



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:02 am GMT

PDB ID : 3S4W
Title : Structure of the FANCI-FANCD2 complex
Authors : Pavletich, N.P.
Deposited on : 2011-05-20
Resolution : 3.41 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

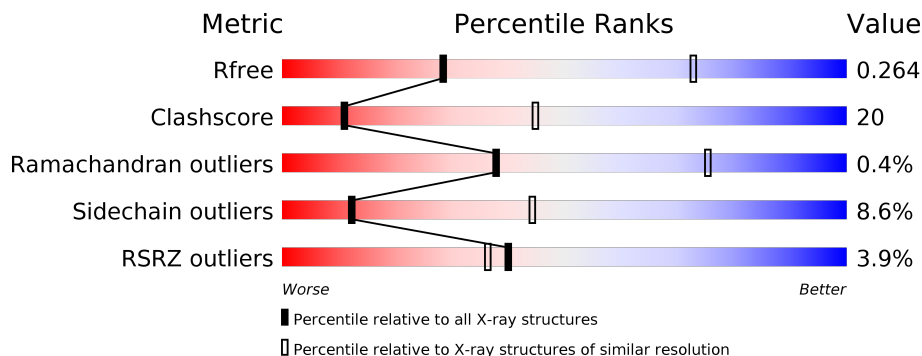
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	1308	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>35%</div> <div>•</div> <div>8%</div> </div> </div>
2	B	1323	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>33%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18671 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 Fanconi anemia group I protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1206	Total	C	N	O	S	0	0	0
			9506	6093	1579	1778	56			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1308	HIS	-	EXPRESSION TAG	UNP Q8K368

- Molecule 2 is a protein called Fanconi anemia group D2 protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1146	Total	C	N	O	S	0	0	0
			9165	5905	1543	1664	53			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	ALA	DELETION	UNP Q80V62
B	?	-	VAL	DELETION	UNP Q80V62
B	?	-	ALA	DELETION	UNP Q80V62
B	?	-	ALA	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	ASN	DELETION	UNP Q80V62
B	?	-	ARG	DELETION	UNP Q80V62

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	GLY	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	THR	DELETION	UNP Q80V62
B	?	-	GLY	DELETION	UNP Q80V62
B	?	-	GLY	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	GLN	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	ALA	DELETION	UNP Q80V62
B	?	-	ASP	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	ASN	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	ALA	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	CYS	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	ASP	DELETION	UNP Q80V62
B	?	-	THR	DELETION	UNP Q80V62
B	?	-	LEU	DELETION	UNP Q80V62
B	?	-	LEU	DELETION	UNP Q80V62
B	?	-	THR	DELETION	UNP Q80V62
B	?	-	GLU	DELETION	UNP Q80V62
B	?	-	ASP	DELETION	UNP Q80V62
B	?	-	THR	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	GLU	DELETION	UNP Q80V62
B	?	-	CYS	DELETION	UNP Q80V62
B	?	-	ASP	DELETION	UNP Q80V62
B	?	-	MET	DELETION	UNP Q80V62
B	?	-	ALA	DELETION	UNP Q80V62
B	?	-	PRO	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	GLY	DELETION	UNP Q80V62
B	?	-	ARG	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	HIS	DELETION	UNP Q80V62
B	?	-	VAL	DELETION	UNP Q80V62
B	?	-	ASP	DELETION	UNP Q80V62

Continued on next page...

