G:142:ASN:HD21	2:G:147:ARG:NE	2.13	0.45
2:G:502:LEU:HD23	2:G:502:LEU:H	1.81	0.45
2:G:634:ILE:O	2:G:637:VAL:HG22	2.17	0.45
1:A:430:ARG:HG3	1:A:495:LYS:HG3	1.98	0.45
1:A:821:GLN:OE1	1:A:823:ILE:HD11	2.16	0.45
1:A:957:VAL:HG23	2:G:1443:VAL:HG12	1.99	0.45
1:A:1606:PRO:HA	1:A:1630:THR:HG23	1.99	0.45
2:G:540:ASP:OD1	2:G:540:ASP:N	2.49	0.45
2:G:646:THR:CG2	2:G:677:GLN:HB2	2.46	0.45
2:G:906:THR:OG1	2:G:925:ARG:NH2	2.49	0.45
2:G:1488:PRO:HA	2:G:1503:ILE:HD13	1.98	0.45
2:G:1669:GLN:HB3	2:G:1809:LEU:HD13	1.99	0.45
2:G:1716:ASN:ND2	2:G:1765:ARG:HA	2.29	0.45
2:G:1819:ALA:HA	2:G:2005:ARG:HD2	1.98	0.45
2:G:273:HIS:HB2	2:G:512:LEU:HD22	1.98	0.45
2:G:479:ILE:O	2:G:483:ILE:HG13	2.16	0.45
2:G:938:TRP:CD2	2:G:944:ARG:HG3	2.51	0.45
2:G:1611:GLN:N	2:G:1652:THR:O	2.35	0.45
2:G:1644:ASN:HB3	2:G:1646:ASP:OD2	2.16	0.45
1:A:1001:VAL:HA	1:A:1004:ILE:HG22	1.98	0.45
1:A:1036:ARG:HH21	1:A:1598:GLN:HE21	1.65	0.45
1:A:1209:ASP:OD2	1:A:1253:GLY:HA2	2.17	0.45
2:G:430:HIS:HA	2:G:433:VAL:HG23	1.99	0.45
2:G:1641:GLU:OE2	2:G:1643:ARG:NE	2.48	0.45
2:G:1712:ASN:OD1	2:G:1712:ASN:N	2.50	0.45
1:A:329:GLU:O	1:A:332:THR:OG1	2.25	0.45
1:A:1020:VAL:HG23	1:A:1402:GLY:O	2.16	0.45
1:A:1046:SER:OG	1:A:1047:LEU:N	2.48	0.45
1:A:1123:GLN:HB3	1:A:1177:LYS:CD	2.45	0.45
1:A:1182:ASP:O	1:A:1184:LEU:HB2	2.16	0.45
1:A:1207:GLN:HE22	1:A:1286:TRP:HZ2	1.65	0.45
1:A:1238:VAL:HG22	1:A:1242:GLU:HB2	1.98	0.45
1:A:1355:GLU:CD	1:A:1360:ARG:HD2	2.37	0.45
2:G:126:TYR:HD2	2:G:127:ILE:HD13	1.80	0.45
2:G:1168:ASN:O	2:G:1172:LYS:HG2	2.17	0.45
2:G:1291:GLU:HA	2:G:1371:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1531:VAL:HG13	2:G:1631:MET:HB2	1.99	0.45
1:A:90:TYR:O	2:G:1533:LEU:HD21	2.17	0.45
1:A:1559:GLU:O	1:A:1563:HIS:N	2.39	0.45
2:G:1357:TYR:CD1	2:G:1406:VAL:HG12	2.52	0.45
2:G:1681:TYR:CE2	2:G:1691:TRP:HB2	2.52	0.45
1:A:413:LEU:HD23	1:A:450:PHE:CE2	2.52	0.45
1:A:739:GLN:HG3	1:A:772:ALA:HB3	1.98	0.45
1:A:819:PRO:HB3	1:A:860:ASN:O	2.16	0.45
1:A:1431:GLU:HB3	1:A:1520:ALA:HB2	1.99	0.45
2:G:2041:ILE:HG12	2:G:2047:LYS:HZ1	1.82	0.45
1:A:27:ARG:NH2	2:G:2015:THR:HA	2.32	0.45
2:G:109:LEU:HD12	2:G:119:THR:HG21	1.98	0.45
2:G:268:LYS:O	2:G:458:PRO:HD2	2.16	0.45
2:G:877:LYS:HG3	2:G:878:ASN:N	2.31	0.45
2:G:938:TRP:CE2	2:G:944:ARG:HG3	2.52	0.45
2:G:1745:LYS:NZ	2:G:1747:LYS:HA	2.32	0.45
1:A:333:LYS:O	1:A:337:VAL:HG13	2.16	0.45
1:A:853:TRP:CE3	1:A:921:PRO:HD3	2.51	0.45
1:A:1026:GLU:OE1	1:A:1594:ASN:ND2	2.47	0.45
1:A:1245:ASN:O	1:A:1298:ILE:HG23	2.17	0.45
1:A:1707:THR:O	1:A:1710:LEU:N	2.46	0.45
2:G:68:VAL:O	2:G:72:VAL:HG23	2.17	0.45
2:G:297:ARG:NE	2:G:447:ASN:HD21	2.15	0.45
2:G:391:LEU:O	2:G:394:ARG:N	2.42	0.45
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.82	0.45
2:G:872:ILE:O	2:G:875:LEU:HB3	2.17	0.45
2:G:1514:ASN:ND2	2:G:1516:VAL:HG22	2.32	0.45
1:A:1418:VAL:HG12	1:A:1647:GLY:HA2	1.99	0.45
2:G:812:LYS:HD3	2:G:812:LYS:HA	1.56	0.45
2:G:1151:HIS:CD2	2:G:1155:LEU:HD12	2.51	0.45
2:G:1669:GLN:HA	2:G:1781:LEU:HD13	1.99	0.45
2:G:1892:ASN:HB2	2:G:1897:GLN:HB3	1.99	0.45
1:A:945:LYS:O	1:A:949:GLU:HG2	2.17	0.44
1:A:981:GLU:OE2	2:G:962:LYS:HB2	2.17	0.44
1:A:1211:ILE:O	1:A:1215:VAL:HG23	2.17	0.44
1:A:1368:PRO:HG2	1:A:1608:ASN:ND2	2.31	0.44
1:A:1717:ASP:OD2	1:A:1739:GLN:HB2	2.17	0.44
2:G:408:PRO:HB3	2:G:833:GLU:OE2	2.17	0.44
2:G:1257:ASP:OD1	2:G:1260:GLN:HB2	2.18	0.44
2:G:1598:ALA:HB2	2:G:1657:ILE:HD11	1.98	0.44
2:G:1767:GLU:HG2	2:G:1768:LYS:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1804:PHE:CG	2:G:1818:LEU:HG	2.52	0.44
2:G:1854:MET:HA	2:G:1901:ALA:HA	1.98	0.44
1:A:330:GLU:HA	1:A:333:LYS:HG2	1.99	0.44
1:A:711:SER:H	1:A:714:VAL:HG12	1.82	0.44
2:G:230:TYR:O	2:G:236:ILE:HG21	2.17	0.44
2:G:437:ASP:OD1	2:G:437:ASP:N	2.50	0.44
2:G:587:ILE:HG13	2:G:589:ARG:H	1.82	0.44
2:G:665:LEU:HD21	2:G:669:LEU:HD12	1.99	0.44
2:G:734:GLY:H	2:G:769:SER:HB3	1.81	0.44
2:G:1539:ILE:HD11	2:G:1628:HIS:HB2	1.97	0.44
2:G:1786:LYS:NZ	2:G:1816:ALA:O	2.50	0.44
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.53	0.44
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.77	0.44
1:A:930:LEU:HD23	1:A:930:LEU:HA	1.71	0.44
2:G:124:LYS:HB2	2:G:179:THR:HA	1.99	0.44
2:G:423:VAL:HG12	2:G:424:ALA:H	1.81	0.44
2:G:1357:TYR:HD1	2:G:1406:VAL:HG12	1.82	0.44
2:G:1713:ASN:ND2	2:G:1771:LEU:HB2	2.33	0.44
2:G:297:ARG:NH1	2:G:301:THR:HG21	2.32	0.44
2:G:330:ASN:HB3	2:G:394:ARG:HH12	1.83	0.44
2:G:543:PHE:HB2	2:G:545:GLN:NE2	2.32	0.44
1:A:1123:GLN:HG2	1:A:1124:GLU:N	2.24	0.44
1:A:1254:VAL:HA	1:A:1257:LEU:HD12	1.99	0.44
1:A:1351:ASN:HB3	1:A:1354:GLU:HG2	2.00	0.44
1:A:1460:LYS:HE3	1:A:1460:LYS:HB3	1.87	0.44
2:G:597:MET:HB2	2:G:601:THR:HG23	2.00	0.44
2:G:604:PRO:HA	2:G:607:VAL:HG12	2.00	0.44
2:G:1624:THR:HA	2:G:1642:THR:HA	2.00	0.44
1:A:11:HIS:HB2	2:G:2001:VAL:HG11	2.00	0.44
1:A:843:LYS:CE	3:A:1901:NAP:HO2N	2.30	0.44
1:A:1086:ASP:O	1:A:1089:VAL:HG12	2.18	0.44
2:G:81:ASP:OD1	2:G:81:ASP:N	2.48	0.44
2:G:615:TYR:CE2	2:G:1074:MET:HB3	2.53	0.44
2:G:821:ILE:HD11	2:G:1055:HIS:ND1	2.32	0.44
2:G:861:GLY:HA2	2:G:898:ASP:O	2.17	0.44
1:A:774:ILE:HD11	1:A:791:ALA:HB2	2.00	0.44
1:A:1087:LYS:HA	1:A:1087:LYS:HD2	1.81	0.44
1:A:1234:MET:O	1:A:1238:VAL:HG12	2.18	0.44
2:G:148:ALA:O	2:G:153:ASN:N	2.50	0.44
2:G:368:ILE:HA	2:G:379:VAL:HG12	2.00	0.44
2:G:608:ALA:HA	2:G:611:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:810:GLU:CD	2:G:1070:ILE:H	2.21	0.44
2:G:2037:PRO:HA	2:G:2040:GLU:OE2	2.17	0.44
1:A:477:ILE:O	1:A:481:LYS:HG3	2.18	0.44
1:A:985:ARG:HB2	2:G:957:ARG:HA	2.00	0.44
1:A:1125:VAL:HG12	1:A:1126:ILE:N	2.18	0.44
1:A:1248:GLY:O	1:A:1331:GLY:HA2	2.17	0.44
2:G:848:SER:OG	2:G:849:GLU:N	2.51	0.44
2:G:1001:ASP:OD2	2:G:1001:ASP:N	2.48	0.44
2:G:1297:VAL:HG23	2:G:1319:MET:HG2	2.00	0.44
2:G:1561:ASN:HD21	2:G:1563:ILE:HG12	1.82	0.44
1:A:658:LEU:HD11	1:A:916:LEU:HD22	1.99	0.44
2:G:457:ILE:C	2:G:469:ARG:HH21	2.21	0.44
2:G:686:PRO:HB3	2:G:690:VAL:HG13	2.00	0.44
2:G:741:HIS:CE1	2:G:855:HIS:NE2	2.86	0.44
2:G:1624:THR:OG1	2:G:1642:THR:HG22	2.18	0.44
1:A:8:GLU:O	1:A:12:ILE:HG12	2.18	0.43
1:A:448:ILE:HD13	1:A:481:LYS:HG2	2.00	0.43
1:A:1298:ILE:HD11	1:A:1323:LYS:HZ1	1.83	0.43
2:G:394:ARG:HA	2:G:397:LYS:CG	2.43	0.43
2:G:461:ASP:OD2	2:G:478:ARG:HD3	2.18	0.43
2:G:736:ARG:NH1	2:G:829:ASP:OD2	2.51	0.43
2:G:1224:ILE:HA	2:G:1235:SER:HA	1.99	0.43
2:G:1299:ASP:OD2	2:G:1556:VAL:HG22	2.18	0.43
2:G:1594:GLU:HG2	2:G:1605:VAL:HG21	2.00	0.43
1:A:402:PHE:HB2	1:A:732:LEU:CD2	2.48	0.43
1:A:1015:LEU:O	1:A:1390:ALA:HB3	2.18	0.43
2:G:123:ILE:HD12	2:G:123:ILE:H	1.82	0.43
2:G:240:LEU:HA	2:G:243:VAL:HG22	2.00	0.43
2:G:517:HIS:HB2	2:G:527:VAL:CG1	2.46	0.43
2:G:1078:HIS:O	2:G:1082:ILE:HG12	2.18	0.43
2:G:1533:LEU:HD23	2:G:1534:GLU:H	1.82	0.43
1:A:1208:VAL:CG1	1:A:1212:THR:HB	2.48	0.43
