



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:57 AM EDT

PDB ID : 1YWK
Title : Crystal structure of 4-deoxy-1-threo-5-hexosulose-uronate ketol-isomerase from *Enterococcus faecalis*
Authors : Fedorov, A.A.; Fedorov, E.V.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2005-02-18
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

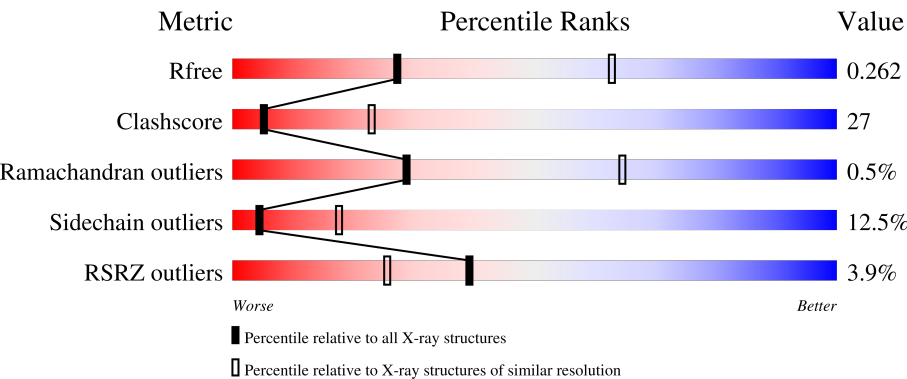
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	
1	C	289	
1	D	289	
1	E	289	

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Mol	Chain	Length	Quality of chain
1	F	289	<div><div></div><div>4%</div><div>46%</div><div>35%</div><div>7%</div><div>12%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12252 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2053	1302	340	396	15			
1	B	254	Total	C	N	O	S	0	0	0
			2042	1296	336	395	15			
1	C	253	Total	C	N	O	S	0	0	0
			2036	1291	338	392	15			
1	D	254	Total	C	N	O	S	0	0	0
			2045	1296	339	395	15			
1	E	254	Total	C	N	O	S	0	0	0
			2042	1296	336	395	15			
1	F	253	Total	C	N	O	S	0	0	0
			2034	1290	335	394	15			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	996	MET	-	cloning artifact	UNP Q838L9
A	997	SER	-	cloning artifact	UNP Q838L9
A	998	LEU	-	cloning artifact	UNP Q838L9
A	999	GLN	-	cloning artifact	UNP Q838L9
A	1000	ASN	-	cloning artifact	UNP Q838L9
A	1277	GLU	-	cloning artifact	UNP Q838L9
A	1278	GLY	-	cloning artifact	UNP Q838L9
A	1279	HIS	-	cloning artifact	UNP Q838L9
A	1280	HIS	-	cloning artifact	UNP Q838L9
A	1281	HIS	-	cloning artifact	UNP Q838L9
A	1282	HIS	-	cloning artifact	UNP Q838L9
A	1283	HIS	-	cloning artifact	UNP Q838L9
A	1284	HIS	-	cloning artifact	UNP Q838L9
B	996	MET	-	cloning artifact	UNP Q838L9
B	997	SER	-	cloning artifact	UNP Q838L9
B	998	LEU	-	cloning artifact	UNP Q838L9
B	999	GLN	-	cloning artifact	UNP Q838L9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1000	ASN	-	cloning artifact	UNP Q838L9
B	1277	GLU	-	cloning artifact	UNP Q838L9
B	1278	GLY	-	cloning artifact	UNP Q838L9
B	1279	HIS	-	cloning artifact	UNP Q838L9
B	1280	HIS	-	cloning artifact	UNP Q838L9
B	1281	HIS	-	cloning artifact	UNP Q838L9
B	1282	HIS	-	cloning artifact	UNP Q838L9
B	1283	HIS	-	cloning artifact	UNP Q838L9
B	1284	HIS	-	cloning artifact	UNP Q838L9
C	996	MET	-	cloning artifact	UNP Q838L9
C	997	SER	-	cloning artifact	UNP Q838L9
C	998	LEU	-	cloning artifact	UNP Q838L9
C	999	GLN	-	cloning artifact	UNP Q838L9
C	1000	ASN	-	cloning artifact	UNP Q838L9
C	1277	GLU	-	cloning artifact	UNP Q838L9
C	1278	GLY	-	cloning artifact	UNP Q838L9
C	1279	HIS	-	cloning artifact	UNP Q838L9
C	1280	HIS	-	cloning artifact	UNP Q838L9
C	1281	HIS	-	cloning artifact	UNP Q838L9
C	1282	HIS	-	cloning artifact	UNP Q838L9
C	1283	HIS	-	cloning artifact	UNP Q838L9
C	1284	HIS	-	cloning artifact	UNP Q838L9
D	996	MET	-	cloning artifact	UNP Q838L9
D	997	SER	-	cloning artifact	UNP Q838L9
D	998	LEU	-	cloning artifact	UNP Q838L9
D	999	GLN	-	cloning artifact	UNP Q838L9
D	1000	ASN	-	cloning artifact	UNP Q838L9
D	1277	GLU	-	cloning artifact	UNP Q838L9
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D	1279	HIS	-	cloning artifact	UNP Q838L9
D	1280	HIS	-	cloning artifact	UNP Q838L9
D	1281	HIS	-	cloning artifact	UNP Q838L9
D	1282	HIS	-	cloning artifact	UNP Q838L9
D	1283	HIS	-	cloning artifact	UNP Q838L9
D	1284	HIS	-	cloning artifact	UNP Q838L9
E	996	MET	-	cloning artifact	UNP Q838L9
E	997	SER	-	cloning artifact	UNP Q838L9
E	998	LEU	-	cloning artifact	UNP Q838L9
E	999	GLN	-	cloning artifact	UNP Q838L9
E	1000	ASN	-	cloning artifact	UNP Q838L9
E	1277	GLU	-	cloning artifact	UNP Q838L9
E	1278	GLY	-	cloning artifact	UNP Q838L9

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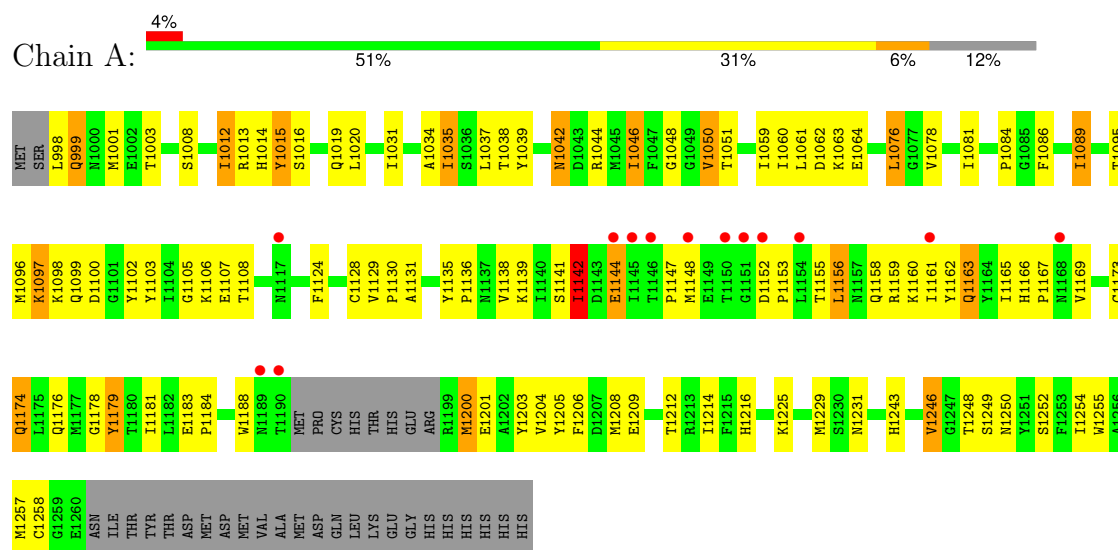
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Chain	Residue	Modelled	Actual	Comment	Reference
E	1279	HIS	-	cloning artifact	UNP Q838L9
E	1280	HIS	-	cloning artifact	UNP Q838L9
E	1281	HIS	-	cloning artifact	UNP Q838L9
E	1282	HIS	-	cloning artifact	UNP Q838L9
E	1283	HIS	-	cloning artifact	UNP Q838L9
E	1284	HIS	-	cloning artifact	UNP Q838L9
F	996	MET	-	cloning artifact	UNP Q838L9
F	997	SER	-	cloning artifact	UNP Q838L9
F	998	LEU	-	cloning artifact	UNP Q838L9
F	999	GLN	-	cloning artifact	UNP Q838L9
F	1000	ASN	-	cloning artifact	UNP Q838L9
F	1277	GLU	-	cloning artifact	UNP Q838L9
F	1278	GLY	-	cloning artifact	UNP Q838L9
F	1279	HIS	-	cloning artifact	UNP Q838L9
F	1280	HIS	-	cloning artifact	UNP Q838L9
F	1281	HIS	-	cloning artifact	UNP Q838L9
F	1282	HIS	-	cloning artifact	UNP Q838L9
F	1283	HIS	-	cloning artifact	UNP Q838L9
F	1284	HIS	-	cloning artifact	UNP Q838L9

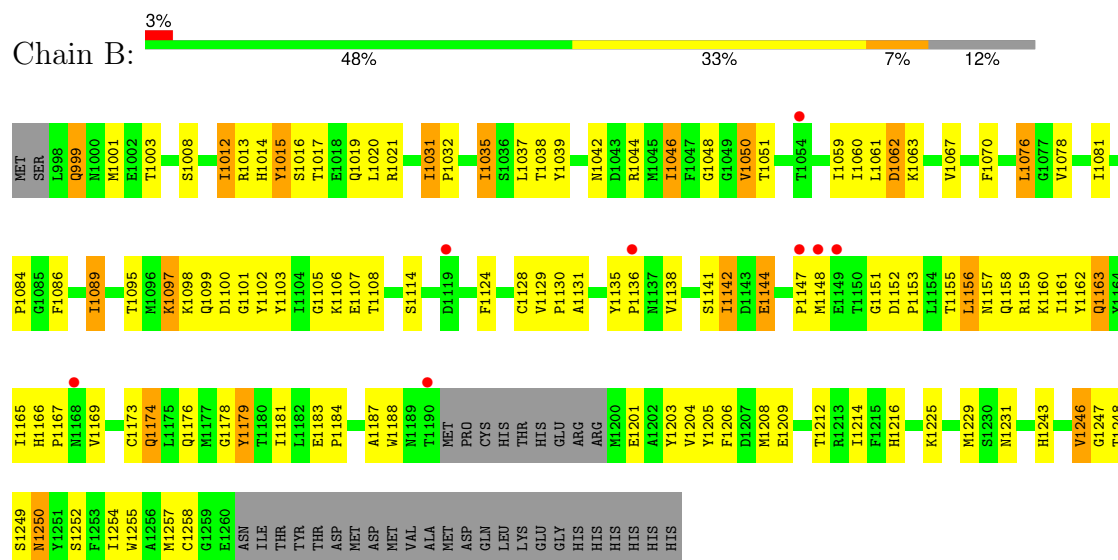
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

