



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:43 am GMT

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.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

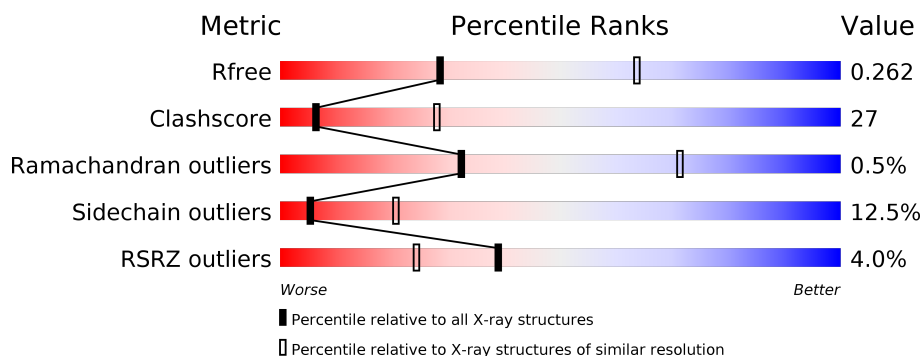
1 Overall quality at a glance

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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (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 on the lower 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 $\leq 5\%$. 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	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>31%</div> <div>6%</div> <div>12%</div> </div> </div>
1	B	289	<div> <div>3%</div> <div> <div></div> <div>48%</div> <div>33%</div> <div>7%</div> <div>12%</div> </div> </div>
1	C	289	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>33%</div> <div>6%</div> <div>12%</div> </div> </div>
1	D	289	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>32%</div> <div>7%</div> <div>12%</div> </div> </div>
1	E	289	<div> <div>5%</div> <div> <div></div> <div>48%</div> <div>34%</div> <div>6%</div> <div>12%</div> </div> </div>
1	F	289	<div> <div>4%</div> <div> <div></div> <div>46%</div> <div>35%</div> <div>7%</div> <div>12%</div> </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

Continued on next page...

Continued from previous page...

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
D	1278	GLY	-	CLONING ARTIFACT	UNP Q838L9
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

Continued on next page...

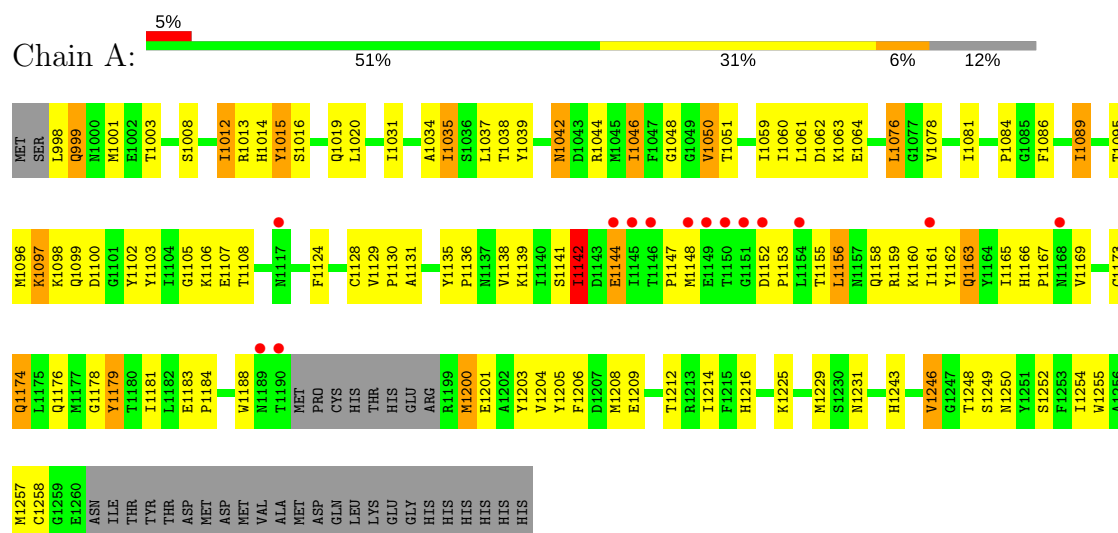
Continued from previous page...