2:G:355:LYS:O	2:G:358:SER:OG	2.31	0.43
2:G:856:LYS:HB2	2:G:862:VAL:HG21	2.00	0.43
2:G:1353:LEU:HD23	2:G:1353:LEU:HA	1.84	0.43
1:A:46:GLU:HA	2:G:1665:VAL:HG23	1.99	0.43
1:A:83:LYS:HD2	1:A:84:ASP:OD1	2.18	0.43
1:A:724:LYS:HE3	1:A:725:TYR:CZ	2.53	0.43
1:A:960:GLU:OE2	1:A:961:THR:HG23	2.19	0.43
2:G:391:LEU:HD23	2:G:394:ARG:HE	1.83	0.43
2:G:1087:HIS:HA	2:G:1092:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:VAL:O	1:A:341:GLN:N	2.42	0.43
1:A:1740:SER:OG	1:A:1742:ASP:OD1	2.27	0.43
2:G:807:ILE:HD11	2:G:822:ALA:HB2	2.01	0.43
2:G:1225:GLU:OE1	2:G:1227:ARG:N	2.52	0.43
2:G:1434:HIS:CD2	2:G:1436:LYS:HE3	2.53	0.43
2:G:1537:ILE:O	2:G:1537:ILE:HG13	2.19	0.43
2:G:1623:LYS:HA	2:G:1623:LYS:HE2	2.00	0.43
2:G:1845:ASP:CG	2:G:1849:ARG:HG2	2.39	0.43
1:A:31:THR:HA	1:A:34:VAL:HG12	2.01	0.43
1:A:440:MET:HE3	1:A:479:ASN:HB3	1.99	0.43
1:A:823:ILE:HD13	1:A:865:CYS:HB3	1.99	0.43
1:A:1101:SER:N	1:A:1104:ARG:HD3	2.32	0.43
2:G:45:THR:OG1	2:G:50:ALA:HB2	2.19	0.43
2:G:525:VAL:C	2:G:526:ARG:HD3	2.39	0.43
2:G:527:VAL:HG13	2:G:541:TYR:HB3	2.00	0.43
2:G:1045:ASP:OD1	2:G:1045:ASP:N	2.46	0.43
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.85	0.43
1:A:841:GLU:OE2	1:A:845:SER:OG	2.37	0.43
2:G:113:ASP:OD1	2:G:113:ASP:N	2.50	0.43
2:G:268:LYS:HE2	2:G:268:LYS:HB3	1.68	0.43
2:G:1869:GLU:HA	2:G:1872:GLN:HG2	2.00	0.43
2:G:2023:LYS:H	2:G:2023:LYS:HD3	1.83	0.43
2:G:256:LEU:HD23	2:G:256:LEU:HA	1.82	0.43
2:G:740:HIS:CE1	2:G:854:ILE:HD11	2.53	0.43
2:G:910:GLN:HE22	2:G:912:ARG:NH2	2.17	0.43
2:G:1428:GLU:OE2	2:G:1470:THR:OG1	2.23	0.43
2:G:1886:VAL:HA	2:G:1901:ALA:O	2.18	0.43
1:A:505:LYS:HA	1:A:954:ARG:HD2	2.01	0.43
1:A:883:ILE:HG13	1:A:884:ILE:HG23	2.01	0.43
2:G:767:PHE:HD2	2:G:771:PHE:CE2	2.37	0.43
2:G:1974:VAL:HG13	2:G:1976:PHE:HD2	1.83	0.43
1:A:430:ARG:CZ	1:A:605:LEU:HD13	2.49	0.43
1:A:694:GLN:O	1:A:698:GLN:HG3	2.19	0.43
1:A:1030:TRP:CZ2	1:A:1102:GLY:HA3	2.54	0.43
1:A:1165:VAL:H	1:A:1165:VAL:HG22	1.63	0.43
2:G:571:LYS:HD3	2:G:571:LYS:HA	1.67	0.43
2:G:1614:ASP:OD1	2:G:1614:ASP:N	2.51	0.43
2:G:1775:GLN:NE2	2:G:1836:MET:SD	2.91	0.43
2:G:1784:MET:HE3	2:G:1784:MET:HB3	1.89	0.43
2:G:1821:VAL:HG23	2:G:1822:MET:HG2	2.00	0.43
2:G:1847:LEU:HD23	2:G:1847:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:LYS:NZ	1:A:716:ASP:OD1	2.51	0.42
1:A:774:ILE:HG22	3:A:1901:NAP:N7A	2.34	0.42
2:G:350:GLN:HA	2:G:353:VAL:HG22	2.00	0.42
2:G:1176:PRO:HA	2:G:1180:MET:HE1	2.01	0.42
2:G:1475:LYS:HG3	2:G:1476:ASN:HD22	1.85	0.42
2:G:1547:PRO:HD3	2:G:1584:PHE:CZ	2.53	0.42
1:A:413:LEU:CD2	1:A:451:MET:HB3	2.49	0.42
1:A:733:ILE:HG22	1:A:735:VAL:HG13	2.01	0.42
1:A:745:VAL:C	1:A:747:ALA:H	2.23	0.42
1:A:1312:VAL:O	1:A:1316:VAL:HG12	2.19	0.42
2:G:16:LEU:HB3	2:G:60:LEU:HD12	2.00	0.42
2:G:48:PHE:HD1	2:G:53:GLU:HB3	1.84	0.42
2:G:569:LEU:HD23	2:G:1090:TYR:CE1	2.52	0.42
2:G:1085:LEU:HA	2:G:1085:LEU:HD23	1.70	0.42
2:G:1383:ASN:HD22	2:G:1388:LYS:HB3	1.83	0.42
2:G:1762:TYR:HE2	2:G:1764:PHE:CE1	2.37	0.42
2:G:1923:ASP:HB2	2:G:1926:GLU:HG3	2.01	0.42
2:G:2039:LYS:HG3	2:G:2040:GLU:N	2.34	0.42
1:A:366:ASP:OD2	1:A:367:THR:N	2.52	0.42
1:A:1165:VAL:HB	1:A:1167:LEU:HD11	2.01	0.42
1:A:1323:LYS:HD3	1:A:1324:ALA:HB2	1.99	0.42
1:A:1443:LEU:HA	1:A:1443:LEU:HD23	1.73	0.42
1:A:1538:VAL:HG12	1:A:1539:ALA:N	2.34	0.42
2:G:198:LEU:HA	2:G:201:THR:HG22	2.00	0.42
2:G:216:LEU:HD12	2:G:216:LEU:H	1.83	0.42
2:G:1181:VAL:O	2:G:1181:VAL:HG23	2.19	0.42
2:G:1447:LYS:HA	2:G:1447:LYS:HD3	1.81	0.42
2:G:1515:PRO:HB2	2:G:1519:PHE:CE2	2.54	0.42
2:G:1923:ASP:O	2:G:1927:LEU:HG	2.20	0.42
1:A:1260:MET:HG3	1:A:1261:PHE:N	2.34	0.42
1:A:1316:VAL:O	1:A:1320:LEU:HD23	2.19	0.42
2:G:7:ARG:N	2:G:22:VAL:O	2.43	0.42
2:G:309:ARG:NE	2:G:442:ASP:OD2	2.28	0.42
2:G:346:GLN:HE21	2:G:368:ILE:HD13	1.84	0.42
2:G:370:LEU:HA	2:G:488:VAL:HG22	2.00	0.42
2:G:1679:ASP:OD1	2:G:1680:LEU:N	2.47	0.42
1:A:338:LEU:HA	1:A:341:GLN:HB2	2.02	0.42
1:A:824:LEU:HB3	1:A:846:LEU:HD23	2.02	0.42
1:A:1070:ARG:HB3	1:A:1072:TYR:CE1	2.55	0.42
1:A:1557:ILE:O	1:A:1561:MET:HG2	2.19	0.42
1:A:1559:GLU:HA	1:A:1562:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:ARG:HG3	2:G:24:THR:HG22	2.01	0.42
2:G:159:ILE:HA	2:G:271:THR:O	2.20	0.42
2:G:865:TRP:CD1	2:G:865:TRP:C	2.93	0.42
2:G:1143:ALA:HB1	2:G:1151:HIS:HA	2.02	0.42
2:G:1175:LYS:O	2:G:1180:MET:HE1	2.20	0.42
2:G:1514:ASN:HB3	2:G:1517:VAL:HG22	2.01	0.42
2:G:1902:GLY:H	2:G:1975:PRO:HB3	1.84	0.42
1:A:538:GLU:OE1	1:A:538:GLU:N	2.45	0.42
1:A:1115:ASN:O	1:A:1118:LYS:N	2.35	0.42
1:A:1223:PHE:HB3	1:A:1228:ILE:O	2.19	0.42
2:G:58:ALA:HA	2:G:95:TYR:CD1	2.54	0.42
2:G:526:ARG:HG2	2:G:558:ASN:H	1.85	0.42
2:G:607:VAL:HG11	2:G:619:LEU:HD13	2.01	0.42
2:G:1236:LEU:HD22	2:G:1265:MET:HE3	2.00	0.42
2:G:1301:THR:HG23	2:G:1306:ASN:ND2	2.35	0.42
2:G:1311:PHE:CE1	2:G:1322:PRO:HA	2.54	0.42
2:G:1673:GLU:N	2:G:1673:GLU:OE1	2.52	0.42
1:A:393:SER:O	1:A:736:PRO:HB2	2.19	0.42
1:A:402:PHE:HB2	1:A:732:LEU:HD23	2.02	0.42
1:A:630:ILE:HG22	1:A:653:ARG:NH2	2.35	0.42
1:A:803:MET:CE	1:A:849:LEU:HD21	2.49	0.42
2:G:598:THR:HA	2:G:620:ALA:HB1	2.00	0.42
2:G:1197:LEU:HD12	2:G:1198:SER:N	2.35	0.42
2:G:1325:PHE:O	2:G:1329:VAL:HG12	2.20	0.42
2:G:1431:TYR:CE1	2:G:1526:THR:HG22	2.52	0.42
2:G:1537:ILE:HG13	2:G:1628:HIS:HB3	2.02	0.42
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.82	0.42
1:A:1152:VAL:CG1	1:A:1154:ILE:HG23	2.49	0.42
1:A:1307:THR:O	1:A:1311:SER:OG	2.33	0.42
1:A:1498:GLU:OE2	1:A:1502:ARG:HD3	2.19	0.42
2:G:14:GLY:HA3	2:G:48:PHE:HZ	1.84	0.42
2:G:670:ARG:NH1	2:G:674:TYR:O	2.53	0.42
2:G:1226:ASN:OD1	2:G:1226:ASN:N	2.48	0.42
2:G:1449:TRP:HZ2	2:G:1519:PHE:HD2	1.67	0.42
2:G:1632:ILE:O	2:G:1635:ARG:HG2	2.19	0.42
1:A:367:THR:HA	1:A:370:GLU:HG3	2.02	0.42
1:A:504:ASP:HB2	1:A:508:ASN:H	1.84	0.42
1:A:1592:MET:HG3	1:A:1641:ILE:HG23	2.02	0.42
2:G:677:GLN:O	2:G:678:PHE:HB3	2.20	0.42
2:G:680:THR:HA	2:G:704:GLY:O	2.20	0.42
2:G:1815:LEU:HB3	2:G:1821:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1962:ARG:HB2	2:G:1968:PRO:HD3	2.02	0.42
1:A:82:SER:OG	1:A:83:LYS:N	2.53	0.42
1:A:1017:ARG:NH1	1:A:1320:LEU:HD12	2.35	0.42
1:A:1375:GLY:O	1:A:1545:SER:OG	2.29	0.42
1:A:1515:ARG:HA	1:A:1515:ARG:HD2	1.79	0.42
1:A:1516:ASP:OD1	1:A:1518:ARG:HG2	2.20	0.42
2:G:238:CYS:O	2:G:275:GLN:NE2	2.53	0.42
2:G:602:VAL:O	2:G:624:TYR:OH	2.32	0.42
2:G:1475:LYS:HE3	2:G:1476:ASN:ND2	2.35	0.42
2:G:1679:ASP:OD1	2:G:1679:ASP:N	2.52	0.42
2:G:1765:ARG:HB3	2:G:1847:LEU:O	2.19	0.42
2:G:1778:GLN:HA	2:G:1809:LEU:HD11	2.01	0.42
1:A:431:GLU:O	1:A:435:GLU:N	2.53	0.41
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.55	0.41
1:A:1680:ARG:H	1:A:1680:ARG:HG2	1.71	0.41
1:A:1734:ASN:HB3	1:A:1736:LYS:HE2	2.00	0.41
2:G:440:ASN:HD21	2:G:477:GLU:HG2	1.83	0.41