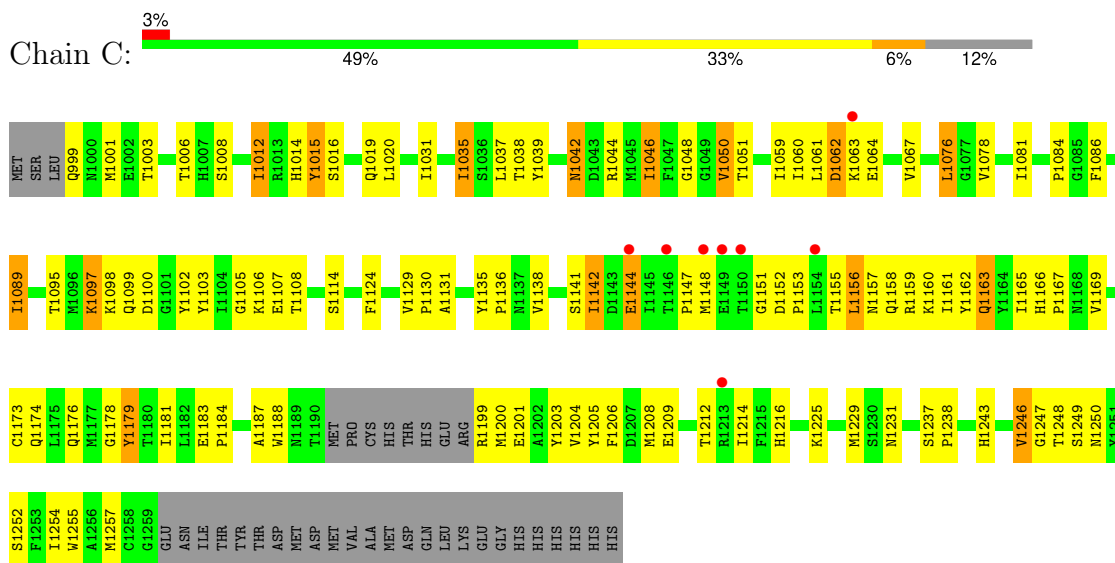
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1



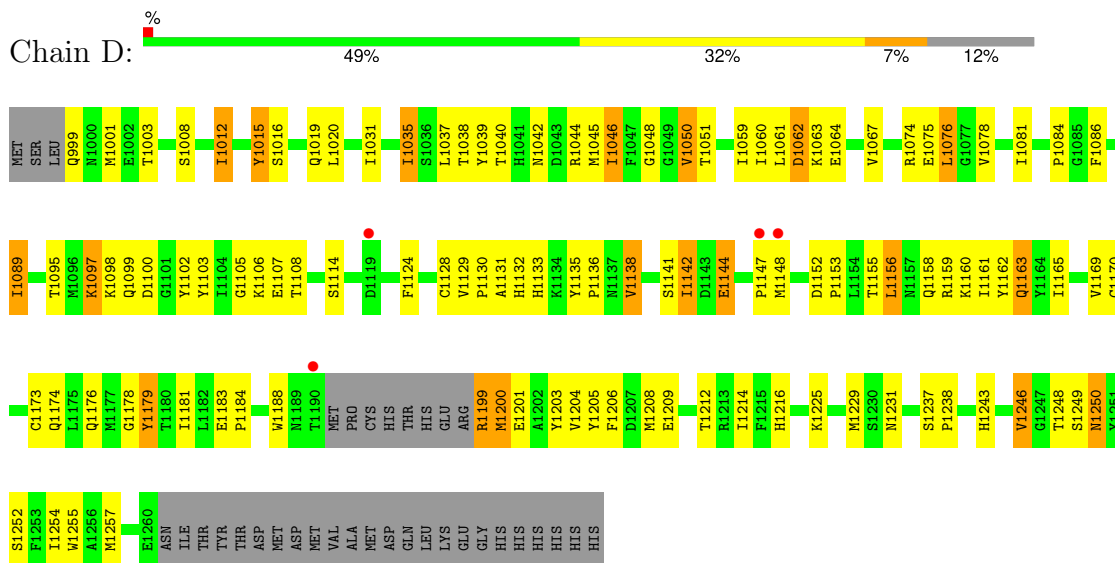
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1



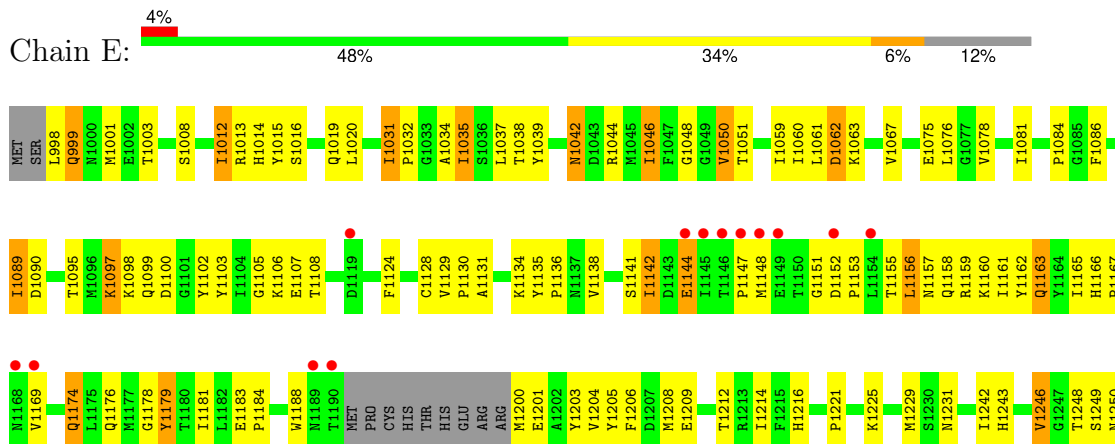
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1



- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1



- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1



Y1251	S1252	F1253	I1254	W1255	A1256	M1257	C1258	E1259	E1260	ASN	ILE	THR	TYR	THR	ASP	ASP	MET	ASP	ASP	ASP	GLN	LEU	LYS	GLU	GLY	HIS	HIS	HIS	HIS	HIS
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● Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1



H1243	Q1163	F1086	MET	SER	LEU	Q999	M1001	E1002	T1003	S1008	I1012	R1013	H1014	Y1015	S1016	Q1019	L1020	V1026	I1031	I1035	S1036	L1037	T1038	Y1039	M1042	D1043	R1044	M1045	I1046	F1047	G1048	G1049	Y1050	T1051	T1054	I1059	I1060	L1061	D1062	K1063	V1067	E1075	L1076	G1077	V1078	I1081	P1084	G1085									
V1246	Q1164	I1089					T1095	M1096	K1097	K1098	Q1099	D1100	G1101	Y1102	Y1103	I1104	G1105	K1106	E1107	T1108	S1114	D1119	M1120	F1124	C1128	V1129	P1130	A1131	H1132	H1133	A1134	Y1135	P1136	N1137	V1138	S1141	T1142	D1143	E1144	I1145	T1146	P1147	M1148	E1149	T1150	G1151	D1152	P1153	L1154	T1155	L1156	N1157	Q1158	R1159	K1160	I1161	Y1162
G1247	H1165						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
S1249	H1166						N1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
M1250	H1167						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
Y1251	H1168						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
S1252	H1169						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
F1253	H1173						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
I1254	H1174						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
W1255	H1175						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
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M1257	H1177						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
C1258	H1178						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
G1259	H1179						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
E1260	H1180						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
ASN	H1181						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
ILE	H1182						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
THR	H1183						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
TYR	H1184						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
THR	H1187						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
THR	H1188						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
ASP	H1189						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
MET	H1190						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
ASP	H1191						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
GLU	H1192						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
ILE	H1182						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
THR	H1183						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200	E1201	A1202	Y1203	V1204	Y1205	F1206	D1207	M1208	E1209	T1212	R1213	I1214	F1215	H1216	P1221	K1225	M1229	S1230	N1231	I1242				
THR	H1184						M1168	V1169	C1173	Q1174	L1175	Q1176	M1177	G1178	Y1179	T1180	I1181	L1182	E1183	P1184	A1187	W1188	N1189	T1190	MET	PRO	CYS	HIS	THR	HIS	GLU	ARG	M1200</																								

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.01Å 107.69Å 191.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 – 2.95 29.69 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.9 (24.90-2.95) 96.8 (29.69-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.241 , 0.265 0.240 , 0.262	Depositor DCC
R_{free} test set	1760 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12252	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0135e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/2105	0.65	0/2850
1	B	0.42	0/2094	0.66	0/2836
1	C	0.41	0/2088	0.65	0/2827
1	D	0.41	0/2097	0.66	0/2839
1	E	0.40	0/2094	0.65	0/2836
1	F	0.41	0/2086	0.65	0/2825
All	All	0.41	0/12564	0.65	0/17013

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2053	0	1970	100	0
1	B	2042	0	1957	100	0
1	C	2036	0	1953	111	0
1	D	2045	0	1959	121	0
1	E	2042	0	1957	111	0
1	F	2034	0	1946	123	0
All	All	12252	0	11742	640	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 27.

