



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 02:51 PM JST

PDB ID : 8WRM
EMDB ID : EMD-37781
Title : XBB.1.5 spike protein in complex with ACE2
Authors : Feng, L.L.; Feng, L.L.
Deposited on : 2023-10-15
Resolution : 4.34 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 : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

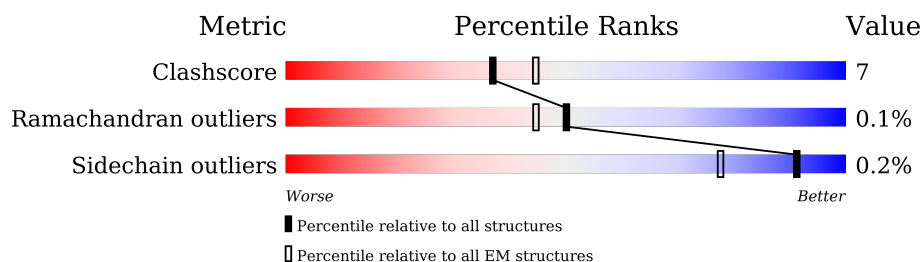
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.34 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	C	1221	
1	F	1221	
1	G	1221	
2	D	594	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29931 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	1066	Total	C	N	O	S	0	0
			8360	5346	1396	1579	39		
1	G	1066	Total	C	N	O	S	0	0
			8359	5344	1396	1580	39		
1	C	1067	Total	C	N	O	S	0	0
			8367	5350	1397	1581	39		

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	19	ILE	THR	variant	UNP P0DTC2
F	26	GLN	PRO	conflict	UNP P0DTC2
F	27	SER	ALA	conflict	UNP P0DTC2
F	83	ALA	VAL	variant	UNP P0DTC2
F	142	ASP	GLY	variant	UNP P0DTC2
F	146	GLN	HIS	variant	UNP P0DTC2
F	183	GLU	GLN	variant	UNP P0DTC2
F	213	GLU	VAL	variant	UNP P0DTC2
F	252	VAL	GLY	variant	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	346	THR	ARG	variant	UNP P0DTC2
F	368	ILE	LEU	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	445	PRO	VAL	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	486	PRO	PHE	variant	UNP P0DTC2
F	490	SER	PHE	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	655	TYR	HIS	variant	UNP P0DTC2
F	764	LYS	ASN	variant	UNP P0DTC2
F	796	TYR	ASP	variant	UNP P0DTC2
F	817	PRO	PHE	conflict	UNP P0DTC2
F	892	PRO	ALA	conflict	UNP P0DTC2
F	899	PRO	ALA	conflict	UNP P0DTC2
F	942	PRO	ALA	conflict	UNP P0DTC2
F	954	HIS	GLN	variant	UNP P0DTC2
F	969	LYS	ASN	variant	UNP P0DTC2
F	986	PRO	LYS	variant	UNP P0DTC2
F	987	PRO	VAL	variant	UNP P0DTC2
F	1141	GLY	-	expression tag	UNP P0DTC2
F	1142	GLY	-	expression tag	UNP P0DTC2
F	1143	SER	-	expression tag	UNP P0DTC2
F	1144	GLY	-	expression tag	UNP P0DTC2
F	1145	GLY	-	expression tag	UNP P0DTC2
F	1146	SER	-	expression tag	UNP P0DTC2
F	1147	TYR	-	expression tag	UNP P0DTC2
F	1148	ILE	-	expression tag	UNP P0DTC2
F	1149	PRO	-	expression tag	UNP P0DTC2
F	1150	GLU	-	expression tag	UNP P0DTC2
F	1151	ALA	-	expression tag	UNP P0DTC2
F	1152	PRO	-	expression tag	UNP P0DTC2
F	1153	ARG	-	expression tag	UNP P0DTC2
F	1154	ASP	-	expression tag	UNP P0DTC2
F	1155	GLY	-	expression tag	UNP P0DTC2
F	1156	GLN	-	expression tag	UNP P0DTC2
F	1157	ALA	-	expression tag	UNP P0DTC2
F	1158	TYR	-	expression tag	UNP P0DTC2
F	1159	VAL	-	expression tag	UNP P0DTC2
F	1160	ARG	-	expression tag	UNP P0DTC2
F	1161	LYS	-	expression tag	UNP P0DTC2
F	1162	ASP	-	expression tag	UNP P0DTC2
F	1163	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1164	GLU	-	expression tag	UNP P0DTC2
F	1165	TRP	-	expression tag	UNP P0DTC2
F	1166	VAL	-	expression tag	UNP P0DTC2
F	1167	LEU	-	expression tag	UNP P0DTC2
F	1168	LEU	-	expression tag	UNP P0DTC2
F	1169	SER	-	expression tag	UNP P0DTC2
F	1170	THR	-	expression tag	UNP P0DTC2
F	1171	PHE	-	expression tag	UNP P0DTC2
F	1172	LEU	-	expression tag	UNP P0DTC2
F	1173	GLY	-	expression tag	UNP P0DTC2
F	1174	ARG	-	expression tag	UNP P0DTC2
F	1175	SER	-	expression tag	UNP P0DTC2
F	1176	LEU	-	expression tag	UNP P0DTC2
F	1177	GLU	-	expression tag	UNP P0DTC2
F	1178	VAL	-	expression tag	UNP P0DTC2
F	1179	LEU	-	expression tag	UNP P0DTC2
F	1180	PHE	-	expression tag	UNP P0DTC2
F	1181	GLN	-	expression tag	UNP P0DTC2
F	1182	GLY	-	expression tag	UNP P0DTC2
F	1183	PRO	-	expression tag	UNP P0DTC2
F	1184	GLY	-	expression tag	UNP P0DTC2
F	1185	TRP	-	expression tag	UNP P0DTC2
F	1186	SER	-	expression tag	UNP P0DTC2
F	1187	HIS	-	expression tag	UNP P0DTC2
F	1188	PRO	-	expression tag	UNP P0DTC2
F	1189	GLN	-	expression tag	UNP P0DTC2
F	1190	PHE	-	expression tag	UNP P0DTC2
F	1191	GLU	-	expression tag	UNP P0DTC2
F	1192	LYS	-	expression tag	UNP P0DTC2
F	1193	GLY	-	expression tag	UNP P0DTC2
F	1194	GLY	-	expression tag	UNP P0DTC2
F	1195	GLY	-	expression tag	UNP P0DTC2
F	1196	SER	-	expression tag	UNP P0DTC2
F	1197	GLY	-	expression tag	UNP P0DTC2
F	1198	GLY	-	expression tag	UNP P0DTC2
F	1199	GLY	-	expression tag	UNP P0DTC2
F	1200	SER	-	expression tag	UNP P0DTC2
F	1201	GLY	-	expression tag	UNP P0DTC2
F	1202	GLY	-	expression tag	UNP P0DTC2
F	1203	SER	-	expression tag	UNP P0DTC2
F	1204	SER	-	expression tag	UNP P0DTC2
F	1205	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1206	TRP	-	expression tag	UNP P0DTC2
F	1207	SER	-	expression tag	UNP P0DTC2
F	1208	HIS	-	expression tag	UNP P0DTC2
F	1209	PRO	-	expression tag	UNP P0DTC2
F	1210	GLN	-	expression tag	UNP P0DTC2
F	1211	PHE	-	expression tag	UNP P0DTC2
F	1212	GLU	-	expression tag	UNP P0DTC2
