



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 3, 2019 – 08:55 PM EST

PDB ID : 6G2D
EMDB ID: : EMD-4342
Title : Citrate-induced acetyl-CoA carboxylase (ACC-Cit) filament at 5.4 Å resolution
Authors : Hunkeler, M.; Hagmann, A.; Stüttfeld, E.; Chami, M.; Stahlberg, H.; Maier, T.
Deposited on : 2018-03-23
Resolution : 5.40 Å (reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

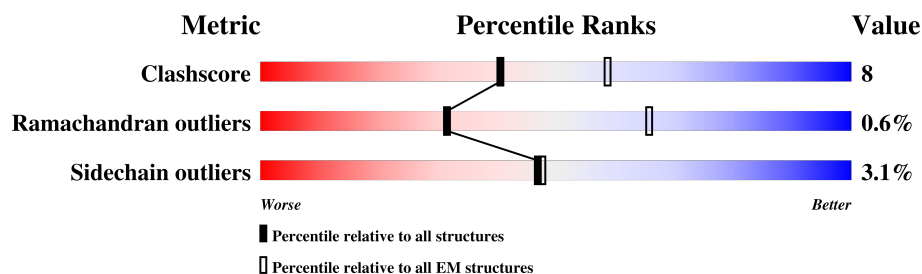
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	B	2407	
1	C	2407	
1	D	2407	
1	F	2407	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 88169 atoms, of which 43991 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 Acetyl-CoA carboxylase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	625	Total	C	H	N	O	S	0	0
			10226	3267	5114	888	922	35		
1	C	2121	Total	C	H	N	O	S	0	0
			33781	10771	16841	2945	3124	100		
1	D	2121	Total	C	H	N	O	S	0	0
			33782	10771	16842	2945	3124	100		
1	F	634	Total	C	H	N	O	S	0	0
			10380	3310	5194	905	936	35		

There are 244 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-60	MET	-	initiating methionine	UNP Q13085
B	-59	ALA	-	expression tag	UNP Q13085
B	-58	HIS	-	expression tag	UNP Q13085
B	-57	HIS	-	expression tag	UNP Q13085
B	-56	HIS	-	expression tag	UNP Q13085
B	-55	HIS	-	expression tag	UNP Q13085
B	-54	HIS	-	expression tag	UNP Q13085
B	-53	HIS	-	expression tag	UNP Q13085
B	-52	HIS	-	expression tag	UNP Q13085
B	-51	HIS	-	expression tag	UNP Q13085
B	-50	HIS	-	expression tag	UNP Q13085
B	-49	HIS	-	expression tag	UNP Q13085
B	-48	GLY	-	expression tag	UNP Q13085
B	-47	SER	-	expression tag	UNP Q13085
B	-46	THR	-	expression tag	UNP Q13085
B	-45	SER	-	expression tag	UNP Q13085
B	-44	GLY	-	expression tag	UNP Q13085
B	-43	SER	-	expression tag	UNP Q13085
B	-42	GLY	-	expression tag	UNP Q13085
B	-41	GLU	-	expression tag	UNP Q13085
B	-40	GLN	-	expression tag	UNP Q13085
B	-39	LYS	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	LEU	-	expression tag	UNP Q13085
B	-37	ILE	-	expression tag	UNP Q13085
B	-36	SER	-	expression tag	UNP Q13085
B	-35	GLU	-	expression tag	UNP Q13085
B	-34	GLU	-	expression tag	UNP Q13085
B	-33	ASP	-	expression tag	UNP Q13085
B	-32	LEU	-	expression tag	UNP Q13085
B	-31	GLY	-	expression tag	UNP Q13085
B	-30	SER	-	expression tag	UNP Q13085
B	-29	THR	-	expression tag	UNP Q13085
B	-28	SER	-	expression tag	UNP Q13085
B	-27	GLY	-	expression tag	UNP Q13085
B	-26	SER	-	expression tag	UNP Q13085
B	-25	GLY	-	expression tag	UNP Q13085
B	-24	ASP	-	expression tag	UNP Q13085
B	-23	TYR	-	expression tag	UNP Q13085
B	-22	LYS	-	expression tag	UNP Q13085
B	-21	ASP	-	expression tag	UNP Q13085
B	-20	ASP	-	expression tag	UNP Q13085
B	-19	ASP	-	expression tag	UNP Q13085
B	-18	ASP	-	expression tag	UNP Q13085
B	-17	LYS	-	expression tag	UNP Q13085
B	-16	LEU	-	expression tag	UNP Q13085
B	-15	THR	-	expression tag	UNP Q13085
B	-14	SER	-	expression tag	UNP Q13085
B	-13	LEU	-	expression tag	UNP Q13085
B	-12	TYR	-	expression tag	UNP Q13085
B	-11	LYS	-	expression tag	UNP Q13085
B	-10	LYS	-	expression tag	UNP Q13085
B	-9	ALA	-	expression tag	UNP Q13085
B	-8	GLY	-	expression tag	UNP Q13085
B	-7	LEU	-	expression tag	UNP Q13085
B	-6	GLU	-	expression tag	UNP Q13085
B	-5	ASN	-	expression tag	UNP Q13085
B	-4	LEU	-	expression tag	UNP Q13085
B	-3	TYR	-	expression tag	UNP Q13085
B	-2	PHE	-	expression tag	UNP Q13085
B	-1	GLN	-	expression tag	UNP Q13085
B	0	GLY	-	expression tag	UNP Q13085
C	-60	MET	-	initiating methionine	UNP Q13085
C	-59	ALA	-	expression tag	UNP Q13085
C	-58	HIS	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-57	HIS	-	expression tag	UNP Q13085
C	-56	HIS	-	expression tag	UNP Q13085
C	-55	HIS	-	expression tag	UNP Q13085
C	-54	HIS	-	expression tag	UNP Q13085
C	-53	HIS	-	expression tag	UNP Q13085
C	-52	HIS	-	expression tag	UNP Q13085
C	-51	HIS	-	expression tag	UNP Q13085
C	-50	HIS	-	expression tag	UNP Q13085
C	-49	HIS	-	expression tag	UNP Q13085
C	-48	GLY	-	expression tag	UNP Q13085
C	-47	SER	-	expression tag	UNP Q13085
C	-46	THR	-	expression tag	UNP Q13085
C	-45	SER	-	expression tag	UNP Q13085
C	-44	GLY	-	expression tag	UNP Q13085
C	-43	SER	-	expression tag	UNP Q13085
C	-42	GLY	-	expression tag	UNP Q13085
C	-41	GLU	-	expression tag	UNP Q13085
C	-40	GLN	-	expression tag	UNP Q13085
C	-39	LYS	-	expression tag	UNP Q13085
C	-38	LEU	-	expression tag	UNP Q13085
C	-37	ILE	-	expression tag	UNP Q13085
C	-36	SER	-	expression tag	UNP Q13085
C	-35	GLU	-	expression tag	UNP Q13085
C	-34	GLU	-	expression tag	UNP Q13085
C	-33	ASP	-	expression tag	UNP Q13085
C	-32	LEU	-	expression tag	UNP Q13085
C	-31	GLY	-	expression tag	UNP Q13085
C	-30	SER	-	expression tag	UNP Q13085
C	-29	THR	-	expression tag	UNP Q13085
C	-28	SER	-	expression tag	UNP Q13085
C	-27	GLY	-	expression tag	UNP Q13085
C	-26	SER	-	expression tag	UNP Q13085
C	-25	GLY	-	expression tag	UNP Q13085
C	-24	ASP	-	expression tag	UNP Q13085
C	-23	TYR	-	expression tag	UNP Q13085
C	-22	LYS	-	expression tag	UNP Q13085
C	-21	ASP	-	expression tag	UNP Q13085
C	-20	ASP	-	expression tag	UNP Q13085
C	-19	ASP	-	expression tag	UNP Q13085
C	-18	ASP	-	expression tag	UNP Q13085
C	-17	LYS	-	expression tag	UNP Q13085
C	-16	LEU	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	THR	-	expression tag	UNP Q13085
C	-14	SER	-	expression tag	UNP Q13085
C	-13	LEU	-	expression tag	UNP Q13085
C	-12	TYR	-	expression tag	UNP Q13085
C	-11	LYS	-	expression tag	UNP Q13085
C	-10	LYS	-	expression tag	UNP Q13085
C	-9	ALA	-	expression tag	UNP Q13085
C	-8	GLY	-	expression tag	UNP Q13085
C	-7	LEU	-	expression tag	UNP Q13085
C	-6	GLU	-	expression tag	UNP Q13085
C	-5	ASN	-	expression tag	UNP Q13085
C	-4	LEU	-	expression tag	UNP Q13085
C	-3	TYR	-	expression tag	UNP Q13085
C	-2	PHE	-	expression tag	UNP Q13085
C	-1	GLN	-	expression tag	UNP Q13085
C	0	GLY	-	expression tag	UNP Q13085
D	-60	MET	-	initiating methionine	UNP Q13085
D	-59	ALA	-	expression tag	UNP Q13085
D	-58	HIS	-	expression tag	UNP Q13085
D	-57	HIS	-	expression tag	UNP Q13085
D	-56	HIS	-	expression tag	UNP Q13085
D	-55	HIS	-	expression tag	UNP Q13085
D	-54	HIS	-	expression tag	UNP Q13085
D	-53	HIS	-	expression tag	UNP Q13085
D	-52	HIS	-	expression tag	UNP Q13085
D	-51	HIS	-	expression tag	UNP Q13085
D	-50	HIS	-	expression tag	UNP Q13085
D	-49	HIS	-	expression tag	UNP Q13085
D	-48	GLY	-	expression tag	UNP Q13085
D	-47	SER	-	expression tag	UNP Q13085
D	-46	THR	-	expression tag	UNP Q13085
D	-45	SER	-	expression tag	UNP Q13085
D	-44	GLY	-	expression tag	UNP Q13085
D	-43	SER	-	expression tag	UNP Q13085
D	-42	GLY	-	expression tag	UNP Q13085
D	-41	GLU	-	expression tag	UNP Q13085
D	-40	GLN	-	expression tag	UNP Q13085
D	-39	LYS	-	expression tag	UNP Q13085
D	-38	LEU	-	expression tag	UNP Q13085
D	-37	ILE	-	expression tag	UNP Q13085
D	-36	SER	-	expression tag	UNP Q13085
D	-35	GLU	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-34	GLU	-	expression tag	UNP Q13085
D	-33	ASP	-	expression tag	UNP Q13085
D	-32	LEU	-	expression tag	UNP Q13085
D	-31	GLY	-	expression tag	UNP Q13085
D	-30	SER	-	expression tag	UNP Q13085
D	-29	THR	-	expression tag	UNP Q13085
D	-28	SER	-	expression tag	UNP Q13085
D	-27	GLY	-	expression tag	UNP Q13085
D	-26	SER	-	expression tag	UNP Q13085
D	-25	GLY	-	expression tag	UNP Q13085
D	-24	ASP	-	expression tag	UNP Q13085
D	-23	TYR	-	expression tag	UNP Q13085
D	-22	LYS	-	expression tag	UNP Q13085
D	-21	ASP	-	expression tag	UNP Q13085
D	-20	ASP	-	expression tag	UNP Q13085
D	-19	ASP	-	expression tag	UNP Q13085
D	-18	ASP	-	expression tag	UNP Q13085
D	-17	LYS	-	expression tag	UNP Q13085
D	-16	LEU	-	expression tag	UNP Q13085
D	-15	THR	-	expression tag	UNP Q13085
D	-14	SER	-	expression tag	UNP Q13085
D	-13	LEU	-	expression tag	UNP Q13085
D	-12	TYR	-	expression tag	UNP Q13085
D	-11	LYS	-	expression tag	UNP Q13085
D	-10	LYS	-	expression tag	UNP Q13085
D	-9	ALA	-	expression tag	UNP Q13085
D	-8	GLY	-	expression tag	UNP Q13085
D	-7	LEU	-	expression tag	UNP Q13085
D	-6	GLU	-	expression tag	UNP Q13085
D	-5	ASN	-	expression tag	UNP Q13085
D	-4	LEU	-	expression tag	UNP Q13085
D	-3	TYR	-	expression tag	UNP Q13085
D	-2	PHE	-	expression tag	UNP Q13085
D	-1	GLN	-	expression tag	UNP Q13085
D	0	GLY	-	expression tag	UNP Q13085
F	-60	MET	-	initiating methionine	UNP Q13085
F	-59	ALA	-	expression tag	UNP Q13085
F	-58	HIS	-	expression tag	UNP Q13085
F	-57	HIS	-	expression tag	UNP Q13085
F	-56	HIS	-	expression tag	UNP Q13085
F	-55	HIS	-	expression tag	UNP Q13085
F	-54	HIS	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-53	HIS	-	expression tag	UNP Q13085
F	-52	HIS	-	expression tag	UNP Q13085
F	-51	HIS	-	expression tag	UNP Q13085
F	-50	HIS	-	expression tag	UNP Q13085
F	-49	HIS	-	expression tag	UNP Q13085
F	-48	GLY	-	expression tag	UNP Q13085
F	-47	SER	-	expression tag	UNP Q13085
F	-46	THR	-	expression tag	UNP Q13085
F	-45	SER	-	expression tag	UNP Q13085
F	-44	GLY	-	expression tag	UNP Q13085
F	-43	SER	-	expression tag	UNP Q13085
F	-42	GLY	-	expression tag	UNP Q13085
F	-41	GLU	-	expression tag	UNP Q13085
F	-40	GLN	-	expression tag	UNP Q13085
F	-39	LYS	-	expression tag	UNP Q13085
F	-38	LEU	-	expression tag	UNP Q13085
F	-37	ILE	-	expression tag	UNP Q13085
F	-36	SER	-	expression tag	UNP Q13085
F	-35	GLU	-	expression tag	UNP Q13085
F	-34	GLU	-	expression tag	UNP Q13085
F	-33	ASP	-	expression tag	UNP Q13085
F	-32	LEU	-	expression tag	UNP Q13085
F	-31	GLY	-	expression tag	UNP Q13085
F	-30	SER	-	expression tag	UNP Q13085
F	-29	THR	-	expression tag	UNP Q13085
F	-28	SER	-	expression tag	UNP Q13085
F	-27	GLY	-	expression tag	UNP Q13085
F	-26	SER	-	expression tag	UNP Q13085
F	-25	GLY	-	expression tag	UNP Q13085
F	-24	ASP	-	expression tag	UNP Q13085
F	-23	TYR	-	expression tag	UNP Q13085
F	-22	LYS	-	expression tag	UNP Q13085
F	-21	ASP	-	expression tag	UNP Q13085
F	-20	ASP	-	expression tag	UNP Q13085
F	-19	ASP	-	expression tag	UNP Q13085
F	-18	ASP	-	expression tag	UNP Q13085
F	-17	LYS	-	expression tag	UNP Q13085
F	-16	LEU	-	expression tag	UNP Q13085
F	-15	THR	-	expression tag	UNP Q13085
F	-14	SER	-	expression tag	UNP Q13085
F	-13	LEU	-	expression tag	UNP Q13085
F	-12	TYR	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	LYS	-	expression tag	UNP Q13085
F	-10	LYS	-	expression tag	UNP Q13085
F	-9	ALA	-	expression tag	UNP Q13085
F	-8	GLY	-	expression tag	UNP Q13085
F	-7	LEU	-	expression tag	UNP Q13085
F	-6	GLU	-	expression tag	UNP Q13085
F	-5	ASN	-	expression tag	UNP Q13085
F	-4	LEU	-	expression tag	UNP Q13085
F	-3	TYR	-	expression tag	UNP Q13085
F	-2	PHE	-	expression tag	UNP Q13085
F	-1	GLN	-	expression tag	UNP Q13085
F	0	GLY	-	expression tag	UNP Q13085