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

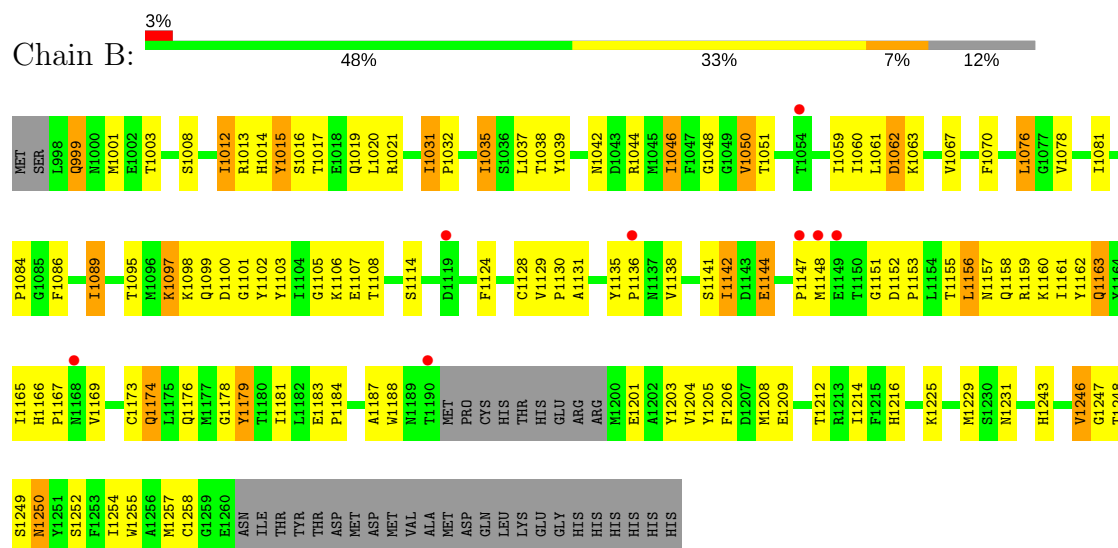
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