2:G:730:LEU:HD23	2:G:730:LEU:HA	1.60	0.41
2:G:1163:LYS:O	2:G:1164:MET:HG3	2.20	0.41
2:G:1263:LYS:NZ	2:G:1338:ILE:O	2.53	0.41
2:G:1306:ASN:OD1	2:G:1308:CYS:HB2	2.20	0.41
2:G:1322:PRO:HB2	2:G:1590:ARG:HH12	1.84	0.41
2:G:56:THR:HG1	2:G:59:GLU:CD	2.19	0.41
2:G:174:ARG:NH1	2:G:222:PRO:HG3	2.35	0.41
2:G:555:LEU:HD21	2:G:557:LYS:HE3	2.02	0.41
2:G:1319:MET:HB3	2:G:1368:VAL:CG2	2.46	0.41
1:A:2:LYS:HB2	1:A:2:LYS:HE2	1.78	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.87	0.41
1:A:807:LYS:HG3	1:A:861:GLN:OE1	2.21	0.41
1:A:1123:GLN:CB	1:A:1177:LYS:HD3	2.48	0.41
2:G:180:TYR:O	2:G:184:VAL:HG22	2.19	0.41
2:G:309:ARG:HB2	2:G:439:ILE:HG12	2.02	0.41
2:G:1127:PHE:HE2	2:G:1184:ILE:HD13	1.85	0.41
2:G:1381:VAL:O	2:G:1422:THR:HG23	2.20	0.41
2:G:1570:ALA:HA	2:G:1575:LEU:HD12	2.03	0.41
2:G:2015:THR:HG23	2:G:2017:LYS:HE2	2.01	0.41
1:A:251:GLN:O	1:A:255:GLY:HA2	2.20	0.41
1:A:417:TYR:OH	1:A:454:HIS:HB3	2.20	0.41
1:A:504:ASP:OD2	1:A:508:ASN:HB3	2.21	0.41
1:A:525:TYR:O	1:A:529:MET:HG2	2.21	0.41
1:A:1238:VAL:HG21	1:A:1325:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:268:LYS:NZ	2:G:497:LYS:O	2.45	0.41
2:G:765:LEU:HD12	2:G:765:LEU:HA	1.83	0.41
2:G:804:ARG:HD2	2:G:1063:THR:HG22	2.02	0.41
2:G:1066:ILE:HD12	2:G:1066:ILE:HA	1.94	0.41
2:G:1475:LYS:HG3	2:G:1476:ASN:ND2	2.35	0.41
1:A:191:GLY:O	1:A:195:GLY:HA2	2.21	0.41
1:A:1140:THR:HA	1:A:1142:GLU:OE1	2.21	0.41
1:A:1148:HIS:CD2	1:A:1167:LEU:CD2	3.03	0.41
1:A:1425:ILE:HD13	1:A:1425:ILE:HA	1.80	0.41
2:G:673:GLY:O	2:G:1164:MET:HG2	2.20	0.41
2:G:875:LEU:HD21	2:G:879:LYS:C	2.41	0.41
2:G:1331:TRP:CD1	2:G:1335:ILE:HD13	2.55	0.41
2:G:1496:LYS:HB2	2:G:1496:LYS:HE3	1.79	0.41
2:G:1576:PRO:HB2	2:G:1617:LEU:HD21	2.00	0.41
2:G:1924:ILE:HG22	2:G:1928:GLN:HE22	1.85	0.41
2:G:748:THR:OG1	2:G:749:PRO:HD3	2.21	0.41
2:G:830:ASP:N	2:G:830:ASP:OD1	2.54	0.41
2:G:1445:ARG:H	2:G:1445:ARG:HG2	1.69	0.41
2:G:1739:GLU:HA	2:G:1747:LYS:O	2.21	0.41
2:G:1989:LYS:HE2	2:G:2037:PRO:HG2	2.03	0.41
1:A:156:ALA:HB1	1:A:161:LYS:O	2.20	0.41
1:A:1496:GLU:O	1:A:1500:GLN:HB2	2.21	0.41
3:A:1901:NAP:O2N	3:A:1901:NAP:C3D	2.69	0.41
2:G:31:SER:O	2:G:35:GLU:HG3	2.21	0.41
2:G:964:LEU:HD13	2:G:964:LEU:HA	1.93	0.41
2:G:1177:SER:H	2:G:1180:MET:HE2	1.86	0.41
2:G:1955:PRO:HB2	2:G:1957:PRO:HD2	2.02	0.41
1:A:79:LEU:HA	1:A:84:ASP:OD2	2.21	0.41
1:A:427:ASN:ND2	1:A:608:ASP:OD1	2.54	0.41
1:A:1676:LYS:O	1:A:1680:ARG:HG2	2.21	0.41
2:G:119:THR:O	2:G:123:ILE:HD12	2.21	0.41
2:G:1301:THR:HG22	2:G:1306:ASN:O	2.21	0.41
2:G:1638:ILE:O	2:G:1654:GLU:HA	2.21	0.41
1:A:34:VAL:HG23	1:A:38:ASP:OD2	2.20	0.41
1:A:61:LEU:HD11	1:A:76:ARG:HD2	2.03	0.41
1:A:439:ILE:HD11	1:A:451:MET:CE	2.50	0.41
1:A:460:GLU:HA	1:A:466:TYR:HB3	2.01	0.41
1:A:490:TYR:HE1	1:A:673:PHE:CE2	2.39	0.41
1:A:771:PHE:HB3	3:A:1901:NAP:C5D	2.40	0.41
1:A:1238:VAL:HG23	1:A:1325:ARG:HG3	2.01	0.41
1:A:1584:PRO:O	1:A:1585:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:74:PRO:HG3	2:G:132:MET:HG3	2.02	0.41
2:G:126:TYR:CD2	2:G:127:ILE:HD13	2.56	0.41
2:G:292:PHE:O	2:G:296:VAL:HG23	2.21	0.41
2:G:309:ARG:CB	2:G:439:ILE:HG12	2.51	0.41
2:G:597:MET:O	2:G:601:THR:N	2.54	0.41
2:G:774:ALA:HB1	2:G:1081:HIS:HD2	1.85	0.41
2:G:803:SER:HB3	2:G:1055:HIS:CE1	2.56	0.41
2:G:926:LEU:HD23	2:G:926:LEU:HA	1.80	0.41
2:G:1011:MET:C	3:G:2102:NAP:H2A	2.40	0.41
2:G:1313:SER:OG	2:G:1314:ARG:N	2.53	0.41
2:G:1484:LYS:HA	2:G:1484:LYS:HD3	1.82	0.41
2:G:1592:LEU:O	2:G:1592:LEU:HD23	2.21	0.41
2:G:1719:ILE:HG21	2:G:1733:TYR:HE2	1.85	0.41
2:G:1721:PHE:HE2	2:G:1755:ILE:HD11	1.86	0.41
2:G:1992:LEU:O	2:G:1996:ILE:HG12	2.21	0.41
1:A:473:GLY:O	1:A:477:ILE:HG23	2.21	0.41
1:A:1024:PHE:HE1	1:A:1401:TYR:CD1	2.38	0.41
1:A:1057:MET:HG2	1:A:1190:PRO:HB2	2.02	0.41
2:G:359:HIS:HB2	2:G:360:LEU:HD12	2.01	0.41
2:G:404:GLN:O	2:G:407:ILE:HG22	2.21	0.41
2:G:1123:ASP:OD1	2:G:1188:ASN:ND2	2.54	0.41
2:G:1680:LEU:HD21	2:G:1687:ALA:HB1	2.03	0.41
2:G:1979:THR:HA	2:G:1982:MET:HG2	2.03	0.41
1:A:419:GLU:O	1:A:424:VAL:N	2.51	0.40
1:A:910:THR:HG22	1:A:912:GLU:H	1.86	0.40
1:A:1065:GLY:O	1:A:1071:PRO:HA	2.20	0.40
1:A:1154:ILE:HD12	1:A:1156:GLU:OE1	2.20	0.40
1:A:1737:ASN:HA	1:A:1740:SER:HB3	2.02	0.40
1:A:1742:ASP:OD1	1:A:1743:SER:N	2.54	0.40
2:G:322:SER:HA	2:G:325:GLU:OE2	2.21	0.40
2:G:666:ILE:HD13	2:G:666:ILE:HA	1.84	0.40
2:G:847:ARG:HH22	2:G:873:PHE:HB2	1.86	0.40
2:G:932:ILE:HG22	2:G:935:THR:H	1.86	0.40
2:G:980:ILE:HG23	2:G:984:PHE:CD1	2.56	0.40
2:G:1241:ASN:O	2:G:1251:ILE:HA	2.21	0.40
2:G:1290:PHE:HB3	2:G:1329:VAL:HG23	2.03	0.40
2:G:1544:SER:O	2:G:1621:ALA:HA	2.21	0.40
1:A:37:LYS:HB2	1:A:65:TYR:OH	2.22	0.40
2:G:89:THR:HG23	2:G:135:ARG:HH22	1.86	0.40
2:G:597:MET:HA	5:G:2101:FMN:N5	2.36	0.40
2:G:1610:CYS:HA	2:G:1653:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:HB2	2:G:2016:ALA:HB1	2.02	0.40
1:A:59:ARG:HH12	2:G:1897:GLN:HE21	1.69	0.40
1:A:630:ILE:HG22	1:A:653:ARG:HH21	1.86	0.40
1:A:849:LEU:HD12	1:A:849:LEU:HA	1.83	0.40
1:A:1227:GLY:O	1:A:1680:ARG:NH2	2.42	0.40
1:A:1391:ASP:OD1	1:A:1392:LEU:N	2.54	0.40
2:G:814:SER:OG	2:G:1040:LEU:HD13	2.21	0.40
2:G:1564:HIS:ND1	2:G:1579:ILE:HG13	2.36	0.40
2:G:1679:ASP:O	2:G:1683:THR:HG23	2.21	0.40
2:G:1773:ALA:O	2:G:1777:THR:HG23	2.21	0.40
2:G:2045:TRP:CE2	2:G:2048:TYR:HB2	2.56	0.40
1:A:56:MET:HA	1:A:59:ARG:HE	1.86	0.40
1:A:455:ILE:HD13	1:A:455:ILE:HA	1.92	0.40
1:A:688:ILE:H	1:A:688:ILE:HG13	1.59	0.40
1:A:960:GLU:OE1	2:G:1447:LYS:NZ	2.36	0.40
1:A:988:ILE:HD13	1:A:1048:GLU:HB3	2.04	0.40
1:A:1089:VAL:HG23	1:A:1093:TYR:CD2	2.52	0.40
1:A:1305:CYS:HA	1:A:1585:LYS:O	2.21	0.40
1:A:1424:GLY:O	1:A:1427:THR:HG22	2.21	0.40
2:G:10:THR:HA	2:G:19:VAL:HA	2.03	0.40
2:G:408:PRO:HG3	2:G:836:TYR:CZ	2.57	0.40
2:G:602:VAL:HG21	2:G:623:GLY:HA3	2.04	0.40
2:G:648:GLY:HA3	2:G:678:PHE:CE2	2.56	0.40
2:G:738:GLY:HA2	2:G:1055:HIS:O	2.22	0.40
2:G:1756:ASN:OD1	2:G:1759:SER:N	2.54	0.40
2:G:1982:MET:O	2:G:1985:VAL:HG22	2.21	0.40
1:A:996:LYS:H	1:A:996:LYS:HG2	1.73	0.40
1:A:1056:ILE:HG21	1:A:1056:ILE:HD13	1.84	0.40
1:A:1064:ASN:HD22	2:G:1001:ASP:HB2	1.86	0.40
2:G:85:ASN:HB2	2:G:135:ARG:NH2	2.36	0.40
2:G:571:LYS:HD2	2:G:575:GLY:C	2.42	0.40
2:G:757:ILE:O	2:G:759:ARG:N	2.54	0.40
2:G:788:LYS:HE2	2:G:789:PHE:HE1	1.86	0.40
2:G:832:TRP:CE3	2:G:833:GLU:HG2	2.56	0.40
2:G:1354:SER:N	2:G:1409:SER:OG	2.55	0.40
2:G:1618:PRO:HB2	2:G:1619:ASN:HD22	1.86	0.40
2:G:1685:LYS:HA	2:G:1688:GLN:NE2	2.37	0.40
2:G:1893:VAL:HG22	2:G:1897:GLN:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1601/1887 (85%)	1433 (90%)	161 (10%)	7 (0%)	30	61
2	G	2029/2073 (98%)	1883 (93%)	146 (7%)	0	100	100
All	All	3630/3960 (92%)	3316 (91%)	307 (8%)	7 (0%)	45	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	A	179	LYS
1	A	195	GLY
1	A	1609	ARG
1	A	180	SER
1	A	851	ASN
1	A	1158	PRO