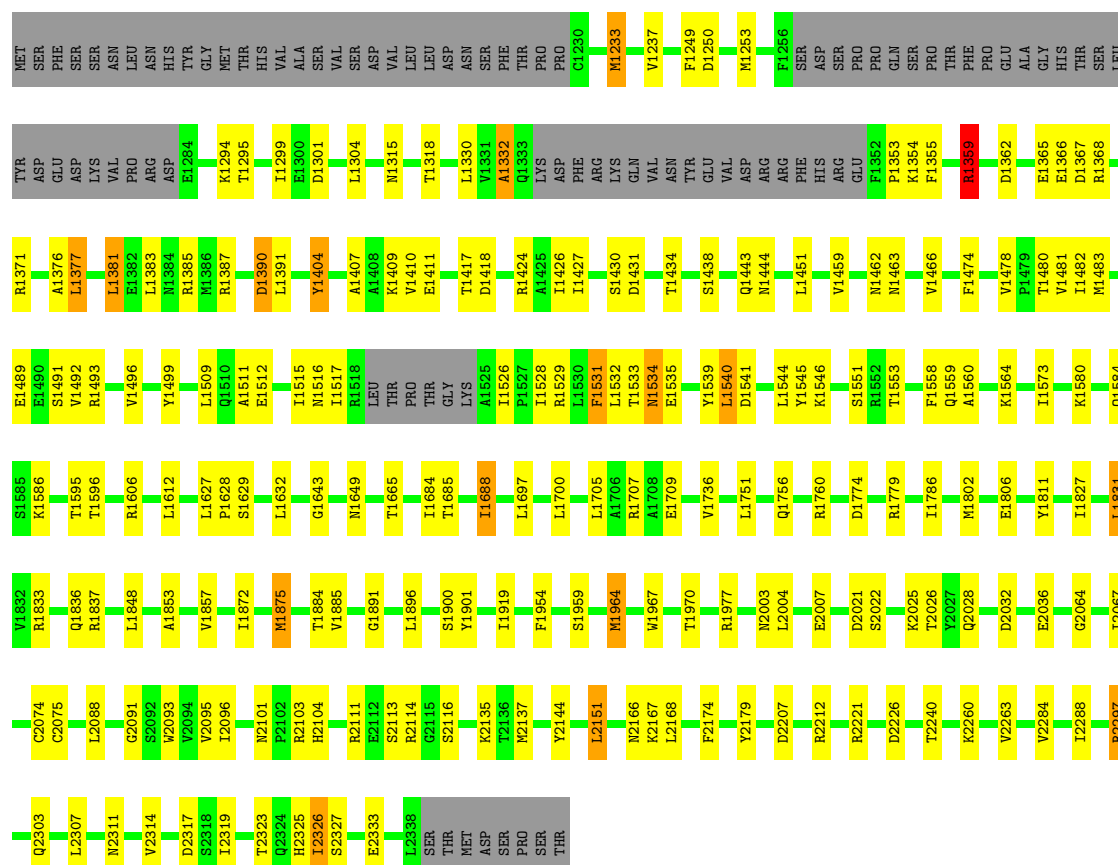



[illegible]

- Molecule 1: Acetyl-CoA carboxylase 1

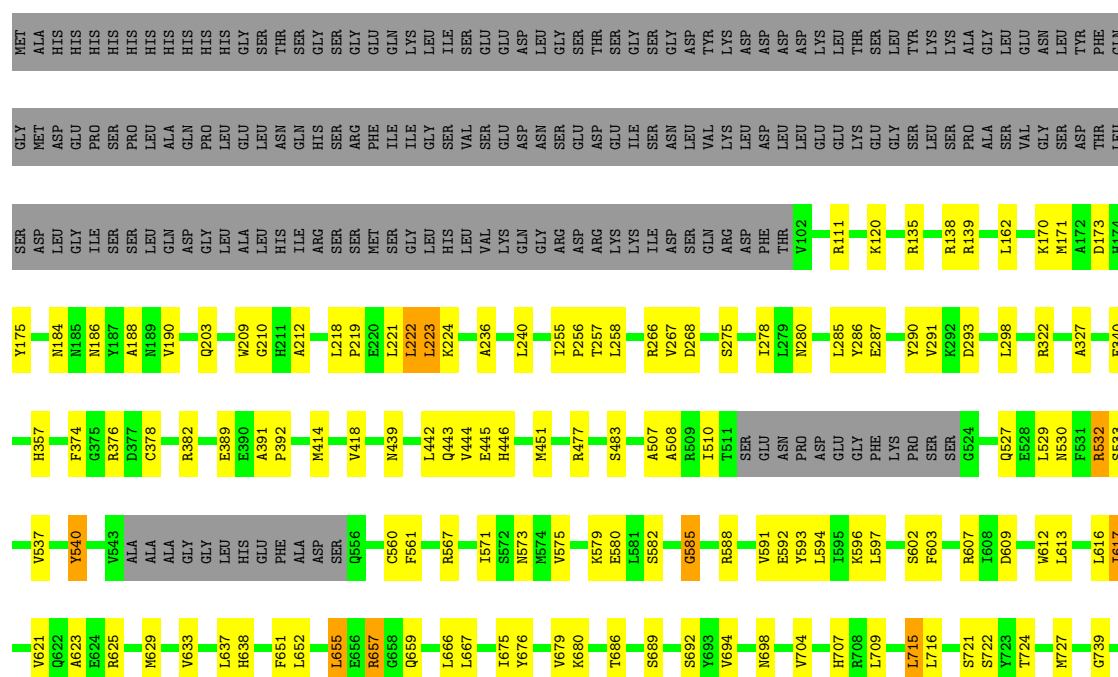
Chain C:  70% 16% • 12%

V1077	A1078	R1080	L1090	P1091	H1096	R1097	M1098	Q1099	S1102	T1108	Y1111	L1123	L1134	F1138	Y1139	H1140	R1146	Y1153	V1154	R1156	M1164	Q1167	Q1170	K1172	D1173	V1177	V1178	F1180	H1188	PRO	ASN	ARG	GLY													
V882	H982	M983	V986	L990	Q993	H994	L995	E996	V997	M1003	Y1006	P1007	K1008	G1009	V1010	R1014	M1017	K1018	S1019	A923	Q924	M1021	N1022	M1026	K1037	N1038	L1039	L1040	V1041	T1042	I1045	D1046	Q1047	L1048	R1051	T1056	D1057	E1058	M1061	T1064	E1065	L1066	T1067	Q1068	A1075	Z1076
V882	T888	L889	P892	L896	H897	E898	D901	T904	P911	P912	X913	Y914	E915	X918	K919	H922	A923	Q924	Y925	A926	L929	T930	L933	Q939	N943	S947	H948	D1046	Q1047	L1048	R1051	N952	K954	N963	Q966	T963	V969	Q970	L971	V972	A975	Z976				
G713	L714	T715	S721	T722	T723	T724	T725	T738	D750	V753	L762	Y765	T766	V767	E768	F774	Q777	D1020	M1021	L809	V814	L815	Q828	R838	S841	L849	H850	F853	D858	R859	L860	V861	M864	Y867	C868	F874	S875	V878								
ASP	QSR	S562	R567	E568	E569	A570	I571	S572	N573	M574	V576	A577	L578	K579	E580	R588	Y593	K596	F603	M629	V633	L637	A640	F651	L652	L655	E656	R657	Q658	Q659	A663	L666	I675	K680	N698	D705	V706	H707								
V409	V415	V418	S419	Y425	L426	L442	H446	E450	B477	S483	T510	SER	GLU	ASN	ASN	GLU	ASN	PRO	ASP	GLY	PHE	PRO	PRO	SER	E528	L529	N530	F531	R532	S533	N534	V537	Y540	A543	ALA	ALA	GLY	GLY	HIS	GLU	PHE					
H185	N186	Y187	A188	N189	V190	D195	Q203	A204	H211	L218	E220	L221	L222	L223	K224	A236	L240	I248	L265	R277	Y286	E287	Y290	V291	K292	D293	A300	V304	R322	E340	R350	Q354	S355	R356	D377	M404	E405	D173	N184							
GLY	ASP	GLU	PRO	SER	PRO	LEU	ALA	GLN	PRO	LEU	ALA	LEU	GLY	ASN	GLY	LEU	HIS	VAL	GLU	ASN	GLU	ILE	SER	GLY	ASP	LEU	ASP	LEU	LEU	LEU	GLU	GLY	LEU	PRO	ALA	ALA	SER	VAL	GLY	ASN	SER	THR	LEU			



• Molecule 1: Acetyl-CoA carboxylase 1

Chain D: 69% 17% 12%



K747	I902	V997	L1108	GLY	ARG	P1485	R1606	I1923	S2116	D2317
E998	M903	E998	I1117	MET	ASP	L1504	L1627	I1923	E2119	S2316
R1014	T904	R1014	I1123	THR	E1284	K1505	P1628	R1935	P2120	I2319
N1017	R909	N1017	L1123	VAL	I1288	L1506	S1629	R1941	E2121	T2323
K1018	R910	K1018	L1124	ALA	I1289	R1507	N1649	R1941	K2135	Q2324
S1019	P911	S1019	T1128	SER	M1290	V1508	N1649	Q1946	K2135	H2325
N1020	P912	N1020	S1129	VAL	V1291	L1509	I1688	Q1949	N2166	I2326
M1021	N913	M1021	S1129	SER	A1292	L1513	I1688	Q1949	K2167	S2327
V1022	V914	V1022	I1130	ASP	I1293	L1514	L1700	L1951	E2173	L2338
N1026	E915	N1026	V1133	VAL	I1299	M1515	R1707	F1954	I2176	SER
Y1027	Y779	Y1027	L1134	LEU	F1300	M1516	R1707	F1954	Q2181	THR
K1037	K920	K1037	F1137	ASP	D1301	R1518	I1714	M1964	Q2181	THR
N1038	A923	N1038	V1145	ASN	D1302	LEU	A1737	M1964	V2184	THR
L1039	Q924	L1039	R1146	SER	R1309	THR	Y1745	V1967	V2184	THR
T1042	A926	T1042	V1154	THR	M1315	THR	Y1745	V1967	R2195	THR
D1046	I929	D1046	R1155	PRO	L1327	GLY	Y1750	V1970	K2209	THR
G1050	T930	G1050	R1156	PRO	L1330	A1525	L1751	V1972	R2212	THR
T1056	V932	T1056	N1164	PRO	V1331	I1526	Y1752	R1977	Y2216	THR
D1057	Q839	D1057	S1165	GLN	A1332	P1527	D1774	N2003	R2221	THR
L1059	N943	L1059	V1166	VAL	Q1333	R1528	R1779	E2007	K2229	THR
L1060	S947	L1060	Q1167	ASP	L1333	R1529	P1794	Q2016	T2240	THR
L1061	N948	L1061	T1175	THR	L1333	F1530	L1797	Q2016	Q2245	THR
L1062	A949	L1062	C1176	GLN	A1332	T1532	M1802	V2017	K2260	THR
L1063	A950	L1063	V1177	VAL	Q1333	M1534	E1806	K2025	V2263	THR
L1064	N952	L1064	Q1181	VAL	L1333	E1535	E1806	K2025	E2275	THR
L1065	L954	L1065	Q1181	GLY	L1333	S1536	Y1811	N2045	T2279	THR
L1066	K848	L1066	L1184	THR	L1333	D1540	I1817	S2050	V2284	THR
L1067	L849	L1067	L1184	THR	L1333	D1541	I1817	S2050	I2288	THR
L1068	H850	L1068	H1188	THR	L1333	L1544	I1817	S2050	S2296	THR
L1069	R851	L1069	H1188	THR	L1333	L1545	I1817	S2050	R2297	THR
L1070	V852	L1070	H1188	THR	L1333	K1546	I1817	S2050	V2300	THR
L1071	N964	L1071	H1188	THR	L1333	K1546	I1817	S2050	I2304	THR
L1072	N968	L1072	H1188	THR	L1333	K1546	I1817	S2050	V2308	THR
L1073	V969	L1073	H1188	THR	L1333	K1546	I1817	S2050	N2311	THR
L1074	Q970	L1074	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1075	L971	L1075	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1076	V972	L1076	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1077	R973	L1077	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1078	R974	L1078	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1079	R974	L1079	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1080	R974	L1080	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1081	R974	L1081	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1082	R974	L1082	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1083	R974	L1083	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1084	R974	L1084	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1085	R974	L1085	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1086	R974	L1086	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1087	R974	L1087	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1088	R974	L1088	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1089	R974	L1089	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1090	R974	L1090	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1091	R974	L1091	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1092	R974	L1092	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1093	R974	L1093	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1094	R974	L1094	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1095	R974	L1095	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1096	R974	L1096	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1097	R974	L1097	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1098	R974	L1098	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1099	R974	L1099	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1100	R974	L1100	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1101	R974	L1101	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1102	R974	L1102	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1103	R974	L1103	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1104	R974	L1104	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1105	R974	L1105	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1106	R974	L1106	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1107	R974	L1107	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1108	R974	L1108	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1109	R974	L1109	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1110	R974	L1110	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1111	R974	L1111	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1112	R974	L1112	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1113	R974	L1113	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1114	R974	L1114	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1115	R974	L1115	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1116	R974	L1116	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1117	R974	L1117	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1118	R974	L1118	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1119	R974	L1119	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1120	R974	L1120	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1121	R974	L1121	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1122	R974	L1122	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1123	R974	L1123	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1124	R974	L1124	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1125	R974	L1125	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1126	R974	L1126	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1127	R974	L1127	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1128	R974	L1128	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1129	R974	L1129	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1130	R974	L1130	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1131	R974	L1131	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1132	R974	L1132	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1133	R974	L1133	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1134	R974	L1134	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1135	R974	L1135	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1136	R974	L1136	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1137	R974	L1137	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1138	R974	L1138	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1139	R974	L1139	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1140	R974	L1140	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1141	R974	L1141	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1142	R974	L1142	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1143	R974	L1143	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1144	R974	L1144	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1145	R974	L1145	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1146	R974	L1146	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1147	R974	L1147	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1148	R974	L1148	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1149	R974	L1149	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1150	R974	L1150	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1151	R974	L1151	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1152	R974	L1152	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1153	R974	L1153	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1154	R974	L1154	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1155	R974	L1155	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1156	R974	L1156	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1157	R974	L1157	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1158	R974	L1158	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1159	R974	L1159	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1160	R974	L1160	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1161	R974	L1161	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1162	R974	L1162	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1163	R974	L1163	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1164	R974	L1164	H1188	THR	L1333	K1546	I1817	S2050	V2314	THR
L1165	R974	L1165	H1188	THR	L1333	K1546	I1817	S2050	V2	