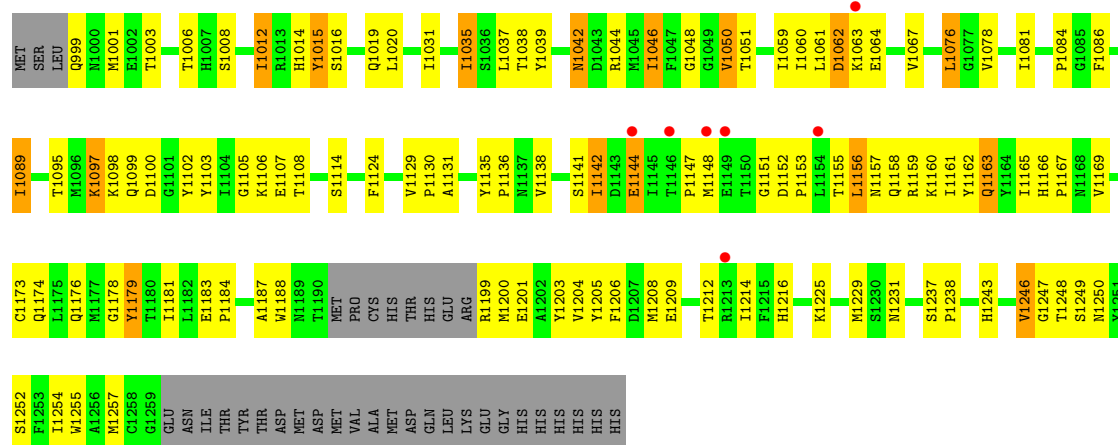


- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1

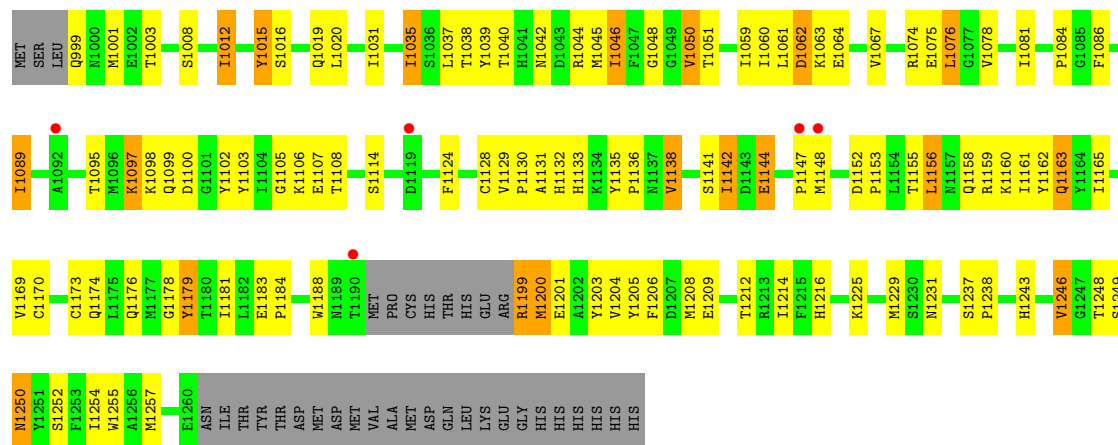


- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1

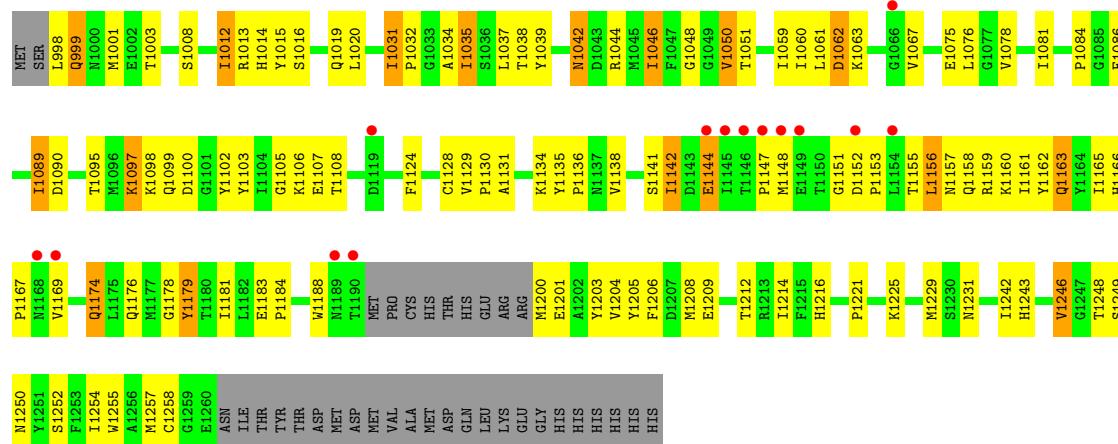




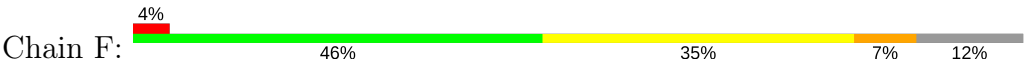
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase 1