All (640) 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:E:999:GLN:HB2	1:E:1035:ILE:HG12	1.33	1.10
1:D:1199:ARG:HH11	1:D:1199:ARG:HB2	1.29	0.96
1:A:1016:SER:H	1:A:1019:GLN:HE21	1.20	0.90
1:C:1016:SER:H	1:C:1019:GLN:HE21	1.16	0.90
1:E:1016:SER:H	1:E:1019:GLN:HE21	1.19	0.88
1:B:1016:SER:H	1:B:1019:GLN:HE21	1.19	0.88
1:D:1016:SER:H	1:D:1019:GLN:HE21	1.23	0.86
1:F:1016:SER:H	1:F:1019:GLN:HE21	1.16	0.86
1:F:999:GLN:HA	1:F:1035:ILE:HG12	1.62	0.82
1:C:1209:GLU:HB2	1:C:1212:THR:HG23	1.62	0.81
1:D:1199:ARG:HB2	1:D:1199:ARG:NH1	1.96	0.81
1:A:1016:SER:OG	1:A:1019:GLN:HG3	1.81	0.81
1:F:1209:GLU:HB2	1:F:1212:THR:HG23	1.63	0.80
1:D:1209:GLU:HB2	1:D:1212:THR:HG23	1.63	0.80
1:E:1209:GLU:HB2	1:E:1212:THR:HG23	1.64	0.79
1:A:1209:GLU:HB2	1:A:1212:THR:HG23	1.63	0.79
1:C:1206:PHE:HE2	1:C:1254:ILE:HG12	1.47	0.79
1:A:1206:PHE:HE2	1:A:1254:ILE:HG12	1.47	0.79
1:E:1016:SER:OG	1:E:1019:GLN:HG3	1.82	0.78
1:A:1178:GLY:HA3	1:A:1255:TRP:CE2	2.20	0.77
1:F:1016:SER:N	1:F:1019:GLN:HE21	1.81	0.77
1:F:1206:PHE:HE2	1:F:1254:ILE:HG12	1.49	0.77
1:D:1132:HIS:H	1:F:1132:HIS:HD2	1.33	0.77
1:E:1016:SER:N	1:E:1019:GLN:HE21	1.83	0.77
1:B:1209:GLU:HB2	1:B:1212:THR:HG23	1.65	0.76
1:A:1016:SER:N	1:A:1019:GLN:HE21	1.83	0.76
1:D:1084:PRO:HD3	1:E:1134:LYS:HE2	1.66	0.76
1:B:1016:SER:N	1:B:1019:GLN:HE21	1.82	0.76
1:D:999:GLN:HE22	1:D:1060:ILE:H	1.31	0.76
1:E:999:GLN:HB2	1:E:1035:ILE:CG1	2.15	0.76
1:B:1206:PHE:HE2	1:B:1254:ILE:HG12	1.48	0.76
1:E:1206:PHE:HE2	1:E:1254:ILE:HG12	1.50	0.76
1:D:1206:PHE:HE2	1:D:1254:ILE:HG12	1.50	0.76
1:C:1016:SER:N	1:C:1019:GLN:HE21	1.83	0.75
1:C:1142:ILE:N	1:C:1142:ILE:HD12	2.02	0.75
1:A:1142:ILE:N	1:A:1142:ILE:HD12	2.02	0.75
1:F:1016:SER:OG	1:F:1019:GLN:HG3	1.87	0.75
1:C:1016:SER:OG	1:C:1019:GLN:HG3	1.87	0.74
1:D:1199:ARG:HH11	1:D:1199:ARG:CB	2.01	0.74
1:D:1016:SER:N	1:D:1019:GLN:HE21	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1142:ILE:HD12	1:E:1142:ILE:N	2.03	0.73
1:F:1084:PRO:HB3	1:F:1097:LYS:HE3	1.71	0.72
1:E:1188:TRP:CZ3	1:E:1246:VAL:HG22	2.23	0.72
1:C:1181:ILE:HG22	1:C:1252:SER:OG	1.90	0.72
1:D:1016:SER:OG	1:D:1019:GLN:HG3	1.89	0.72
1:C:999:GLN:HE22	1:C:1060:ILE:H	1.37	0.71
1:D:1152:ASP:OD1	1:D:1153:PRO:HD2	1.91	0.71
1:A:1188:TRP:CZ3	1:A:1246:VAL:HG22	2.25	0.71
1:D:1084:PRO:HG3	1:E:1134:LYS:HD3	1.72	0.71
1:D:1132:HIS:HD2	1:F:1132:HIS:H	1.38	0.71
1:B:1016:SER:OG	1:B:1019:GLN:HG3	1.91	0.71
1:F:1142:ILE:N	1:F:1142:ILE:HD12	2.06	0.70
1:A:1084:PRO:HB3	1:A:1097:LYS:HE3	1.74	0.70
1:C:1016:SER:H	1:C:1019:GLN:NE2	1.90	0.70
1:E:1156:LEU:N	1:E:1156:LEU:HD23	2.06	0.70
1:C:1084:PRO:HB3	1:C:1097:LYS:HE3	1.73	0.70
1:F:1181:ILE:HG22	1:F:1252:SER:OG	1.92	0.70
1:A:1160:LYS:HE3	1:A:1181:ILE:HD11	1.74	0.69
1:D:1160:LYS:HE3	1:D:1181:ILE:HD11	1.74	0.69
1:C:1160:LYS:HE3	1:C:1181:ILE:HD11	1.75	0.69
1:E:1016:SER:H	1:E:1019:GLN:NE2	1.90	0.69
1:B:1084:PRO:HB3	1:B:1097:LYS:HE3	1.75	0.69
1:E:1160:LYS:HE3	1:E:1181:ILE:HD11	1.75	0.69
1:F:1016:SER:H	1:F:1019:GLN:NE2	1.90	0.68
1:B:1035:ILE:HD12	1:B:1059:ILE:HG12	1.76	0.68
1:B:1160:LYS:HE3	1:B:1181:ILE:HD11	1.74	0.68
1:C:1156:LEU:N	1:C:1156:LEU:HD23	2.08	0.68
1:D:1097:LYS:HE2	1:D:1097:LYS:HA	1.76	0.68
1:F:1035:ILE:HD12	1:F:1059:ILE:HG12	1.76	0.68
1:D:1156:LEU:HD23	1:D:1156:LEU:N	2.08	0.68
1:F:1097:LYS:HE2	1:F:1097:LYS:HA	1.76	0.68
1:C:1035:ILE:HD12	1:C:1059:ILE:HG12	1.76	0.68
1:B:1142:ILE:HD12	1:B:1142:ILE:N	2.09	0.68
1:B:1152:ASP:OD1	1:B:1153:PRO:HD2	1.93	0.67
1:E:1152:ASP:OD1	1:E:1153:PRO:HD2	1.94	0.67
1:A:1178:GLY:HA3	1:A:1255:TRP:CZ2	2.30	0.67
1:E:1084:PRO:HB3	1:E:1097:LYS:HE3	1.75	0.67
1:F:1160:LYS:HE3	1:F:1181:ILE:HD11	1.76	0.67
1:A:1156:LEU:N	1:A:1156:LEU:HD23	2.08	0.67
1:E:1181:ILE:HG22	1:E:1252:SER:OG	1.94	0.67
1:B:1181:ILE:HG22	1:B:1252:SER:OG	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1152:ASP:OD1	1:C:1153:PRO:HD2	1.95	0.67
1:F:1001:MET:HE2	1:F:1046:ILE:HB	1.76	0.67
1:C:1206:PHE:CE2	1:C:1254:ILE:HG12	2.30	0.66
1:D:1132:HIS:H	1:F:1132:HIS:CD2	2.13	0.66
1:A:1152:ASP:OD1	1:A:1153:PRO:HD2	1.95	0.66
1:F:1206:PHE:CE2	1:F:1254:ILE:HG12	2.31	0.66
1:A:1001:MET:HE2	1:A:1046:ILE:HB	1.76	0.66
1:B:1206:PHE:CE2	1:B:1254:ILE:HG12	2.31	0.66
1:A:1206:PHE:CE2	1:A:1254:ILE:HG12	2.30	0.66
1:B:1097:LYS:HE2	1:B:1097:LYS:HA	1.76	0.66
1:C:1158:GLN:HG2	1:C:1183:GLU:OE1	1.97	0.65
1:D:1205:TYR:OH	1:D:1216:HIS:HD2	1.79	0.65
1:A:1097:LYS:HE2	1:A:1097:LYS:HA	1.77	0.65
1:B:1163:GLN:HA	1:B:1163:GLN:HE21	1.60	0.65
1:A:1016:SER:H	1:A:1019:GLN:NE2	1.90	0.65
1:D:1035:ILE:HD12	1:D:1059:ILE:HG12	1.78	0.65
1:B:1156:LEU:HD23	1:B:1156:LEU:N	2.11	0.65
1:C:1148:MET:O	1:C:1161:ILE:HG12	1.97	0.65
1:D:1084:PRO:HB3	1:D:1097:LYS:HE3	1.77	0.65
1:F:1163:GLN:HE21	1:F:1163:GLN:HA	1.62	0.65
1:D:1132:HIS:CD2	1:F:1132:HIS:H	2.14	0.65
1:F:1156:LEU:N	1:F:1156:LEU:HD23	2.11	0.65
1:A:1035:ILE:HD12	1:A:1059:ILE:HG12	1.76	0.65
1:B:1016:SER:H	1:B:1019:GLN:NE2	1.91	0.65
1:F:1159:ARG:HG2	1:F:1159:ARG:HH11	1.62	0.65
1:E:1035:ILE:HD12	1:E:1059:ILE:HG12	1.78	0.64
1:A:1176:GLN:HB2	1:A:1257:MET:HG3	1.78	0.64
1:C:1163:GLN:HA	1:C:1163:GLN:HE21	1.62	0.64
1:D:1206:PHE:CE2	1:D:1254:ILE:HG12	2.32	0.64
1:E:1148:MET:O	1:E:1161:ILE:HG12	1.97	0.64
1:E:1105:GLY:O	1:E:1108:THR:HG23	1.96	0.64
1:E:1158:GLN:HG2	1:E:1183:GLU:OE1	1.98	0.64
1:E:999:GLN:HE22	1:E:1060:ILE:H	1.45	0.64
1:E:1163:GLN:HE21	1:E:1163:GLN:HA	1.61	0.64
1:A:1163:GLN:HE21	1:A:1163:GLN:HA	1.62	0.64
1:C:1039:TYR:OH	1:C:1044:ARG:HG2	1.96	0.64
1:E:1097:LYS:HA	1:E:1097:LYS:HE2	1.78	0.63
1:C:1159:ARG:HG2	1:C:1159:ARG:HH11	1.64	0.63
1:C:1097:LYS:HA	1:C:1097:LYS:HE2	1.80	0.63
1:D:1001:MET:HE2	1:D:1046:ILE:HB	1.79	0.63
1:D:1158:GLN:HG2	1:D:1183:GLU:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1158:GLN:HG2	1:F:1183:GLU:OE1	1.97	0.63
1:B:1020:LEU:HD11	1:B:1225:LYS:HD3	1.79	0.63
1:D:1076:LEU:HD21	1:D:1078:VAL:CG2	2.29	0.63
1:A:1158:GLN:HG2	1:A:1183:GLU:OE1	1.97	0.63
1:D:1132:HIS:CG	1:F:1173:CYS:HB3	2.33	0.63
1:F:1076:LEU:HD21	1:F:1078:VAL:CG2	2.29	0.63
1:D:1142:ILE:N	1:D:1142:ILE:HD12	2.13	0.63
1:F:1020:LEU:HD11	1:F:1225:LYS:HD3	1.79	0.63
1:A:1097:LYS:O	1:A:1100:ASP:HB2	1.99	0.63
1:A:1039:TYR:OH	1:A:1044:ARG:HG2	1.99	0.62
1:B:1158:GLN:HG2	1:B:1183:GLU:OE1	1.97	0.62
1:E:1001:MET:HE2	1:E:1046:ILE:HB	1.80	0.62
1:E:1178:GLY:HA3	1:E:1255:TRP:CE2	2.35	0.62
1:D:1163:GLN:HE21	1:D:1163:GLN:HA	1.63	0.62
1:C:1076:LEU:HD21	1:C:1078:VAL:CG2	2.30	0.62
1:E:1159:ARG:HG2	1:E:1159:ARG:HH11	1.63	0.62
1:A:1148:MET:O	1:A:1161:ILE:HG12	1.98	0.62
1:C:1188:TRP:CZ3	1:C:1246:VAL:HG22	2.35	0.62
1:C:1001:MET:HA	1:C:1037:LEU:O	2.00	0.62
1:D:1039:TYR:OH	1:D:1044:ARG:HG2	1.98	0.62
1:D:1173:CYS:HB3	1:F:1132:HIS:CG	2.35	0.62
1:E:1206:PHE:CE2	1:E:1254:ILE:HG12	2.33	0.62
1:F:1097:LYS:NZ	1:F:1098:LYS:H	1.98	0.62
1:F:1178:GLY:HA3	1:F:1255:TRP:CE2	2.35	0.62
1:B:1148:MET:O	1:B:1161:ILE:HG12	1.99	0.62
1:C:1001:MET:HE2	1:C:1046:ILE:HB	1.82	0.62
1:D:1178:GLY:HA3	1:D:1255:TRP:CE2	2.34	0.62
1:D:1097:LYS:NZ	1:D:1098:LYS:H	1.98	0.62
1:F:1148:MET:O	1:F:1161:ILE:HG12	2.00	0.62
1:F:1152:ASP:OD1	1:F:1153:PRO:HD2	1.99	0.62
1:B:1039:TYR:OH	1:B:1044:ARG:HG2	2.00	0.61
1:C:1178:GLY:HA3	1:C:1255:TRP:CE2	2.34	0.61
1:F:1039:TYR:OH	1:F:1044:ARG:HG2	2.00	0.61
1:D:1148:MET:O	1:D:1161:ILE:HG12	2.00	0.61
1:E:1076:LEU:HD21	1:E:1078:VAL:CG2	2.30	0.61
1:F:1205:TYR:OH	1:F:1216:HIS:HD2	1.84	0.61
1:E:1020:LEU:HD11	1:E:1225:LYS:HD3	1.82	0.61
1:C:1020:LEU:HD11	1:C:1225:LYS:HD3	1.82	0.61
1:A:1097:LYS:NZ	1:A:1098:LYS:H	1.99	0.61
1:B:1097:LYS:NZ	1:B:1098:LYS:H	1.99	0.60
1:E:1097:LYS:NZ	1:E:1098:LYS:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:ARG:HG2	1:A:1159:ARG:HH11	1.65	0.60
1:B:1153:PRO:HD3	1:B:1158:GLN:OE1	2.01	0.60
1:C:1205:TYR:OH	1:C:1216:HIS:HD2	1.84	0.60
1:F:1097:LYS:O	1:F:1100:ASP:HB2	2.01	0.60
1:E:1039:TYR:OH	1:E:1044:ARG:HG2	2.02	0.60
1:B:1178:GLY:HA3	1:B:1255:TRP:CE2	2.37	0.60
1:E:1208:MET:HG2	1:E:1231:ASN:OD1	2.01	0.60
1:A:1208:MET:HG2	1:A:1231:ASN:OD1	2.02	0.60
1:B:1205:TYR:OH	1:B:1216:HIS:HD2	1.85	0.60
1:C:1097:LYS:O	1:C:1100:ASP:HB2	2.02	0.60
1:B:1097:LYS:O	1:B:1100:ASP:HB2	2.01	0.60
1:D:1016:SER:H	1:D:1019:GLN:NE2	1.94	0.60
1:D:1105:GLY:O	1:D:1108:THR:HG23	2.01	0.60
1:C:1097:LYS:NZ	1:C:1098:LYS:H	2.00	0.59
1:E:1201:GLU:HG2	1:E:1257:MET:HB3	1.85	0.59
1:B:1001:MET:HE2	1:B:1046:ILE:HB	1.85	0.59
1:A:999:GLN:HE22	1:A:1060:ILE:H	1.50	0.59
1:A:1076:LEU:HD21	1:A:1078:VAL:CG2	2.32	0.59
1:D:1133:HIS:HD2	1:F:1133:HIS:HD2	1.49	0.59
1:E:1097:LYS:O	1:E:1100:ASP:HB2	2.02	0.59
1:A:1105:GLY:O	1:A:1108:THR:HG23	2.03	0.59
1:C:1153:PRO:HD3	1:C:1158:GLN:OE1	2.03	0.59
1:E:1188:TRP:CH2	1:E:1246:VAL:HG22	2.37	0.59
1:F:1200:MET:SD	1:F:1200:MET:C	2.81	0.59
1:D:1097:LYS:O	1:D:1100:ASP:HB2	2.01	0.59
1:B:999:GLN:HG2	1:B:1035:ILE:HG12	1.85	0.59
1:B:1076:LEU:HD21	1:B:1078:VAL:CG2	2.33	0.59
1:B:1105:GLY:O	1:B:1108:THR:HG23	2.02	0.59
1:F:1008:SER:O	1:F:1012:ILE:HG22	2.03	0.58
1:C:1105:GLY:O	1:C:1108:THR:HG23	2.02	0.58
1:D:1201:GLU:HG2	1:D:1257:MET:HB3	1.85	0.58
1:D:1208:MET:HG2	1:D:1231:ASN:OD1	2.04	0.58
1:F:1153:PRO:HD3	1:F:1158:GLN:OE1	2.03	0.58
1:D:1008:SER:O	1:D:1012:ILE:HG22	2.04	0.58
1:D:1132:HIS:HD2	1:F:1132:HIS:N	2.01	0.58
1:D:1153:PRO:HD3	1:D:1158:GLN:OE1	2.04	0.58
1:B:1188:TRP:CZ3	1:B:1246:VAL:HG22	2.39	0.58
1:C:1106:LYS:HG2	1:C:1107:GLU:HG3	1.85	0.58
1:F:1214:ILE:HD11	1:F:1229:MET:SD	2.43	0.58
1:A:1153:PRO:HD3	1:A:1158:GLN:OE1	2.04	0.58
1:F:1106:LYS:HG2	1:F:1107:GLU:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:SER:O	1:B:1012:ILE:HG22	2.04	0.57
1:E:1001:MET:HA	1:E:1037:LEU:O	2.03	0.57
1:E:1153:PRO:HD3	1:E:1158:GLN:OE1	2.04	0.57
1:D:1001:MET:HA	1:D:1037:LEU:O	2.04	0.57
1:F:1129:VAL:HG13	1:F:1130:PRO:HD2	1.86	0.57
1:D:1129:VAL:HG13	1:D:1130:PRO:HD2	1.85	0.57
1:E:1214:ILE:HD11	1:E:1229:MET:SD	2.44	0.57
1:A:1214:ILE:HD11	1:A:1229:MET:SD	2.44	0.57
1:B:1201:GLU:HG2	1:B:1257:MET:HB3	1.86	0.57
1:C:1042:ASN:HB3	1:C:1200:MET:HG2	1.86	0.57
1:C:1208:MET:HG2	1:C:1231:ASN:OD1	2.05	0.57
1:B:1208:MET:HG2	1:B:1231:ASN:OD1	2.04	0.57
1:B:1046:ILE:HG13	1:B:1046:ILE:O	2.04	0.56
1:F:1201:GLU:HG2	1:F:1257:MET:HB3	1.86	0.56
1:E:1188:TRP:CE2	1:E:1246:VAL:HG13	2.39	0.56