4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	B	0.42	0/5209	0.95	13/7030 (0.2%)
1	C	0.40	1/17302 (0.0%)	0.88	34/23432 (0.1%)
1	D	0.42	2/17302 (0.0%)	0.94	59/23432 (0.3%)
1	F	0.42	0/5284	0.96	12/7131 (0.2%)
All	All	0.41	3/45097 (0.0%)	0.92	118/61025 (0.2%)

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	B	0	8
1	C	0	16
1	D	0	16
1	F	0	10
All	All	0	50

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1526	ILE	C-N	7.03	1.47	1.34
1	D	1527	PRO	CB-CG	-5.58	1.22	1.50
1	C	1138	PHE	CA-C	5.14	1.66	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	971	LEU	CA-CB-CG	13.49	146.33	115.30
1	D	1526	ILE	C-N-CD	-13.29	91.36	120.60
1	D	585	GLY	N-CA-C	12.22	143.64	113.10
1	D	222	LEU	CA-CB-CG	10.98	140.56	115.30
1	D	1527	PRO	C-N-CA	10.94	149.04	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	LEU	CA-CB-CG	9.88	138.01	115.30
1	D	1381	LEU	CA-CB-CG	9.12	136.27	115.30
1	F	933	LEU	CA-CB-CG	9.12	136.26	115.30
1	D	1382	GLU	C-N-CA	8.96	144.11	121.70
1	D	1527	PRO	CA-N-CD	-8.85	99.11	111.50
1	D	1079	LEU	CA-CB-CG	8.80	135.54	115.30
1	D	1085	LEU	CB-CG-CD2	8.72	125.83	111.00
1	D	1384	ASN	C-N-CA	8.24	142.31	121.70
1	D	971	LEU	CA-CB-CG	7.96	133.61	115.30
1	D	1478	VAL	CG1-CB-CG2	7.77	123.33	110.90
1	D	1250	ASP	CB-CG-OD1	7.71	125.24	118.30
1	F	1090	LEU	CA-CB-CG	7.71	133.03	115.30
1	D	1423	VAL	CG1-CB-CG2	7.55	122.99	110.90
1	C	2179	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	F	933	LEU	CB-CG-CD1	7.47	123.70	111.00
1	C	2151	LEU	CB-CG-CD2	-7.42	98.39	111.00
1	D	974	ARG	CA-CB-CG	7.41	129.70	113.40
1	C	1079	LEU	CA-CB-CG	7.34	132.18	115.30
1	C	286	TYR	CA-CB-CG	7.17	127.02	113.40
1	C	1367	ASP	CB-CG-OD1	7.14	124.73	118.30
1	C	1359	ARG	CA-CB-CG	7.13	129.08	113.40
1	C	983	MET	CA-CB-CG	7.01	125.22	113.30
1	D	1134	LEU	CB-CA-C	7.00	123.51	110.20
1	B	971	LEU	CA-CB-CG	6.96	131.30	115.30
1	C	1831	LEU	CA-CB-CG	6.88	131.13	115.30
1	D	1391	LEU	CB-CG-CD2	6.87	122.67	111.00
1	C	2179	TYR	CB-CG-CD1	6.85	125.11	121.00
1	D	1288	ILE	CG1-CB-CG2	6.84	126.44	111.40
1	D	983	MET	CA-CB-CG	6.83	124.91	113.30
1	D	1451	LEU	CA-CB-CG	6.80	130.95	115.30
1	D	286	TYR	CA-CB-CG	6.77	126.26	113.40
1	D	1130	ILE	CG1-CB-CG2	6.71	126.16	111.40
1	C	223	LEU	CA-CB-CG	6.67	130.64	115.30
1	D	1449	LEU	CB-CG-CD1	6.61	122.24	111.00
1	D	1124	ILE	CG1-CB-CG2	6.49	125.69	111.40
1	D	223	LEU	CA-CB-CG	6.48	130.20	115.30
1	D	1368	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	1158	TYR	CA-CB-CG	6.36	125.49	113.40
1	D	1539	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	C	540	TYR	CB-CG-CD1	-6.24	117.26	121.00
1	F	858	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	1964	MET	CA-CB-CG	6.16	123.77	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	952	LEU	CA-CB-CG	6.16	129.47	115.30
1	C	2151	LEU	CB-CG-CD1	6.14	121.44	111.00
1	D	1964	MET	CA-CB-CG	6.13	123.73	113.30
1	D	897	LEU	CA-CB-CG	6.12	129.37	115.30
1	D	1517	ILE	C-N-CA	6.09	136.94	121.70
1	F	896	LEU	CA-CB-CG	6.08	129.28	115.30
1	F	1449	LEU	CB-CG-CD1	6.03	121.25	111.00
1	C	858	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	1367	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	1964	MET	CB-CG-SD	5.98	130.33	112.40
1	D	374	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	D	1504	TRP	CB-CA-C	5.91	122.21	110.40
1	C	889	LEU	CA-CB-CG	5.86	128.77	115.30
1	C	1140	HIS	CB-CA-C	5.78	121.97	110.40
1	C	933	LEU	CA-CB-CG	5.78	128.60	115.30
1	C	588	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	F	1233	MET	CA-CB-CG	5.73	123.04	113.30
1	C	1368	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	899	LEU	CA-CB-CG	5.72	128.47	115.30
1	D	637	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	D	111	ARG	CA-CB-CG	5.67	125.87	113.40
1	D	540	TYR	CB-CG-CD1	-5.66	117.61	121.00
1	B	1140	HIS	CB-CA-C	5.62	121.64	110.40
1	C	540	TYR	CB-CG-CD2	5.62	124.37	121.00
1	D	1403	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	1508	VAL	CG1-CB-CG2	-5.57	101.99	110.90
1	D	666	LEU	CB-CG-CD1	5.56	120.45	111.00
1	C	1404	TYR	CA-CB-CG	5.55	123.95	113.40
1	D	1130	ILE	C-N-CA	5.54	135.56	121.70
1	D	1509	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	858	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	1090	LEU	CA-CB-CG	5.48	127.89	115.30
1	D	374	PHE	CB-CG-CD2	5.47	124.63	120.80
1	B	1318	THR	OG1-CB-CG2	5.46	122.56	110.00
1	D	657	ARG	CA-CB-CG	5.46	125.41	113.40
1	C	1531	PHE	CB-CG-CD2	5.45	124.62	120.80
1	C	815	LEU	CA-CB-CG	5.43	127.80	115.30
1	C	715	LEU	CA-CB-CG	5.42	127.78	115.30
1	D	666	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	B	1442	LEU	CA-CB-CG	5.37	127.65	115.30
1	D	1403	LEU	CB-CG-CD1	5.36	120.12	111.00
1	C	867	TYR	CA-CB-CG	-5.36	103.21	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1232	ARG	CG-CD-NE	5.36	123.05	111.80
1	D	1368	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	990	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	896	LEU	CA-CB-CG	5.33	127.56	115.30
1	D	974	ARG	N-CA-CB	5.31	120.15	110.60
1	D	1451	LEU	CB-CG-CD1	5.29	119.99	111.00
1	D	1485	PRO	N-CA-C	5.28	125.83	112.10
1	D	952	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	1079	LEU	CA-CB-CG	5.24	127.36	115.30
1	C	1390	ASP	N-CA-C	-5.24	96.85	111.00
1	D	540	TYR	CB-CG-CD2	5.23	124.14	121.00
1	C	1090	LEU	CA-CB-CG	5.22	127.32	115.30
1	B	1568	LEU	CB-CG-CD2	5.21	119.86	111.00
1	D	1128	THR	OG1-CB-CG2	5.20	121.97	110.00
1	B	1428	ARG	N-CA-CB	-5.19	101.25	110.60
1	D	1250	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	F	1368	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	F	1137	PHE	C-N-CA	-5.16	108.81	121.70
1	D	382	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	1233	MET	CA-CB-CG	5.10	121.97	113.30
1	C	1531	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	F	971	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	896	LEU	CA-CB-CG	5.04	126.89	115.30
1	D	561	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	F	909	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	561	PHE	CB-CG-CD1	5.02	124.31	120.80
1	C	990	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	1367	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	896	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1171	LEU	Peptide
1	B	1173	ASP	Peptide
1	B	1249	PHE	Peptide
1	B	1315	ASN	Peptide
1	B	1332	ALA	Peptide
1	B	1360	ALA	Peptide
1	B	1466	VAL	Peptide
1	B	1564	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	1047	GLN	Peptide
1	C	1171	LEU	Peptide
1	C	1173	ASP	Peptide
1	C	1249	PHE	Peptide
1	C	1315	ASN	Peptide
1	C	1332	ALA	Peptide
1	C	1362	ASP	Peptide
1	C	1377	LEU	Peptide
1	C	1466	VAL	Peptide
1	C	1564	LYS	Peptide
1	C	277	ARG	Peptide
1	C	588	ARG	Peptide
1	C	750	ASP	Peptide
1	C	924	GLN	Peptide
1	C	952	LEU	Peptide
1	C	954	ARG	Peptide
1	D	1108	ILE	Peptide
1	D	1130	ILE	Peptide
1	D	1184	LEU	Peptide
1	D	1249	PHE	Peptide
1	D	1315	ASN	Peptide
1	D	1332	ALA	Peptide
1	D	1360	ALA	Peptide
1	D	1376	ALA	Peptide
1	D	1526	ILE	Peptide
1	D	1527	PRO	Peptide
1	D	210	GLY	Peptide
1	D	617	ILE	Peptide
1	D	924	GLN	Peptide
1	D	951	THR	Peptide
1	D	953	ASN	Peptide
1	D	956	SER	Peptide
1	F	1140	HIS	Peptide
1	F	1171	LEU	Peptide
1	F	1172	LYS	Peptide
1	F	1249	PHE	Peptide
1	F	1315	ASN	Peptide
1	F	1332	ALA	Peptide
1	F	1376	ALA	Peptide
1	F	1377	LEU	Peptide
1	F	1564	LYS	Peptide
1	F	924	GLN	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	B	5112	5114	5134	108	0
1	C	16940	16841	16897	255	0
1	D	16940	16842	16897	282	0
1	F	5186	5194	5214	113	0
All	All	44178	43991	44142	728	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 8.