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	A	1230/1566 (78%)	1223 (99%)	7 (1%)	84	95
2	G	1772/1810 (98%)	1757 (99%)	15 (1%)	79	93
All	All	3002/3376 (89%)	2980 (99%)	22 (1%)	80	94

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	394	PHE
1	A	505	LYS
1	A	712	LYS
1	A	894	ARG
1	A	1035	THR
1	A	1307	THR
2	G	63	LYS
2	G	76	LYS
2	G	140	LYS
2	G	297	ARG
2	G	395	LYS
2	G	415	LYS
2	G	419	ARG
2	G	809	LYS
2	G	993	GLN
2	G	1023	ARG
2	G	1315	PRO
2	G	1439	LYS
2	G	1680	LEU
2	G	1704	PHE
2	G	1765	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	11	HIS
1	A	411	GLN
1	A	465	ASN
1	A	479	ASN
1	A	669	ASN
1	A	830	HIS
1	A	1115	ASN
1	A	1146	HIS
1	A	1188	GLN
1	A	1207	GLN
1	A	1239	HIS
1	A	1272	ASN
1	A	1380	GLN
1	A	1507	GLN
1	A	1558	ASN
1	A	1598	GLN

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Mol	Chain	Res	Type
1	A	1601	ASN
1	A	1689	HIS
1	A	1734	ASN
2	G	34	GLN
2	G	99	ASN
2	G	142	ASN
2	G	273	HIS
2	G	275	GLN
2	G	343	ASN
2	G	354	ASN
2	G	404	GLN
2	G	428	HIS
2	G	440	ASN
2	G	612	ASN
2	G	650	ASN
2	G	715	GLN
2	G	723	HIS
2	G	740	HIS
2	G	741	HIS
2	G	747	HIS
2	G	900	GLN
2	G	910	GLN
2	G	985	ASN
2	G	993	GLN
2	G	1012	GLN
2	G	1046	GLN
2	G	1148	ASN
2	G	1302	HIS
2	G	1352	HIS
2	G	1355	ASN
2	G	1383	ASN
2	G	1424	GLN
2	G	1476	ASN
2	G	1514	ASN
2	G	1535	ASN
2	G	1581	HIS
2	G	1619	ASN
2	G	1674	GLN
2	G	1716	ASN
2	G	1839	GLN
2	G	1868	GLN
2	G	1896	GLN

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Mol	Chain	Res	Type
2	G	1897	GLN
2	G	1920	GLN
2	G	1939	HIS
2	G	2027	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FMN	G	2101	-	33,33,33	1.23	5 (15%)	48,50,50	1.28	8 (16%)
3	NAP	A	1901	-	46,52,52	2.56	25 (54%)	61,80,80	2.33	16 (26%)
4	PNS	A	1902	1	1,4,21	0.65	0	0,4,29	-	-
3	NAP	G	2102	-	46,52,52	0.84	1 (2%)	61,80,80	1.10	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FMN	G	2101	-	-	3/18/18/18	0/3/3/3
3	NAP	A	1901	-	-	6/31/67/67	0/5/5/5
4	PNS	A	1902	1	-	0/0/2/27	-
3	NAP	G	2102	-	-	6/31/67/67	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1901	NAP	C3N-C7N	-5.46	1.42	1.50
3	A	1901	NAP	PN-O3	-4.93	1.54	1.59
3	A	1901	NAP	O4D-C4D	-4.91	1.34	1.45
3	A	1901	NAP	C2N-N1N	-4.21	1.30	1.35
3	A	1901	NAP	C4A-N3A	-4.18	1.30	1.35
3	A	1901	NAP	C4N-C3N	-4.07	1.33	1.39
3	A	1901	NAP	O7N-C7N	-4.02	1.16	1.24
3	A	1901	NAP	C2N-C3N	-3.72	1.33	1.39
3	A	1901	NAP	P2B-O2B	-3.15	1.54	1.59
5	G	2101	FMN	C4A-N5	2.99	1.37	1.30
3	A	1901	NAP	C5A-N7A	-2.90	1.29	1.39
3	A	1901	NAP	PN-O2N	-2.80	1.42	1.55
3	A	1901	NAP	C2A-N1A	-2.78	1.29	1.33
3	A	1901	NAP	P2B-O3X	-2.72	1.44	1.54
3	A	1901	NAP	P2B-O2X	-2.71	1.44	1.54
3	A	1901	NAP	C1B-N9A	-2.70	1.43	1.49
3	A	1901	NAP	C3D-C4D	-2.53	1.46	1.53
3	A	1901	NAP	C7N-N7N	-2.53	1.28	1.33
3	A	1901	NAP	O4B-C4B	-2.48	1.39	1.45
3	A	1901	NAP	C3B-C4B	-2.43	1.46	1.53
3	A	1901	NAP	O4B-C1B	-2.39	1.37	1.40
3	A	1901	NAP	PN-O5D	-2.35	1.50	1.59
5	G	2101	FMN	C9A-N10	-2.29	1.37	1.41
3	A	1901	NAP	PN-O1N	-2.28	1.42	1.50
5	G	2101	FMN	C10-N1	2.17	1.37	1.33
3	A	1901	NAP	C6A-N1A	-2.15	1.28	1.36
5	G	2101	FMN	C4A-C10	-2.13	1.37	1.44
3	A	1901	NAP	C6N-N1N	-2.11	1.30	1.35
5	G	2101	FMN	C9A-C5A	-2.10	1.37	1.41
3	A	1901	NAP	O5D-C5D	-2.06	1.36	1.44
3	G	2102	NAP	O4D-C1D	2.00	1.43	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	NAP	C4D-O4D-C1D	-9.30	101.40	109.92
3	A	1901	NAP	O3D-C3D-C4D	-5.30	95.86	111.08
3	A	1901	NAP	C6N-N1N-C2N	-5.22	117.44	121.88
3	A	1901	NAP	O4B-C1B-N9A	-4.76	102.43	108.75
3	A	1901	NAP	P2B-O2B-C2B	-4.64	111.04	123.43
3	A	1901	NAP	O4B-C4B-C3B	-4.40	96.42	105.15
3	A	1901	NAP	O4B-C1B-C2B	-4.14	99.54	106.61
3	A	1901	NAP	N3A-C2A-N1A	-3.77	123.55	128.67
3	G	2102	NAP	N3A-C2A-N1A	-3.66	123.71	128.67
5	G	2101	FMN	C4-N3-C2	-3.50	119.42	125.64
3	A	1901	NAP	O2A-PA-O3	3.34	116.30	107.27
3	A	1901	NAP	C5B-C4B-C3B	-2.81	105.08	115.21
5	G	2101	FMN	C4A-C4-N3	2.79	120.34	113.25
3	A	1901	NAP	O3X-P2B-O2B	-2.71	95.30	105.85
3	A	1901	NAP	C5N-C4N-C3N	-2.61	117.80	120.36
5	G	2101	FMN	O4-C4-C4A	-2.59	119.69	126.53
3	G	2102	NAP	C4A-C5A-N7A	-2.57	106.62	109.34
5	G	2101	FMN	C5A-C9A-N10	2.47	120.20	117.97
3	A	1901	NAP	O3X-P2B-O2X	2.44	116.93	107.80
3	A	1901	NAP	O5B-PA-O1A	-2.36	99.57	108.94
5	G	2101	FMN	C9A-C5A-N5	-2.30	120.01	122.45
5	G	2101	FMN	C4'-C3'-C2'	-2.28	109.78	113.57
5	G	2101	FMN	C4A-C10-N10	2.25	119.70	116.48
3	A	1901	NAP	O5B-C5B-C4B	2.22	116.54	108.99
3	A	1901	NAP	O3-PA-O1A	-2.20	104.08	110.70
5	G	2101	FMN	C10-C4A-N5	-2.13	120.46	124.81
3	G	2102	NAP	C4B-O4B-C1B	2.12	111.87	109.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	NAP	C5B-O5B-PA-O1A
3	A	1901	NAP	C5D-O5D-PN-O3
3	A	1901	NAP	C5D-O5D-PN-O2N
3	A	1901	NAP	C4D-C5D-O5D-PN
3	G	2102	NAP	C5D-O5D-PN-O1N
3	A	1901	NAP	C3B-C4B-C5B-O5B
3	A	1901	NAP	O4B-C4B-C5B-O5B
5	G	2101	FMN	C5'-O5'-P-O1P
3	G	2102	NAP	C3B-C4B-C5B-O5B
3	G	2102	NAP	C5B-O5B-PA-O3
3	G	2102	NAP	C4D-C5D-O5D-PN