1:B:1103:TYR:HB2	1:B:1165:ILE:HD12	1.88	0.56
1:E:1046:ILE:O	1:E:1046:ILE:HG13	2.04	0.56
1:E:1205:TYR:OH	1:E:1216:HIS:HD2	1.86	0.56
1:F:1188:TRP:CZ3	1:F:1246:VAL:HG22	2.40	0.56
1:B:1106:LYS:HG2	1:B:1107:GLU:HG3	1.86	0.56
1:A:1001:MET:HA	1:A:1037:LEU:O	2.05	0.56
1:C:1008:SER:O	1:C:1012:ILE:HG22	2.05	0.56
1:D:1132:HIS:HB2	1:F:1132:HIS:HB2	1.87	0.56
1:F:1001:MET:HA	1:F:1037:LEU:O	2.06	0.56
1:F:1103:TYR:HB2	1:F:1165:ILE:HD12	1.88	0.56
1:F:1208:MET:HG2	1:F:1231:ASN:OD1	2.06	0.56
1:D:1103:TYR:HB2	1:D:1165:ILE:HD12	1.88	0.56
1:E:1156:LEU:HD23	1:E:1156:LEU:H	1.69	0.56
1:C:1129:VAL:HG13	1:C:1130:PRO:HD2	1.87	0.55
1:D:1159:ARG:HG2	1:D:1159:ARG:HH11	1.71	0.55
1:E:999:GLN:CB	1:E:1035:ILE:HG12	2.22	0.55
1:A:1205:TYR:OH	1:A:1216:HIS:HD2	1.88	0.55
1:C:1199:ARG:NH1	1:C:1257:MET:HE1	2.21	0.55
1:D:1045:MET:SD	1:D:1200:MET:HE1	2.46	0.55
1:A:1188:TRP:CH2	1:A:1246:VAL:HG22	2.41	0.55
1:D:1132:HIS:N	1:F:1132:HIS:HD2	2.01	0.55
1:C:1188:TRP:CH2	1:C:1246:VAL:HG22	2.42	0.55
1:D:1156:LEU:HD23	1:D:1156:LEU:H	1.70	0.55
1:A:1008:SER:O	1:A:1012:ILE:HG22	2.05	0.55
1:A:1081:ILE:HD12	1:A:1206:PHE:CZ	2.41	0.55
1:D:1178:GLY:HA3	1:D:1255:TRP:CZ2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1156:LEU:HD23	1:B:1156:LEU:H	1.71	0.55
1:F:1046:ILE:O	1:F:1046:ILE:HG13	2.05	0.55
1:A:1201:GLU:HG2	1:A:1257:MET:HB3	1.88	0.55
1:D:1181:ILE:HG22	1:D:1252:SER:OG	2.07	0.55
1:D:1099:GLN:NE2	1:E:1090:ASP:O	2.40	0.55
1:E:1106:LYS:HG2	1:E:1107:GLU:HG3	1.89	0.55
1:E:1129:VAL:HG13	1:E:1130:PRO:HD2	1.89	0.55
1:A:1046:ILE:HG13	1:A:1046:ILE:O	2.07	0.54
1:A:1188:TRP:CE2	1:A:1246:VAL:HG13	2.41	0.54
1:C:1046:ILE:HG13	1:C:1046:ILE:O	2.06	0.54
1:D:1084:PRO:HG3	1:E:1134:LYS:CD	2.37	0.54
1:F:1105:GLY:O	1:F:1108:THR:HG23	2.06	0.54
1:A:1203:TYR:OH	1:A:1243:HIS:HB3	2.07	0.54
1:C:1156:LEU:HD23	1:C:1156:LEU:H	1.71	0.54
1:D:1204:VAL:HG13	1:D:1204:VAL:O	2.08	0.54
1:F:1147:PRO:HB3	1:F:1162:TYR:CZ	2.43	0.54
1:A:1147:PRO:HB3	1:A:1162:TYR:CZ	2.43	0.54
1:A:1250:ASN:N	1:A:1250:ASN:HD22	2.05	0.54
1:A:1089:ILE:O	1:A:1089:ILE:HG13	2.07	0.54
1:A:1106:LYS:HG2	1:A:1107:GLU:HG3	1.88	0.54
1:D:1147:PRO:HB3	1:D:1162:TYR:CZ	2.42	0.54
1:D:1046:ILE:O	1:D:1046:ILE:HG13	2.07	0.54
1:D:1106:LYS:HG2	1:D:1107:GLU:HG3	1.90	0.54
1:E:1250:ASN:N	1:E:1250:ASN:HD22	2.06	0.54
1:D:1081:ILE:HD12	1:D:1206:PHE:CZ	2.43	0.54
1:A:1129:VAL:HG13	1:A:1130:PRO:HD2	1.88	0.54
1:A:1246:VAL:HG11	1:C:1246:VAL:HG11	1.90	0.54
1:B:1147:PRO:HB3	1:B:1162:TYR:CZ	2.43	0.54
1:C:1214:ILE:C	1:C:1214:ILE:HD12	2.28	0.54
1:E:1008:SER:O	1:E:1012:ILE:HG22	2.07	0.54
1:E:1176:GLN:HB2	1:E:1257:MET:HG3	1.90	0.54
1:B:1204:VAL:CG1	1:B:1254:ILE:HB	2.38	0.53
1:B:1250:ASN:HD22	1:B:1250:ASN:N	2.06	0.53
1:C:1201:GLU:HG2	1:C:1257:MET:HB3	1.88	0.53
1:D:1060:ILE:O	1:D:1060:ILE:HG13	2.08	0.53
1:E:1214:ILE:C	1:E:1214:ILE:HD12	2.28	0.53
1:A:1020:LEU:HD11	1:A:1225:LYS:HD3	1.90	0.53
1:B:1037:LEU:HD13	1:B:1046:ILE:CD1	2.38	0.53
1:C:1103:TYR:HB2	1:C:1165:ILE:HD12	1.91	0.53
1:E:1103:TYR:HB2	1:E:1165:ILE:HD12	1.89	0.53
1:E:1203:TYR:OH	1:E:1243:HIS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1084:PRO:HB3	1:F:1097:LYS:CE	2.37	0.53
1:A:1214:ILE:C	1:A:1214:ILE:HD12	2.29	0.53
1:D:1020:LEU:HD11	1:D:1225:LYS:HD3	1.91	0.53
1:D:1188:TRP:CZ3	1:D:1246:VAL:HG22	2.43	0.53
1:D:1250:ASN:N	1:D:1250:ASN:HD22	2.06	0.53
1:A:1156:LEU:HD23	1:A:1156:LEU:H	1.73	0.53
1:B:1214:ILE:HD12	1:B:1214:ILE:C	2.30	0.53
1:C:1250:ASN:N	1:C:1250:ASN:HD22	2.07	0.53
1:D:1074:ARG:NH2	1:F:1260:GLU:OE2	2.40	0.53
1:D:1084:PRO:CD	1:E:1134:LYS:HE2	2.38	0.53
1:D:1089:ILE:HG13	1:D:1089:ILE:O	2.09	0.53
1:B:1214:ILE:HD11	1:B:1229:MET:SD	2.49	0.53
1:D:1200:MET:HE3	1:D:1201:GLU:CA	2.38	0.53
1:E:1188:TRP:CD2	1:E:1246:VAL:HG13	2.44	0.53
1:A:1060:ILE:O	1:A:1060:ILE:HG13	2.09	0.52
1:C:1147:PRO:HB3	1:C:1162:TYR:CZ	2.44	0.52
1:B:1129:VAL:HG13	1:B:1130:PRO:HD2	1.91	0.52
1:B:1159:ARG:HH11	1:B:1159:ARG:HG2	1.73	0.52
1:A:1142:ILE:N	1:A:1142:ILE:CD1	2.69	0.52
1:B:1001:MET:HA	1:B:1037:LEU:O	2.09	0.52
1:D:1214:ILE:HD11	1:D:1229:MET:SD	2.48	0.52
1:E:1050:VAL:HG13	1:E:1124:PHE:HB2	1.91	0.52
1:B:1250:ASN:N	1:B:1250:ASN:ND2	2.57	0.52
1:D:1214:ILE:HD12	1:D:1214:ILE:C	2.30	0.52
1:B:1089:ILE:O	1:B:1089:ILE:HG13	2.09	0.52
1:C:1060:ILE:O	1:C:1060:ILE:HG13	2.08	0.52
1:C:1142:ILE:HD12	1:C:1142:ILE:H	1.73	0.52
1:E:1147:PRO:HB3	1:E:1162:TYR:CZ	2.45	0.52
1:A:1204:VAL:CG1	1:A:1254:ILE:HB	2.39	0.52
1:B:1050:VAL:HG13	1:B:1124:PHE:HB2	1.91	0.52
1:C:1214:ILE:HG13	1:C:1229:MET:HB2	1.92	0.52
1:F:1204:VAL:CG1	1:F:1254:ILE:HB	2.40	0.52
1:A:1037:LEU:HD13	1:A:1046:ILE:HD11	1.91	0.52
1:A:1181:ILE:HG22	1:A:1252:SER:OG	2.09	0.52
1:B:1037:LEU:HD13	1:B:1046:ILE:HD11	1.91	0.51
1:A:1142:ILE:HD12	1:A:1142:ILE:H	1.76	0.51
1:A:1250:ASN:N	1:A:1250:ASN:ND2	2.57	0.51
1:C:1037:LEU:HD13	1:C:1046:ILE:HD11	1.93	0.51
1:E:1204:VAL:CG1	1:E:1254:ILE:HB	2.40	0.51
1:A:1084:PRO:HB3	1:A:1097:LYS:CE	2.38	0.51
1:C:1050:VAL:HG13	1:C:1124:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:TYR:HB2	1:A:1165:ILE:HD12	1.93	0.51
1:C:1089:ILE:HG13	1:C:1089:ILE:O	2.09	0.51
1:A:1050:VAL:HG13	1:A:1124:PHE:HB2	1.92	0.51
1:B:1203:TYR:OH	1:B:1243:HIS:HB3	2.11	0.51
1:E:1250:ASN:N	1:E:1250:ASN:ND2	2.58	0.51
1:F:1050:VAL:HG13	1:F:1124:PHE:HB2	1.93	0.51
1:F:1250:ASN:N	1:F:1250:ASN:HD22	2.09	0.51
1:B:1060:ILE:O	1:B:1060:ILE:HG13	2.10	0.51
1:B:1188:TRP:CH2	1:B:1246:VAL:HG22	2.46	0.51
1:C:1250:ASN:N	1:C:1250:ASN:ND2	2.58	0.51
1:E:1141:SER:O	1:E:1144:GLU:HG2	2.11	0.51
1:F:1081:ILE:HD12	1:F:1206:PHE:CZ	2.46	0.51
1:B:999:GLN:HE21	1:B:1060:ILE:H	1.59	0.51
1:C:1084:PRO:HB3	1:C:1097:LYS:CE	2.38	0.51
1:F:1212:THR:HG21	1:F:1249:SER:HB3	1.92	0.51
1:F:1214:ILE:HG13	1:F:1229:MET:HB2	1.93	0.51
1:C:1188:TRP:CE2	1:C:1246:VAL:HG13	2.45	0.51
1:D:1203:TYR:OH	1:D:1243:HIS:HB3	2.10	0.51
1:E:1142:ILE:HD12	1:E:1142:ILE:H	1.75	0.51
1:E:1089:ILE:HG13	1:E:1089:ILE:O	2.11	0.51
1:E:1081:ILE:HD12	1:E:1206:PHE:CZ	2.46	0.50
1:C:1037:LEU:HD13	1:C:1046:ILE:CD1	2.42	0.50
1:D:1037:LEU:HD13	1:D:1046:ILE:HD11	1.93	0.50
1:F:1214:ILE:C	1:F:1214:ILE:HD12	2.31	0.50
1:A:1037:LEU:HD13	1:A:1046:ILE:CD1	2.41	0.50
1:A:1212:THR:HG21	1:A:1249:SER:HB3	1.92	0.50
1:C:1204:VAL:CG1	1:C:1254:ILE:HB	2.42	0.50
1:E:1060:ILE:HG13	1:E:1060:ILE:O	2.10	0.50
1:F:1046:ILE:C	1:F:1046:ILE:HD12	2.32	0.50
1:D:1204:VAL:CG1	1:D:1254:ILE:HB	2.41	0.50
1:F:1141:SER:O	1:F:1144:GLU:HG2	2.12	0.50
1:C:1178:GLY:HA3	1:C:1255:TRP:CZ2	2.47	0.50
1:D:1212:THR:HG21	1:D:1249:SER:HB3	1.94	0.50
1:D:1250:ASN:N	1:D:1250:ASN:ND2	2.59	0.50
1:F:1037:LEU:HD13	1:F:1046:ILE:HD11	1.93	0.50
1:C:1199:ARG:HD2	1:C:1257:MET:HE3	1.94	0.50
1:E:1084:PRO:HB3	1:E:1097:LYS:CE	2.39	0.50
1:E:1178:GLY:HA3	1:E:1255:TRP:CZ2	2.47	0.50
1:B:1212:THR:HG21	1:B:1249:SER:HB3	1.93	0.50
1:F:1203:TYR:OH	1:F:1243:HIS:HB3	2.11	0.50
1:E:1212:THR:HG21	1:E:1249:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1204:VAL:O	1:F:1204:VAL:HG13	2.11	0.49
1:B:1204:VAL:HG13	1:B:1204:VAL:O	2.11	0.49
1:E:1037:LEU:HD13	1:E:1046:ILE:HD11	1.94	0.49
1:F:1156:LEU:HD23	1:F:1156:LEU:H	1.75	0.49
1:A:1014:HIS:CD2	1:C:1019:GLN:NE2	2.80	0.49
1:B:1035:ILE:CD1	1:B:1059:ILE:HG12	2.42	0.49
1:C:1081:ILE:HD12	1:C:1206:PHE:CZ	2.48	0.49
1:F:1037:LEU:HD13	1:F:1046:ILE:CD1	2.41	0.49
1:F:1178:GLY:HA3	1:F:1255:TRP:CZ2	2.47	0.49
1:A:1188:TRP:CD2	1:A:1246:VAL:HG13	2.47	0.49
1:E:1046:ILE:HD12	1:E:1046:ILE:C	2.33	0.49
1:A:1214:ILE:HG13	1:A:1229:MET:HB2	1.93	0.49
1:C:1214:ILE:HD11	1:C:1229:MET:SD	2.53	0.49
1:D:1050:VAL:HG13	1:D:1124:PHE:HB2	1.94	0.49
1:F:1098:LYS:HG2	1:F:1099:GLN:HG2	1.94	0.49
1:E:1214:ILE:HG13	1:E:1229:MET:HB2	1.95	0.49
1:D:1098:LYS:HG2	1:D:1099:GLN:HG2	1.95	0.49
1:E:1174:GLN:NE2	1:E:1258:CYS:HB2	2.28	0.49
1:B:1214:ILE:HG13	1:B:1229:MET:HB2	1.94	0.49
1:C:1200:MET:SD	1:C:1200:MET:C	2.91	0.49
1:C:1141:SER:O	1:C:1144:GLU:HG2	2.12	0.48
1:D:1037:LEU:HD13	1:D:1046:ILE:CD1	2.43	0.48
1:B:1084:PRO:HB3	1:B:1097:LYS:CE	2.42	0.48
1:C:1012:ILE:HG12	1:C:1012:ILE:O	2.14	0.48
1:C:1046:ILE:HD12	1:C:1046:ILE:C	2.33	0.48
1:A:1098:LYS:HG2	1:A:1099:GLN:HG2	1.94	0.48
1:F:1012:ILE:HG12	1:F:1012:ILE:O	2.13	0.48
1:F:1060:ILE:HG13	1:F:1060:ILE:O	2.13	0.48
1:F:1142:ILE:HD12	1:F:1142:ILE:H	1.77	0.48
1:A:1014:HIS:HB3	1:C:1014:HIS:O	2.14	0.48
1:B:1141:SER:O	1:B:1144:GLU:HG2	2.14	0.48
1:D:1046:ILE:C	1:D:1046:ILE:HD12	2.33	0.48
1:D:1141:SER:O	1:D:1144:GLU:HG2	2.13	0.48
1:E:1086:PHE:CE1	1:E:1095:THR:HG22	2.48	0.48
1:C:1098:LYS:HG2	1:C:1099:GLN:HG2	1.96	0.48
1:A:1141:SER:O	1:A:1144:GLU:HG2	2.13	0.48
1:F:1250:ASN:N	1:F:1250:ASN:ND2	2.61	0.48
1:F:1089:ILE:HG13	1:F:1089:ILE:O	2.13	0.48
1:C:1142:ILE:N	1:C:1142:ILE:CD1	2.69	0.48
1:D:999:GLN:HA	1:D:1035:ILE:HG12	1.96	0.48
1:D:1035:ILE:CD1	1:D:1059:ILE:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1086:PHE:CE1	1:D:1095:THR:HG22	2.48	0.48
1:D:1106:LYS:O	1:D:1107:GLU:HB2	2.14	0.48
1:C:999:GLN:HG3	1:C:1035:ILE:HD11	1.95	0.47
1:C:1212:THR:HG21	1:C:1249:SER:HB3	1.95	0.47
1:D:1084:PRO:HB3	1:D:1097:LYS:CE	2.43	0.47
1:E:1098:LYS:HG2	1:E:1099:GLN:HG2	1.96	0.47
1:C:1204:VAL:HG13	1:C:1204:VAL:O	2.14	0.47
1:D:1176:GLN:HB2	1:D:1257:MET:HG3	1.96	0.47
1:E:1037:LEU:HD13	1:E:1046:ILE:CD1	2.44	0.47
1:A:1035:ILE:CD1	1:A:1059:ILE:HG12	2.43	0.47
1:A:1086:PHE:CE1	1:A:1095:THR:HG22	2.50	0.47
1:D:1183:GLU:HG2	1:D:1184:PRO:HD2	1.96	0.47
1:D:1200:MET:HE3	1:D:1201:GLU:HA	1.97	0.47
1:E:1106:LYS:O	1:E:1107:GLU:HB2	2.15	0.47
1:E:1204:VAL:O	1:E:1204:VAL:HG13	2.15	0.47
1:C:1176:GLN:HB2	1:C:1257:MET:HG3	1.95	0.47
1:E:1183:GLU:HG2	1:E:1184:PRO:HD2	1.97	0.47
1:F:1081:ILE:HD12	1:F:1206:PHE:CE1	2.49	0.47
1:C:1203:TYR:OH	1:C:1243:HIS:HB3	2.14	0.47
1:D:1097:LYS:CE	1:D:1098:LYS:H	2.28	0.47
1:D:1188:TRP:CH2	1:D:1246:VAL:HG22	2.49	0.47
1:D:1214:ILE:HG13	1:D:1229:MET:HB2	1.96	0.47
1:F:1035:ILE:CD1	1:F:1059:ILE:HG12	2.42	0.47
1:A:1204:VAL:HG13	1:A:1204:VAL:O	2.15	0.47
1:B:1046:ILE:HD12	1:B:1046:ILE:C	2.35	0.47
1:D:1086:PHE:HE1	1:D:1095:THR:HG22	1.80	0.47
1:B:1178:GLY:HA3	1:B:1255:TRP:CZ2	2.50	0.47
1:C:1106:LYS:O	1:C:1107:GLU:HB2	2.15	0.47
1:C:1035:ILE:CD1	1:C:1059:ILE:HG12	2.43	0.47
1:D:1200:MET:O	1:D:1200:MET:HG3	2.14	0.47
1:F:1179:TYR:HE2	1:F:1181:ILE:HG23	1.79	0.47