All (728) 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:C:1511:ALA:HB3	1:C:1532:LEU:HD12	1.36	1.07
1:C:721:SER:OG	1:D:173:ASP:O	1.92	0.86
1:C:1533:THR:OG1	1:C:1541:ASP:O	1.94	0.84
1:D:357:HIS:ND1	1:D:378:CYS:SG	2.50	0.83
1:C:1387:ARG:O	1:C:1409:LYS:NZ	2.12	0.81
1:C:173:ASP:O	1:D:721:SER:OG	1.98	0.81
1:F:1123:LEU:O	1:F:1156:ARG:NH1	2.15	0.80
1:D:477:ARG:NE	1:D:483:SER:O	2.14	0.77
1:B:1512:GLU:OE1	1:B:1529:ARG:NH2	2.18	0.77
1:C:1003:ASN:O	1:C:1008:LYS:NZ	2.17	0.77
1:B:864:MET:O	1:B:1037:LYS:NZ	2.16	0.77
1:B:1123:LEU:O	1:B:1156:ARG:NH1	2.18	0.77
1:D:1900:SER:OG	1:D:1977:ARG:NH2	2.18	0.76
1:D:1533:THR:OG1	1:D:1541:ASP:O	2.02	0.76
1:C:2317:ASP:OD2	1:D:2297:ARG:NH2	2.19	0.76
1:B:898:GLU:OE1	1:B:975:TYR:OH	2.01	0.75
1:C:864:MET:O	1:C:1037:LYS:NZ	2.19	0.75
1:F:1082:ARG:NH2	1:F:1458:GLU:OE1	2.19	0.75
1:B:1038:ASN:HD22	1:B:1073:THR:HG22	1.52	0.75
1:D:1424:ARG:NH2	1:D:1577:TYR:OH	2.20	0.74
1:D:1833:ARG:NH1	1:D:1836:GLN:OE1	2.21	0.74
1:D:1447:GLU:O	1:D:1451:LEU:HD13	1.87	0.74
1:D:1954:PHE:O	1:D:2212:ARG:NH1	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1512:GLU:OE1	1:F:1529:ARG:NH2	2.20	0.74
1:D:1022:ASN:O	1:D:1026:ASN:ND2	2.20	0.74
1:F:1022:ASN:O	1:F:1026:ASN:ND2	2.20	0.74
1:B:1140:HIS:O	1:B:1146:ARG:NH2	2.20	0.74
1:C:1900:SER:OG	1:C:1977:ARG:NH2	2.20	0.74
1:F:1038:ASN:ND2	1:F:1073:THR:O	2.20	0.73
1:D:1099:GLN:O	1:D:1102:SER:OG	2.02	0.73
1:F:901:ASP:O	1:F:904:THR:OG1	2.06	0.73
1:D:588:ARG:NH2	1:D:739:GLY:O	2.21	0.73
1:C:1837:ARG:NH2	1:C:2036:GLU:OE2	2.22	0.73
1:D:943:ASN:O	1:D:947:SER:OG	2.06	0.73
1:D:873:PHE:O	1:D:876:SER:OG	2.06	0.72
1:F:1531:PHE:O	1:F:1543:SER:OG	2.07	0.72
1:C:1811:TYR:OH	1:C:2032:ASP:OD1	2.08	0.72
1:C:1041:VAL:HG11	1:C:1077:VAL:HG22	1.70	0.72
1:D:1707:ARG:NE	1:D:1806:GLU:OE2	2.23	0.71
1:D:1534:ASN:ND2	1:D:1539:TYR:O	2.24	0.71
1:C:322:ARG:NH2	1:C:340:GLU:OE2	2.23	0.71
1:C:477:ARG:NE	1:C:483:SER:O	2.17	0.71
1:F:1387:ARG:O	1:F:1409:LYS:NZ	2.23	0.71
1:D:828:GLN:OE1	1:D:830:GLU:N	2.22	0.71
1:D:1046:ASP:O	1:D:1050:GLY:HA3	1.91	0.71
1:C:139:ARG:NH2	1:D:533:SER:O	2.24	0.71
1:B:1091:PRO:O	1:B:1096:ARG:NH1	2.24	0.70
1:D:2300:VAL:O	1:D:2304:ILE:HD12	1.91	0.70
1:D:255:ILE:HG23	1:D:258:LEU:HD12	1.71	0.70
1:C:2091:GLY:O	1:C:2095:VAL:HG22	1.91	0.70
1:D:2229:LYS:NZ	1:D:2245:GLN:OE1	2.22	0.70
1:D:596:LYS:NZ	1:D:621:VAL:O	2.25	0.70
1:D:1123:LEU:O	1:D:1156:ARG:NH1	2.25	0.70
1:D:357:HIS:HD1	1:D:378:CYS:HG	1.38	0.69
1:D:532:ARG:NH2	1:D:580:GLU:OE2	2.24	0.69
1:D:623:ALA:O	1:D:625:ARG:NH1	2.25	0.69
1:D:376:ARG:NH2	1:D:443:GLN:OE1	2.26	0.69
1:B:1014:ARG:O	1:B:1018:LYS:HA	1.93	0.69
1:C:121:VAL:HG22	1:C:204:ALA:HB3	1.74	0.69
1:D:901:ASP:O	1:D:904:THR:OG1	2.09	0.69
1:C:1833:ARG:NH1	1:C:1836:GLN:OE1	2.25	0.69
1:D:1038:ASN:ND2	1:D:1073:THR:O	2.25	0.69
1:D:530:ASN:ND2	1:D:537:VAL:O	2.26	0.69
1:D:1811:TYR:OH	1:D:2032:ASP:OD1	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:ASN:O	1:B:1026:ASN:ND2	2.26	0.68
1:C:567:ARG:NH2	1:C:603:PHE:O	2.26	0.68
1:C:530:ASN:O	1:C:532:ARG:NH2	2.27	0.68
1:C:1079:LEU:HB3	1:C:1462:ASN:HD22	1.58	0.68
1:B:892:PRO:HG2	1:B:929:ILE:HD11	1.76	0.68
1:B:939:GLN:O	1:B:943:ASN:ND2	2.27	0.68
1:D:322:ARG:NH2	1:D:340:GLU:OE2	2.27	0.68
1:C:580:GLU:OE1	1:D:135:ARG:NH2	2.27	0.67
1:C:1022:ASN:O	1:C:1026:ASN:ND2	2.27	0.67
1:D:138:ARG:NH2	1:D:171:MET:O	2.27	0.67
1:C:1123:LEU:O	1:C:1156:ARG:NH1	2.29	0.66
1:D:287:GLU:O	1:D:290:TYR:O	2.12	0.66
1:C:655:LEU:O	1:C:1014:ARG:NH1	2.29	0.66
1:C:1427:ILE:O	1:C:1478:VAL:HG22	1.94	0.66
1:D:1082:ARG:NH1	1:D:1455:ASP:OD1	2.29	0.66
1:D:804:ARG:NH2	1:D:1745:TYR:OH	2.28	0.66
1:C:248:ILE:HG13	1:C:265:LEU:HD13	1.78	0.65
1:D:1020:ASP:OD1	1:D:1021:MET:N	2.29	0.65
1:F:1020:ASP:OD1	1:F:1021:MET:N	2.29	0.65
1:C:190:VAL:HG13	1:C:218:LEU:HD23	1.79	0.65
1:D:1177:VAL:HG13	1:D:1237:VAL:HG22	1.77	0.65
1:C:1020:ASP:OD1	1:C:1021:MET:N	2.30	0.65
1:C:1836:GLN:OE1	1:C:2028:GLN:NE2	2.29	0.65
1:C:892:PRO:HB2	1:C:929:ILE:HD11	1.78	0.65
1:B:1534:ASN:ND2	1:B:1539:TYR:O	2.29	0.65
1:C:1140:HIS:O	1:C:1146:ARG:NH2	2.30	0.64
1:D:1445:GLU:O	1:D:1449:LEU:HD13	1.97	0.64
1:F:1014:ARG:O	1:F:1018:LYS:HA	1.97	0.64
1:F:1533:THR:OG1	1:F:1541:ASP:O	2.16	0.64
1:C:1434:THR:OG1	1:C:1482:ILE:O	2.11	0.64
1:F:1382:GLU:OE2	1:F:1529:ARG:NH2	2.31	0.64
1:B:930:THR:OG1	1:D:1166:VAL:O	2.16	0.63
1:D:939:GLN:O	1:D:943:ASN:ND2	2.31	0.63
1:C:901:ASP:O	1:C:904:THR:OG1	2.17	0.63
1:D:926:ALA:O	1:D:929:ILE:HG22	1.98	0.63
1:C:2021:ASP:OD1	1:C:2022:SER:N	2.31	0.63
1:D:1700:LEU:HD22	1:D:1802:MET:CE	2.28	0.63
1:D:1457:LEU:HD23	1:D:1457:LEU:O	1.98	0.63
1:D:2021:ASP:OD1	1:D:2022:SER:N	2.31	0.63
1:B:1496:VAL:HG11	1:B:1540:LEU:HD11	1.79	0.63
1:F:1083:GLN:O	1:F:1087:ALA:HB2	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:838:ARG:O	1:C:841:SER:OG	2.10	0.62
1:D:2166:ASN:OD1	1:D:2167:LYS:N	2.32	0.62
1:C:571:ILE:O	1:C:575:VAL:HG23	1.99	0.62
1:B:996:ARG:NH1	1:B:1027:TYR:OH	2.33	0.62
1:D:186:ASN:OD1	1:D:186:ASN:N	2.33	0.62
1:D:760:GLY:O	1:D:809:LEU:N	2.32	0.62
1:C:355:SER:OG	1:C:426:LEU:HD11	1.99	0.62
1:D:1530:LEU:HD12	1:D:1544:LEU:HD12	1.82	0.62
1:F:1534:ASN:ND2	1:F:1539:TYR:O	2.33	0.62
1:C:705:ASP:OD1	1:C:705:ASP:N	2.30	0.62
1:F:1172:LYS:O	1:F:1175:THR:OG1	2.12	0.62
1:F:898:GLU:OE1	1:F:975:TYR:OH	2.15	0.62
1:C:1014:ARG:O	1:C:1018:LYS:HA	1.98	0.62
1:C:1366:GLU:OE1	1:C:1371:ARG:NH2	2.32	0.62
1:F:1046:ASP:O	1:F:1050:GLY:HA3	2.00	0.62
1:D:190:VAL:HG22	1:D:218:LEU:HD21	1.82	0.62
1:F:1158:TYR:OH	1:F:1326:ARG:NH1	2.33	0.61
1:F:858:ASP:OD1	1:F:859:ASN:N	2.33	0.61
1:F:918:ILE:O	1:F:922:MET:HG2	1.99	0.61
1:D:184:ASN:HA	1:D:188:ALA:HB3	1.82	0.61
1:B:1020:ASP:OD1	1:B:1021:MET:N	2.32	0.61
1:C:120:LYS:N	1:C:203:GLN:OE1	2.32	0.61
1:C:1434:THR:HG23	1:C:1481:VAL:HB	1.83	0.61
1:D:1606:ARG:NH1	1:D:1628:PRO:O	2.32	0.61
1:D:982:HIS:O	1:D:986:VAL:HG12	2.00	0.61
1:C:1047:GLN:O	1:C:1048:LEU:HD22	1.99	0.61
1:C:858:ASP:OD1	1:C:859:ASN:N	2.33	0.61
1:D:1039:LEU:O	1:D:1042:THR:OG1	2.16	0.61
1:F:850:HIS:HB2	1:F:897:LEU:HD23	1.82	0.61
1:F:1014:ARG:NH1	1:F:1018:LYS:O	2.33	0.61
1:F:1079:LEU:HG	1:F:1459:VAL:HG22	1.83	0.61
1:B:1492:VAL:O	1:B:1496:VAL:HG12	2.00	0.61
1:B:902:ILE:HD13	1:B:971:LEU:HD22	1.82	0.61
1:D:1946:GLN:NE2	1:D:1949:GLN:OE1	2.34	0.61
1:D:1237:VAL:HB	1:D:1291:VAL:HG12	1.83	0.60
1:F:1545:TYR:OH	1:F:1567:PRO:O	2.19	0.60
1:C:404:MET:O	1:C:425:TYR:OH	2.19	0.60
1:D:1820:VAL:HG11	1:D:1846:LEU:HD21	1.82	0.60
1:D:212:ALA:HB1	1:D:218:LEU:HD11	1.82	0.60
1:B:1511:ALA:HB3	1:B:1532:LEU:HD12	1.83	0.60
1:D:1403:LEU:HB3	1:D:1423:VAL:HG23	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:850:HIS:HB2	1:C:897:LEU:HD23	1.83	0.60
1:F:1092:SER:HB3	1:F:1095:LEU:HD23	1.84	0.60
1:B:1046:ASP:O	1:B:1050:GLY:HA3	2.02	0.60
1:B:961:PHE:O	1:B:965:THR:HG22	2.01	0.60
1:F:1163:LEU:HD13	1:F:1182:PHE:HB3	1.83	0.60
1:C:1492:VAL:O	1:C:1496:VAL:HG12	2.01	0.60
1:C:2166:ASN:OD1	1:C:2167:LYS:N	2.34	0.60
1:D:1085:LEU:O	1:D:1088:SER:OG	2.19	0.60
1:B:1370:TYR:HE1	1:B:1383:LEU:HD23	1.67	0.59
1:D:1967:TRP:O	1:D:2025:LYS:NZ	2.32	0.59
1:B:1177:VAL:HG13	1:B:1237:VAL:HG22	1.83	0.59
1:B:858:ASP:OD1	1:B:859:ASN:N	2.35	0.59
1:C:1534:ASN:ND2	1:C:1539:TYR:O	2.36	0.59
1:C:2074:CYS:O	1:C:2101:ASN:ND2	2.35	0.59
1:B:1374:GLU:O	1:B:1376:ALA:N	2.35	0.59
1:C:1385:ARG:NE	1:C:1573:ILE:O	2.36	0.59
1:C:1606:ARG:NH1	1:C:1628:PRO:O	2.36	0.59
1:D:389:GLU:HB2	1:D:507:ALA:HB3	1.85	0.59
1:D:508:ALA:HB3	1:D:560:CYS:SG	2.43	0.59
1:D:275:SER:OG	1:D:414:MET:O	2.14	0.59
1:D:1836:GLN:OE1	1:D:2028:GLN:NE2	2.36	0.59
1:C:1330:LEU:HD12	1:C:1355:PHE:CE1	2.38	0.59
1:C:1700:LEU:HD22	1:C:1802:MET:CE	2.32	0.59
1:C:1967:TRP:O	1:C:2025:LYS:NZ	2.34	0.59
1:C:707:HIS:CG	1:D:162:LEU:HD21	2.36	0.59
1:B:1481:VAL:O	1:B:1517:ILE:HG22	2.02	0.58
1:C:926:ALA:O	1:C:929:ILE:HG22	2.02	0.58
1:D:567:ARG:NH2	1:D:603:PHE:O	2.34	0.58
1:C:1632:LEU:HD12	1:C:1665:THR:O	2.02	0.58
1:F:1445:GLU:O	1:F:1449:LEU:HD13	2.03	0.58
1:C:1377:LEU:HD12	1:C:1426:ILE:HD11	1.84	0.58
1:C:1684:ILE:O	1:C:1688:ILE:HA	2.03	0.58
1:F:1099:GLN:O	1:F:1102:SER:OG	2.16	0.58
1:F:1373:LEU:HD13	1:F:1374:GLU:N	2.18	0.58
1:D:2107:MET:SD	1:D:2107:MET:N	2.76	0.58
1:D:721:SER:HG	1:D:722:SER:H	1.51	0.58
1:B:1167:GLN:OE1	1:B:1167:GLN:N	2.37	0.58
1:C:1167:GLN:N	1:C:1167:GLN:OE1	2.37	0.58
1:F:1094:GLU:O	1:F:1095:LEU:HD22	2.04	0.58
1:C:849:LEU:HD22	1:C:888:THR:CG2	2.34	0.57
1:D:686:THR:O	1:D:694:VAL:HG12	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1166:VAL:HG22	1:B:1180:PHE:CD1	2.39	0.57
1:D:1457:LEU:HD22	1:D:1506:LEU:CD1	2.33	0.57
1:F:1492:VAL:O	1:F:1496:VAL:HG12	2.04	0.57
1:B:1047:GLN:O	1:B:1048:LEU:HD22	2.04	0.57
1:C:240:LEU:HD21	1:C:415:VAL:HG11	1.85	0.57
1:C:725:THR:HG22	1:C:738:ILE:HG23	1.86	0.57
1:D:2091:GLY:O	1:D:2095:VAL:HG22	2.03	0.57
1:B:1154:VAL:HG11	1:B:1180:PHE:CZ	2.39	0.57
1:C:949:ALA:O	1:C:952:LEU:HD22	2.05	0.57
1:C:715:LEU:HD13	1:D:175:TYR:OH	2.05	0.57
1:D:947:SER:O	1:D:950:ALA:HB3	2.05	0.57
1:D:1700:LEU:HD22	1:D:1802:MET:HE1	1.87	0.57
1:C:993:GLN:O	1:C:997:VAL:HG22	2.04	0.57
1:B:1253:MET:SD	1:B:1253:MET:N	2.78	0.57
1:B:1421:PHE:CE2	1:B:1460:ALA:HB1	2.40	0.57
1:C:1045:ILE:O	1:C:1048:LEU:C	2.43	0.57
1:D:993:GLN:O	1:D:997:VAL:HG22	2.05	0.57
1:F:864:MET:SD	1:F:993:GLN:NE2	2.78	0.57
1:C:569:GLU:OE2	1:C:573:ASN:ND2	2.29	0.56
1:C:418:VAL:O	1:C:419:SER:OG	2.17	0.56
1:D:1239:PHE:CE1	1:D:1248:ILE:HD11	2.40	0.56
1:C:2174:PHE:O	1:D:804:ARG:NH2	2.38	0.56
1:B:966:GLN:O	1:B:969:VAL:HG12	2.05	0.56
1:D:1504:TRP:O	1:D:1507:ARG:NH1	2.33	0.56
1:C:248:ILE:CG1	1:C:265:LEU:HD13	2.36	0.56
1:D:1737:ALA:HB3	1:D:1750:TYR:O	2.05	0.56
1:D:391:ALA:HB3	1:D:392:PRO:HD3	1.88	0.56
1:F:1113:HIS:O	1:F:1116:CYS:N	2.39	0.56
1:D:287:GLU:O	1:D:290:TYR:C	2.43	0.56
1:C:939:GLN:O	1:C:943:ASN:ND2	2.39	0.56
1:D:721:SER:OG	1:D:722:SER:N	2.39	0.56
1:F:1052:ASP:OD2	1:F:1054:THR:OG1	2.23	0.56
1:F:1391:LEU:HD13	1:F:1404:TYR:OH	2.06	0.56
1:C:2297:ARG:NH2	1:D:2317:ASP:OD2	2.39	0.56
1:D:1383:LEU:HD13	1:D:1383:LEU:O	2.06	0.56
1:D:2016:GLN:HE21	1:D:2045:ASN:HD21	1.53	0.56
1:F:898:GLU:O	1:F:902:ILE:HD12	2.06	0.56
1:B:1184:LEU:HD22	1:B:1187:SER:HB3	1.88	0.55
1:C:1736:VAL:HG22	1:C:1751:LEU:CD2	2.36	0.55
1:D:709:LEU:HD11	1:D:715:LEU:HG	1.86	0.55
1:B:1531:PHE:O	1:B:1543:SER:OG	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:PHE:O	1:B:878:VAL:HG22	2.06	0.55
1:C:184:ASN:HA	1:C:188:ALA:HB3	1.89	0.55
1:D:418:VAL:O	1:D:418:VAL:HG12	2.06	0.55
1:D:629:MET:O	1:D:633:VAL:HG23	2.07	0.55
1:C:1253:MET:HE1	1:C:1318:THR:HG22	1.87	0.55
1:C:721:SER:OG	1:C:722:SER:N	2.39	0.55
1:C:753:VAL:HG13	1:C:814:VAL:HG13	1.88	0.55
1:D:1481:VAL:O	1:D:1517:ILE:HG22	2.06	0.55
1:C:2297:ARG:HG2	1:D:2314:VAL:HG12	1.88	0.55
1:F:1167:GLN:N	1:F:1167:GLN:OE1	2.40	0.55
1:C:1381:LEU:HD13	1:C:1383:LEU:HD22	1.89	0.55
1:C:132:LYS:NZ	1:C:450:GLU:OE1	2.40	0.55
1:C:2174:PHE:O	1:D:1745:TYR:OH	2.24	0.55
1:C:1901:TYR:OH	1:C:1959:SER:O	2.19	0.55
1:D:704:VAL:HB	1:D:716:LEU:HD11	1.89	0.55
1:D:759:ALA:HB2	1:D:811:PRO:HD3	1.89	0.55
1:F:1233:MET:HB3	1:F:1287:HIS:HD1	1.72	0.55
1:D:767:VAL:HG12	1:D:768:GLU:H	1.71	0.54