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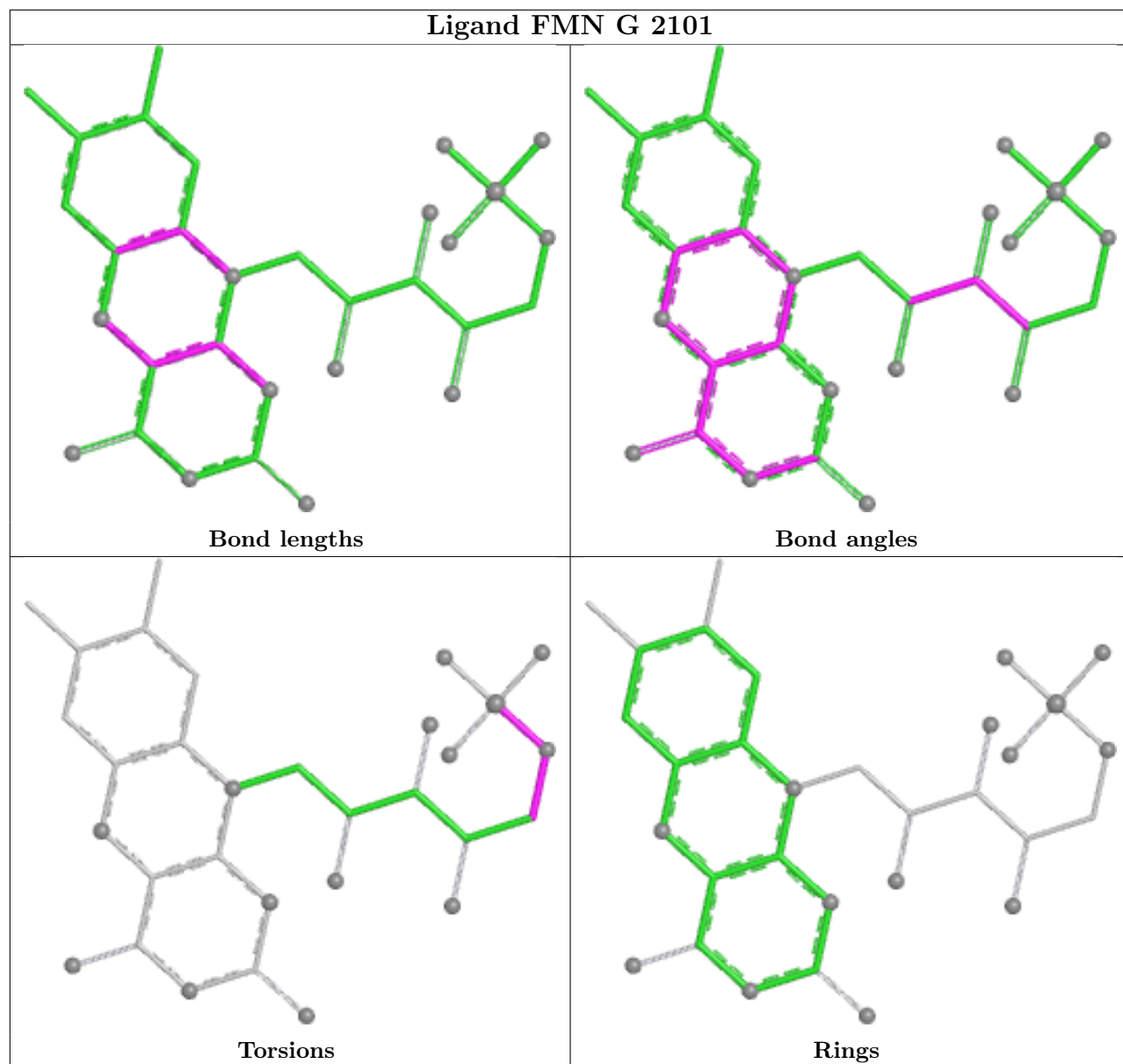
Mol	Chain	Res	Type	Atoms
5	G	2101	FMN	C4'-C5'-O5'-P
5	G	2101	FMN	C5'-O5'-P-O2P
3	G	2102	NAP	PA-O3-PN-O2N
3	G	2102	NAP	C2B-O2B-P2B-O1X

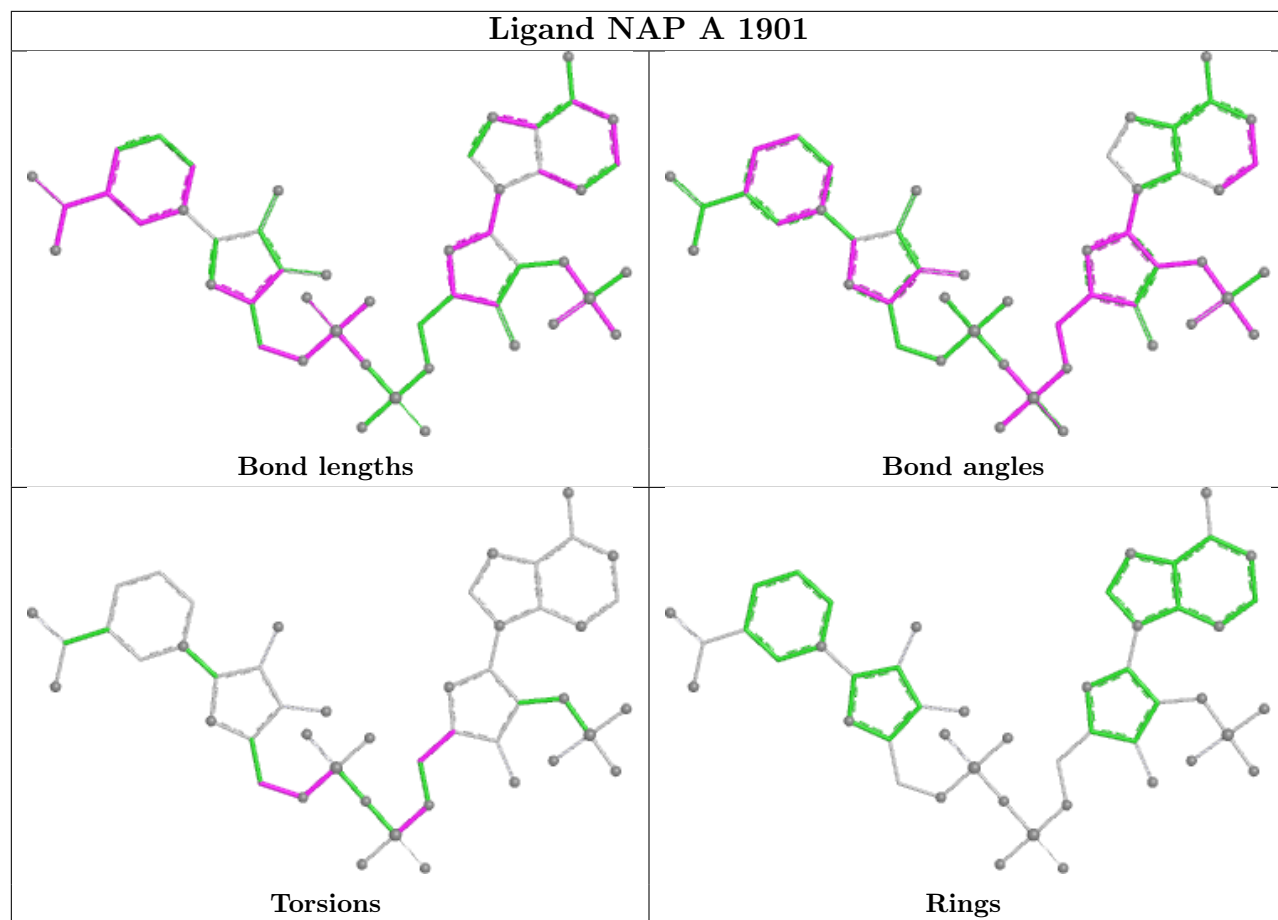
There are no ring outliers.