F	1213	LYS	-	expression tag	UNP P0DTC2
F	1214	HIS	-	expression tag	UNP P0DTC2
F	1215	HIS	-	expression tag	UNP P0DTC2
F	1216	HIS	-	expression tag	UNP P0DTC2
F	1217	HIS	-	expression tag	UNP P0DTC2
F	1218	HIS	-	expression tag	UNP P0DTC2
F	1219	HIS	-	expression tag	UNP P0DTC2
F	1220	HIS	-	expression tag	UNP P0DTC2
F	1221	HIS	-	expression tag	UNP P0DTC2
G	19	ILE	THR	variant	UNP P0DTC2
G	26	GLN	PRO	conflict	UNP P0DTC2
G	27	SER	ALA	conflict	UNP P0DTC2
G	83	ALA	VAL	variant	UNP P0DTC2
G	142	ASP	GLY	variant	UNP P0DTC2
G	146	GLN	HIS	variant	UNP P0DTC2
G	183	GLU	GLN	variant	UNP P0DTC2
G	213	GLU	VAL	variant	UNP P0DTC2
G	252	VAL	GLY	variant	UNP P0DTC2
G	339	HIS	GLY	variant	UNP P0DTC2
G	346	THR	ARG	variant	UNP P0DTC2
G	368	ILE	LEU	variant	UNP P0DTC2
G	371	PHE	SER	variant	UNP P0DTC2
G	373	PRO	SER	variant	UNP P0DTC2
G	375	PHE	SER	variant	UNP P0DTC2
G	376	ALA	THR	variant	UNP P0DTC2
G	405	ASN	ASP	variant	UNP P0DTC2
G	408	SER	ARG	variant	UNP P0DTC2
G	417	ASN	LYS	variant	UNP P0DTC2
G	440	LYS	ASN	variant	UNP P0DTC2
G	445	PRO	VAL	variant	UNP P0DTC2
G	446	SER	GLY	variant	UNP P0DTC2
G	460	LYS	ASN	variant	UNP P0DTC2
G	477	ASN	SER	variant	UNP P0DTC2
G	478	LYS	THR	variant	UNP P0DTC2
G	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	486	PRO	PHE	variant	UNP P0DTC2
G	490	SER	PHE	variant	UNP P0DTC2
G	498	ARG	GLN	variant	UNP P0DTC2
G	501	TYR	ASN	variant	UNP P0DTC2
G	505	HIS	TYR	variant	UNP P0DTC2
G	614	GLY	ASP	variant	UNP P0DTC2
G	655	TYR	HIS	variant	UNP P0DTC2
G	764	LYS	ASN	variant	UNP P0DTC2
G	796	TYR	ASP	variant	UNP P0DTC2
G	817	PRO	PHE	conflict	UNP P0DTC2
G	892	PRO	ALA	conflict	UNP P0DTC2
G	899	PRO	ALA	conflict	UNP P0DTC2
G	942	PRO	ALA	conflict	UNP P0DTC2
G	954	HIS	GLN	variant	UNP P0DTC2
G	969	LYS	ASN	variant	UNP P0DTC2
G	986	PRO	LYS	variant	UNP P0DTC2
G	987	PRO	VAL	variant	UNP P0DTC2
G	1141	GLY	-	expression tag	UNP P0DTC2
G	1142	GLY	-	expression tag	UNP P0DTC2
G	1143	SER	-	expression tag	UNP P0DTC2
G	1144	GLY	-	expression tag	UNP P0DTC2
G	1145	GLY	-	expression tag	UNP P0DTC2
G	1146	SER	-	expression tag	UNP P0DTC2
G	1147	TYR	-	expression tag	UNP P0DTC2
G	1148	ILE	-	expression tag	UNP P0DTC2
G	1149	PRO	-	expression tag	UNP P0DTC2
G	1150	GLU	-	expression tag	UNP P0DTC2
G	1151	ALA	-	expression tag	UNP P0DTC2
G	1152	PRO	-	expression tag	UNP P0DTC2
G	1153	ARG	-	expression tag	UNP P0DTC2
G	1154	ASP	-	expression tag	UNP P0DTC2
G	1155	GLY	-	expression tag	UNP P0DTC2
G	1156	GLN	-	expression tag	UNP P0DTC2
G	1157	ALA	-	expression tag	UNP P0DTC2
G	1158	TYR	-	expression tag	UNP P0DTC2
G	1159	VAL	-	expression tag	UNP P0DTC2
G	1160	ARG	-	expression tag	UNP P0DTC2
G	1161	LYS	-	expression tag	UNP P0DTC2
G	1162	ASP	-	expression tag	UNP P0DTC2
G	1163	GLY	-	expression tag	UNP P0DTC2
G	1164	GLU	-	expression tag	UNP P0DTC2
G	1165	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1166	VAL	-	expression tag	UNP P0DTC2
G	1167	LEU	-	expression tag	UNP P0DTC2
G	1168	LEU	-	expression tag	UNP P0DTC2
G	1169	SER	-	expression tag	UNP P0DTC2
G	1170	THR	-	expression tag	UNP P0DTC2
G	1171	PHE	-	expression tag	UNP P0DTC2
G	1172	LEU	-	expression tag	UNP P0DTC2
G	1173	GLY	-	expression tag	UNP P0DTC2
G	1174	ARG	-	expression tag	UNP P0DTC2
G	1175	SER	-	expression tag	UNP P0DTC2
G	1176	LEU	-	expression tag	UNP P0DTC2
G	1177	GLU	-	expression tag	UNP P0DTC2
G	1178	VAL	-	expression tag	UNP P0DTC2
G	1179	LEU	-	expression tag	UNP P0DTC2
G	1180	PHE	-	expression tag	UNP P0DTC2
G	1181	GLN	-	expression tag	UNP P0DTC2
G	1182	GLY	-	expression tag	UNP P0DTC2
G	1183	PRO	-	expression tag	UNP P0DTC2
G	1184	GLY	-	expression tag	UNP P0DTC2
G	1185	TRP	-	expression tag	UNP P0DTC2
G	1186	SER	-	expression tag	UNP P0DTC2
G	1187	HIS	-	expression tag	UNP P0DTC2
G	1188	PRO	-	expression tag	UNP P0DTC2
G	1189	GLN	-	expression tag	UNP P0DTC2
G	1190	PHE	-	expression tag	UNP P0DTC2
G	1191	GLU	-	expression tag	UNP P0DTC2
G	1192	LYS	-	expression tag	UNP P0DTC2
G	1193	GLY	-	expression tag	UNP P0DTC2
G	1194	GLY	-	expression tag	UNP P0DTC2
G	1195	GLY	-	expression tag	UNP P0DTC2
G	1196	SER	-	expression tag	UNP P0DTC2
G	1197	GLY	-	expression tag	UNP P0DTC2
G	1198	GLY	-	expression tag	UNP P0DTC2
G	1199	GLY	-	expression tag	UNP P0DTC2
G	1200	SER	-	expression tag	UNP P0DTC2
G	1201	GLY	-	expression tag	UNP P0DTC2
G	1202	GLY	-	expression tag	UNP P0DTC2
G	1203	SER	-	expression tag	UNP P0DTC2
G	1204	SER	-	expression tag	UNP P0DTC2
G	1205	ALA	-	expression tag	UNP P0DTC2
G	1206	TRP	-	expression tag	UNP P0DTC2
G	1207	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1208	HIS	-	expression tag	UNP P0DTC2
G	1209	PRO	-	expression tag	UNP P0DTC2
G	1210	GLN	-	expression tag	UNP P0DTC2
G	1211	PHE	-	expression tag	UNP P0DTC2
G	1212	GLU	-	expression tag	UNP P0DTC2
G	1213	LYS	-	expression tag	UNP P0DTC2
G	1214	HIS	-	expression tag	UNP P0DTC2