1:C:162:LEU:HD21	1:D:707:HIS:HB3	1.88	0.54
1:D:442:LEU:HD11	1:D:446:HIS:CG	2.43	0.54
1:F:1420:ARG:NH2	1:F:1578:VAL:O	2.41	0.54
1:C:1885:VAL:HG11	1:C:1891:GLY:HA2	1.88	0.54
1:D:1430:SER:OG	1:D:1431:ASP:N	2.40	0.54
1:D:1527:PRO:CB	1:D:1528:ILE:HG12	2.38	0.54
1:C:911:PRO:O	1:C:914:VAL:HG12	2.07	0.54
1:D:612:TRP:O	1:D:616:LEU:HD23	2.08	0.54
1:F:1079:LEU:HD11	1:F:1462:ASN:HD22	1.72	0.54
1:C:408:ALA:HB2	1:C:425:TYR:OH	2.07	0.54
1:D:724:THR:O	1:D:739:GLY:N	2.40	0.54
1:F:1546:LYS:N	1:F:1559:GLN:O	2.40	0.54
1:C:528:GLU:HG3	1:D:532:ARG:HB3	1.90	0.53
1:B:992:ARG:HA	1:B:995:LEU:HB3	1.89	0.53
1:C:1134:LEU:HD21	1:C:1153:TYR:HB2	1.90	0.53
1:C:1707:ARG:NE	1:C:1806:GLU:OE2	2.38	0.53
1:C:762:LEU:HD11	1:C:809:LEU:HD12	1.89	0.53
1:C:767:VAL:HG12	1:C:768:GLU:H	1.73	0.53
1:D:1737:ALA:HB2	1:D:1752:TYR:CD1	2.43	0.53
1:D:659:GLN:NE2	1:D:2007:GLU:OE2	2.42	0.53
1:F:939:GLN:OE1	1:F:943:ASN:ND2	2.26	0.53
1:B:1496:VAL:HG21	1:B:1540:LEU:HD13	1.90	0.53
1:D:911:PRO:O	1:D:914:VAL:HG12	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1580:LYS:O	1:C:1584:GLN:NE2	2.41	0.53
1:D:1366:GLU:OE1	1:D:1371:ARG:NH1	2.40	0.53
1:D:809:LEU:HD22	1:D:815:LEU:HD21	1.91	0.53
1:C:1430:SER:OG	1:C:1431:ASP:N	2.41	0.53
1:C:2088:LEU:HD12	1:C:2093:TRP:HE3	1.74	0.53
1:C:2103:ARG:NH1	1:C:2226:ASP:OD1	2.41	0.53
1:D:686:THR:HG21	1:D:870:PRO:HD3	1.91	0.53
1:B:1546:LYS:N	1:B:1559:GLN:O	2.42	0.53
1:C:354:GLN:NE2	1:C:355:SER:O	2.41	0.53
1:D:1184:LEU:HD11	1:D:1232:ARG:NH2	2.23	0.53
1:D:1421:PHE:CE2	1:D:1457:LEU:HD21	2.44	0.53
1:D:219:PRO:HA	1:D:222:LEU:HD23	1.91	0.52
1:D:715:LEU:O	1:D:715:LEU:HD12	2.09	0.52
1:F:926:ALA:O	1:F:929:ILE:HG22	2.09	0.52
1:F:993:GLN:O	1:F:997:VAL:HG22	2.10	0.52
1:C:982:HIS:O	1:C:986:VAL:HG12	2.08	0.52
1:C:1099:GLN:O	1:C:1102:SER:OG	2.19	0.52
1:C:1359:ARG:N	1:C:1365:GLU:O	2.42	0.52
1:B:1370:TYR:CE1	1:B:1383:LEU:HD23	2.45	0.52
1:C:1091:PRO:O	1:C:1096:ARG:NH1	2.42	0.52
1:C:170:LYS:HG2	1:D:724:THR:HG21	1.91	0.52
1:F:1107:ALA:HB1	1:F:1116:CYS:HB2	1.91	0.52
1:B:850:HIS:HB2	1:B:897:LEU:HD23	1.92	0.52
1:C:1041:VAL:CG1	1:C:1077:VAL:HG22	2.40	0.52
1:C:1509:LEU:HD12	1:C:1534:ASN:O	2.10	0.52
1:B:1124:ILE:C	1:B:1125:LEU:HD22	2.30	0.52
1:B:898:GLU:O	1:B:902:ILE:HD12	2.10	0.52
1:C:1108:ILE:O	1:C:1111:TYR:N	2.43	0.52
1:D:1480:THR:O	1:D:1480:THR:OG1	2.28	0.52
1:C:724:THR:HG21	1:D:170:LYS:HG3	1.91	0.52
1:D:1014:ARG:O	1:D:1018:LYS:HA	2.09	0.52
1:D:1167:GLN:OE1	1:D:1167:GLN:N	2.42	0.52
1:F:1079:LEU:CD1	1:F:1462:ASN:HD22	2.23	0.52
1:C:1064:THR:O	1:C:1068:GLN:NE2	2.40	0.52
1:C:2022:SER:O	1:C:2026:THR:OG1	2.20	0.52
1:F:1178:VAL:HG12	1:F:1236:MET:HB3	1.92	0.52
1:F:1421:PHE:CZ	1:F:1460:ALA:HB1	2.45	0.52
1:B:1056:THR:O	1:B:1058:GLU:N	2.40	0.52
1:C:1586:LYS:NZ	1:C:1685:THR:OG1	2.20	0.52
1:D:510:ILE:HD11	1:D:540:TYR:O	2.10	0.52
1:B:1014:ARG:NH1	1:B:1021:MET:SD	2.83	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1295:THR:OG1	1:B:1332:ALA:O	2.28	0.51
1:C:724:THR:HG21	1:D:170:LYS:CG	2.40	0.51
1:D:1627:LEU:HD22	1:D:1628:PRO:HD2	1.92	0.51
1:D:923:ALA:O	1:D:926:ALA:HB3	2.10	0.51
1:C:849:LEU:HD22	1:C:888:THR:HG22	1.91	0.51
1:C:971:LEU:HD22	1:C:975:TYR:CZ	2.45	0.51
1:F:947:SER:O	1:F:950:ALA:HB3	2.10	0.51
1:C:918:ILE:O	1:C:922:MET:HG2	2.10	0.51
1:C:947:SER:O	1:C:950:ALA:HB3	2.10	0.51
1:F:1431:ASP:OD1	1:F:1480:THR:N	2.40	0.51
1:D:1535:GLU:HG3	1:D:1536:SER:H	1.76	0.51
1:F:1457:LEU:HB3	1:F:1506:LEU:HD23	1.92	0.51
1:C:1299:ILE:O	1:C:1301:ASP:N	2.44	0.51
1:C:1756:GLN:O	1:C:1760:ARG:NH1	2.44	0.51
1:C:293:ASP:N	1:C:293:ASP:OD1	2.43	0.51
1:C:304:VAL:O	1:C:350:ARG:NH2	2.42	0.51
1:C:966:GLN:O	1:C:969:VAL:HG12	2.10	0.51
1:D:120:LYS:N	1:D:203:GLN:OE1	2.44	0.51
1:D:1470:CYS:HA	1:D:1509:LEU:HD23	1.92	0.51
1:D:293:ASP:N	1:D:293:ASP:OD1	2.44	0.51
1:D:676:TYR:N	1:D:679:VAL:O	2.42	0.51
1:C:186:ASN:N	1:C:186:ASN:OD1	2.42	0.51
1:D:209:TRP:CZ2	1:D:444:VAL:HG23	2.46	0.51
1:C:1551:SER:OG	1:C:1553:THR:O	2.28	0.51
1:C:1853:ALA:O	1:C:1857:VAL:HG23	2.09	0.51
1:D:592:GLU:OE1	1:D:625:ARG:NH1	2.43	0.51
1:B:968:ILE:O	1:B:972:VAL:HG12	2.12	0.50
1:C:878:VAL:O	1:C:882:VAL:HG23	2.11	0.50
1:C:1786:ILE:O	1:D:2195:ARG:NE	2.44	0.50
1:B:1151:GLU:OE2	1:D:932:VAL:HG12	2.12	0.50
1:D:949:ALA:O	1:D:952:LEU:HD22	2.11	0.50
1:C:356:ARG:NH2	1:C:377:ASP:OD2	2.43	0.50
1:F:1323:GLY:C	1:F:1324:ILE:HD12	2.32	0.50
1:C:1046:ASP:OD1	1:C:1080:ARG:NH2	2.44	0.50
1:C:1517:ILE:HG13	1:C:1526:ILE:HD11	1.93	0.50
1:C:1443:GLN:NE2	1:C:1491:SER:OG	2.44	0.50
1:F:902:ILE:HD13	1:F:971:LEU:HD22	1.93	0.50
1:C:1294:LYS:O	1:C:1295:THR:OG1	2.27	0.50
1:C:300:ALA:O	1:C:304:VAL:HG22	2.12	0.50
1:C:874:PHE:O	1:C:878:VAL:HG22	2.12	0.50
1:B:1578:VAL:HG12	1:B:1580:LYS:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1391:LEU:HD22	1:C:1404:TYR:OH	2.11	0.49
1:C:2096:ILE:O	1:C:2096:ILE:HG22	2.12	0.49
1:B:1330:LEU:HD12	1:B:1355:PHE:HE1	1.77	0.49
1:B:1295:THR:HG21	1:B:1331:VAL:HB	1.95	0.49
1:D:1108:ILE:HD13	1:D:1145:VAL:HB	1.94	0.49
1:D:675:ILE:HA	1:D:680:LYS:HA	1.94	0.49
1:D:1941:ARG:O	1:D:1951:LEU:N	2.39	0.49
1:F:1480:THR:OG1	1:F:1480:THR:O	2.29	0.49
1:B:1148:ALA:O	1:B:1152:VAL:HG23	2.13	0.49
1:C:2303:GLN:O	1:C:2307:LEU:HD23	2.12	0.49
1:C:898:GLU:OE1	1:C:975:TYR:OH	2.29	0.49
1:C:1330:LEU:HD21	1:C:1353:PRO:HB3	1.95	0.49
1:C:1627:LEU:HD22	1:C:1628:PRO:HD2	1.93	0.49
1:D:898:GLU:O	1:D:902:ILE:HD12	2.13	0.49
1:F:933:LEU:HD13	1:F:933:LEU:O	2.12	0.49
1:C:913:ASN:OD1	1:C:914:VAL:N	2.45	0.49
1:C:971:LEU:HD22	1:C:975:TYR:CE2	2.48	0.49
1:D:2311:ASN:O	1:D:2314:VAL:HG22	2.13	0.49
1:C:1493:ARG:NH1	1:C:1540:LEU:HD21	2.28	0.49
1:C:1595:THR:OG1	1:C:1596:THR:N	2.45	0.49
1:D:1714:ILE:HD12	1:D:1817:ILE:HB	1.95	0.49
1:D:255:ILE:O	1:D:257:THR:N	2.44	0.49
1:D:591:VAL:HA	1:D:594:LEU:HD12	1.94	0.49
1:D:2260:LYS:O	1:D:2263:VAL:HG12	2.13	0.48
1:F:922:MET:HG3	1:F:923:ALA:N	2.27	0.48
1:D:266:ARG:H	1:D:285:LEU:HD21	1.78	0.48
1:D:1853:ALA:O	1:D:1857:VAL:HG23	2.13	0.48
1:F:1375:PRO:O	1:F:1378:ALA:HB2	2.13	0.48
1:C:1061:ASN:O	1:C:1064:THR:HG22	2.14	0.48
1:F:1164:ASN:C	1:F:1165:SER:HG	2.15	0.48
1:F:1319:LEU:HD21	1:F:1361:ARG:HB2	1.96	0.48
1:D:1527:PRO:HB3	1:D:1528:ILE:HG12	1.94	0.48
1:D:2096:ILE:O	1:D:2096:ILE:HG22	2.13	0.48
1:F:1071:LYS:O	1:F:1074:ASN:C	2.51	0.48
1:F:1517:ILE:HG13	1:F:1526:ILE:HD11	1.95	0.48
1:C:1180:PHE:O	1:C:1233:MET:HB2	2.13	0.48
1:B:1471:ASN:ND2	1:B:1507:ARG:O	2.46	0.48
1:C:721:SER:HG	1:C:722:SER:H	1.61	0.48
1:C:765:TYR:OH	1:C:799:ILE:HG21	2.14	0.48
1:D:968:ILE:O	1:D:972:VAL:HG12	2.14	0.48
1:F:1061:ASN:O	1:F:1064:THR:HG22	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1165:SER:HB2	1:F:1181:GLN:HB2	1.96	0.48
1:D:753:VAL:HG13	1:D:814:VAL:HG13	1.95	0.48
1:F:1143:GLN:HE21	1:F:1170:GLN:NE2	2.10	0.48
1:C:1827:ILE:HD13	1:D:2094:VAL:HG11	1.96	0.47
1:D:1079:LEU:HD11	1:D:1462:ASN:HB3	1.96	0.47
1:D:913:ASN:OD1	1:D:914:VAL:N	2.47	0.47
1:C:1098:ASN:OD1	1:F:1098:ASN:ND2	2.46	0.47
1:C:1418:ASP:OD2	1:C:1584:GLN:NE2	2.47	0.47
1:F:1391:LEU:HB2	1:F:1404:TYR:HE2	1.79	0.47
1:F:878:VAL:O	1:F:882:VAL:HG23	2.14	0.47
1:C:1045:ILE:O	1:C:1048:LEU:O	2.31	0.47
1:D:2325:HIS:O	1:D:2326:ILE:HG23	2.14	0.47
1:C:510:ILE:HD11	1:C:540:TYR:O	2.15	0.47
1:C:2284:VAL:O	1:C:2284:VAL:HG12	2.14	0.47
1:F:852:VAL:CG1	1:F:888:THR:HG21	2.45	0.47
1:F:906:VAL:HG13	1:F:909:ARG:HE	1.80	0.47
1:B:1092:SER:HB3	1:B:1095:LEU:HB3	1.96	0.47
1:B:1093:TYR:CE1	1:B:1133:VAL:HG22	2.50	0.47
1:C:1090:LEU:HD22	1:C:1090:LEU:O	2.14	0.47
1:C:236:ALA:O	1:C:240:LEU:HB2	2.15	0.47
1:D:1239:PHE:CZ	1:D:1248:ILE:HD11	2.49	0.47
1:C:1045:ILE:HG21	1:C:1080:ARG:HB3	1.95	0.47
1:C:1534:ASN:HD22	1:C:1535:GLU:N	2.13	0.47
1:B:1105:LEU:HD21	1:B:1145:VAL:HG11	1.97	0.47
1:B:926:ALA:O	1:B:929:ILE:HG22	2.14	0.47
1:D:1534:ASN:HD22	1:D:1535:GLU:H	1.63	0.47
1:D:255:ILE:HG23	1:D:258:LEU:HB2	1.97	0.47
1:B:1333:GLN:OE1	1:B:1352:PHE:N	2.48	0.47
1:B:1535:GLU:HG3	1:B:1536:SER:H	1.80	0.47
1:D:1774:ASP:O	1:D:1779:ARG:NH1	2.48	0.47
1:D:1824:ALA:HB3	1:D:1846:LEU:HD13	1.97	0.47
1:F:1253:MET:N	1:F:1253:MET:SD	2.87	0.47
1:F:1359:ARG:NH2	1:F:1367:ASP:OD2	2.47	0.47
1:F:1408:ALA:HB2	1:F:1418:ASP:HB2	1.95	0.47
1:B:1061:ASN:O	1:B:1064:THR:HG22	2.15	0.47
1:B:1064:THR:O	1:B:1068:GLN:NE2	2.43	0.47
1:B:1154:VAL:HG11	1:B:1180:PHE:CE2	2.50	0.47
1:B:993:GLN:O	1:B:997:VAL:HG22	2.15	0.47
1:C:2260:LYS:O	1:C:2263:VAL:HG12	2.14	0.47
1:D:1061:ASN:O	1:D:1064:THR:HG22	2.15	0.47
1:D:1442:LEU:HA	1:D:1442:LEU:HD13	1.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1066:LEU:O	1:F:1069:LEU:HD13	2.14	0.47
1:B:1391:LEU:HD12	1:B:1391:LEU:O	2.16	0.46
1:C:1039:LEU:O	1:C:1042:THR:OG1	2.14	0.46
1:C:2064:GLY:O	1:C:2067:ILE:HG13	2.16	0.46
1:D:996:ARG:NH1	1:D:1027:TYR:OH	2.47	0.46
1:C:2093:TRP:CD1	1:D:1797:LEU:HD13	2.49	0.46
1:C:1512:GLU:OE1	1:C:1529:ARG:NH2	2.48	0.46
1:C:287:GLU:O	1:C:290:TYR:O	2.32	0.46
1:D:1534:ASN:HD22	1:D:1535:GLU:N	2.13	0.46
1:D:2113:SER:O	1:D:2114:ARG:NH1	2.41	0.46
1:C:919:LYS:HA	1:C:922:MET:HG2	1.97	0.46
1:D:255:ILE:HD11	1:D:266:ARG:HE	1.80	0.46
1:D:1164:ASN:O	1:D:1165:SER:OG	2.32	0.46
1:F:1391:LEU:HB2	1:F:1404:TYR:CE2	2.50	0.46
1:B:1090:LEU:HD22	1:B:1090:LEU:O	2.15	0.46
1:B:1302:ASP:O	1:B:1306:ALA:HB2	2.16	0.46
1:D:389:GLU:HG3	1:D:445:GLU:HG2	1.97	0.46
1:D:2284:VAL:O	1:D:2284:VAL:HG12	2.15	0.46
1:D:593:TYR:O	1:D:597:LEU:HD23	2.16	0.46
1:F:1418:ASP:OD2	1:F:1420:ARG:NH1	2.49	0.46
1:F:1511:ALA:HB3	1:F:1532:LEU:HD12	1.98	0.46
1:B:1289:LEU:HB3	1:B:1324:ILE:HD11	1.98	0.46
1:C:219:PRO:HA	1:C:222:LEU:HD23	1.98	0.46
1:D:1330:LEU:HD22	1:D:1355:PHE:CE1	2.51	0.46
1:C:1006:TYR:O	1:C:1010:VAL:HG23	2.15	0.46
1:C:2095:VAL:HG23	1:C:2096:ILE:HG12	1.97	0.46
1:C:762:LEU:CD1	1:C:809:LEU:HD12	2.45	0.46
1:D:638:HIS:ND1	1:D:727:MET:HB2	2.31	0.46
1:F:1301:ASP:OD1	1:F:1302:ASP:N	2.48	0.46
1:B:1496:VAL:HG21	1:B:1540:LEU:CD1	2.44	0.46
1:C:2111:ARG:NH1	1:C:2207:ASP:OD1	2.49	0.46
1:C:2319:ILE:O	1:C:2323:THR:N	2.47	0.46
1:D:849:LEU:HD22	1:D:888:THR:HG22	1.97	0.46
1:F:1154:VAL:HG13	1:F:1180:PHE:CE1	2.50	0.46
1:B:1424:ARG:HA	1:B:1474:PHE:HB3	1.98	0.46
1:B:1431:ASP:C	1:B:1432:LEU:HD12	2.36	0.46
1:C:969:VAL:HA	1:C:972:VAL:HG12	1.98	0.46
1:D:1434:THR:HG22	1:D:1482:ILE:HG23	1.97	0.46
1:B:943:ASN:O	1:B:947:SER:OG	2.28	0.45
1:D:1352:PHE:HB3	1:D:1353:PRO:HD3	1.98	0.45
1:D:1421:PHE:CD2	1:D:1457:LEU:HD21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1424:ARG:HG2	1:D:1474:PHE:HB3	1.99	0.45
1:D:920:LYS:O	1:D:923:ALA:HB3	2.14	0.45
1:C:1051:ARG:NH2	1:F:1109:ASP:O	2.50	0.45
1:B:1411:GLU:OE2	1:B:1412:VAL:HG22	2.16	0.45
1:D:256:PRO:O	1:D:257:THR:OG1	2.35	0.45
1:F:923:ALA:O	1:F:926:ALA:HB3	2.17	0.45
1:C:1056:THR:O	1:C:1058:GLU:N	2.42	0.45
1:C:1480:THR:O	1:C:1480:THR:OG1	2.31	0.45
1:C:1612:LEU:HD22	1:C:1896:LEU:HB3	1.99	0.45
1:C:248:ILE:HG12	1:C:265:LEU:HD22	1.99	0.45
1:D:2319:ILE:O	1:D:2323:THR:N	2.47	0.45
1:B:936:PHE:O	1:B:938:SER:N	2.42	0.45
1:D:221:LEU:HA	1:D:224:LYS:HG2	1.97	0.45
1:D:2296:SER:O	1:D:2300:VAL:HG23	2.16	0.45
1:C:637:LEU:HA	1:C:640:ALA:HB3	1.98	0.45
1:D:1299:ILE:O	1:D:1299:ILE:HG22	2.16	0.45
1:C:1451:LEU:HD21	1:C:1499:TYR:CE2	2.51	0.45