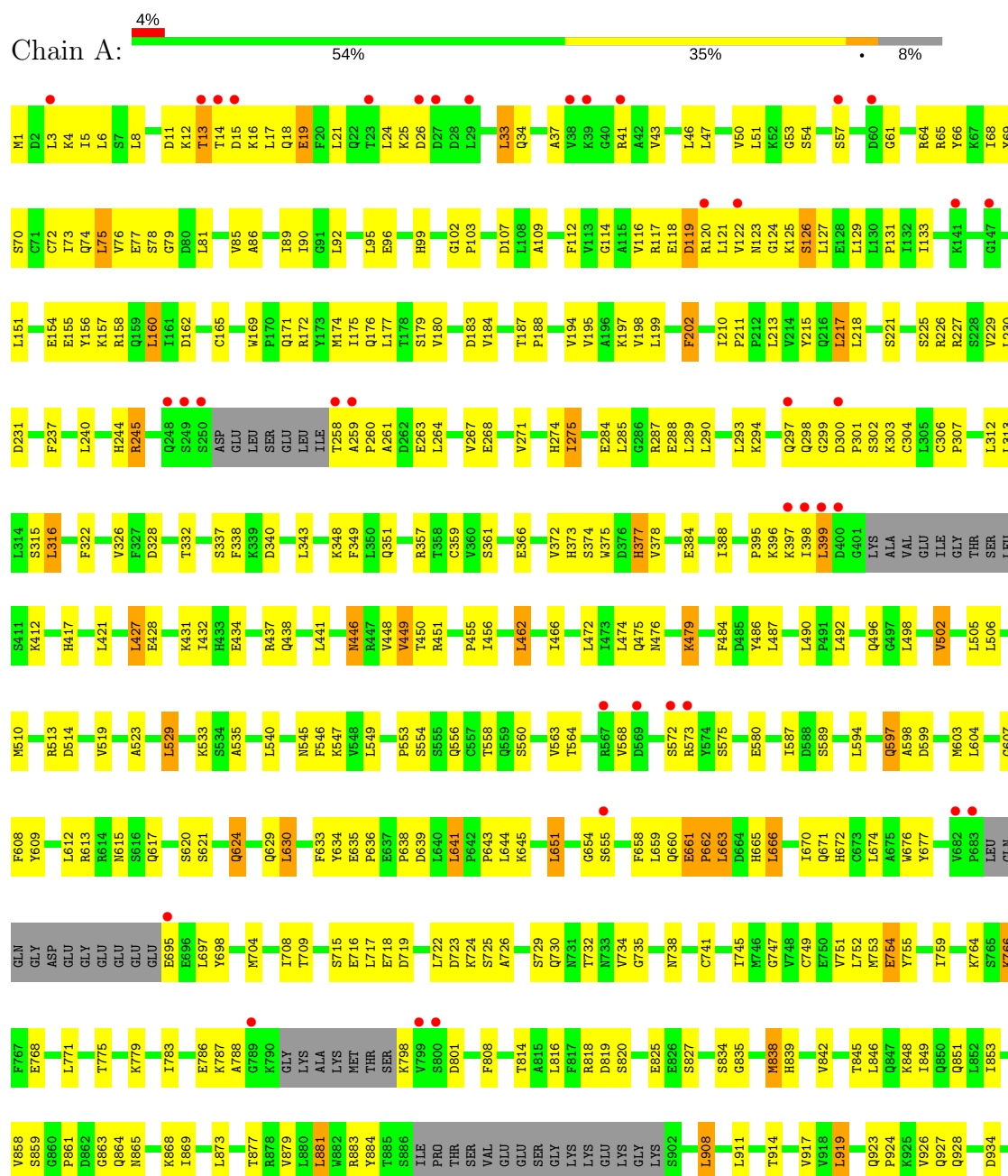
Continued from previous page...