G	1215	HIS	-	expression tag	UNP P0DTC2
G	1216	HIS	-	expression tag	UNP P0DTC2
G	1217	HIS	-	expression tag	UNP P0DTC2
G	1218	HIS	-	expression tag	UNP P0DTC2
G	1219	HIS	-	expression tag	UNP P0DTC2
G	1220	HIS	-	expression tag	UNP P0DTC2
G	1221	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	26	GLN	PRO	conflict	UNP P0DTC2
C	27	SER	ALA	conflict	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1141	GLY	-	expression tag	UNP P0DTC2
C	1142	GLY	-	expression tag	UNP P0DTC2
C	1143	SER	-	expression tag	UNP P0DTC2
C	1144	GLY	-	expression tag	UNP P0DTC2
C	1145	GLY	-	expression tag	UNP P0DTC2
C	1146	SER	-	expression tag	UNP P0DTC2
C	1147	TYR	-	expression tag	UNP P0DTC2
C	1148	ILE	-	expression tag	UNP P0DTC2
C	1149	PRO	-	expression tag	UNP P0DTC2
C	1150	GLU	-	expression tag	UNP P0DTC2
C	1151	ALA	-	expression tag	UNP P0DTC2
C	1152	PRO	-	expression tag	UNP P0DTC2
C	1153	ARG	-	expression tag	UNP P0DTC2
C	1154	ASP	-	expression tag	UNP P0DTC2
C	1155	GLY	-	expression tag	UNP P0DTC2
C	1156	GLN	-	expression tag	UNP P0DTC2
C	1157	ALA	-	expression tag	UNP P0DTC2
C	1158	TYR	-	expression tag	UNP P0DTC2
C	1159	VAL	-	expression tag	UNP P0DTC2
C	1160	ARG	-	expression tag	UNP P0DTC2
C	1161	LYS	-	expression tag	UNP P0DTC2
C	1162	ASP	-	expression tag	UNP P0DTC2
C	1163	GLY	-	expression tag	UNP P0DTC2
C	1164	GLU	-	expression tag	UNP P0DTC2
C	1165	TRP	-	expression tag	UNP P0DTC2
C	1166	VAL	-	expression tag	UNP P0DTC2
C	1167	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1168	LEU	-	expression tag	UNP P0DTC2
C	1169	SER	-	expression tag	UNP P0DTC2
C	1170	THR	-	expression tag	UNP P0DTC2
C	1171	PHE	-	expression tag	UNP P0DTC2
C	1172	LEU	-	expression tag	UNP P0DTC2
C	1173	GLY	-	expression tag	UNP P0DTC2
C	1174	ARG	-	expression tag	UNP P0DTC2
C	1175	SER	-	expression tag	UNP P0DTC2
C	1176	LEU	-	expression tag	UNP P0DTC2
C	1177	GLU	-	expression tag	UNP P0DTC2
C	1178	VAL	-	expression tag	UNP P0DTC2
C	1179	LEU	-	expression tag	UNP P0DTC2
C	1180	PHE	-	expression tag	UNP P0DTC2
C	1181	GLN	-	expression tag	UNP P0DTC2
C	1182	GLY	-	expression tag	UNP P0DTC2
C	1183	PRO	-	expression tag	UNP P0DTC2
C	1184	GLY	-	expression tag	UNP P0DTC2
C	1185	TRP	-	expression tag	UNP P0DTC2
C	1186	SER	-	expression tag	UNP P0DTC2
C	1187	HIS	-	expression tag	UNP P0DTC2
C	1188	PRO	-	expression tag	UNP P0DTC2
C	1189	GLN	-	expression tag	UNP P0DTC2
C	1190	PHE	-	expression tag	UNP P0DTC2
C	1191	GLU	-	expression tag	UNP P0DTC2
C	1192	LYS	-	expression tag	UNP P0DTC2
C	1193	GLY	-	expression tag	UNP P0DTC2
C	1194	GLY	-	expression tag	UNP P0DTC2
C	1195	GLY	-	expression tag	UNP P0DTC2
C	1196	SER	-	expression tag	UNP P0DTC2
C	1197	GLY	-	expression tag	UNP P0DTC2
C	1198	GLY	-	expression tag	UNP P0DTC2
C	1199	GLY	-	expression tag	UNP P0DTC2
C	1200	SER	-	expression tag	UNP P0DTC2
C	1201	GLY	-	expression tag	UNP P0DTC2
C	1202	GLY	-	expression tag	UNP P0DTC2
C	1203	SER	-	expression tag	UNP P0DTC2
C	1204	SER	-	expression tag	UNP P0DTC2
C	1205	ALA	-	expression tag	UNP P0DTC2
C	1206	TRP	-	expression tag	UNP P0DTC2
C	1207	SER	-	expression tag	UNP P0DTC2
C	1208	HIS	-	expression tag	UNP P0DTC2
C	1209	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1210	GLN	-	expression tag	UNP P0DTC2
C	1211	PHE	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	LYS	-	expression tag	UNP P0DTC2
C	1214	HIS	-	expression tag	UNP P0DTC2
C	1215	HIS	-	expression tag	UNP P0DTC2
C	1216	HIS	-	expression tag	UNP P0DTC2
C	1217	HIS	-	expression tag	UNP P0DTC2
C	1218	HIS	-	expression tag	UNP P0DTC2
C	1219	HIS	-	expression tag	UNP P0DTC2
C	1220	HIS	-	expression tag	UNP P0DTC2
C	1221	HIS	-	expression tag	UNP P0DTC2

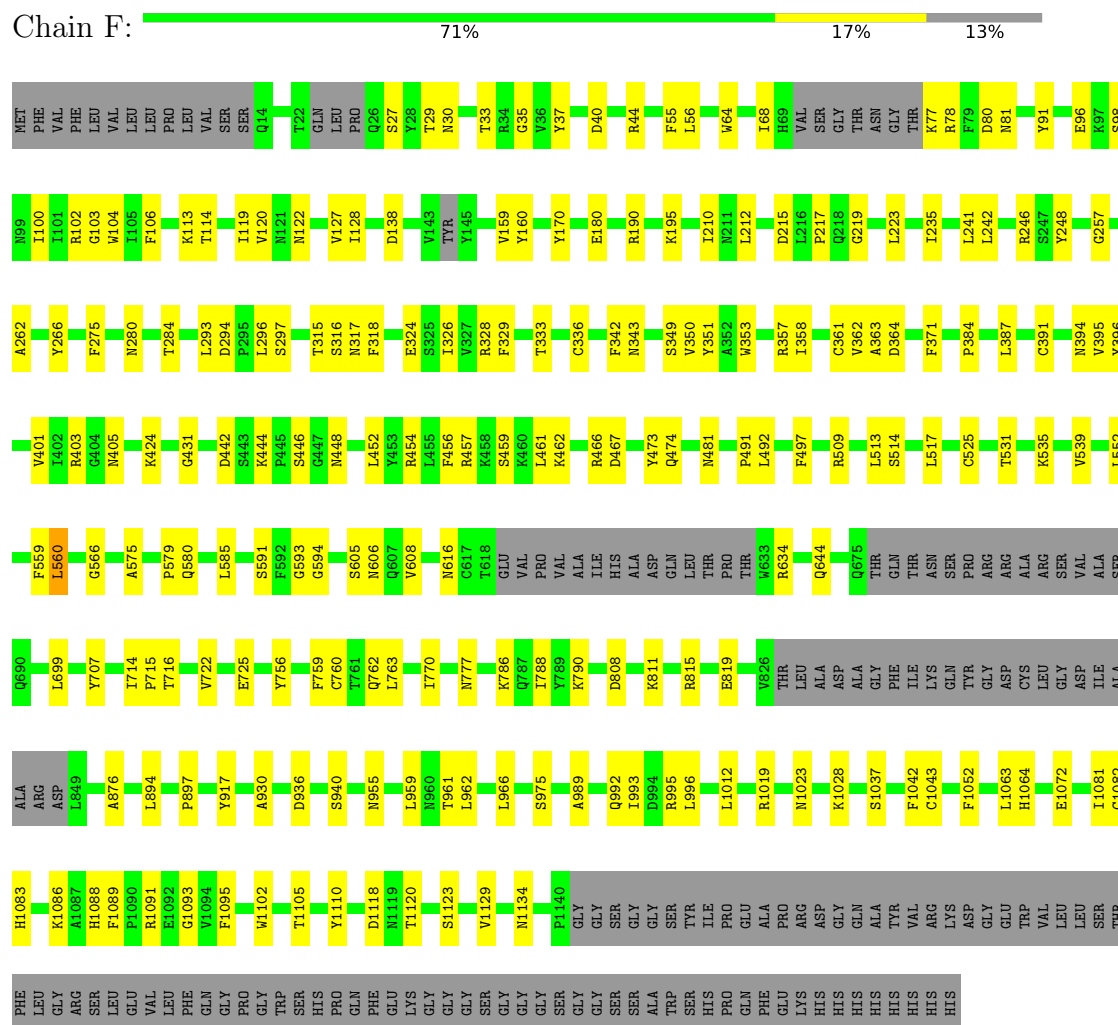
- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	594	Total	C	N	O	S	0	0
			4845	3099	803	914	29		

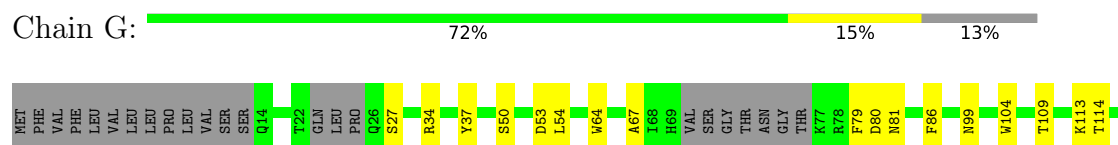
3 Residue-property plots [i](#)

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. 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. 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: Spike glycoprotein



• Molecule 1: Spike glycoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136454	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.28	0/8568	0.59	2/11658 (0.0%)
1	F	0.27	0/8561	0.58	1/11648 (0.0%)
1	G	0.28	0/8560	0.57	0/11647
2	D	0.27	0/4981	0.55	1/6767 (0.0%)
All	All	0.28	0/30670	0.57	4/41720 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	560	LEU	CA-CB-CG	6.64	130.57	115.30
2	D	376	MET	CA-CB-CG	5.47	122.60	113.30
1	C	582	LEU	CA-CB-CG	5.36	127.62	115.30
1	C	54	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	8367	0	8181	145	0
1	F	8360	0	8174	131	0
1	G	8359	0	8168	120	0
2	D	4845	0	4625	57	0
All	All	29931	0	29148	436	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 7.