1:A:998:LEU:O	1:A:1034:ALA:HB1	2.15	0.46
1:B:1081:ILE:HD12	1:B:1206:PHE:CZ	2.49	0.46
1:B:1086:PHE:CE1	1:B:1095:THR:HG22	2.51	0.46
1:B:1103:TYR:HB2	1:B:1165:ILE:CD1	2.45	0.46
1:C:1103:TYR:HB2	1:C:1165:ILE:CD1	2.45	0.46
1:F:1020:LEU:HD11	1:F:1225:LYS:CD	2.45	0.46
1:A:1086:PHE:HE1	1:A:1095:THR:HG22	1.81	0.46
1:B:1151:GLY:HA2	1:B:1157:ASN:ND2	2.30	0.46
1:B:1188:TRP:CE2	1:B:1246:VAL:HG13	2.50	0.46
1:D:1133:HIS:CD2	1:F:1133:HIS:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1135:TYR:HB3	1:C:1136:PRO:HD2	1.97	0.46
1:E:1086:PHE:HE1	1:E:1095:THR:HG22	1.80	0.46
1:F:1075:GLU:HG2	1:F:1131:ALA:HB2	1.96	0.46
1:F:1097:LYS:CE	1:F:1098:LYS:H	2.28	0.46
1:F:1142:ILE:N	1:F:1142:ILE:CD1	2.72	0.46
1:C:1179:TYR:HE2	1:C:1181:ILE:HG23	1.80	0.46
1:A:1106:LYS:O	1:A:1107:GLU:HB2	2.15	0.46
1:C:1086:PHE:CE1	1:C:1095:THR:HG22	2.51	0.46
1:B:1012:ILE:O	1:B:1012:ILE:HG12	2.15	0.46
1:B:1098:LYS:HG2	1:B:1099:GLN:HG2	1.96	0.46
1:B:1204:VAL:HG12	1:B:1254:ILE:HB	1.98	0.46
1:B:1183:GLU:HG2	1:B:1184:PRO:HD2	1.96	0.46
1:D:1135:TYR:HB3	1:D:1136:PRO:HD2	1.98	0.46
1:E:1042:ASN:HB3	1:E:1200:MET:HG3	1.98	0.46
1:C:1183:GLU:HG2	1:C:1184:PRO:HD2	1.98	0.46
1:E:1166:HIS:ND1	1:E:1167:PRO:HD2	2.31	0.46
1:E:1184:PRO:HA	1:E:1250:ASN:OD1	2.14	0.46
1:F:1188:TRP:CH2	1:F:1246:VAL:HG22	2.50	0.46
1:A:1183:GLU:HG2	1:A:1184:PRO:HD2	1.98	0.46
1:E:1179:TYR:HE2	1:E:1181:ILE:HG23	1.80	0.46
1:F:1086:PHE:CE1	1:F:1095:THR:HG22	2.51	0.46
1:B:1097:LYS:CE	1:B:1098:LYS:H	2.30	0.45
1:F:1179:TYR:CE2	1:F:1181:ILE:HG23	2.51	0.45
1:B:1166:HIS:ND1	1:B:1167:PRO:HD2	2.31	0.45
1:C:1184:PRO:HA	1:C:1250:ASN:OD1	2.16	0.45
1:F:1187:ALA:HB1	1:F:1247:GLY:H	1.81	0.45
1:C:1184:PRO:HA	1:C:1250:ASN:CG	2.36	0.45
1:E:1046:ILE:HG13	1:E:1128:CYS:HB3	1.98	0.45
1:F:1103:TYR:HB2	1:F:1165:ILE:CD1	2.46	0.45
1:A:1179:TYR:HE2	1:A:1181:ILE:HG23	1.82	0.45
1:B:1179:TYR:HE2	1:B:1181:ILE:HG23	1.82	0.45
1:D:1173:CYS:HB3	1:F:1132:HIS:CD2	2.51	0.45
1:E:1142:ILE:N	1:E:1142:ILE:CD1	2.70	0.45
1:E:1159:ARG:HG2	1:E:1159:ARG:NH1	2.31	0.45
1:F:1176:GLN:HB2	1:F:1257:MET:HG3	1.98	0.45
1:A:1046:ILE:C	1:A:1046:ILE:HD12	2.37	0.45
1:B:1176:GLN:HB2	1:B:1257:MET:HG3	1.99	0.45
1:E:1097:LYS:CE	1:E:1098:LYS:H	2.29	0.45
1:F:1086:PHE:HE1	1:F:1095:THR:HG22	1.80	0.45
1:B:1106:LYS:O	1:B:1107:GLU:HB2	2.17	0.45
1:C:1166:HIS:ND1	1:C:1167:PRO:HD2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1131:ALA:HB1	1:C:1173:CYS:SG	2.57	0.45
1:C:1187:ALA:HB1	1:C:1247:GLY:H	1.82	0.45
1:E:1103:TYR:HB2	1:E:1165:ILE:CD1	2.47	0.45
1:A:1204:VAL:HG12	1:A:1254:ILE:HB	1.97	0.45
1:D:1075:GLU:HG2	1:D:1131:ALA:HB2	1.99	0.45
1:E:1037:LEU:HD23	1:E:1048:GLY:HA3	1.98	0.45
1:A:1015:TYR:HA	1:A:1019:GLN:NE2	2.32	0.44
1:C:1179:TYR:CE2	1:C:1181:ILE:HG23	2.52	0.44
1:E:1035:ILE:CD1	1:E:1059:ILE:HG12	2.45	0.44
1:F:1046:ILE:HG13	1:F:1128:CYS:HB3	1.98	0.44
1:F:1183:GLU:HG2	1:F:1184:PRO:HD2	1.99	0.44
1:B:1086:PHE:HE1	1:B:1095:THR:HG22	1.82	0.44
1:B:1212:THR:CG2	1:B:1249:SER:HB3	2.48	0.44
1:C:1086:PHE:HE1	1:C:1095:THR:HG22	1.83	0.44
1:C:1097:LYS:CE	1:C:1098:LYS:H	2.30	0.44
1:E:1042:ASN:HB3	1:E:1200:MET:CG	2.46	0.44
1:A:1046:ILE:HG13	1:A:1128:CYS:HB3	1.98	0.44
1:B:1015:TYR:HA	1:B:1019:GLN:NE2	2.33	0.44
1:E:1031:ILE:HA	1:E:1032:PRO:HD2	1.82	0.44
1:A:1166:HIS:ND1	1:A:1167:PRO:HD2	2.33	0.44
1:A:1174:GLN:NE2	1:A:1258:CYS:HB2	2.33	0.44
1:F:1106:LYS:O	1:F:1107:GLU:HB2	2.17	0.44
1:F:1166:HIS:ND1	1:F:1167:PRO:HD2	2.31	0.44
1:A:1179:TYR:CE2	1:A:1181:ILE:HG23	2.53	0.44
1:D:1103:TYR:HB2	1:D:1165:ILE:CD1	2.47	0.44
1:E:1012:ILE:HG12	1:E:1012:ILE:O	2.17	0.44
1:E:1081:ILE:HD12	1:E:1206:PHE:CE1	2.53	0.44
1:F:1131:ALA:HB1	1:F:1173:CYS:SG	2.58	0.44
1:F:1212:THR:CG2	1:F:1249:SER:HB3	2.48	0.44
1:F:1204:VAL:HG12	1:F:1254:ILE:HB	1.99	0.44
1:B:1179:TYR:CE2	1:B:1181:ILE:HG23	2.52	0.44
1:A:1178:GLY:HA3	1:A:1255:TRP:NE1	2.31	0.43
1:E:1135:TYR:HB3	1:E:1136:PRO:HD2	2.00	0.43
1:E:1221:PRO:HB3	1:E:1242:ILE:HD11	2.00	0.43
1:A:1097:LYS:CE	1:A:1098:LYS:H	2.31	0.43
1:D:1212:THR:CG2	1:D:1249:SER:HB3	2.47	0.43
1:E:1179:TYR:HE2	1:E:1181:ILE:CG2	2.31	0.43
1:F:1147:PRO:HB3	1:F:1162:TYR:CE1	2.53	0.43
1:D:1046:ILE:HG13	1:D:1128:CYS:HB3	2.00	0.43
1:F:1179:TYR:HE2	1:F:1181:ILE:CG2	2.31	0.43
1:B:1187:ALA:HB1	1:B:1247:GLY:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1204:VAL:HG12	1:C:1254:ILE:HB	2.00	0.43
1:D:1138:VAL:HG11	1:D:1170:CYS:HB2	2.01	0.43
1:E:1179:TYR:CE2	1:E:1181:ILE:HG23	2.53	0.43
1:A:1135:TYR:HB3	1:A:1136:PRO:HD2	2.00	0.43
1:B:1046:ILE:HG13	1:B:1128:CYS:HB3	2.01	0.43
1:B:1179:TYR:HE2	1:B:1181:ILE:CG2	2.31	0.43
1:C:999:GLN:HA	1:C:1035:ILE:HG12	2.00	0.43
1:E:1188:TRP:CH2	1:E:1246:VAL:CG2	3.01	0.43
1:A:1212:THR:CG2	1:A:1249:SER:HB3	2.48	0.43
1:E:1204:VAL:HG12	1:E:1254:ILE:HB	2.00	0.43
1:E:1212:THR:CG2	1:E:1249:SER:HB3	2.48	0.43
1:F:1159:ARG:HG2	1:F:1159:ARG:NH1	2.30	0.43
1:C:1147:PRO:HB3	1:C:1162:TYR:CE1	2.54	0.43
1:E:1075:GLU:HG2	1:E:1131:ALA:HB2	2.01	0.43
1:C:1209:GLU:HB2	1:C:1212:THR:CG2	2.42	0.43
1:D:1015:TYR:HA	1:D:1019:GLN:NE2	2.34	0.43
1:D:1129:VAL:HG13	1:D:1130:PRO:CD	2.48	0.43
1:A:1081:ILE:HD12	1:A:1206:PHE:CE1	2.54	0.43
1:A:1131:ALA:HB1	1:A:1173:CYS:SG	2.59	0.43
1:A:1179:TYR:HE2	1:A:1181:ILE:CG2	2.32	0.43
1:C:1179:TYR:HE2	1:C:1181:ILE:CG2	2.31	0.43
1:D:1132:HIS:CD2	1:F:1131:ALA:HA	2.54	0.43
1:D:1133:HIS:HD2	1:F:1133:HIS:CD2	2.32	0.43
1:D:1204:VAL:HG12	1:D:1254:ILE:HB	2.00	0.43
1:A:1147:PRO:HB3	1:A:1162:TYR:CE1	2.54	0.42
1:A:1159:ARG:HG2	1:A:1159:ARG:NH1	2.33	0.42
1:D:1086:PHE:HB2	1:D:1114:SER:OG	2.19	0.42
1:F:1037:LEU:HD23	1:F:1048:GLY:HA3	2.00	0.42
1:F:1187:ALA:O	1:F:1246:VAL:HA	2.19	0.42
1:C:1015:TYR:HA	1:C:1019:GLN:NE2	2.34	0.42
1:B:1013:ARG:HG2	1:B:1014:HIS:CE1	2.53	0.42
1:D:1179:TYR:HE2	1:D:1181:ILE:HG23	1.84	0.42
1:B:1062:ASP:HB2	1:B:1067:VAL:O	2.19	0.42
1:B:1142:ILE:HD12	1:B:1142:ILE:H	1.82	0.42
1:B:1184:PRO:HA	1:B:1250:ASN:CG	2.40	0.42
1:D:1179:TYR:CE2	1:D:1181:ILE:HG23	2.54	0.42
1:F:1062:ASP:HB2	1:F:1067:VAL:O	2.20	0.42
1:F:1063:LYS:HB2	1:F:1063:LYS:NZ	2.35	0.42
1:C:1178:GLY:O	1:C:1254:ILE:HA	2.20	0.42
1:E:1184:PRO:HA	1:E:1250:ASN:CG	2.40	0.42
1:F:1188:TRP:HB3	1:F:1190:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1147:PRO:HB3	1:E:1162:TYR:CE1	2.55	0.42
1:E:1151:GLY:HA2	1:E:1157:ASN:ND2	2.34	0.42
1:A:1012:ILE:O	1:A:1012:ILE:HG12	2.20	0.42
1:C:1086:PHE:HB2	1:C:1114:SER:OG	2.20	0.42
1:C:1214:ILE:CD1	1:C:1216:HIS:HB2	2.50	0.42
1:D:1012:ILE:O	1:D:1012:ILE:HG12	2.19	0.42
1:D:1132:HIS:CD2	1:F:1132:HIS:CD2	3.08	0.42
1:F:1015:TYR:HA	1:F:1019:GLN:NE2	2.35	0.42
1:F:1086:PHE:HB2	1:F:1114:SER:OG	2.20	0.42
1:F:1188:TRP:CE2	1:F:1246:VAL:HG13	2.54	0.42
1:B:1031:ILE:HA	1:B:1032:PRO:HD2	1.82	0.42
1:C:1151:GLY:HA2	1:C:1157:ASN:ND2	2.35	0.42
1:C:1214:ILE:HD12	1:C:1214:ILE:O	2.20	0.42
1:B:1214:ILE:CD1	1:B:1216:HIS:HB2	2.50	0.42
1:D:1188:TRP:CE2	1:D:1246:VAL:HG13	2.55	0.42
1:A:1013:ARG:HG2	1:A:1014:HIS:CE1	2.55	0.41
1:A:1096:MET:CE	1:A:1139:LYS:HE3	2.50	0.41
1:C:1081:ILE:HD12	1:C:1206:PHE:CE1	2.55	0.41
1:D:1044:ARG:HD2	1:F:1043:ASP:OD1	2.20	0.41
1:F:1026:VAL:HG21	1:F:1038:THR:HG21	2.02	0.41
1:A:1042:ASN:HB3	1:A:1200:MET:HG2	2.01	0.41
1:C:1062:ASP:HB2	1:C:1067:VAL:O	2.19	0.41
1:D:1037:LEU:HD23	1:D:1048:GLY:HA3	2.01	0.41
1:A:1037:LEU:HD23	1:A:1048:GLY:HA3	2.03	0.41
1:B:1078:VAL:O	1:B:1101:GLY:HA2	2.20	0.41
1:C:1159:ARG:HG2	1:C:1159:ARG:NH1	2.31	0.41
1:D:1081:ILE:HD12	1:D:1206:PHE:CE1	2.54	0.41
1:A:1188:TRP:CH2	1:A:1246:VAL:CG2	3.04	0.41
1:B:1174:GLN:NE2	1:B:1258:CYS:HB2	2.35	0.41
1:C:1212:THR:CG2	1:C:1249:SER:HB3	2.50	0.41
1:D:1062:ASP:HB2	1:D:1067:VAL:O	2.19	0.41
1:D:1179:TYR:HE2	1:D:1181:ILE:CG2	2.34	0.41
1:E:999:GLN:HB2	1:E:1035:ILE:CD1	2.50	0.41
1:E:1062:ASP:HB2	1:E:1067:VAL:O	2.21	0.41
1:B:1147:PRO:HB3	1:B:1162:TYR:CE1	2.56	0.41
1:C:1037:LEU:HD23	1:C:1048:GLY:HA3	2.02	0.41
1:C:1129:VAL:HG13	1:C:1130:PRO:CD	2.51	0.41
1:E:998:LEU:HG	1:E:1034:ALA:HB2	2.03	0.41
1:B:1017:THR:O	1:B:1021:ARG:HG3	2.21	0.41
1:B:1135:TYR:HB3	1:B:1136:PRO:HD2	2.02	0.41
1:E:1178:GLY:O	1:E:1254:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1221:PRO:HB3	1:F:1242:ILE:HD11	2.03	0.41
1:B:1020:LEU:HD11	1:B:1225:LYS:CD	2.49	0.41
1:B:1178:GLY:O	1:B:1254:ILE:HA	2.21	0.41
1:E:1013:ARG:HG2	1:E:1014:HIS:CE1	2.56	0.41
1:E:1214:ILE:CD1	1:E:1216:HIS:HB2	2.50	0.41
1:D:1040:THR:HG23	1:D:1040:THR:O	2.21	0.41
1:F:1098:LYS:O	1:F:1099:GLN:HB2	2.21	0.41
1:F:1184:PRO:HA	1:F:1250:ASN:ND2	2.36	0.41
1:A:1014:HIS:HB3	1:C:1014:HIS:HB3	2.04	0.40
1:B:999:GLN:HG2	1:B:1035:ILE:CD1	2.51	0.40
1:B:1086:PHE:HB2	1:B:1114:SER:OG	2.21	0.40
1:C:1006:THR:HG22	1:C:1042:ASN:OD1	2.21	0.40
1:D:1214:ILE:CD1	1:D:1216:HIS:HB2	2.51	0.40
1:F:1013:ARG:HG2	1:F:1014:HIS:CE1	2.56	0.40
1:F:1135:TYR:HB3	1:F:1136:PRO:HD2	2.03	0.40
1:F:1143:ASP:O	1:F:1145:ILE:N	2.54	0.40
1:C:1237:SER:HA	1:C:1238:PRO:HD2	1.95	0.40
1:F:1097:LYS:HE2	1:F:1097:LYS:CA	2.50	0.40
1:C:1064:GLU:H	1:C:1064:GLU:CD	2.25	0.40
1:D:1064:GLU:H	1:D:1064:GLU:CD	2.25	0.40
1:F:1084:PRO:CB	1:F:1097:LYS:HE3	2.46	0.40
1:F:1174:GLN:NE2	1:F:1258:CYS:HB2	2.36	0.40
1:A:1064:GLU:H	1:A:1064:GLU:CD	2.24	0.40
1:B:1037:LEU:HD23	1:B:1048:GLY:HA3	2.02	0.40
1:B:1131:ALA:HB1	1:B:1173:CYS:SG	2.62	0.40
1:D:1237:SER:HA	1:D:1238:PRO:HD2	1.96	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/289 (87%)	232 (92%)	17 (7%)	2 (1%)	19	53
1	B	250/289 (86%)	229 (92%)	19 (8%)	2 (1%)	19	53
1	C	249/289 (86%)	233 (94%)	15 (6%)	1 (0%)	34	69
1	D	250/289 (86%)	230 (92%)	19 (8%)	1 (0%)	34	69
1	E	250/289 (86%)	232 (93%)	17 (7%)	1 (0%)	34	69
1	F	249/289 (86%)	229 (92%)	19 (8%)	1 (0%)	34	69
All	All	1499/1734 (86%)	1385 (92%)	106 (7%)	8 (0%)	29	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1144	GLU
1	B	1144	GLU
1	C	1144	GLU
1	E	1144	GLU
1	F	1144	GLU
1	D	1144	GLU
1	B	1070	PHE
1	A	1142	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/259 (88%)	198 (87%)	29 (13%)	4	17
1	B	226/259 (87%)	197 (87%)	29 (13%)	4	17
1	C	225/259 (87%)	198 (88%)	27 (12%)	5	19
1	D	226/259 (87%)	196 (87%)	30 (13%)	4	15
1	E	226/259 (87%)	199 (88%)	27 (12%)	5	20
1	F	225/259 (87%)	197 (88%)	28 (12%)	4	18
All	All	1355/1554 (87%)	1185 (88%)	170 (12%)	4	17