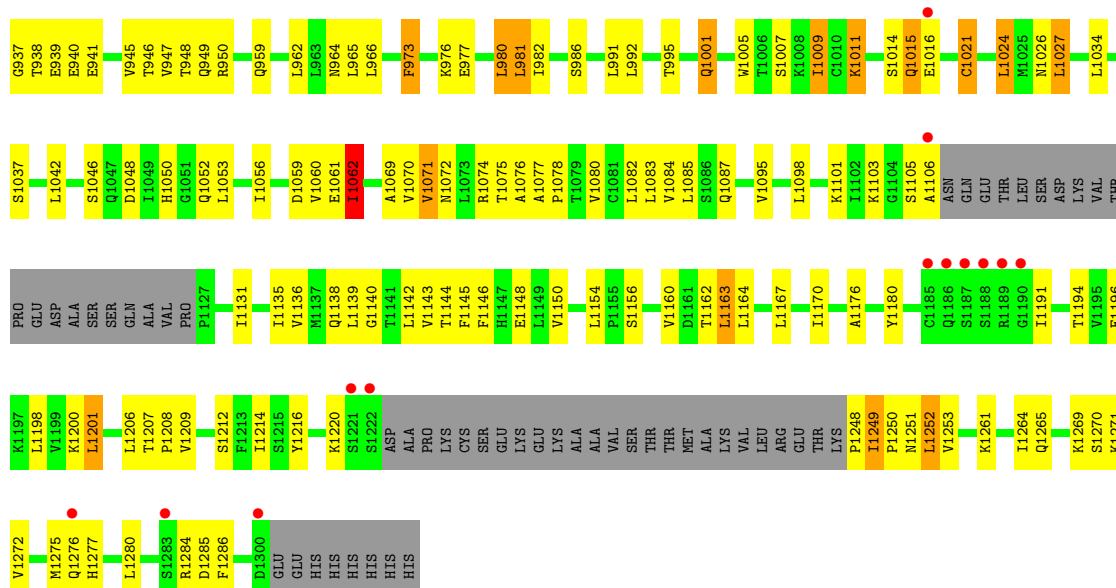
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	GLU	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	THR	DELETION	UNP Q80V62
B	?	-	GLY	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	