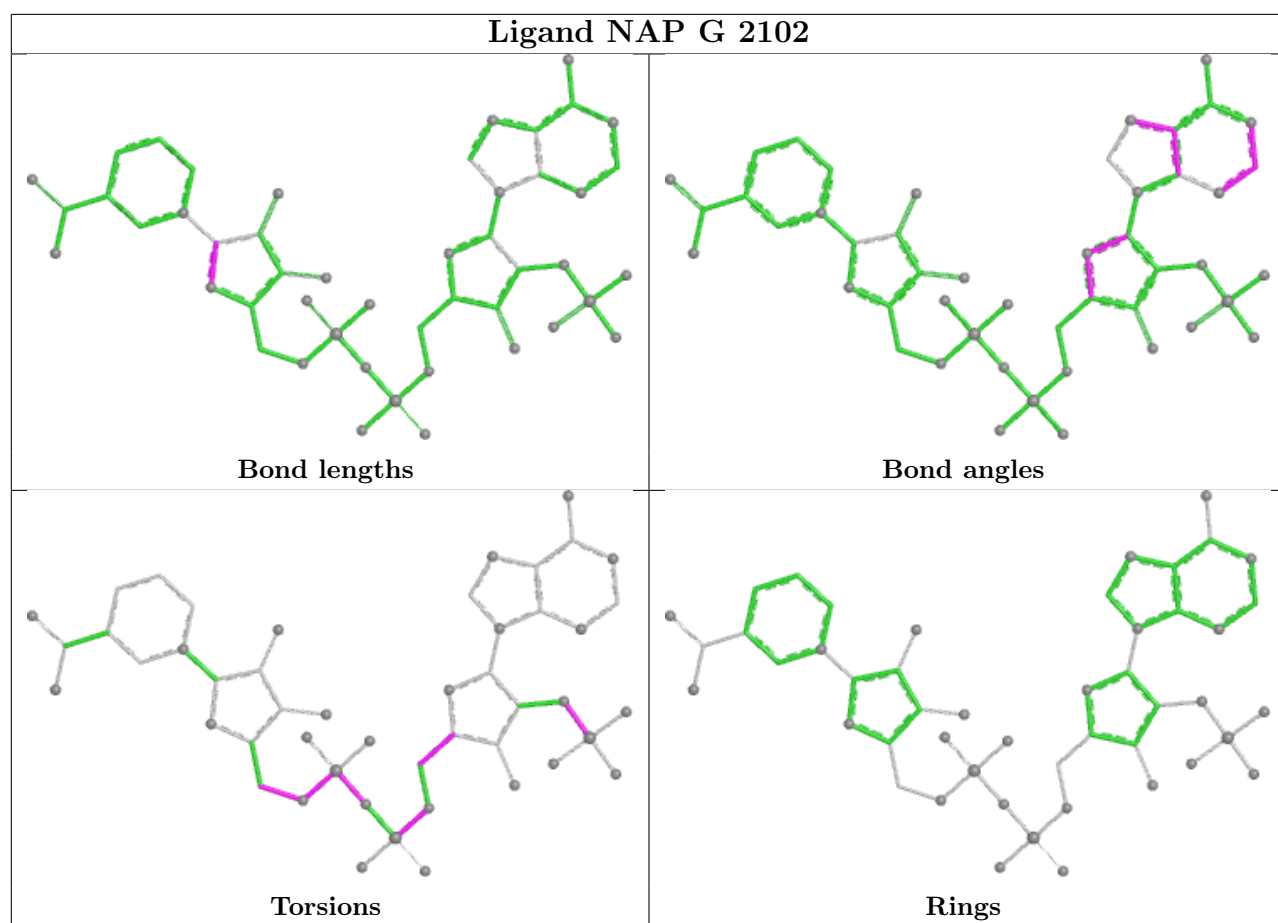
3 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2101	FMN	3	0
3	A	1901	NAP	19	0
3	G	2102	NAP	27	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

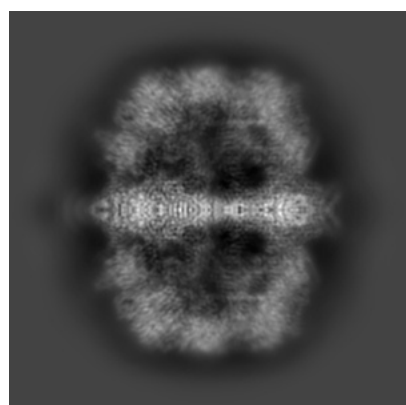
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20656. These allow visual inspection of the internal detail of the map and identification of artifacts.

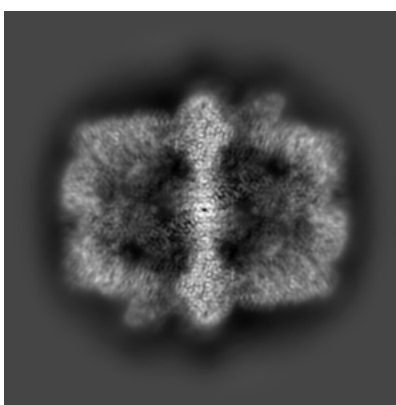
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

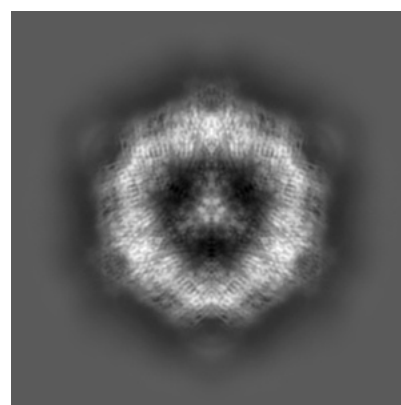
6.1.1 Primary map



X



Y

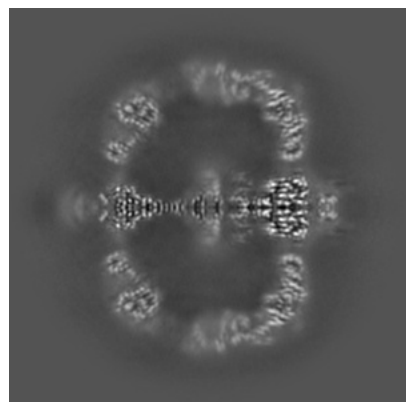


Z

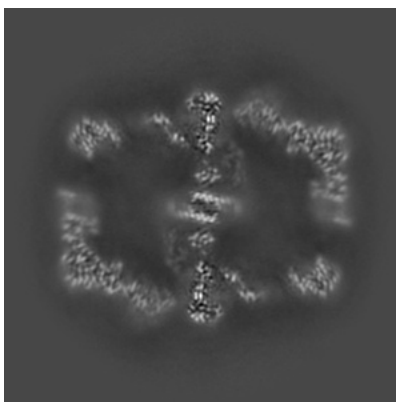
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

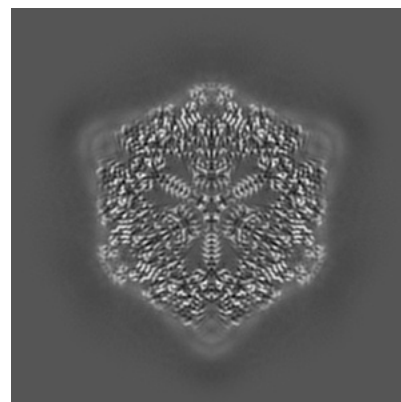
6.2.1 Primary map



X Index: 176



Y Index: 176

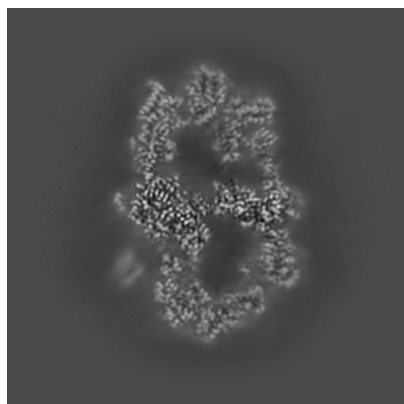


Z Index: 176

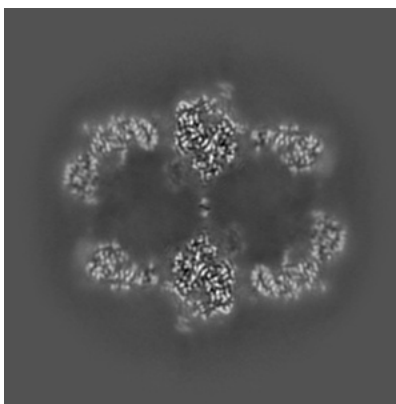
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

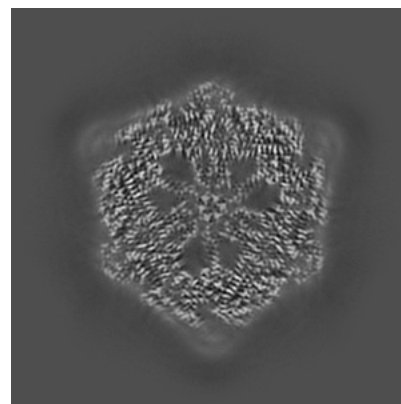
6.3.1 Primary map



X Index: 237



Y Index: 140

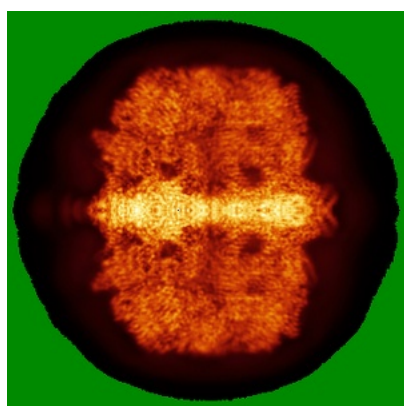


Z Index: 172

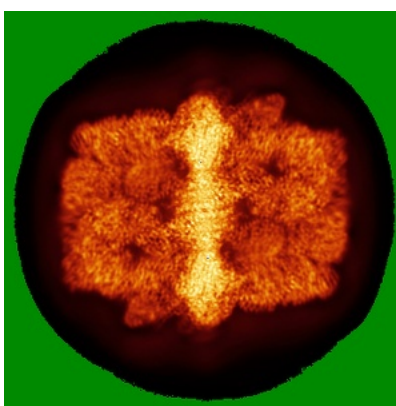
The images above show the largest variance slices of the map in three orthogonal directions.

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

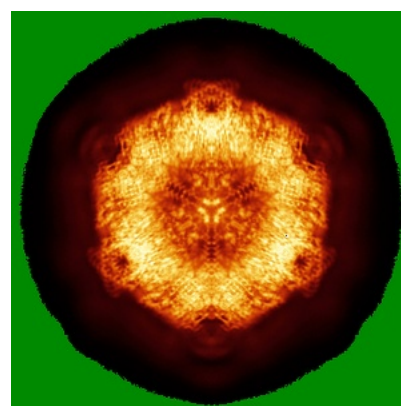
6.4.1 Primary map



X



Y

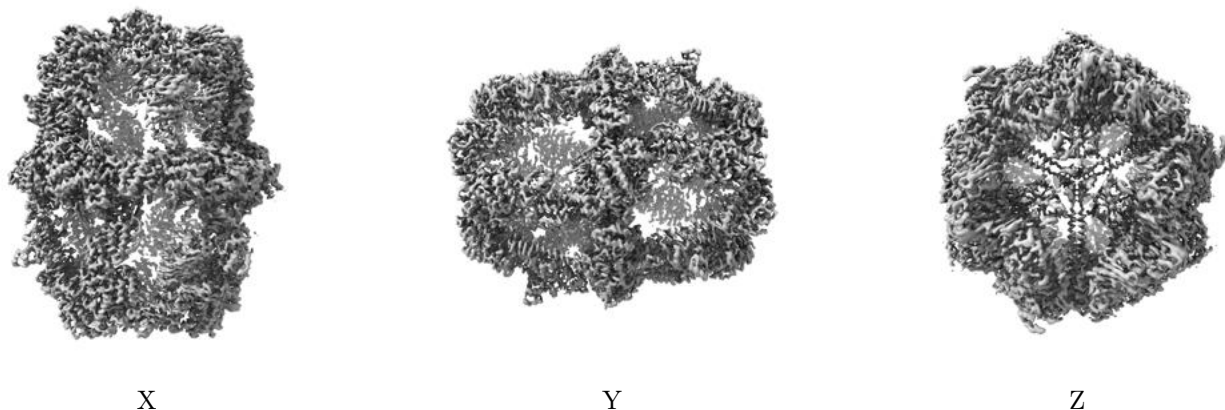


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.706. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