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	999	GLN
1	A	1003	THR
1	A	1012	ILE
1	A	1015	TYR
1	A	1031	ILE
1	A	1035	ILE
1	A	1038	THR
1	A	1042	ASN
1	A	1046	ILE
1	A	1050	VAL
1	A	1051	THR
1	A	1061	LEU
1	A	1062	ASP
1	A	1063	LYS
1	A	1076	LEU
1	A	1089	ILE
1	A	1097	LYS
1	A	1102	TYR
1	A	1138	VAL
1	A	1142	ILE
1	A	1155	THR
1	A	1156	LEU
1	A	1163	GLN
1	A	1169	VAL
1	A	1174	GLN
1	A	1179	TYR
1	A	1200	MET
1	A	1246	VAL
1	A	1248	THR
1	B	999	GLN
1	B	1003	THR
1	B	1012	ILE
1	B	1015	TYR
1	B	1031	ILE
1	B	1035	ILE
1	B	1038	THR
1	B	1042	ASN
1	B	1046	ILE
1	B	1050	VAL
1	B	1051	THR
1	B	1061	LEU
1	B	1062	ASP

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Mol	Chain	Res	Type
1	B	1063	LYS
1	B	1076	LEU
1	B	1089	ILE
1	B	1097	LYS
1	B	1102	TYR
1	B	1138	VAL
1	B	1142	ILE
1	B	1155	THR
1	B	1156	LEU
1	B	1163	GLN
1	B	1169	VAL
1	B	1174	GLN
1	B	1179	TYR
1	B	1246	VAL
1	B	1248	THR
1	B	1250	ASN
1	C	1003	THR
1	C	1012	ILE
1	C	1015	TYR
1	C	1031	ILE
1	C	1035	ILE
1	C	1038	THR
1	C	1042	ASN
1	C	1046	ILE
1	C	1050	VAL
1	C	1051	THR
1	C	1061	LEU
1	C	1062	ASP
1	C	1063	LYS
1	C	1076	LEU
1	C	1089	ILE
1	C	1097	LYS
1	C	1102	TYR
1	C	1138	VAL
1	C	1142	ILE
1	C	1155	THR
1	C	1156	LEU
1	C	1163	GLN
1	C	1169	VAL
1	C	1174	GLN
1	C	1179	TYR
1	C	1246	VAL