All (436) 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)
1:F:431:GLY:HA3	1:F:513:LEU:O	1.69	0.93
1:C:431:GLY:HA3	1:C:513:LEU:O	1.73	0.88
1:C:81:ASN:HB3	1:C:138:ASP:HB3	1.71	0.72
1:F:1052:PHE:HB2	1:F:1063:LEU:HB2	1.72	0.72
1:G:80:ASP:H	1:G:262:ALA:HB2	1.55	0.71
1:C:714:ILE:HD12	1:C:715:PRO:HD2	1.73	0.71
2:D:261:CYS:SG	2:D:262:LEU:N	2.65	0.70
1:F:353:TRP:HE1	1:F:454:ARG:HH22	1.37	0.70
1:F:1019:ARG:HH12	1:F:1023:ASN:HB2	1.57	0.69
1:F:98:SER:HA	1:F:180:GLU:H	1.58	0.68
1:G:731:MET:SD	1:G:774:GLN:NE2	2.65	0.67
1:C:452:LEU:HD21	1:C:492:LEU:HD23	1.77	0.67
1:F:403:ARG:HH21	1:F:405:ASN:HD21	1.42	0.66
1:G:226:LEU:HG	1:G:227:VAL:HG23	1.76	0.66
1:C:37:TYR:HB3	1:C:223:LEU:HD23	1.77	0.66
1:C:448:ASN:HB2	1:C:497:PHE:HB2	1.77	0.66
2:D:482:ARG:NH2	2:D:607:SER:O	2.29	0.66
1:F:961:THR:OG1	1:G:762:GLN:NE2	2.29	0.66
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.77	0.66
1:F:993:ILE:HG13	1:F:996:LEU:HD21	1.79	0.65
1:C:457:ARG:HH22	1:C:461:LEU:HB2	1.62	0.64
1:F:80:ASP:H	1:F:262:ALA:HB2	1.62	0.64
1:F:212:LEU:HD21	1:F:217:PRO:HB3	1.80	0.63
1:G:318:PHE:H	1:G:593:GLY:HA3	1.62	0.63
1:G:143:VAL:H	1:G:246:ARG:HG2	1.63	0.63
1:G:557:LYS:HD3	1:G:559:PHE:H	1.63	0.63
1:F:790:LYS:HZ2	1:C:704:SER:HB3	1.64	0.63
1:C:80:ASP:H	1:C:262:ALA:HB2	1.64	0.62
1:C:35:GLY:HA3	1:C:56:LEU:HD12	1.82	0.62
1:F:336:CYS:HB3	1:F:363:ALA:HB2	1.82	0.62
1:G:81:ASN:HB3	1:G:138:ASP:HB3	1.82	0.62
1:C:566:GLY:HA3	1:C:575:ALA:HB3	1.81	0.61
1:G:1086:LYS:NZ	1:G:1087:ALA:O	2.31	0.61
1:F:448:ASN:HB2	1:F:497:PHE:HB2	1.81	0.61
1:F:37:TYR:HB3	1:F:223:LEU:HD23	1.83	0.61
1:G:80:ASP:HB2	1:G:262:ALA:H	1.66	0.61
1:G:752:LEU:O	1:G:755:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:ASN:ND2	1:G:360:ASN:O	2.35	0.60
1:C:979:ASP:O	1:C:983:ARG:HB2	2.01	0.60
1:F:35:GLY:HA3	1:F:56:LEU:HD12	1.83	0.60
1:G:212:LEU:HD21	1:G:217:PRO:HB3	1.82	0.60
1:G:53:ASP:O	1:G:272:PRO:HA	2.02	0.60
1:G:1114:ILE:O	1:G:1119:ASN:ND2	2.33	0.60
1:G:738:CYS:H	1:G:764:LYS:HZ3	1.49	0.59
1:C:27:SER:OG	1:C:64:TRP:O	2.20	0.59
1:C:457:ARG:HH12	1:C:461:LEU:HD13	1.65	0.59
1:F:394:ASN:ND2	1:G:200:TYR:OH	2.35	0.59
1:G:553:THR:HB	1:G:586:ASP:HB2	1.85	0.59
1:C:14:GLN:HB2	1:C:158:ARG:HE	1.67	0.59
1:C:244:LEU:HD23	1:C:246:ARG:HH22	1.68	0.59
2:D:184:VAL:HG22	2:D:464:PHE:HE1	1.68	0.59
1:C:146:GLN:HE21	1:C:249:LEU:HD13	1.68	0.59
1:C:742:ILE:HD11	1:C:997:ILE:HA	1.85	0.59
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.85	0.59
1:F:27:SER:OG	1:F:64:TRP:O	2.20	0.58
1:C:67:ALA:HA	1:C:264:ALA:HB2	1.85	0.58
1:C:148:ASN:ND2	1:C:153:MET:SD	2.76	0.58
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.33	0.58
1:F:989:ALA:O	1:F:993:ILE:N	2.36	0.58
1:G:120:VAL:HB	1:G:127:VAL:HB	1.85	0.58
1:G:37:TYR:OH	1:G:195:LYS:NZ	2.36	0.58
1:C:80:ASP:HB2	1:C:262:ALA:H	1.68	0.58
2:D:165:TRP:HD1	2:D:270:MET:HE3	1.70	0.57
1:G:67:ALA:HA	1:G:264:ALA:HB2	1.85	0.57
1:C:729:VAL:HG21	1:C:781:VAL:HG11	1.86	0.57
1:G:1080:ALA:HB3	1:G:1132:ILE:HD12	1.86	0.57
1:G:27:SER:OG	1:G:64:TRP:O	2.22	0.57
2:D:571:GLU:HA	2:D:575:GLY:H	1.70	0.57
1:G:969:LYS:HZ3	1:G:974:SER:HA	1.69	0.56
1:F:80:ASP:HB2	1:F:262:ALA:H	1.69	0.56
1:C:442:ASP:O	1:C:448:ASN:ND2	2.38	0.56
1:G:422:ASN:ND2	1:G:454:ARG:O	2.39	0.56
1:C:195:LYS:HG2	1:C:197:ILE:HG12	1.86	0.56
2:D:226:VAL:HG21	2:D:513:ILE:HD11	1.87	0.56
1:F:552:LEU:HD22	1:F:585:LEU:HD13	1.88	0.56
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.37	0.56
1:F:120:VAL:HB	1:F:127:VAL:HB	1.87	0.56
1:F:396:TYR:O	1:F:513:LEU:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:LEU:HA	1:G:362:VAL:H	1.70	0.56
1:G:552:LEU:HD12	1:G:585:LEU:HD12	1.87	0.56
1:C:100:ILE:HG22	1:C:242:LEU:HD12	1.87	0.56
1:F:715:PRO:HD3	1:G:894:LEU:HD21	1.87	0.56
1:F:318:PHE:H	1:F:593:GLY:HA3	1.71	0.56
1:C:722:VAL:HA	1:C:1064:HIS:O	2.05	0.56
1:G:475:ALA:HB1	2:D:24:GLN:HB2	1.88	0.55
2:D:267:LEU:HD11	2:D:487:VAL:HG11	1.87	0.55
1:C:302:THR:O	1:C:304:LYS:NZ	2.39	0.55
1:C:969:LYS:HZ3	1:C:974:SER:HA	1.71	0.55
1:F:535:LYS:NZ	1:F:552:LEU:O	2.35	0.55
1:F:917:TYR:HB3	1:C:1129:VAL:HG23	1.88	0.55