GLU	DELETION	UNP Q80V62
B	?	-	GLY	DELETION	UNP Q80V62

3 Residue-property plots

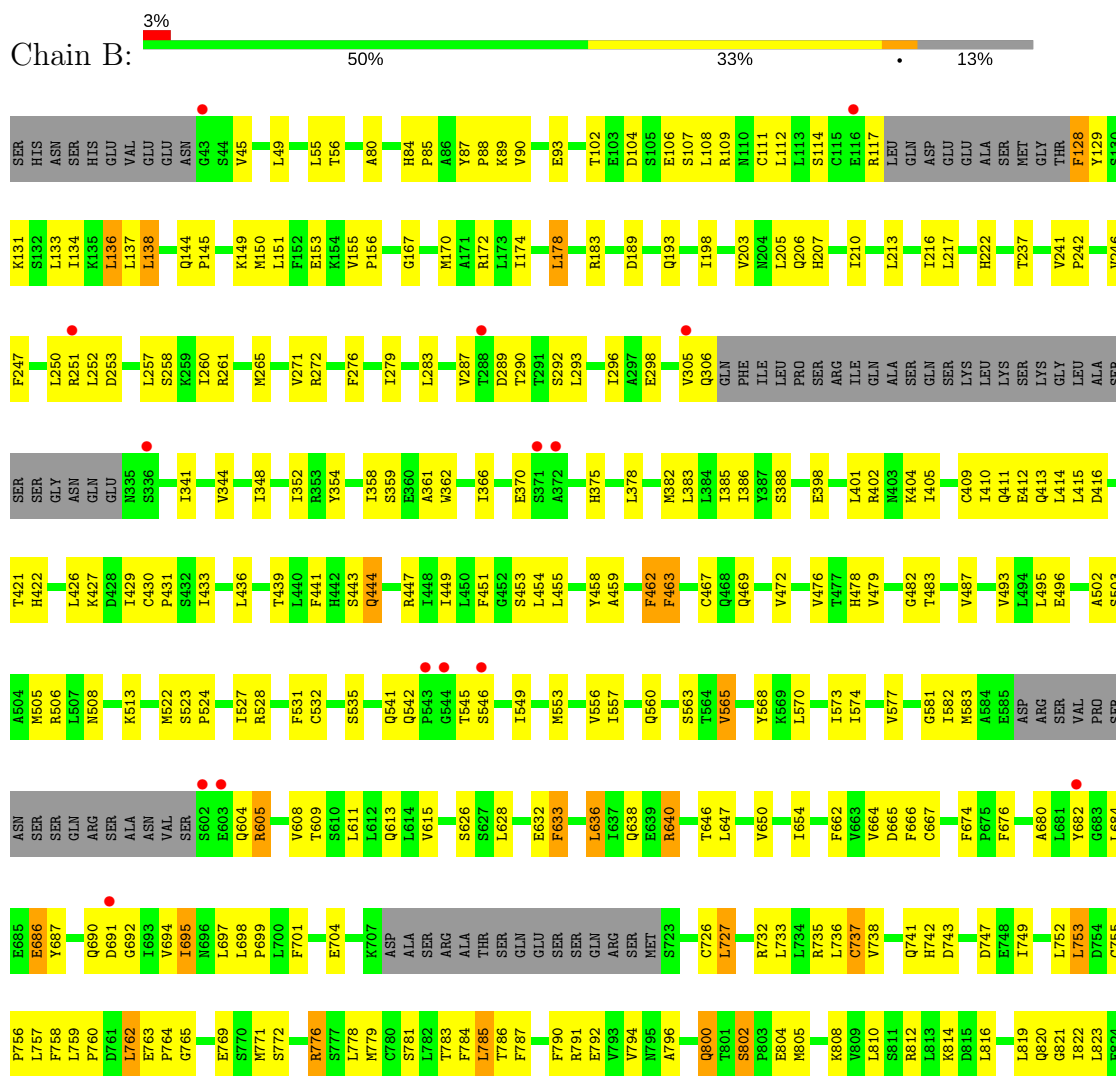
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Fanconi anemia group I protein homolog