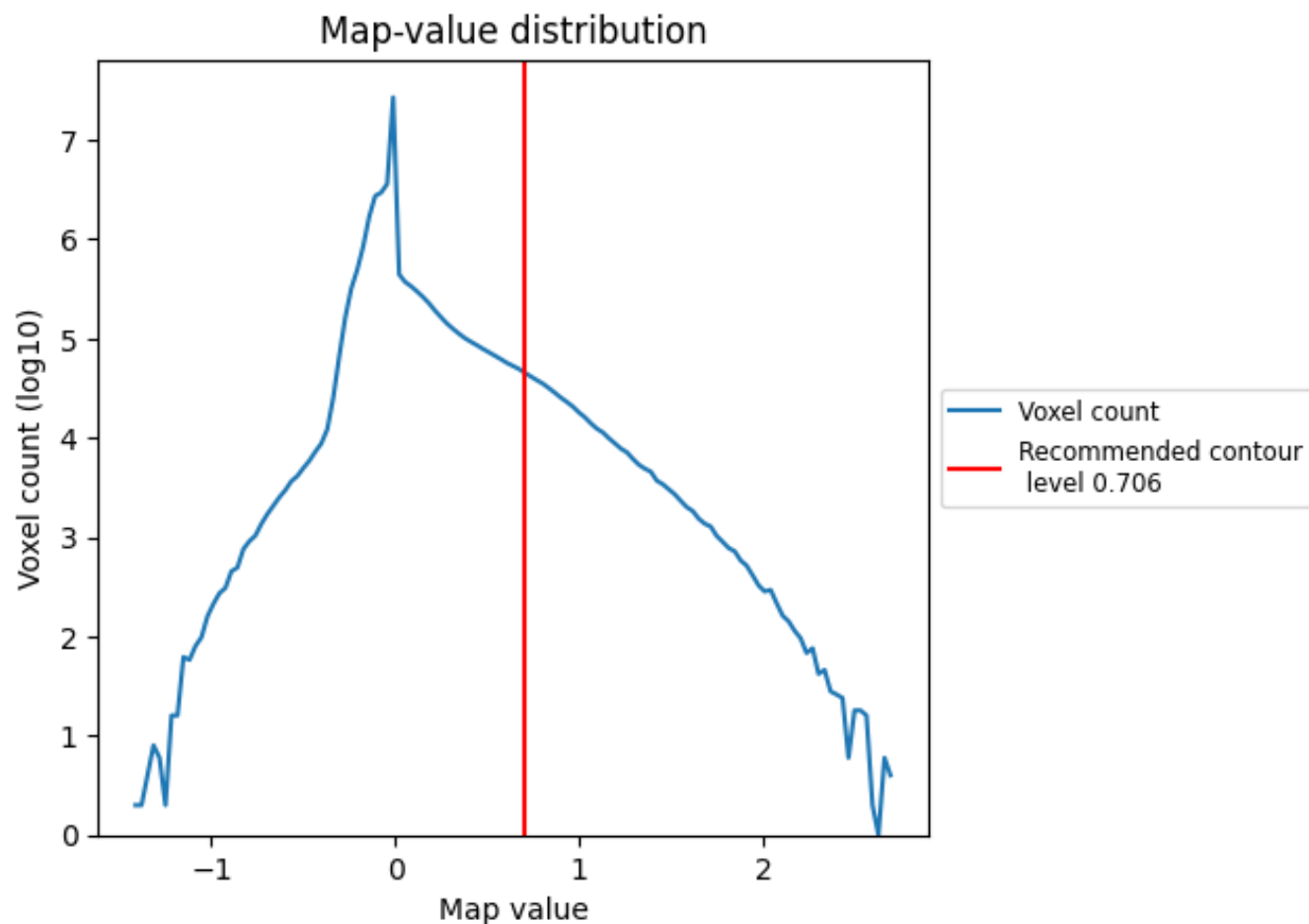
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

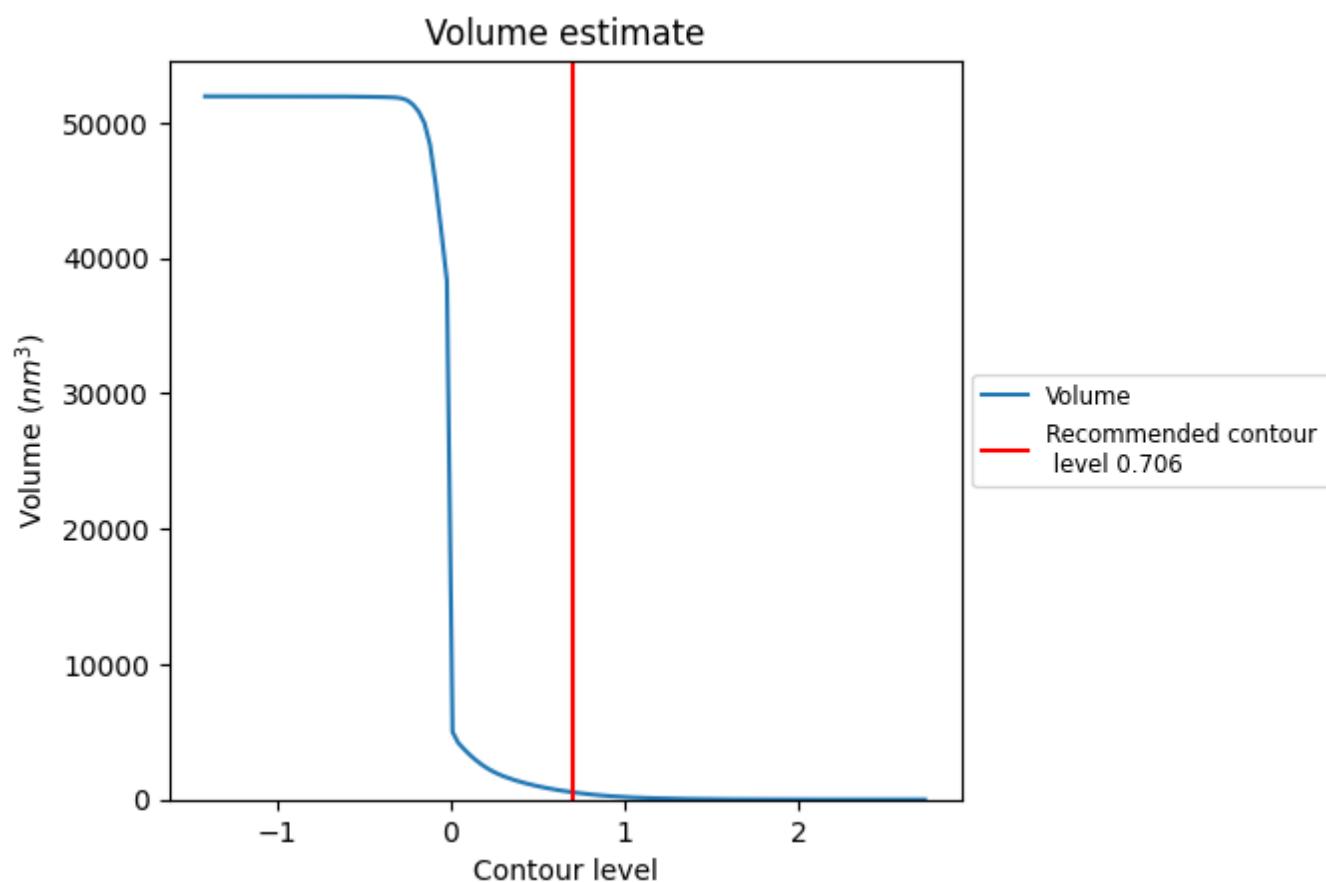
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

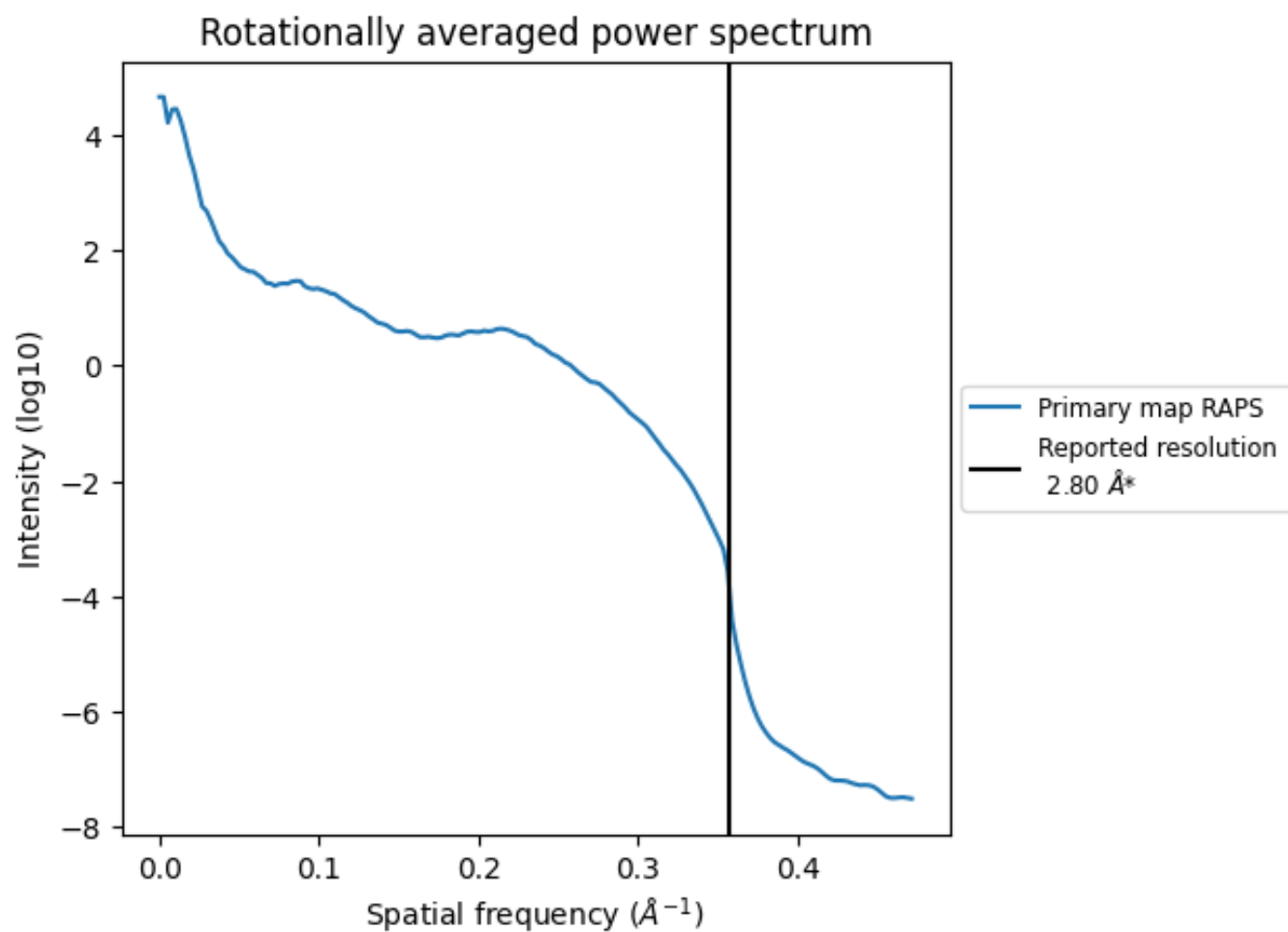
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 531 nm³; this corresponds to an approximate mass of 480 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation ⓘ