1:C:419:ALA:O	1:C:424:LYS:NZ	2.39	0.55
2:D:96:GLN:HG2	2:D:391:LEU:HD22	1.88	0.55
2:D:230:PHE:HA	2:D:233:ILE:HG22	1.88	0.55
1:F:457:ARG:NH1	1:F:467:ASP:OD2	2.40	0.55
1:C:966:LEU:O	1:C:975:SER:OG	2.25	0.55
2:D:83:TYR:O	2:D:101:GLN:NE2	2.38	0.55
1:F:1095:PHE:HB3	1:F:1102:TRP:HE1	1.71	0.55
1:F:566:GLY:HA3	1:F:575:ALA:HB3	1.88	0.55
2:D:56:GLU:N	2:D:56:GLU:OE2	2.40	0.55
1:G:179:LEU:HD12	1:G:180:GLU:HB2	1.89	0.55
1:F:316:SER:OG	1:F:317:ASN:N	2.41	0.54
1:C:452:LEU:HD11	1:C:492:LEU:HB3	1.89	0.54
1:G:1123:SER:OG	1:C:914:ASN:ND2	2.39	0.54
1:C:112:SER:HB3	1:C:134:GLN:HG2	1.89	0.54
1:G:454:ARG:NH2	1:G:469:SER:O	2.40	0.54
2:D:204:ARG:HA	2:D:222:LEU:HD22	1.90	0.54
1:C:82:PRO:O	1:C:237:ARG:NH2	2.40	0.54
1:C:329:PHE:O	1:C:580:GLN:NE2	2.41	0.54
1:G:34:ARG:HH12	1:G:219:GLY:H	1.54	0.54
1:C:14:GLN:OE1	1:C:158:ARG:NH2	2.39	0.54
1:C:118:LEU:HG	1:C:129:LYS:HB2	1.89	0.54
1:C:212:LEU:HD21	1:C:217:PRO:HB3	1.89	0.54
1:F:353:TRP:HB2	1:F:466:ARG:HH22	1.73	0.53
2:D:476:LYS:O	2:D:480:MET:HB2	2.08	0.53
1:C:300:LYS:HD3	1:C:306:PHE:HA	1.89	0.53
1:F:992:GLN:OE1	1:F:995:ARG:NH2	2.41	0.53
1:F:106:PHE:HB3	1:F:235:ILE:HG12	1.91	0.53
1:F:315:THR:HG22	1:F:316:SER:H	1.73	0.53
1:G:589:PRO:HG2	1:C:855:PHE:HD1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ASN:O	1:C:102:ARG:NH2	2.41	0.53
1:C:277:LEU:HD21	1:C:285:ILE:HG12	1.89	0.53
1:C:617:CYS:O	1:C:633:TRP:N	2.42	0.53
1:C:1105:THR:OG1	1:C:1109:PHE:O	2.27	0.53
1:F:280:ASN:OD1	1:F:284:THR:N	2.42	0.53
1:F:788:ILE:HG13	1:F:876:ALA:HB2	1.91	0.53
1:G:559:PHE:HZ	1:G:575:ALA:HB1	1.75	0.53
1:F:103:GLY:HA3	1:F:241:LEU:HB2	1.92	0.52
1:G:328:ARG:HH21	1:G:533:LEU:HB3	1.74	0.52
1:C:79:PHE:HB3	1:C:258:TRP:HB3	1.90	0.52
1:C:416:GLY:H	1:C:419:ALA:HB3	1.74	0.52
1:C:611:LEU:HD12	1:C:650:LEU:HD12	1.90	0.52
1:F:591:SER:O	1:F:634:ARG:NH2	2.34	0.52
1:F:1093:GLY:HA3	1:F:1105:THR:O	2.10	0.52
1:F:128:ILE:HB	1:F:170:TYR:HB3	1.92	0.52
1:C:725:GLU:OE2	1:C:1064:HIS:NE2	2.42	0.52
1:G:34:ARG:NH1	1:G:219:GLY:O	2.43	0.52
1:C:147:LYS:HB2	1:C:155:SER:HA	1.91	0.51
1:C:858:LEU:HD13	1:C:959:LEU:HD22	1.92	0.51
1:F:96:GLU:O	1:F:190:ARG:NH2	2.43	0.51
1:F:1081:ILE:HB	1:F:1088:HIS:HB2	1.92	0.51
1:C:897:PRO:HB2	1:C:900:MET:HG2	1.93	0.51
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.91	0.51
1:F:351:TYR:O	1:F:454:ARG:NH1	2.44	0.51
1:G:99:ASN:OD1	1:G:190:ARG:NH1	2.41	0.51
1:C:55:PHE:HB2	1:C:275:PHE:CE2	2.46	0.51
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.44	0.51
1:F:1082:CYS:HB2	1:F:1134:ASN:HA	1.93	0.51
1:G:449:TYR:OH	1:G:498:ARG:NH2	2.43	0.51
1:C:141:LEU:HB3	1:C:158:ARG:HD2	1.93	0.51
2:D:99:ALA:HB3	2:D:391:LEU:HD11	1.92	0.51
2:D:338:ASN:OD1	2:D:339:VAL:N	2.44	0.51
2:D:524:GLN:HG2	2:D:583:PRO:HG2	1.92	0.51
1:G:109:THR:HG21	1:G:113:LYS:HB3	1.93	0.51
1:C:350:VAL:HG21	1:C:418:ILE:HD12	1.93	0.51
1:F:591:SER:H	1:F:634:ARG:HH12	1.59	0.50
1:C:82:PRO:O	1:C:239:GLN:NE2	2.43	0.50
1:C:456:PHE:H	1:C:491:PRO:HB3	1.76	0.50
1:F:280:ASN:ND2	1:F:284:THR:OG1	2.45	0.50
1:F:770:ILE:HD11	1:F:1012:LEU:HD13	1.93	0.50
1:G:605:SER:OG	1:G:606:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1086:LYS:HE3	1:G:1122:VAL:HG13	1.93	0.50
1:C:355:ARG:NH2	1:C:465:GLU:O	2.44	0.50
1:C:409:GLN:HA	1:C:414:GLN:HE22	1.75	0.50
1:F:294:ASP:O	1:F:297:SER:OG	2.29	0.50
1:G:1116:THR:HG23	1:G:1118:ASP:H	1.76	0.50
1:G:79:PHE:N	1:G:259:THR:O	2.43	0.50
1:G:1092:GLU:OE2	1:G:1107:ARG:NE	2.38	0.50
1:C:102:ARG:HD3	1:C:122:ASN:HA	1.93	0.50
1:C:432:CYS:SG	1:C:433:VAL:N	2.85	0.50
1:F:329:PHE:O	1:F:580:GLN:NE2	2.42	0.50
1:C:65:PHE:HZ	1:C:84:LEU:HD11	1.77	0.50
1:F:452:LEU:HD13	1:F:492:LEU:HD23	1.93	0.49
1:C:54:LEU:HD22	1:C:272:PRO:HB3	1.94	0.49
1:F:715:PRO:HA	1:F:1072:GLU:HA	1.94	0.49
1:G:145:TYR:HE1	1:G:152:TRP:HE1	1.60	0.49
1:C:316:SER:OG	1:C:317:ASN:N	2.44	0.49
1:G:1028:LYS:NZ	1:G:1042:PHE:O	2.45	0.49
1:F:1089:PHE:O	1:F:1120:THR:OG1	2.29	0.49
1:C:299:THR:HG22	1:C:308:VAL:HG11	1.94	0.49
1:G:104:TRP:HB2	1:G:119:ILE:HB	1.93	0.49
1:G:141:LEU:HD22	1:G:157:PHE:HA	1.93	0.49
2:D:235:PRO:O	2:D:238:GLU:HB3	2.12	0.49