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Mol	Chain	Res	Type
1	C	1248	THR
1	D	1003	THR
1	D	1012	ILE
1	D	1015	TYR
1	D	1031	ILE
1	D	1035	ILE
1	D	1038	THR
1	D	1042	ASN
1	D	1046	ILE
1	D	1050	VAL
1	D	1051	THR
1	D	1061	LEU
1	D	1062	ASP
1	D	1063	LYS
1	D	1076	LEU
1	D	1089	ILE
1	D	1097	LYS
1	D	1102	TYR
1	D	1138	VAL
1	D	1142	ILE
1	D	1155	THR
1	D	1156	LEU
1	D	1163	GLN
1	D	1169	VAL
1	D	1174	GLN
1	D	1179	TYR
1	D	1199	ARG
1	D	1200	MET
1	D	1246	VAL
1	D	1248	THR
1	D	1250	ASN
1	E	999	GLN
1	E	1003	THR
1	E	1012	ILE
1	E	1015	TYR
1	E	1031	ILE
1	E	1035	ILE
1	E	1038	THR
1	E	1042	ASN
1	E	1046	ILE
1	E	1050	VAL
1	E	1051	THR

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Mol	Chain	Res	Type
1	E	1061	LEU
1	E	1062	ASP
1	E	1063	LYS
1	E	1089	ILE
1	E	1097	LYS
1	E	1102	TYR
1	E	1138	VAL
1	E	1142	ILE
1	E	1155	THR
1	E	1156	LEU
1	E	1163	GLN
1	E	1169	VAL
1	E	1174	GLN
1	E	1179	TYR
1	E	1246	VAL
1	E	1248	THR
1	F	999	GLN
1	F	1003	THR
1	F	1012	ILE
1	F	1015	TYR
1	F	1031	ILE
1	F	1035	ILE
1	F	1038	THR
1	F	1042	ASN
1	F	1046	ILE
1	F	1050	VAL
1	F	1051	THR
1	F	1061	LEU
1	F	1062	ASP
1	F	1063	LYS
1	F	1076	LEU
1	F	1089	ILE
1	F	1097	LYS
1	F	1102	TYR
1	F	1138	VAL
1	F	1142	ILE
1	F	1155	THR
1	F	1156	LEU
1	F	1163	GLN
1	F	1169	VAL
1	F	1174	GLN
1	F	1179	TYR