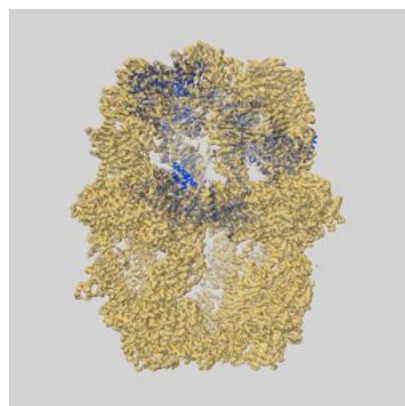
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

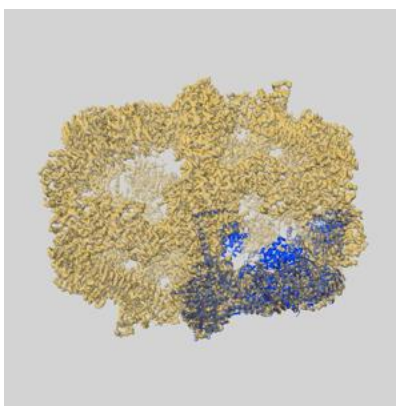
This section contains information regarding the fit between EMDB map EMD-20656 and PDB model 6U5U. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

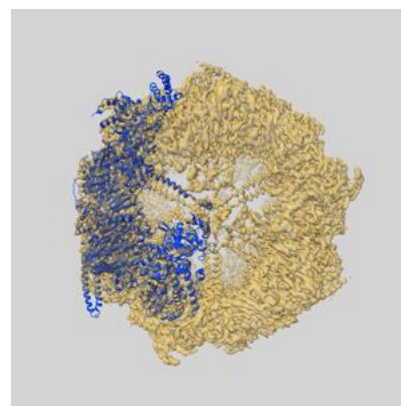
9.1.1 Map-model overlay [i](#)



X

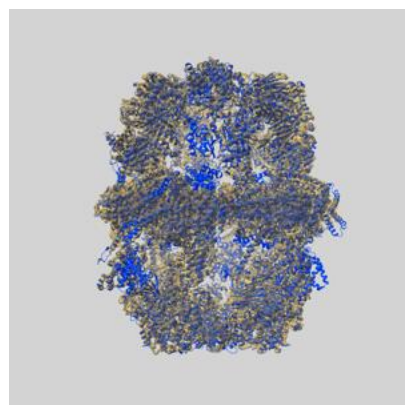


Y

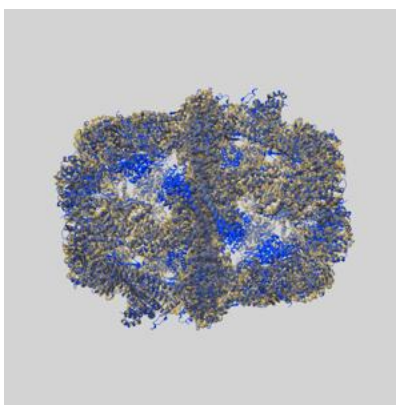


Z

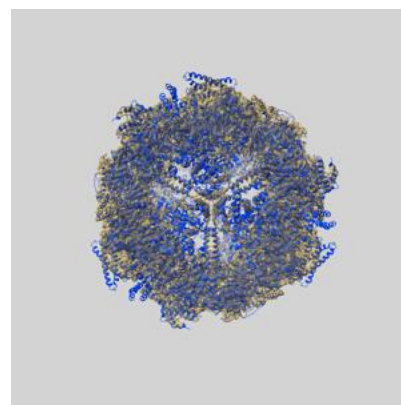
9.1.2 Map-model assembly overlay [i](#)



X



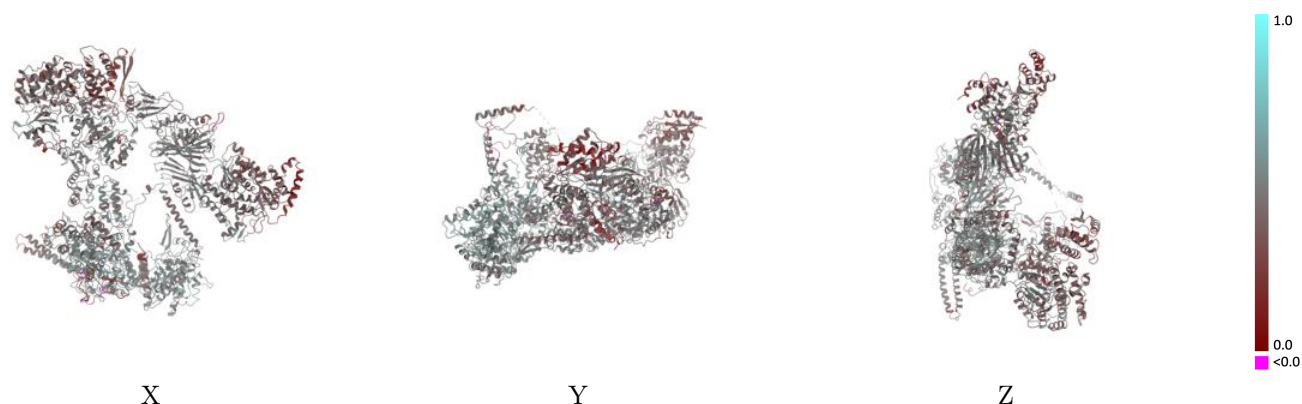
Y



Z

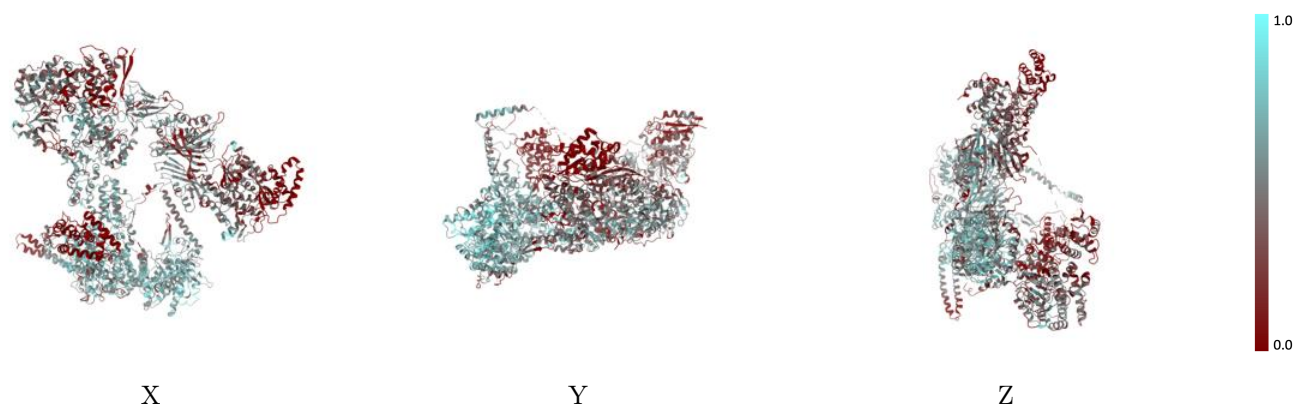
The images above show the 3D surface view of the map at the recommended contour level 0.706 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



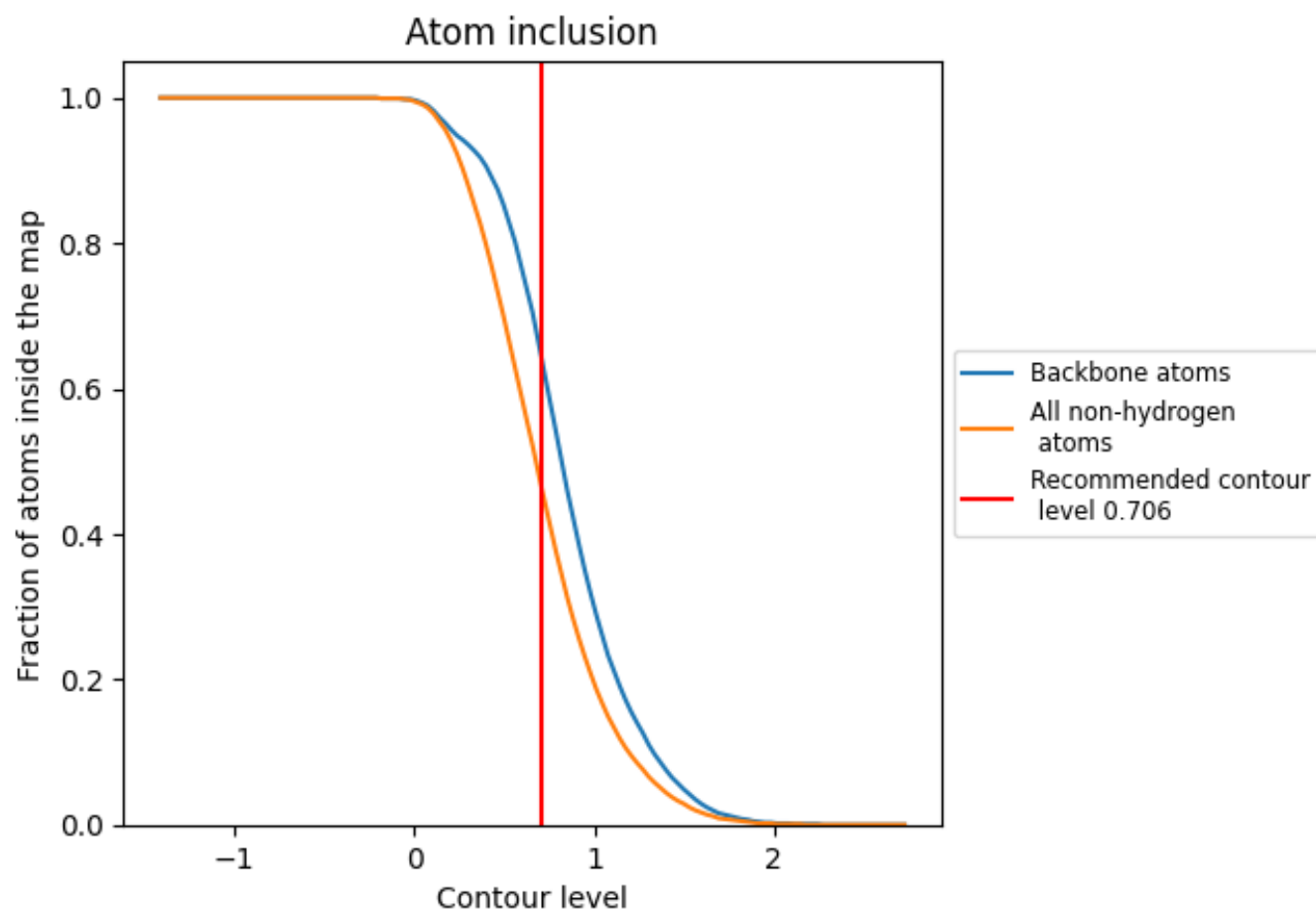
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.706).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 46% 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 (0.706) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4650	<div></div> 0.4490
A	<div></div> 0.5460	<div></div> 0.4800
G	<div></div> 0.4030	<div></div> 0.4260