1:D:2017:VAL:HG11	1:D:2050:SER:HB3	1.98	0.45
1:F:1154:VAL:HG13	1:F:1180:PHE:CZ	2.51	0.45
1:D:1064:THR:O	1:D:1068:GLN:NE2	2.44	0.45
1:D:1071:LYS:O	1:D:1074:ASN:C	2.55	0.45
1:F:913:ASN:OD1	1:F:914:VAL:N	2.49	0.45
1:F:939:GLN:O	1:F:943:ASN:ND2	2.50	0.45
1:D:1330:LEU:HD11	1:D:1353:PRO:CB	2.46	0.45
1:F:1330:LEU:HD13	1:F:1355:PHE:CD1	2.52	0.45
1:F:919:LYS:HA	1:F:922:MET:HG2	1.98	0.45
1:C:2113:SER:O	1:C:2114:ARG:NH1	2.44	0.45
1:D:1134:LEU:HD23	1:D:1137:PHE:CE1	2.51	0.45
1:D:818:MET:N	1:D:818:MET:SD	2.90	0.45
1:F:1481:VAL:O	1:F:1517:ILE:HG22	2.17	0.45
1:C:1515:ILE:CG2	1:C:1528:ILE:HD11	2.47	0.44
1:C:774:PHE:N	1:C:777:GLN:OE1	2.47	0.44
1:D:1309:ARG:NH1	1:D:1366:GLU:OE2	2.49	0.44
1:D:1545:TYR:HA	1:D:1560:ALA:HA	1.98	0.44
1:B:1166:VAL:HG22	1:B:1180:PHE:HD1	1.81	0.44
1:C:1177:VAL:HG13	1:C:1237:VAL:HG22	2.00	0.44
1:C:715:LEU:HD13	1:D:175:TYR:CZ	2.52	0.44
1:B:1055:LEU:HD13	1:B:1056:THR:N	2.33	0.44
1:C:190:VAL:HG13	1:C:218:LEU:CD2	2.47	0.44
1:C:575:VAL:HG12	1:C:579:LYS:NZ	2.33	0.44
1:D:298:LEU:HD22	1:D:327:ALA:HB1	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:909:ARG:HH11	1:D:964:ASN:HB3	1.82	0.44
1:F:1177:VAL:HG13	1:F:1237:VAL:HG22	1.98	0.44
1:C:922:MET:HG3	1:C:923:ALA:N	2.32	0.44
1:C:995:LEU:HD12	1:C:1066:LEU:HD22	1.98	0.44
1:D:1517:ILE:HG12	1:D:1527:PRO:CD	2.48	0.44
1:D:767:VAL:HG12	1:D:768:GLU:N	2.32	0.44
1:C:1705:LEU:HD11	1:C:1709:GLU:OE2	2.17	0.44
1:C:767:VAL:HG12	1:C:768:GLU:N	2.32	0.44
1:D:1919:ILE:HG21	1:D:2216:TYR:CD2	2.53	0.44
1:D:848:LYS:O	1:D:852:VAL:HG23	2.17	0.44
1:C:858:ASP:HA	1:C:861:VAL:HG12	1.99	0.44
1:D:1060:LEU:HA	1:D:1063:LEU:HB2	1.99	0.44
1:D:1545:TYR:OH	1:D:1567:PRO:O	2.24	0.44
1:B:933:LEU:HB3	1:D:1117:ILE:HG12	1.99	0.44
1:F:852:VAL:HG11	1:F:888:THR:HG21	2.00	0.44
1:B:1360:ALA:HB2	1:B:1365:GLU:HA	2.00	0.44
1:B:1545:TYR:HA	1:B:1560:ALA:HA	2.00	0.44
1:C:1167:GLN:NE2	1:C:1179:GLU:OE1	2.51	0.44
1:C:1919:ILE:HD12	1:C:1919:ILE:H	1.82	0.44
1:D:1301:ASP:OD1	1:D:1302:ASP:N	2.51	0.44
1:D:638:HIS:CE1	1:D:727:MET:HB2	2.53	0.44
1:F:1481:VAL:HG22	1:F:1515:ILE:HD11	1.99	0.44
1:B:886:MET:SD	1:B:1048:LEU:HD21	2.58	0.44
1:B:961:PHE:CE2	1:B:965:THR:HG21	2.52	0.44
1:C:1390:ASP:N	1:C:1407:ALA:O	2.33	0.44
1:C:1872:ILE:HB	1:C:1884:THR:HG21	1.99	0.44
1:C:849:LEU:HD22	1:C:888:THR:HG21	2.00	0.44
1:D:1369:ILE:CD1	1:D:1391:LEU:HD21	2.47	0.44
1:F:1424:ARG:HG2	1:F:1474:PHE:HB3	2.00	0.44
1:B:1482:ILE:O	1:B:1482:ILE:HG22	2.18	0.43
1:D:1700:LEU:HD22	1:D:1802:MET:HE3	1.96	0.43
1:D:2288:ILE:H	1:D:2288:ILE:HD12	1.83	0.43
1:C:1643:GLY:HA3	1:C:1697:LEU:HD21	2.00	0.43
1:C:442:LEU:HD11	1:C:446:HIS:CG	2.53	0.43
1:D:1421:PHE:CD2	1:D:1457:LEU:HD11	2.53	0.43
1:B:939:GLN:OE1	1:B:976:ARG:NH1	2.50	0.43
1:C:963:MET:HA	1:C:966:GLN:HG2	2.01	0.43
1:D:2173:GLU:HA	1:D:2176:ILE:HD12	1.99	0.43
1:F:969:VAL:HA	1:F:972:VAL:HG12	1.99	0.43
1:C:1170:GLN:C	1:C:1171:LEU:HD12	2.39	0.43
1:C:2288:ILE:H	1:C:2288:ILE:HD12	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:LEU:H	1:C:540:TYR:HA	1.84	0.43
1:D:1164:ASN:OD1	1:D:1164:ASN:N	2.52	0.43
1:D:1457:LEU:HD13	1:D:1506:LEU:HD11	2.01	0.43
1:D:571:ILE:O	1:D:575:VAL:HG23	2.18	0.43
1:B:1038:ASN:ND2	1:B:1074:ASN:OD1	2.51	0.43
1:C:629:MET:O	1:C:633:VAL:HG23	2.18	0.43
1:C:707:HIS:CD2	1:C:715:LEU:HD11	2.52	0.43
1:B:980:ARG:O	1:B:984:LYS:HG3	2.19	0.43
1:C:1294:LYS:HA	1:C:1332:ALA:HB3	2.01	0.43
1:C:1079:LEU:HB2	1:C:1459:VAL:HG22	2.00	0.43
1:C:574:MET:O	1:C:577:ALA:HB3	2.19	0.43
1:B:856:VAL:HG21	1:B:884:ARG:HB3	1.99	0.43
1:C:1410:VAL:HG12	1:C:1411:GLU:N	2.34	0.43
1:D:1177:VAL:HG13	1:D:1237:VAL:CG2	2.45	0.43
1:D:1935:ARG:NH2	1:D:1972:VAL:HG11	2.33	0.43
1:C:923:ALA:O	1:C:926:ALA:HB3	2.19	0.43
1:D:1528:ILE:HA	1:D:1545:TYR:O	2.18	0.43
1:B:1480:THR:O	1:B:1480:THR:OG1	2.28	0.43
1:B:919:LYS:HA	1:B:922:MET:HG2	2.00	0.43
1:C:1546:LYS:N	1:C:1559:GLN:O	2.52	0.43
1:C:442:LEU:HD11	1:C:446:HIS:CB	2.49	0.43
1:C:659:GLN:NE2	1:C:2007:GLU:OE2	2.52	0.43
1:C:933:LEU:HD21	1:F:1155:ARG:HD2	2.01	0.43
1:C:968:ILE:O	1:C:972:VAL:HG12	2.19	0.43
1:D:1528:ILE:CA	1:D:1545:TYR:O	2.67	0.43
1:B:1418:ASP:OD2	1:B:1420:ARG:NH1	2.52	0.43
1:C:1164:ASN:N	1:C:1164:ASN:OD1	2.49	0.43
1:C:2311:ASN:O	1:C:2314:VAL:HG22	2.19	0.43
1:D:1434:THR:CG2	1:D:1482:ILE:HG23	2.49	0.43
1:D:895:PRO:O	1:D:899:LEU:HD23	2.19	0.43
1:D:969:VAL:HA	1:D:972:VAL:HG12	2.00	0.43
1:B:1155:ARG:O	1:B:1159:ILE:HB	2.19	0.42
1:B:878:VAL:O	1:B:882:VAL:HG23	2.19	0.42
1:D:2119:GLU:OE1	1:D:2121:GLU:N	2.51	0.42
1:B:1237:VAL:HB	1:B:1291:VAL:HG12	2.01	0.42
1:C:1875:MET:SD	1:C:1875:MET:N	2.92	0.42
1:C:713:GLY:C	1:C:714:LEU:HD12	2.39	0.42
1:D:1046:ASP:OD2	1:D:1080:ARG:NH1	2.52	0.42
1:D:2181:GLN:O	1:D:2184:VAL:HG22	2.19	0.42
1:C:528:GLU:HG2	1:C:540:TYR:HB3	2.00	0.42
1:D:1330:LEU:HD13	1:D:1355:PHE:CD1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:LYS:O	1:B:1041:VAL:HG23	2.19	0.42
1:C:659:GLN:NE2	1:C:2004:LEU:O	2.51	0.42
1:C:663:ALA:O	1:C:666:LEU:HD23	2.18	0.42
1:C:930:THR:HG22	1:C:930:THR:O	2.19	0.42
1:C:528:GLU:CG	1:D:532:ARG:HB3	2.50	0.42
1:F:963:MET:HA	1:F:966:GLN:HG2	2.01	0.42
1:B:1165:SER:HB2	1:B:1181:GLN:HB2	2.00	0.42
1:C:1154:VAL:HG13	1:C:1180:PHE:CE1	2.55	0.42
1:C:1627:LEU:HD12	1:C:1629:SER:OG	2.19	0.42
1:D:1134:LEU:HD23	1:D:1137:PHE:HE1	1.84	0.42
1:D:1165:SER:HB2	1:D:1181:GLN:HB3	2.01	0.42
1:D:1481:VAL:HG22	1:D:1515:ILE:HD11	2.02	0.42
1:D:2064:GLY:O	1:D:2067:ILE:HG13	2.19	0.42
1:D:609:ASP:OD1	1:D:612:TRP:N	2.52	0.42
1:D:766:ILE:HG22	1:D:779:TYR:C	2.39	0.42
1:C:1545:TYR:HA	1:C:1560:ALA:HA	2.02	0.42
1:D:1239:PHE:HB3	1:D:1293:ILE:HG22	2.02	0.42
1:D:613:LEU:O	1:D:617:ILE:HD12	2.20	0.42
1:B:1066:LEU:HD11	1:B:1077:VAL:CG1	2.50	0.42
1:C:287:GLU:O	1:C:290:TYR:C	2.58	0.42
1:C:537:VAL:HG13	1:C:562:SER:HB2	2.01	0.42
1:C:675:ILE:HA	1:C:680:LYS:HA	2.01	0.42
1:F:1062:ILE:H	1:F:1062:ILE:HD12	1.85	0.42
1:F:885:LEU:HD11	1:F:889:LEU:HD12	2.01	0.42
1:F:896:LEU:HA	1:F:899:LEU:HD23	2.01	0.42
1:C:534:ASN:HB3	1:C:537:VAL:HG23	2.01	0.42
1:D:1845:HIS:C	1:D:1846:LEU:HD22	2.40	0.42
1:D:864:MET:O	1:D:1037:LYS:NZ	2.51	0.42
1:F:1180:PHE:HB2	1:F:1234:GLY:HA3	2.02	0.42
1:F:1390:ASP:HB2	1:F:1409:LYS:HB3	2.01	0.42
1:F:1377:LEU:CD1	1:F:1426:ILE:HD11	2.49	0.42
1:D:1410:VAL:HG12	1:D:1411:GLU:N	2.34	0.42
1:D:1919:ILE:HD12	1:D:1919:ILE:H	1.85	0.42
1:D:527:GLN:CD	1:D:529:LEU:HD21	2.40	0.42
1:F:1164:ASN:N	1:F:1164:ASN:OD1	2.51	0.42
1:F:1299:ILE:O	1:F:1299:ILE:HG22	2.19	0.42
1:F:1454:MET:HB2	1:F:1506:LEU:HD21	2.00	0.42
1:F:1549:THR:HG22	1:F:1554:ALA:HA	2.00	0.42
1:D:1923:ILE:O	1:D:2209:LYS:NZ	2.53	0.42
1:D:2095:VAL:HG23	1:D:2096:ILE:HG12	2.02	0.42
1:D:894:LEU:HB3	1:D:895:PRO:HD3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:930:THR:O	1:D:930:THR:HG22	2.20	0.42
1:F:1306:ALA:HA	1:F:1309:ARG:HE	1.84	0.42
1:F:965:THR:HG23	1:F:965:THR:O	2.20	0.42
1:D:1066:LEU:O	1:D:1069:LEU:HD13	2.20	0.41
1:D:1071:LYS:O	1:D:1074:ASN:N	2.53	0.41
1:D:1627:LEU:HD12	1:D:1629:SER:OG	2.19	0.41
1:D:2275:GLU:O	1:D:2279:THR:HG23	2.20	0.41
1:F:939:GLN:CD	1:F:943:ASN:HD21	2.19	0.41
1:B:1294:LYS:O	1:B:1295:THR:OG1	2.33	0.41
1:C:1954:PHE:O	1:C:2212:ARG:NH1	2.52	0.41
1:C:221:LEU:HA	1:C:224:LYS:HG2	2.02	0.41
1:C:164:ALA:HB1	1:C:525:THR:HG21	2.02	0.41
1:D:1474:PHE:C	1:D:1475:LEU:HD12	2.41	0.41
1:D:1517:ILE:H	1:D:1527:PRO:HD2	1.84	0.41
1:D:1515:ILE:O	1:D:1527:PRO:HG2	2.20	0.41
1:D:278:ILE:CG2	1:D:280:ASN:HD22	2.33	0.41
1:B:1164:ASN:OD1	1:B:1164:ASN:N	2.48	0.41
1:D:1133:VAL:HG11	1:D:1332:ALA:HB2	2.01	0.41
1:C:1424:ARG:HG2	1:C:1474:PHE:HB3	2.03	0.41
1:C:1489:GLU:HA	1:C:1492:VAL:HG12	2.02	0.41
1:C:1534:ASN:HD22	1:C:1535:GLU:H	1.66	0.41
1:C:2075:CYS:O	1:C:2104:HIS:NE2	2.53	0.41
1:D:1056:THR:O	1:D:1058:GLU:N	2.51	0.41
1:D:1527:PRO:HB2	1:D:1528:ILE:HG12	2.02	0.41
1:F:1424:ARG:HA	1:F:1474:PHE:HB3	2.02	0.41
1:F:1535:GLU:HG3	1:F:1536:SER:H	1.85	0.41
1:B:1534:ASN:HD22	1:B:1535:GLU:N	2.18	0.41
1:B:878:VAL:HB	1:B:1040:LEU:HD11	2.03	0.41
1:D:1457:LEU:HD22	1:D:1506:LEU:HD11	2.01	0.41
1:D:255:ILE:CD1	1:D:266:ARG:HE	2.34	0.41
1:B:1410:VAL:HG12	1:B:1411:GLU:N	2.36	0.41
1:C:1827:ILE:O	1:C:1831:LEU:HD13	2.21	0.41
1:C:657:ARG:HE	1:C:2007:GLU:CG	2.34	0.41
1:D:1405:LEU:HD12	1:D:1421:PHE:HE1	1.86	0.41
1:D:2323:THR:HG22	1:D:2323:THR:O	2.21	0.41
1:D:579:LYS:O	1:D:582:SER:OG	2.34	0.41
1:B:1506:LEU:N	1:B:1506:LEU:HD12	2.36	0.41
1:B:1388:ASN:HD22	1:B:1576:PRO:HB2	1.86	0.41
1:C:1075:ALA:O	1:C:1079:LEU:HD12	2.20	0.41
1:C:1528:ILE:HB	1:C:1544:LEU:HD21	2.03	0.41
1:D:1595:THR:OG1	1:D:1596:THR:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:585:GLY:HA2	1:D:588:ARG:HD2	2.01	0.41
1:D:651:PHE:O	1:D:655:LEU:HB2	2.21	0.41
1:C:195:ASP:OD2	1:D:851:ARG:NH2	2.54	0.41
1:B:1009:CYS:O	1:B:1013:LEU:HD23	2.21	0.41
1:C:1480:THR:HA	1:C:1516:ASN:O	2.21	0.41
1:C:2323:THR:HG22	1:C:2323:THR:O	2.20	0.41
1:C:2325:HIS:O	1:C:2326:ILE:HG23	2.20	0.41
1:C:651:PHE:O	1:C:655:LEU:HB2	2.21	0.41
1:D:1154:VAL:HG22	1:D:1236:MET:SD	2.61	0.41
1:D:537:VAL:HG21	1:D:573:ASN:HB3	2.01	0.41
1:F:1293:ILE:HD11	1:F:1331:VAL:HG12	2.03	0.41
1:C:2144:TYR:CD1	1:C:2168:LEU:HD11	2.55	0.41
1:D:1133:VAL:HG23	1:D:1353:PRO:CG	2.51	0.41
1:D:529:LEU:H	1:D:540:TYR:HA	1.86	0.41
1:F:1410:VAL:HG12	1:F:1411:GLU:N	2.36	0.41
1:C:967:SER:O	1:C:971:LEU:HB2	2.21	0.41
1:D:1184:LEU:HD11	1:D:1232:ARG:CZ	2.51	0.41
1:D:2304:ILE:O	1:D:2308:VAL:HG23	2.21	0.41
1:D:602:SER:OG	1:D:607:ARG:NH2	2.53	0.41
1:B:1533:THR:OG1	1:B:1541:ASP:O	2.31	0.41
1:B:997:VAL:HG23	1:B:998:GLU:N	2.36	0.41
1:C:1545:TYR:CG	1:C:1558:PHE:HB3	2.56	0.41
1:C:405:GLU:O	1:C:409:VAL:HG23	2.21	0.41
1:C:593:TYR:HA	1:C:596:LYS:HZ2	1.86	0.41
1:B:1055:LEU:HD12	1:B:1060:LEU:HG	2.02	0.40
1:C:173:ASP:O	1:D:722:SER:N	2.42	0.40
1:D:1794:PRO:HB3	1:D:1797:LEU:HD12	2.03	0.40
1:D:236:ALA:O	1:D:240:LEU:HB2	2.21	0.40
1:D:992:ARG:HA	1:D:995:LEU:HB3	2.03	0.40
1:F:1324:ILE:N	1:F:1324:ILE:HD12	2.36	0.40
1:C:1774:ASP:O	1:C:1779:ARG:NH1	2.54	0.40
1:D:612:TRP:C	1:D:616:LEU:HD23	2.42	0.40
1:B:1387:ARG:HE	1:B:1576:PRO:HG3	1.86	0.40
1:D:1289:LEU:O	1:D:1327:LEU:HA	2.21	0.40
1:D:2323:THR:HG23	1:D:2326:ILE:HD11	2.02	0.40
1:D:267:VAL:HG12	1:D:268:ASP:N	2.36	0.40
1:D:971:LEU:HA	1:D:974:ARG:HD3	2.03	0.40
1:B:1297:CYS:SG	1:B:1298:ASP:N	2.94	0.40
1:C:533:SER:O	1:D:139:ARG:NE	2.52	0.40
1:D:796:SER:O	1:D:820:LEU:HD22	2.22	0.40
1:D:997:VAL:HG23	1:D:998:GLU:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1382:GLU:O	1:F:1424:ARG:NH2	2.53	0.40
1:F:922:MET:HG3	1:F:923:ALA:H	1.86	0.40
1:B:1302:ASP:O	1:B:1306:ALA:CB	2.70	0.40
1:C:1299:ILE:H	1:C:1299:ILE:HD12	1.86	0.40
1:C:1434:THR:HG21	1:C:1483:MET:HB2	2.02	0.40
1:D:1546:LYS:O	1:D:1558:PHE:HA	2.22	0.40
1:D:689:SER:HB3	1:D:692:SER:HB2	2.04	0.40
1:D:983:MET:O	1:D:987:VAL:HG12	2.22	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	B	609/2407 (25%)	522 (86%)	81 (13%)	6 (1%)	17	59
1	C	2107/2407 (88%)	1908 (91%)	191 (9%)	8 (0%)	36	77
1	D	2107/2407 (88%)	1901 (90%)	193 (9%)	13 (1%)	27	70
1	F	620/2407 (26%)	521 (84%)	91 (15%)	8 (1%)	13	54
All	All	5443/9628 (56%)	4852 (89%)	556 (10%)	35 (1%)	31	70