1:G:985:ASP:N	1:G:985:ASP:OD1	2.45	0.49
1:G:316:SER:OG	1:G:317:ASN:N	2.45	0.49
1:G:645:THR:HG23	1:G:648:GLY:H	1.78	0.49
1:F:396:TYR:HB2	1:F:514:SER:O	2.12	0.49
1:C:53:ASP:O	1:C:272:PRO:HA	2.13	0.49
1:G:966:LEU:O	1:G:975:SER:OG	2.31	0.49
1:C:16:VAL:HB	1:C:141:LEU:HD22	1.94	0.49
1:F:605:SER:OG	1:F:606:ASN:N	2.45	0.48
2:D:21:ILE:HG12	2:D:84:PRO:HD2	1.95	0.48
1:F:1037:SER:OG	1:F:1043:CYS:SG	2.68	0.48
1:G:212:LEU:HD12	1:G:214:ARG:H	1.78	0.48
1:G:961:THR:HA	1:G:964:LYS:HG2	1.95	0.48
1:C:663:ASP:OD1	1:C:663:ASP:N	2.44	0.48
2:D:49:ASN:HA	2:D:52:THR:HG22	1.94	0.48
2:D:365:THR:HG22	2:D:367:ASP:H	1.77	0.48
1:G:215:ASP:OD1	1:G:266:TYR:OH	2.31	0.48
1:G:277:LEU:HD21	1:G:285:ILE:HD12	1.95	0.48
1:C:151:SER:OG	1:C:152:TRP:N	2.44	0.48
1:C:54:LEU:HB3	1:C:270:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LYS:HD3	1:C:664:ILE:HD11	1.96	0.48
1:F:357:ARG:NH2	1:F:358:ILE:O	2.39	0.48
1:G:128:ILE:HB	1:G:170:TYR:HB3	1.96	0.48
1:G:246:ARG:NH1	1:G:255:SER:OG	2.47	0.48
1:G:1091:ARG:HH12	1:G:1119:ASN:HA	1.79	0.48
1:C:53:ASP:OD1	1:C:53:ASP:N	2.47	0.48
2:D:515:TYR:HD2	2:D:518:ARG:HH21	1.61	0.48
1:G:131:CYS:HA	1:G:166:CYS:HB3	1.96	0.48
1:C:788:ILE:HG13	1:C:876:ALA:HB2	1.94	0.48
2:D:284:PRO:HG3	2:D:440:LEU:HD13	1.96	0.48
1:G:466:ARG:HD2	1:G:468:ILE:HD11	1.94	0.48
1:C:791:THR:HG21	1:C:806:LEU:HD11	1.95	0.47
2:D:205:GLY:HA2	2:D:219:ARG:HG2	1.96	0.47
1:F:391:CYS:HA	1:F:525:CYS:HB3	1.95	0.47
1:F:442:ASP:O	1:F:448:ASN:ND2	2.47	0.47
1:F:722:VAL:HA	1:F:1064:HIS:O	2.14	0.47
1:C:553:THR:HB	1:C:586:ASP:HB2	1.95	0.47
1:F:364:ASP:N	1:F:364:ASP:OD1	2.46	0.47
1:G:869:MET:SD	1:G:869:MET:N	2.73	0.47
1:G:1103:PHE:CD2	1:G:1112:PRO:HB3	2.49	0.47
1:C:353:TRP:H	1:C:466:ARG:HH22	1.61	0.47
1:C:555:SER:HB2	1:C:584:ILE:HB	1.96	0.47
1:C:659:SER:HB3	1:C:698:SER:HB3	1.96	0.47
2:D:573:VAL:HG13	2:D:574:VAL:HG23	1.96	0.47
1:C:103:GLY:HA3	1:C:241:LEU:HB2	1.96	0.47
1:C:147:LYS:HE3	1:C:156:GLU:H	1.80	0.47
2:D:260:GLY:HA3	2:D:610:TRP:HE3	1.79	0.47
1:F:808:ASP:OD2	1:F:811:LYS:N	2.48	0.47
1:G:353:TRP:O	1:G:466:ARG:NE	2.46	0.47
1:G:566:GLY:HA3	1:G:575:ALA:HB3	1.96	0.47
1:C:122:ASN:ND2	1:C:125:ASN:O	2.48	0.47
1:C:139:PRO:HB2	1:C:241:LEU:HD11	1.97	0.47
1:C:343:ASN:HB3	1:C:371:PHE:HZ	1.80	0.47
2:D:226:VAL:HG13	2:D:516:TYR:CZ	2.50	0.47
1:F:77:LYS:HG3	1:F:78:ARG:H	1.80	0.47
1:F:357:ARG:HH22	1:F:395:VAL:H	1.63	0.47
2:D:385:TYR:OH	2:D:401:HIS:NE2	2.40	0.47
1:G:708:SER:HB3	1:G:711:SER:HB3	1.97	0.47
2:D:335:ASP:OD1	2:D:335:ASP:N	2.48	0.47
1:F:966:LEU:O	1:F:975:SER:OG	2.32	0.47
1:G:1107:ARG:HD3	1:C:904:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:699:LEU:HD21	1:G:869:MET:HB2	1.98	0.46
2:D:183:TYR:CE1	2:D:187:LYS:HD2	2.51	0.46
1:F:759:PHE:HA	1:F:762:GLN:HE22	1.80	0.46
1:C:473:TYR:HD2	1:C:488:CYS:HA	1.80	0.46
1:F:936:ASP:O	1:F:940:SER:HB3	2.16	0.46
1:C:364:ASP:OD2	1:C:365:TYR:N	2.48	0.46
1:C:786:LYS:HA	1:C:786:LYS:HD3	1.70	0.46
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.97	0.46
2:D:238:GLU:OE2	2:D:605:GLY:N	2.44	0.46
1:F:120:VAL:HG12	1:F:122:ASN:HD22	1.80	0.46
1:F:897:PRO:HA	1:C:707:TYR:HE1	1.81	0.46
1:F:1091:ARG:NH1	1:F:1118:ASP:O	2.45	0.46
1:G:357:ARG:HH21	1:G:396:TYR:HE1	1.64	0.46
2:D:567:THR:HB	2:D:577:LYS:HE2	1.96	0.46
1:F:210:ILE:HG21	1:F:217:PRO:HG2	1.98	0.46
1:F:326:ILE:HG23	1:F:531:THR:HG23	1.98	0.46
1:G:192:PHE:HA	1:G:204:TYR:O	2.14	0.46
1:G:712:ILE:O	1:G:1074:ASN:HA	2.14	0.46
1:F:401:VAL:HG22	1:F:509:ARG:HD3	1.96	0.46
1:G:54:LEU:HD22	1:G:272:PRO:HB3	1.98	0.46
1:C:328:ARG:HG2	1:C:579:PRO:HD2	1.97	0.46
1:F:296:LEU:HB3	1:F:608:VAL:HG11	1.97	0.46
1:F:384:PRO:HA	1:F:387:LEU:HD23	1.97	0.46
1:C:574:ASP:HA	1:C:587:ILE:HB	1.97	0.46
1:F:894:LEU:HD13	1:C:715:PRO:HD3	1.98	0.45
1:G:785:VAL:HG22	1:G:787:GLN:H	1.80	0.45
1:G:1091:ARG:NH1	1:G:1119:ASN:HA	2.31	0.45
1:F:342:PHE:HB3	1:F:371:PHE:CE2	2.51	0.45
1:G:50:SER:HB2	1:G:276:LEU:HB2	1.98	0.45
1:G:420:ASP:OD1	1:G:420:ASP:N	2.50	0.45
1:G:574:ASP:HA	1:G:587:ILE:HB	1.97	0.45
1:F:56:LEU:HD11	1:F:91:TYR:CG	2.52	0.45
1:F:328:ARG:HG2	1:F:579:PRO:HD2	1.98	0.45