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



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



H1243	Q1163	F1086	MET
V1246	Y1164	I1089	SER
G1247	I1165		LEU
T1248	H1166		Q999
S1249	P1167	T1095	N1000
N1250	M1168	K1096	M1001
Y1251	V1169	K1097	E1002
S1252	C1173	K1098	T1003
F1253	Q1174	Q1099	S1008
I1254	L1175	D1100	
W1255	L1176	G1101	I1012
A1256	M1177	Y1102	R1013
M1257	G1178	Y1103	H1014
C1258	Y1179	I1104	Y1015
G1259	T1180	G1105	S1016
E1260	I1181	K1106	
ASN	L1182	E1107	Q1019
ILE	E1183	T1108	L1020
THR	P1184	S1114	
TYR			V1026
THR	A1187	D1119	
ASP	W1188	N1120	I1031
MET	M1189		
ASP	T1190	F1124	I1035
MET	MET		S1036
VAL	PRO	C1128	L1037
ALA	CYS	V1129	T1038
MET	HIS	P1130	Y1039
ASP	THR	A1131	
GLN	HIS	H1132	N1042
LEU	GLU	H1133	D1043
LYS	ARG	K1134	R1044
GLU	ARG	Y1135	M1045
GLY	M1200	P1136	I1046
HIS	E1201	N1137	F1047
HIS	A1202	V1138	G1048
HIS	Y1203		G1049
HIS	V1204		V1050
HIS	Y1205	S1141	T1051
HIS	F1206	I1142	
HIS	D1207	E1144	T1054
	M1208	I1145	
	E1209	T1146	
		P1147	I1059
	T1212	M1148	L1060
	R1213	E1149	L1061
	I1214	T1150	D1062
	F1215	G1151	K1063
	H1216	D1152	
		P1153	V1067
		L1154	
	P1221	E1075	
	K1225	L1076	
		G1077	
	M1229	V1078	
	S1230		I1081
	N1231	K1160	
		I1161	P1084
	I1242	Y1162	G1085

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	1722 reflections (4.95%)	DCC
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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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:HD12	1:C:1142:ILE:N	2.02	0.75
1:A:1142:ILE:HD12	1:A:1142:ILE:N	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:CB	1:D:1199:ARG:HH11	2.01	0.74
1:D:1016:SER:N	1:D:1019:GLN:HE21	1.85	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1142:ILE:N	1:E:1142:ILE:HD12	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:HD12	1:F:1142:ILE:N	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:HD23	1:C:1156:LEU:N	2.08	0.68
1:D:1097:LYS:HA	1:D:1097:LYS:HE2	1.76	0.68
1:F:1035:ILE:HD12	1:F:1059:ILE:HG12	1.76	0.68
1:D:1156:LEU:N	1:D:1156:LEU:HD23	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:HD23	1:A:1156:LEU:N	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

Continued on next page...

Continued from previous page...

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:HA	1:A:1097:LYS:HE2	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:HA	1:F:1163:GLN:HE21	1.62	0.65
1:D:1132:HIS:CD2	1:F:1132:HIS:H	2.14	0.65
1:F:1156:LEU:HD23	1:F:1156:LEU:N	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:HE21	1:C:1163:GLN:HA	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:HA	1:A:1163:GLN:HE21	1.62	0.64
1:C:1039:TYR:OH	1:C:1044:ARG:HG2	1.96	0.64
1:E:1097:LYS:HE2	1:E:1097:LYS:HA	1.78	0.63
1:C:1159:ARG:HH11	1:C:1159:ARG:HG2	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

Continued on next page...

Continued from previous page...

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:F:1076:LEU:HD21	1:F:1078:VAL:CG2	2.29	0.63
1:D:1132:HIS:CG	1:F:1173:CYS:HB3	2.33	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: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:D:1173:CYS:HB3	1:F:1132:HIS:CG	2.35	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

Continued on next page...

Continued from previous page...

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:C	1:F:1200:MET:SD	2.81	0.59
1:D:1097:LYS:O	1:D:1100:ASP:HB2	2.01	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:B:999:GLN:HG2	1:B:1035:ILE:HG12	1.85	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

Continued on next page...

Continued from previous page...

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:1205:TYR:OH	1:E:1216:HIS:HD2	1.86	0.56
1:E:1046:ILE:O	1:E:1046:ILE:HG13	2.04	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:F:1001:MET:HA	1:F:1037:LEU:O	2.06	0.56
1:D:1132:HIS:HB2	1:F:1132:HIS:HB2	1.87	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:H	1:E:1156:LEU:HD23	1.69	0.56
1:C:1129:VAL:HG13	1:C:1130:PRO:HD2	1.87	0.55
1:D:1159:ARG:HH11	1:D:1159:ARG:HG2	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:H	1:D:1156:LEU:HD23	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

Continued on next page...

Continued from previous page...