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1087	ALA
1	B	1304	LEU
1	B	1365	GLU
1	C	1304	LEU
1	D	1527	PRO
1	F	1087	ALA
1	C	211	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	291	VAL
1	D	667	LEU
1	D	867	TYR
1	F	1172	LYS
1	B	937	PRO
1	C	291	VAL
1	C	868	CYS
1	C	1376	ALA
1	D	1564	LYS
1	D	1580	LYS
1	D	1376	ALA
1	D	1400	LYS
1	D	1560	ALA
1	D	1581	ASP
1	F	937	PRO
1	F	994	TYR
1	F	1113	HIS
1	F	1173	ASP
1	C	419	SER
1	F	938	SER
1	F	1376	ALA
1	B	1360	ALA
1	C	853	PHE
1	D	1146	ARG
1	D	1360	ALA
1	C	1688	ILE
1	D	1688	ILE
1	B	1412	VAL

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	B	571/2108 (27%)	552 (97%)	19 (3%)	41	67
1	C	1855/2108 (88%)	1806 (97%)	49 (3%)	49	73
1	D	1855/2108 (88%)	1800 (97%)	55 (3%)	44	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	579/2108 (28%)	552 (95%)	27 (5%)	29	59
All	All	4860/8432 (58%)	4710 (97%)	150 (3%)	47	68