1:G:970:PHE:HE1	1:C:756:TYR:HA	1.80	0.45
1:G:788:ILE:HG13	1:G:876:ALA:HB2	1.99	0.45
1:C:110:LEU:HB3	1:C:135:PHE:HB2	1.98	0.45
2:D:198:ASP:HB3	2:D:201:ASP:H	1.81	0.45
1:F:100:ILE:HG22	1:F:242:LEU:HD12	1.97	0.45
1:C:318:PHE:H	1:C:593:GLY:HA3	1.82	0.45
2:D:355:ASP:OD2	2:D:357:ARG:NH2	2.49	0.45
2:D:527:GLU:HB3	2:D:539:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:722:VAL:HG12	1:G:930:ALA:HB1	1.98	0.45
1:G:738:CYS:N	1:G:764:LYS:HZ3	2.15	0.45
1:G:1039:ARG:NE	1:C:1031:GLU:OE2	2.49	0.45
1:C:591:SER:H	1:C:634:ARG:HH12	1.65	0.45
2:D:267:LEU:HB3	2:D:275:TRP:HE1	1.82	0.45
1:F:725:GLU:OE1	1:F:1064:HIS:NE2	2.48	0.45
1:F:1129:VAL:HG22	1:G:917:TYR:HB3	1.98	0.45
1:C:177:MET:HG2	1:C:178:ASP:H	1.81	0.45
1:F:215:ASP:OD1	1:F:266:TYR:OH	2.33	0.45
1:G:215:ASP:HB3	1:G:216:LEU:H	1.59	0.45
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.99	0.45
2:D:334:THR:OG1	2:D:335:ASP:N	2.49	0.45
1:F:102:ARG:HD3	1:F:122:ASN:HA	1.98	0.44
1:F:333:THR:HG22	1:F:362:VAL:HG21	1.99	0.44
1:G:420:ASP:HA	1:G:424:LYS:HE2	1.99	0.44
1:C:96:GLU:OE2	1:C:100:ILE:N	2.50	0.44
2:D:240:LEU:HD21	2:D:591:LEU:HD21	1.99	0.44
1:G:393:THR:O	1:G:523:THR:OG1	2.35	0.44
1:G:906:PHE:HB3	1:G:911:VAL:HB	1.99	0.44
1:C:326:ILE:HG23	1:C:531:THR:HG23	1.99	0.44
1:F:786:LYS:HA	1:F:786:LYS:HD3	1.82	0.44
1:C:138:ASP:N	1:C:138:ASP:OD1	2.51	0.44
1:C:146:GLN:NE2	1:C:249:LEU:HB2	2.32	0.44
1:C:1115:ILE:HG22	1:C:1137:VAL:HG23	2.00	0.44
1:F:336:CYS:HB2	1:F:361:CYS:HB2	1.78	0.44
1:F:457:ARG:HH22	1:F:461:LEU:HD13	1.81	0.44
1:F:559:PHE:HB3	1:F:560:LEU:H	1.51	0.44
1:C:424:LYS:HD3	1:C:424:LYS:HA	1.84	0.44
1:F:1028:LYS:NZ	1:F:1042:PHE:O	2.51	0.44
1:G:567:ARG:HD2	1:G:571:ASP:HA	2.00	0.44
1:G:1129:VAL:HG22	1:G:1132:ILE:HD11	1.99	0.44
1:C:805:ILE:HD13	1:C:1052:PHE:CE2	2.53	0.44
1:F:113:LYS:HG3	1:F:114:THR:HG23	1.98	0.44
1:F:815:ARG:HB3	1:F:819:GLU:HB3	2.00	0.44
2:D:260:GLY:HA2	2:D:482:ARG:NH2	2.32	0.44
1:C:179:LEU:HD12	1:C:180:GLU:HB2	1.99	0.43
1:C:744:GLY:H	1:C:977:LEU:HD13	1.83	0.43
1:C:819:GLU:OE2	1:C:1055:SER:N	2.51	0.43
2:D:419:LYS:HB2	2:D:424:LEU:HD23	1.99	0.43
1:F:68:ILE:H	1:F:78:ARG:HH22	1.66	0.43
1:C:311:GLY:HA2	1:C:664:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:909:ILE:HD13	1:C:1038:LYS:HZ1	1.83	0.43
1:F:159:VAL:HG23	1:F:160:TYR:CD2	2.53	0.43
1:F:342:PHE:HB3	1:F:371:PHE:HE2	1.82	0.43
1:F:959:LEU:O	1:F:962:LEU:HB3	2.18	0.43
1:F:1123:SER:O	1:F:1123:SER:OG	2.36	0.43
1:G:375:PHE:N	1:G:435:ALA:O	2.52	0.43
2:D:174:LYS:HA	2:D:174:LYS:HD2	1.87	0.43
1:F:81:ASN:HB3	1:F:138:ASP:HB3	2.01	0.43
1:F:756:TYR:HB3	1:F:759:PHE:CD1	2.54	0.43
1:G:80:ASP:OD1	1:G:81:ASN:N	2.52	0.43
1:G:411:ALA:HB3	1:G:414:GLN:HB2	2.00	0.43
2:D:187:LYS:NZ	2:D:509:ASP:OD1	2.34	0.43
1:F:349:SER:OG	1:F:350:VAL:N	2.51	0.43
1:C:80:ASP:OD1	1:C:81:ASN:N	2.50	0.43
1:C:294:ASP:OD1	1:C:294:ASP:N	2.51	0.43
1:C:506:GLN:OE1	1:C:507:PRO:HD2	2.18	0.43
1:C:616:ASN:HA	1:C:644:GLN:HE22	1.84	0.43
1:C:1114:ILE:O	1:C:1119:ASN:ND2	2.52	0.43
2:D:274:PHE:HB3	2:D:276:THR:HG22	2.00	0.43
1:F:474:GLN:OE1	1:F:481:ASN:N	2.48	0.43
1:G:203:ILE:HB	1:G:227:VAL:HB	2.00	0.43
2:D:476:LYS:O	2:D:480:MET:CB	2.66	0.43
1:F:102:ARG:HH11	1:F:122:ASN:HA	1.83	0.42
1:F:456:PHE:HB2	1:F:491:PRO:HA	2.00	0.42
1:C:436:TRP:NE1	1:C:509:ARG:HB2	2.34	0.42
1:F:33:THR:OG1	1:F:219:GLY:O	2.36	0.42
1:F:760:CYS:HA	1:F:763:LEU:HB2	2.01	0.42
1:G:950:ASP:OD1	1:G:950:ASP:N	2.51	0.42
1:C:106:PHE:HB3	1:C:235:ILE:HD12	2.01	0.42
1:F:444:LYS:HG2	1:F:446:SER:H	1.84	0.42
1:G:448:ASN:HB3	1:G:497:PHE:H	1.85	0.42
1:C:280:ASN:OD1	1:C:284:THR:N	2.53	0.42
1:C:424:LYS:HE3	1:C:460:LYS:HD2	2.00	0.42
2:D:589:GLU:HG2	2:D:590:PRO:HD3	2.01	0.42
1:F:40:ASP:OD2	1:F:44:ARG:NH2	2.52	0.42
1:C:560:LEU:H	1:C:563:GLN:HB3	1.84	0.42
1:C:724:THR:HG22	1:C:1063:LEU:HD23	2.00	0.42
1:F:55:PHE:HB2	1:F:275:PHE:CE2	2.54	0.42
1:G:985:ASP:HB2	1:G:987:PRO:HD2	2.02	0.42
1:F:40:ASP:OD1	1:F:40:ASP:N	2.51	0.42
1:G:334:ASN:O	1:G:362:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:998:THR:HA	1:G:1001:LEU:HG	2.02	0.42
1:C:334:ASN:HD21	1:C:361:CYS:HA	1.85	0.42