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Mol	Chain	Res	Type
1	F	1246	VAL
1	F	1248	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	999	GLN
1	A	1014	HIS
1	A	1019	GLN
1	A	1041	HIS
1	A	1163	GLN
1	A	1168	ASN
1	A	1174	GLN
1	A	1216	HIS
1	A	1243	HIS
1	A	1250	ASN
1	B	999	GLN
1	B	1019	GLN
1	B	1041	HIS
1	B	1099	GLN
1	B	1163	GLN
1	B	1168	ASN
1	B	1174	GLN
1	B	1216	HIS
1	B	1226	HIS
1	B	1243	HIS
1	B	1250	ASN
1	C	999	GLN
1	C	1014	HIS
1	C	1019	GLN
1	C	1041	HIS
1	C	1163	GLN
1	C	1168	ASN
1	C	1174	GLN
1	C	1216	HIS
1	C	1243	HIS
1	C	1250	ASN
1	D	999	GLN
1	D	1019	GLN
1	D	1041	HIS
1	D	1099	GLN
1	D	1132	HIS

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Mol	Chain	Res	Type
1	D	1133	HIS
1	D	1163	GLN
1	D	1168	ASN
1	D	1174	GLN
1	D	1216	HIS
1	D	1226	HIS
1	D	1243	HIS
1	D	1250	ASN
1	E	999	GLN
1	E	1019	GLN
1	E	1041	HIS
1	E	1163	GLN
1	E	1168	ASN
1	E	1174	GLN
1	E	1216	HIS
1	E	1243	HIS
1	E	1250	ASN
1	F	1019	GLN
1	F	1041	HIS
1	F	1132	HIS
1	F	1133	HIS
1	F	1163	GLN
1	F	1168	ASN
1	F	1174	GLN
1	F	1216	HIS
1	F	1226	HIS
1	F	1243	HIS
1	F	1250	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	255/289 (88%)	0.18	13 (5%)	28 17	13, 37, 69, 99	0
1	B	254/289 (87%)	0.12	8 (3%)	49 32	15, 36, 64, 98	0
1	C	253/289 (87%)	0.10	8 (3%)	47 31	19, 41, 67, 98	0
1	D	254/289 (87%)	0.12	4 (1%)	72 55	13, 39, 64, 95	0
1	E	254/289 (87%)	0.07	13 (5%)	28 17	11, 36, 73, 95	0
1	F	253/289 (87%)	0.22	13 (5%)	28 17	19, 42, 70, 96	0
All	All	1523/1734 (87%)	0.14	59 (3%)	39 25	11, 39, 68, 99	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1148	MET	7.2
1	A	1146	THR	6.3
1	C	1148	MET	6.2
1	A	1144	GLU	6.0
1	E	1146	THR	6.0
1	A	1148	MET	5.3
1	F	1149	GLU	4.9
1	A	1151	GLY	4.6
1	F	1148	MET	4.6
1	A	1154	LEU	4.5
1	A	1145	ILE	4.4
1	C	1146	THR	4.4
1	A	1152	ASP	4.4
1	F	1154	LEU	4.3
1	A	1150	THR	4.2
1	F	1119	ASP	3.8
1	E	1154	LEU	3.8
1	E	1119	ASP	3.6
1	D	1148	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	1150	THR	3.4
1	F	1145	ILE	3.4
1	F	1146	THR	3.3
1	E	1149	GLU	3.2
1	E	1144	GLU	3.2
1	F	1168	ASN	3.1
1	B	1149	GLU	3.1
1	B	1119	ASP	2.9
1	C	1144	GLU	2.9
1	A	1168	ASN	2.9
1	E	1168	ASN	2.8
1	B	1190	THR	2.7
1	B	1148	MET	2.6
1	C	1063	LYS	2.6
1	B	1054	THR	2.5
1	A	1161	ILE	2.5
1	B	1147	PRO	2.5
1	D	1147	PRO	2.5
1	F	1063	LYS	2.5
1	D	1190	THR	2.4
1	E	1169	VAL	2.4
1	C	1149	GLU	2.4
1	D	1119	ASP	2.4
1	E	1152	ASP	2.4
1	F	1120	ASN	2.3
1	F	1054	THR	2.2
1	F	1190	THR	2.2
1	A	1117	ASN	2.2
1	E	1190	THR	2.2
1	A	1189	ASN	2.2
1	C	1154	LEU	2.2
1	E	1189	ASN	2.2
1	F	1142	ILE	2.2
1	B	1168	ASN	2.1
1	C	1213	ARG	2.0
1	E	1145	ILE	2.0
1	E	1147	PRO	2.0
1	A	1190	THR	2.0
1	B	1136	PRO	2.0
1	C	1150	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.