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:HG13	1:F:1046:ILE:O	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:O	1:A:1046:ILE:HG13	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:H	1:C:1156:LEU:HD23	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:B:1147:PRO:HB3	1:B:1162:TYR:CZ	2.43	0.54
1:C:1214:ILE:HD12	1:C:1214:ILE:C	2.28	0.54
1:A:1246:VAL:HG11	1:C:1246:VAL:HG11	1.90	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:HG13	1:D:1060:ILE:O	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

Continued on next page...

Continued from previous page...

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:HD22	1:C:1250:ASN:N	2.07	0.53
1:D:1089:ILE:HG13	1:D:1089:ILE:O	2.09	0.53
1:D:1084:PRO:CD	1:E:1134:LYS:HE2	2.38	0.53
1:D:1074:ARG:NH2	1:F:1260:GLU:OE2	2.40	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:HG13	1:C:1060:ILE:O	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

Continued on next page...

Continued from previous page...

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:O	1:C:1089:ILE:HG13	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:HD22	1:F:1250:ASN:N	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:ND2	1:C:1250:ASN:N	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:1214:ILE:HG13	1:F:1229:MET:HB2	1.93	0.51
1:F:1212:THR:HG21	1:F:1249:SER:HB3	1.92	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:O	1:E:1089:ILE:HG13	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:HD12	1:F:1214:ILE:C	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:O	1:E:1060:ILE:HG13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1204:VAL:HG13	1:F:1204:VAL:O	2.11	0.49
1:B:1204:VAL:O	1:B:1204:VAL:HG13	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:B:1035:ILE:CD1	1:B:1059:ILE:HG12	2.42	0.49
1:A:1014:HIS:CD2	1:C:1019:GLN:NE2	2.80	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:C	1:C:1046:ILE:HD12	2.33	0.48
1:A:1098:LYS:HG2	1:A:1099:GLN:HG2	1.94	0.48
1:F:1012:ILE:O	1:F:1012:ILE:HG12	2.13	0.48
1:F:1060:ILE:O	1:F:1060:ILE:HG13	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:HD12	1:D:1046:ILE:C	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:O	1:F:1089:ILE:HG13	2.13	0.48
1:C:1142:ILE:CD1	1:C:1142:ILE:N	2.69	0.48
1:D:1035:ILE:CD1	1:D:1059:ILE:HG12	2.43	0.48
1:D:1086:PHE:CE1	1:D:1095:THR:HG22	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1106:LYS:O	1:D:1107:GLU:HB2	2.14	0.48
1:D:999:GLN:HA	1:D:1035:ILE:HG12	1.96	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:O	1:C:1204:VAL:HG13	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: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:D:1188:TRP:CH2	1:D:1246:VAL:HG22	2.49	0.47
1:A:1204:VAL:O	1:A:1204:VAL:HG13	2.15	0.47
1:B:1046:ILE:C	1:B:1046:ILE:HD12	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:HG3	1:D:1200:MET:O	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: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:B:1081:ILE:HD12	1:B:1206:PHE:CZ	2.49	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

Continued on next page...

Continued from previous page...

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:1097:LYS:CE	1:F:1098:LYS:H	2.28	0.46
1:F:1075:GLU:HG2	1:F:1131:ALA:HB2	1.96	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:HG12	1:B:1012:ILE:O	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: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:D:1173:CYS:HB3	1:F:1132:HIS:CD2	2.51	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

Continued on next page...

Continued from previous page...

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:O	1:E:1012:ILE:HG12	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

Continued on next page...

Continued from previous page...

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: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:D:1132:HIS:CD2	1:F:1131:ALA:HA	2.54	0.43
1:A:1159:ARG:HG2	1:A:1159:ARG:NH1	2.33	0.42
1:A:1147:PRO:HB3	1:A:1162:TYR:CE1	2.54	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:1063:LYS:NZ	1:F:1063:LYS:HB2	2.35	0.42
1:F:1062:ASP:HB2	1:F:1067:VAL:O	2.20	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

Continued on next page...

Continued from previous page...

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: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:D:1132:HIS:CD2	1:F:1132:HIS:CD2	3.08	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:1062:ASP:HB2	1:E:1067:VAL:O	2.21	0.41
1:E:999:GLN:HB2	1:E:1035:ILE:CD1	2.50	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

Continued on next page...