• Molecule 2: Fanconi anemia group D2 protein homolog



GLY					
R1346	Q1347	D1348	T1349	R1350	L1351
					T1352
K1353					
H1354					V1355
					P1356
K1359					
K1360					
S1361					
L1362					
E1363					
L1364					
L1365					
M1372					
L1373					
V1374					
L1375					
N1376					
M1377					
C1378					
R1379					
E1380					
A1381					
L1384					
G1385					
T1386					
L1387					
D1391					
LEU					
GLN					
GLY					
GLU					
GLU					
ILE					
ILE					
SER					
GLN					
ASP					
PRO					
SER					
SER					
SER					
GLU					
L1331					
SER					
ASN					
ALA					
GLU					
ASP					
SER					
GLU					
ASP					
SER					
GLU					
ASP					
SER					
GLU					
ASP					
SER					
GLU					
ASP					
L1195					
I1198					
V1204					
G1205					
V1206					
P1207					
E1208					
S1211					
A1212					
P1213					
LYS					
ASP					
ALA					
ALA					
S1218					
S1219					
T1220					
F1221					
P1222					
T1223					
L1224					
T1225					
R1226					
H1227					
T1228					
F1229					
F1232					
F1233					
M1236					
M1237					
L1240					
E1241					
V1244					
K1245					
G1246					
L1247					
GLN					
ALA					
GLY					
THR					
A1252					
A1253					
Q1257					
V1258					
H1259					
E1260					
K1261					
E1262					
L1263					
L1264					
Y1265					
W1266					
H1267					
N1173					
P1174					
L1184					
Y1187					
T1191					
D1192					
K1158					
K1148					
Q1149					
L1153					
A1154					
S1155					
K1081					
S1080					
Q1079					
H1078					
T1077					
F1076					
G1075					
L1070					
ASN					
PRO					
VAL					
ALA					
S1143					
K1142					
L1136					
L1136					
C1128					
T1049					
ALA					
ARG					
ALA					
ALA					
LYS					
ASP					
ASP					
H1120					
H1121					
S1122					
V1123					
P1124					
E1052					
C1059					
Y1060					
Q1061					
K1062					
L1063					
PHE					
CYS					
ILE					
ARG					
GLN					
ARG					
E925					
L926					
D927					
I928					
E929					
F930					
F931					
S932					
H1003					
Q1004					
V1007					
V1011					
H1012					
C1013					
V1014					
V1015					
Q1016					
L1017					
L1018					
T1019					
P1020					
M1021					
C1022					
L1025					
E1026					
H1029					
E1017					
L1106					
L1105					
P1104					
Q1103					
D1102					
Q1101					
E1100					
M1099					
Q1098					
K1097					
E1090					
V1091					
L1092					
S1093					
M1094					
L1085					
H1086					
S1087					
C1162					
R1163					
A1164					
W1165					
P1166					
HIS					
GLY					
GLU					
LYS					
GLU					
K1172					
N1173					
P1174					
L1184					
Y1187					
T1191					
D1192					
E1107					
L1106					
L1105					
P1104					
Q1103					
D1102					
Q1101					
E1100					
M1099					
Q1098					
K1097					
E1090					
V1091					
L1092					
S1093					
M1094					
L1085					
H1086					
S1087					
C1162					
R1163					
A1164					
W1165					
P1166					
HIS					
GLY					
GLU					
LYS					
GLU					
K1172					
N1173					
P1174					
L1184					
Y1187					
T1191					
D1192					
E1107					
L1106					
L1105					
P1104					
Q1103					
D1102					
Q1101					
E1100					
M1099					
Q1098					
K1097					
E1090					
V1091					
L1092					
S1093					
M1094					
L1085					
H1086					
S1087					
C1162					
R1163					
A1164					
W1165					
P1166					
HIS					
GLY					
GLU					
LYS					
GLU					
K1172					
N1173					
P1174					
L1184					
Y1187					
T1191					
D1192					
E1107					
L1106					
L1105					
P1104					
Q1103					
D1102					
Q1101					
E1100					
M1099					
Q1098					
K1097					
E1090					
V1091					
L1092					
S1093					
M1094					
L1085					
H1086					
S1087					
C1162					
R1163					