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	857	LEU
1	B	889	LEU
1	B	897	LEU
1	B	947	SER
1	B	1090	LEU
1	B	1309	ARG
1	B	1354	LYS
1	B	1359	ARG
1	B	1368	ARG
1	B	1381	LEU
1	B	1417	THR
1	B	1438	SER
1	B	1444	ASN
1	B	1463	ASN
1	B	1531	PHE
1	B	1534	ASN
1	B	1540	LEU
1	B	1546	LYS
1	B	1577	TYR
1	C	223	LEU
1	C	529	LEU
1	C	637	LEU
1	C	652	LEU
1	C	655	LEU
1	C	698	ASN
1	C	705	ASP
1	C	828	GLN
1	C	875	SER
1	C	897	LEU
1	C	915	GLU
1	C	933	LEU
1	C	947	SER
1	C	954	ARG
1	C	983	MET
1	C	1008	LYS
1	C	1017	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1065	GLU
1	C	1066	LEU
1	C	1079	LEU
1	C	1090	LEU
1	C	1096	ARG
1	C	1250	ASP
1	C	1354	LYS
1	C	1359	ARG
1	C	1381	LEU
1	C	1417	THR
1	C	1438	SER
1	C	1444	ASN
1	C	1463	ASN
1	C	1531	PHE
1	C	1534	ASN
1	C	1540	LEU
1	C	1649	ASN
1	C	1848	LEU
1	C	1875	MET
1	C	1964	MET
1	C	1970	THR
1	C	2003	ASN
1	C	2116	SER
1	C	2135	LYS
1	C	2137	MET
1	C	2151	LEU
1	C	2221	ARG
1	C	2240	THR
1	C	2297	ARG
1	C	2326	ILE
1	C	2327	SER
1	C	2333	GLU
1	D	223	LEU
1	D	439	ASN
1	D	451	MET
1	D	532	ARG
1	D	652	LEU
1	D	655	LEU
1	D	657	ARG
1	D	698	ASN
1	D	715	LEU
1	D	747	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	791	LEU
1	D	897	LEU
1	D	899	LEU
1	D	915	GLU
1	D	947	SER
1	D	954	ARG
1	D	974	ARG
1	D	1017	ASN
1	D	1079	LEU
1	D	1096	ARG
1	D	1170	GLN
1	D	1175	THR
1	D	1233	MET
1	D	1236	MET
1	D	1250	ASP
1	D	1354	LYS
1	D	1377	LEU
1	D	1381	LEU
1	D	1391	LEU
1	D	1403	LEU
1	D	1417	THR
1	D	1438	SER
1	D	1444	ASN
1	D	1449	LEU
1	D	1451	LEU
1	D	1463	ASN
1	D	1475	LEU
1	D	1478	VAL
1	D	1513	LEU
1	D	1531	PHE
1	D	1534	ASN
1	D	1540	LEU
1	D	1575	THR
1	D	1649	ASN
1	D	1875	MET
1	D	1964	MET
1	D	1970	THR
1	D	2003	ASN
1	D	2116	SER
1	D	2135	LYS
1	D	2221	ARG
1	D	2240	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2297	ARG
1	D	2326	ILE
1	D	2327	SER
1	F	851	ARG
1	F	864	MET
1	F	897	LEU
1	F	899	LEU
1	F	909	ARG
1	F	915	GLU
1	F	933	LEU
1	F	947	SER
1	F	1065	GLU
1	F	1066	LEU
1	F	1090	LEU
1	F	1096	ARG
1	F	1244	ASP
1	F	1250	ASP
1	F	1289	LEU
1	F	1319	LEU
1	F	1326	ARG
1	F	1354	LYS
1	F	1381	LEU
1	F	1417	THR
1	F	1438	SER
1	F	1444	ASN
1	F	1449	LEU
1	F	1463	ASN
1	F	1478	VAL
1	F	1534	ASN
1	F	1540	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	862	ASN
1	B	865	ASN
1	B	943	ASN
1	B	964	ASN
1	B	966	GLN
1	B	1033	GLN
1	B	1038	ASN
1	B	1114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1287	HIS
1	B	1313	GLN
1	B	1315	ASN
1	B	1333	GLN
1	B	1388	ASN
1	B	1443	GLN
1	B	1444	ASN
1	B	1463	ASN
1	B	1476	ASN
1	B	1534	ASN
1	B	1565	GLN
1	B	1569	HIS
1	C	165	ASN
1	C	225	ASN
1	C	280	ASN
1	C	354	GLN
1	C	698	ASN
1	C	859	ASN
1	C	862	ASN
1	C	943	ASN
1	C	966	GLN
1	C	1017	ASN
1	C	1026	ASN
1	C	1119	ASN
1	C	1429	HIS
1	C	1443	GLN
1	C	1444	ASN
1	C	1462	ASN
1	C	1463	ASN
1	C	1476	ASN
1	C	1534	ASN
1	C	2003	ASN
1	C	2028	GLN
1	C	2045	ASN
1	D	225	ASN
1	D	280	ASN
1	D	354	GLN
1	D	698	ASN
1	D	707	HIS
1	D	862	ASN
1	D	943	ASN
1	D	964	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	966	GLN
1	D	1017	ASN
1	D	1026	ASN
1	D	1114	GLN
1	D	1443	GLN
1	D	1444	ASN
1	D	1463	ASN
1	D	1534	ASN
1	D	1946	GLN
1	D	2003	ASN
1	D	2028	GLN
1	D	2045	ASN
1	F	859	ASN
1	F	862	ASN
1	F	865	ASN
1	F	1170	GLN
1	F	1181	GLN
1	F	1402	HIS
1	F	1444	ASN
1	F	1462	ASN
1	F	1463	ASN
1	F	1534	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.