Continued from previous page...

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: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: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: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: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:A:1014:HIS:HB3	1:C:1014:HIS:HB3	2.04	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:CA	1:F:1097:LYS:HE2	2.50	0.40
1:C:1064:GLU:H	1:C:1064:GLU:CD	2.25	0.40
1:D:1064:GLU:CD	1:D:1064:GLU:H	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:CD	1:A:1064:GLU:H	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

5.3.1 Protein backbone

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%)	22	61
1	B	250/289 (86%)	229 (92%)	19 (8%)	2 (1%)	22	61
1	C	249/289 (86%)	233 (94%)	15 (6%)	1 (0%)	38	75
1	D	250/289 (86%)	230 (92%)	19 (8%)	1 (0%)	38	75
1	E	250/289 (86%)	232 (93%)	17 (7%)	1 (0%)	38	75
1	F	249/289 (86%)	229 (92%)	19 (8%)	1 (0%)	38	75
All	All	1499/1734 (86%)	1385 (92%)	106 (7%)	8 (0%)	32	71

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%)	5	20
1	B	226/259 (87%)	197 (87%)	29 (13%)	5	20
1	C	225/259 (87%)	198 (88%)	27 (12%)	6	23
1	D	226/259 (87%)	196 (87%)	30 (13%)	4	18
1	E	226/259 (87%)	199 (88%)	27 (12%)	6	23
1	F	225/259 (87%)	197 (88%)	28 (12%)	5	21
All	All	1355/1554 (87%)	1185 (88%)	170 (12%)	5	20

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Some 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

Continued on next page...

Continued from previous page...

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	14 (5%)	26 15	13, 37, 69, 99	0
1	B	254/289 (87%)	0.12	8 (3%)	49 31	15, 36, 64, 98	0
1	C	253/289 (87%)	0.10	7 (2%)	53 35	19, 41, 67, 98	0
1	D	254/289 (87%)	0.12	5 (1%)	65 46	13, 39, 64, 95	0
1	E	254/289 (87%)	0.07	14 (5%)	26 15	11, 36, 73, 95	0
1	F	253/289 (87%)	0.22	13 (5%)	29 18	19, 42, 70, 96	0
All	All	1523/1734 (87%)	0.14	61 (4%)	39 24	11, 39, 68, 99	0

All (61) 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	6.1
1	E	1146	THR	6.0
1	A	1148	MET	5.3
1	F	1149	GLU	4.9
1	A	1154	LEU	4.6
1	A	1151	GLY	4.6
1	F	1148	MET	4.5
1	C	1146	THR	4.4
1	A	1145	ILE	4.4
1	A	1152	ASP	4.4
1	F	1154	LEU	4.4
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	1145	ILE	3.4
1	F	1150	THR	3.4
1	F	1146	THR	3.2
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	3.0
1	C	1144	GLU	3.0
1	A	1168	ASN	2.8
1	E	1168	ASN	2.8
1	B	1190	THR	2.7
1	C	1063	LYS	2.6
1	B	1148	MET	2.6
1	B	1054	THR	2.5
1	B	1147	PRO	2.5
1	F	1063	LYS	2.5
1	A	1161	ILE	2.5
1	D	1147	PRO	2.4
1	D	1190	THR	2.4
1	E	1169	VAL	2.4
1	E	1152	ASP	2.3
1	D	1119	ASP	2.3
1	C	1149	GLU	2.3
1	F	1120	ASN	2.3
1	F	1054	THR	2.2
1	F	1190	THR	2.2
1	E	1190	THR	2.2
1	C	1154	LEU	2.2
1	A	1117	ASN	2.2
1	A	1189	ASN	2.2
1	E	1189	ASN	2.2
1	F	1142	ILE	2.1
1	B	1168	ASN	2.1
1	A	1190	THR	2.1
1	E	1066	GLY	2.1
1	C	1213	ARG	2.0
1	B	1136	PRO	2.0
1	E	1145	ILE	2.0
1	D	1092	ALA	2.0
1	A	1149	GLU	2.0
1	E	1147	PRO	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 carbohydrates 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.