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.80Å 110.40Å 350.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 3.41 20.02 – 3.41	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.86-3.41) 88.9 (20.02-3.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.240 , 0.272 0.231 , 0.264	Depositor DCC
R_{free} test set	1638 reflections (4.03%)	DCC
Wilson B-factor (Å ²)	90.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.5	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	0.93	EDS
Total number of atoms	18671	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.28	0/9655	0.47	0/13038
2	B	0.26	0/9336	0.46	0/12621
All	All	0.27	0/18991	0.46	0/25659

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1062	ILE	Peptide
2	B	1094	ASN	Peptide
2	B	1284	ASP	Peptide
2	B	290	THR	Peptide

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	9506	0	9792	373	0
2	B	9165	0	9297	394	0
All	All	18671	0	19089	759	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 20.

All (759) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:698:LEU:HD22	2:B:760:PRO:HD3	1.38	1.04
1:A:764:LYS:HG2	1:A:827:SER:HB3	1.40	1.02
2:B:1123:VAL:HG13	2:B:1128:CYS:HB2	1.48	0.95
1:A:1071:VAL:HG13	1:A:1076:ALA:HB2	1.49	0.95
2:B:426:LEU:HD23	2:B:429:ILE:HD12	1.51	0.93
2:B:1195:LEU:HB2	2:B:1266:TRP:HZ3	1.37	0.88
2:B:763:GLU:HB2	2:B:764:PRO:HD3	1.52	0.88
2:B:836:PRO:HD3	2:B:914:VAL:HG23	1.55	0.88
2:B:916:LEU:O	2:B:919:TYR:HD2	1.59	0.85
1:A:1136:VAL:HG11	1:A:1194:THR:HG22	1.57	0.85
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.59	0.85
2:B:749:ILE:HG23	2:B:752:LEU:HD12	1.59	0.85
1:A:1077:ALA:HB3	1:A:1078:PRO:HD3	1.60	0.81
1:A:3:LEU:HD23	1:A:6:LEU:HD12	1.64	0.80
1:A:306:CYS:HB2	1:A:307:PRO:HD2	1.66	0.78
2:B:771:MET:O	2:B:776:ARG:NH1	2.16	0.78
1:A:877:THR:OG1	1:A:914:THR:HG21	1.83	0.78
1:A:399:LEU:HB2	1:A:455:PRO:HG3	1.64	0.78
2:B:1315:PHE:HA	2:B:1322:VAL:HG21	1.65	0.77
2:B:411:GLN:HE22	2:B:1077:THR:HG21	1.50	0.77
1:A:34:GLN:O	1:A:37:ALA:N	2.18	0.76
2:B:763:GLU:HB2	2:B:764:PRO:CD	2.15	0.76
2:B:665:ASP:HA	2:B:692:GLY:O	1.84	0.76
2:B:1191:THR:HG22	2:B:1192:ASP:H	1.49	0.75
2:B:1277:LEU:HD13	2:B:1288:VAL:HG13	1.68	0.74
2:B:296:ILE:HD12	2:B:361:ALA:HB3	1.70	0.74
2:B:523:SER:HB2	2:B:524:PRO:HD2	1.69	0.74
2:B:776:ARG:HH21	2:B:779:MET:HG3	1.53	0.74
2:B:102:THR:HG23	2:B:108:LEU:HD13	1.70	0.73
1:A:1103:LYS:HG2	1:A:1180:TYR:HD1	1.51	0.73
2:B:697:LEU:HD23	2:B:759:LEU:HD21	1.69	0.72
1:A:1142:LEU:HA	1:A:1145:PHE:HB3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ILE:HG22	1:A:752:LEU:HD11	1.71	0.72
2:B:735:ARG:HD2	2:B:796:ALA:HA	1.71	0.72