1:C:357:ARG:NH2	1:C:396:TYR:OH	2.41	0.42
1:G:1129:VAL:HG23	1:C:917:TYR:HB3	2.01	0.42
1:F:343:ASN:HB3	1:F:371:PHE:HZ	1.84	0.42
1:G:819:GLU:OE2	1:G:1055:SER:N	2.52	0.42
1:C:349:SER:OG	1:C:350:VAL:N	2.51	0.42
1:F:68:ILE:HB	1:F:78:ARG:NH1	2.35	0.42
1:F:457:ARG:NE	1:F:459:SER:O	2.52	0.42
1:F:707:TYR:HE1	1:G:897:PRO:HA	1.85	0.42
1:F:714:ILE:HD13	1:F:714:ILE:HA	1.89	0.42
1:G:564:GLN:HB2	1:G:577:ARG:HB2	2.02	0.42
2:D:482:ARG:NH1	2:D:606:TRP:HB2	2.35	0.42
1:G:86:PHE:N	1:G:236:THR:O	2.43	0.42
2:D:407:ILE:HG23	2:D:522:GLN:HB2	2.01	0.42
1:C:438:SER:HB3	1:C:509:ARG:HG2	2.01	0.41
2:D:188:ASN:OD1	2:D:192:ARG:NH1	2.53	0.41
1:C:94:SER:HB2	1:C:265:TYR:HA	2.00	0.41
2:D:539:LEU:HD22	2:D:587:TYR:HB2	2.00	0.41
1:G:64:TRP:HE1	1:G:264:ALA:HB1	1.86	0.41
1:G:877:LEU:HD23	1:G:877:LEU:HA	1.90	0.41
1:C:326:ILE:O	1:C:541:PHE:HA	2.19	0.41
1:G:436:TRP:HE1	1:G:509:ARG:NH2	2.19	0.41
1:G:960:ASN:HA	1:G:963:VAL:HG12	2.02	0.41
1:F:293:LEU:HG	1:F:294:ASP:H	1.85	0.41
1:F:324:GLU:HG2	1:F:539:VAL:HG23	2.02	0.41
1:F:462:LYS:HA	1:F:462:LYS:HD3	1.94	0.41
1:C:923:ILE:O	1:C:927:PHE:N	2.43	0.41
2:D:493:HIS:NE2	2:D:497:TYR:HB2	2.36	0.41
1:F:77:LYS:N	1:F:257:GLY:O	2.54	0.41
1:F:517:LEU:HD23	1:F:517:LEU:HA	1.91	0.41
1:F:716:THR:HG22	1:F:1110:TYR:HB3	2.03	0.41
1:G:605:SER:OG	1:G:607:GLN:OE1	2.39	0.41
1:C:226:LEU:HG	1:C:227:VAL:HG23	2.03	0.41
1:C:428:ASP:OD1	1:C:428:ASP:N	2.53	0.41
1:G:747:THR:O	1:G:750:SER:OG	2.33	0.41
1:G:767:LEU:HA	1:G:770:ILE:HG22	2.02	0.41
1:C:353:TRP:O	1:C:466:ARG:NH1	2.53	0.41
1:C:869:MET:SD	1:C:869:MET:N	2.89	0.41
1:F:722:VAL:HG12	1:F:930:ALA:HB1	2.03	0.41
1:F:68:ILE:O	1:F:78:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:ASN:HA	1:F:594:GLY:H	1.86	0.40
1:F:473:TYR:O	1:F:474:GLN:NE2	2.55	0.40
1:F:616:ASN:HA	1:F:644:GLN:HE22	1.85	0.40
1:G:341:VAL:HG22	1:G:356:LYS:HD3	2.04	0.40
1:G:347:PHE:CE2	1:G:509:ARG:HD2	2.56	0.40
1:G:530:SER:OG	1:G:531:THR:N	2.54	0.40
1:G:878:LEU:HA	1:G:881:THR:HG22	2.03	0.40
1:C:191:GLU:HG2	1:C:206:LYS:HB3	2.03	0.40
2:D:267:LEU:HB3	2:D:275:TRP:NE1	2.36	0.40
2:D:475:LYS:NZ	2:D:495:GLU:OE1	2.53	0.40
1:F:424:LYS:H	1:F:461:LEU:HD23	1.86	0.40
1:C:78:ARG:HE	1:C:261:GLY:HA3	1.86	0.40
2:D:165:TRP:CD1	2:D:270:MET:HE3	2.53	0.40
2:D:530:CYS:HB3	2:D:542:CYS:HB3	1.90	0.40
1:F:29:THR:OG1	1:F:30:ASN:N	2.53	0.40
1:F:37:TYR:OH	1:F:195:LYS:NZ	2.37	0.40
1:F:104:TRP:HB2	1:F:119:ILE:HB	2.03	0.40
1:G:455:LEU:HD22	1:G:493:GLN:HE22	1.87	0.40
1:G:738:CYS:HB3	1:G:760:CYS:HB2	1.89	0.40
1:C:747:THR:O	1:C:750:SER:OG	2.31	0.40
1:G:993:ILE:O	1:G:997:ILE:HG12	2.22	0.40
1:C:129:LYS:NZ	1:C:169:GLU:HA	2.36	0.40
2:D:306:ARG:HH12	2:D:310:GLU:HG2	1.85	0.40
1:F:777:ASN:HD21	1:F:1019:ARG:HD2	1.86	0.40
1:F:1083:HIS:O	1:F:1086:LYS:HG2	2.21	0.40
1:G:113:LYS:HG3	1:G:114:THR:HG23	2.03	0.40
1:G:905:ARG:O	1:G:1036:GLN:NE2	2.52	0.40
1:C:17:ASN:ND2	1:C:138:ASP:OD1	2.38	0.40
1:C:636:TYR:HB3	1:C:637:SER:H	1.77	0.40
2:D:304:ALA:HA	2:D:362:THR:HG21	2.03	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	1053/1221 (86%)	947 (90%)	106 (10%)	0	100	100
1	F	1052/1221 (86%)	959 (91%)	92 (9%)	1 (0%)	48	82
1	G	1052/1221 (86%)	960 (91%)	91 (9%)	1 (0%)	48	82
2	D	592/594 (100%)	565 (95%)	26 (4%)	1 (0%)	44	78
All	All	3749/4257 (88%)	3431 (92%)	315 (8%)	3 (0%)	50	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	303	ASP
1	F	248	TYR
1	G	443	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	935/1056 (88%)	933 (100%)	2 (0%)	92	94
1	F	934/1056 (88%)	932 (100%)	2 (0%)	92	94
1	G	934/1056 (88%)	931 (100%)	3 (0%)	91	92
2	D	525/525 (100%)	525 (100%)	0	100	100
All	All	3328/3693 (90%)	3321 (100%)	7 (0%)	91	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	246	ARG
1	F	955	ASN
1	G	190	ARG
1	G	895	GLN
1	G	955	ASN

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Mol	Chain	Res	Type
1	C	190	ARG
1	C	955	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	762	GLN
1	C	448	ASN
1	C	1106	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](#)

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.