2:B:1223:THR:HG22	2:B:1228:THR:HG21	1.70	0.72
1:A:202:PHE:CE1	1:A:210:ILE:HG23	2.25	0.72
1:A:818:ARG:NH1	1:A:825:GLU:OE1	2.22	0.72
2:B:1206:VAL:N	2:B:1207:PRO:HD2	2.04	0.72
2:B:1277:LEU:HA	2:B:1280:MET:HB2	1.70	0.72
1:A:18:GLN:HG2	1:A:53:GLY:O	1.90	0.72
1:A:373:HIS:O	1:A:374:SER:OG	2.06	0.72
2:B:765:GLY:O	2:B:769:GLU:HG3	1.90	0.71
2:B:104:ASP:HB3	2:B:107:SER:HB2	1.72	0.71
1:A:275:ILE:HD11	1:A:312:LEU:HD11	1.73	0.71
2:B:469:GLN:HA	2:B:508:ASN:ND2	2.06	0.71
2:B:49:LEU:HD11	2:B:80:ALA:HB1	1.72	0.71
1:A:361:SER:HA	1:A:421:LEU:HD11	1.73	0.71
1:A:1048:ASP:HB3	1:A:1071:VAL:HG11	1.73	0.70
2:B:581:GLY:HA2	2:B:636:LEU:HD13	1.73	0.70
1:A:1053:LEU:HD21	1:A:1077:ALA:HB2	1.70	0.70
1:A:448:VAL:HA	1:A:456:ILE:HG21	1.74	0.70
1:A:1136:VAL:HG12	1:A:1198:LEU:HD12	1.74	0.70
2:B:1025:LEU:O	2:B:1029:HIS:HD2	1.75	0.70
1:A:1285:ASP:OD1	1:A:1286:PHE:N	2.21	0.70
1:A:338:PHE:CE2	1:A:417:HIS:HB3	2.27	0.69
2:B:800:GLN:HB3	2:B:805:MET:HG2	1.74	0.69
2:B:1233:PHE:CZ	2:B:1273:PHE:HB3	2.27	0.69
2:B:258:SER:HA	2:B:261:ARG:HH11	1.55	0.69
2:B:636:LEU:O	2:B:636:LEU:HD12	1.92	0.69
1:A:838:MET:HA	1:A:838:MET:HE2	1.74	0.69
2:B:742:HIS:O	2:B:743:ASP:HB2	1.92	0.68
1:A:598:ALA:HB2	1:A:660:GLN:HA	1.75	0.68
1:A:641:LEU:HG	1:A:715:SER:HB3	1.75	0.68
1:A:662:PRO:HB2	1:A:665:HIS:HB2	1.75	0.68
1:A:959:GLN:HB2	1:A:1005:TRP:CZ2	2.29	0.68
2:B:1107:GLU:O	2:B:1111:GLN:HG2	1.94	0.68
2:B:1015:VAL:HG22	2:B:1070:LEU:HD11	1.76	0.68
1:A:449:VAL:HA	1:A:490:LEU:HD21	1.75	0.68
2:B:155:VAL:N	2:B:156:PRO:HD2	2.08	0.68
1:A:1053:LEU:HD11	1:A:1077:ALA:HA	1.76	0.67
2:B:1285:SER:CB	2:B:1288:VAL:HB	2.24	0.67
2:B:352:ILE:HD11	2:B:385:ILE:HG22	1.74	0.67
2:B:1116:LEU:HB2	2:B:1136:LEU:HD21	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1195:LEU:HB2	2:B:1266:TRP:CZ3	2.27	0.67
2:B:1330:GLN:O	2:B:1334:ARG:HG3	1.94	0.67
2:B:210:ILE:HG22	2:B:246:VAL:HG21	1.77	0.67
1:A:558:THR:HB	1:A:563:VAL:HG23	1.75	0.67
1:A:121:LEU:C	1:A:123:ASN:H	1.96	0.66
2:B:1236:MET:HB3	2:B:1273:PHE:CE2	2.30	0.66
1:A:202:PHE:HE1	1:A:210:ILE:HG23	1.60	0.65
2:B:666:PHE:CG	2:B:666:PHE:O	2.49	0.65
1:A:349:PHE:CZ	1:A:1138:GLN:HG3	2.32	0.65
1:A:85:VAL:O	1:A:89:ILE:HG13	1.96	0.65
2:B:545:THR:HG22	2:B:546:SER:H	1.61	0.65
1:A:1270:SER:OG	1:A:1271:LYS:N	2.28	0.65
2:B:1061:GLN:HG3	2:B:1128:CYS:SG	2.37	0.65
1:A:258:THR:N	1:A:261:ALA:HB3	2.12	0.65
2:B:1090:GLU:HA	2:B:1093:SER:HB3	1.79	0.65
2:B:412:GLU:HG2	2:B:454:LEU:HD11	1.79	0.65
2:B:583:MET:HG3	2:B:608:VAL:HG22	1.77	0.65
2:B:784:PHE:HD1	2:B:823:LEU:HD11	1.62	0.65
2:B:826:TYR:O	2:B:830:ILE:HG22	1.96	0.65
2:B:178:LEU:HB3	2:B:216:ILE:HG23	1.78	0.64
2:B:45:VAL:HG21	2:B:93:GLU:HG2	1.80	0.64
2:B:763:GLU:CB	2:B:764:PRO:HD3	2.25	0.64
1:A:1070:VAL:O	1:A:1071:VAL:HB	1.98	0.64
2:B:411:GLN:NE2	2:B:1077:THR:HG21	2.12	0.64
1:A:174:MET:HE2	1:A:213:LEU:HD11	1.80	0.63
1:A:633:PHE:HB3	1:A:663:LEU:HD11	1.79	0.63
2:B:1020:PRO:O	2:B:1021:MET:HE3	1.98	0.63
2:B:131:LYS:HG3	2:B:136:LEU:HD22	1.80	0.63
2:B:914:VAL:HG22	2:B:922:PHE:CE1	2.33	0.63
2:B:1326:LEU:HD11	2:B:1372:MET:HG2	1.81	0.63
2:B:1342:HIS:HE1	2:B:1344:LYS:HB2	1.64	0.63
1:A:127:LEU:HB3	1:A:180:VAL:HG21	1.79	0.63
2:B:454:LEU:O	2:B:458:TYR:HD1	1.82	0.63
2:B:830:ILE:HD13	2:B:834:VAL:HG22	1.81	0.63
2:B:735:ARG:HD2	2:B:796:ALA:CA	2.28	0.63
1:A:109:ALA:HB2	1:A:133:ILE:HG21	1.81	0.62
2:B:1342:HIS:CE1	2:B:1344:LYS:HB2	2.33	0.62
2:B:802:SER:OG	2:B:804:GLU:HG2	1.98	0.62
2:B:203:VAL:HA	2:B:206:GLN:HG2	1.79	0.62
2:B:925:GLU:CD	2:B:925:GLU:H	2.03	0.62
2:B:1285:SER:HB2	2:B:1288:VAL:HB	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:LEU:H	1:A:1280:LEU:HD23	1.64	0.62
1:A:873:LEU:HD22	1:A:914:THR:HG23	1.81	0.62
2:B:528:ARG:HD2	2:B:632:GLU:OE1	1.99	0.62
1:A:21:LEU:O	1:A:64:ARG:NH2	2.33	0.62
2:B:528:ARG:HH22	2:B:1000:SER:HB2	1.65	0.62
2:B:55:LEU:CD2	2:B:133:LEU:HD13	2.29	0.62
1:A:946:THR:HG22	1:A:947:VAL:H	1.66	0.61
2:B:1022:CYS:HA	2:B:1025:LEU:HB2	1.82	0.61
2:B:1326:LEU:CD1	2:B:1372:MET:HG2	2.30	0.61
2:B:638:GLN:HB3	2:B:736:LEU:HD13	1.82	0.61
1:A:33:LEU:HA	1:A:75:LEU:HD11	1.83	0.61
2:B:1085:LEU:HD11	2:B:1142:LYS:HE3	1.82	0.61
2:B:963:LEU:HD23	2:B:1059:CYS:SG	2.41	0.61
1:A:66:TYR:CE1	1:A:107:ASP:HB3	2.35	0.61
2:B:502:ALA:O	2:B:506:ARG:HG2	2.00	0.61
2:B:830:ILE:O	2:B:830:ILE:HG23	2.01	0.61
2:B:836:PRO:HD3	2:B:914:VAL:CG2	2.29	0.61
1:A:1014:SER:HB2	1:A:1072:ASN:HD21	1.66	0.60
1:A:1198:LEU:HA	1:A:1201:LEU:HB2	1.81	0.60
1:A:835:GLY:HA2	1:A:838:MET:HB2	1.82	0.60
1:A:199:LEU:HD23	1:A:202:PHE:HE2	1.66	0.60
2:B:1059:CYS:O	2:B:1063:LEU:HG	2.01	0.60
2:B:344:VAL:O	2:B:348:ILE:HG13	2.02	0.60
2:B:735:ARG:HD2	2:B:796:ALA:CB	2.32	0.60
1:A:395:PRO:HB3	1:A:398:ILE:HD12	1.83	0.60
1:A:816:LEU:HD13	1:A:838:MET:CE	2.32	0.60
2:B:779:MET:HB3	2:B:826:TYR:CZ	2.37	0.60
1:A:1265:GLN:O	1:A:1269:LYS:HB2	2.01	0.59
1:A:594:LEU:CD2	1:A:604:LEU:HD23	2.32	0.59
1:A:908:LEU:HD13	1:A:980:LEU:HD21	1.83	0.59
2:B:640:ARG:H	2:B:640:ARG:HD2	1.68	0.59
2:B:1017:LEU:O	2:B:1021:MET:HG3	2.01	0.59
2:B:611:LEU:O	2:B:615:VAL:HG23	2.02	0.59
1:A:226:ARG:HB2	1:A:288:GLU:HG2	1.84	0.59
2:B:430:CYS:HB3	2:B:431:PRO:HD3	1.83	0.59
2:B:772:SER:HA	2:B:776:ARG:HD2	1.84	0.59
1:A:510:MET:HA	1:A:513:ARG:NH1	2.18	0.59
1:A:754:GLU:OE1	1:A:808:PHE:HB2	2.02	0.59
1:A:838:MET:HA	1:A:838:MET:CE	2.33	0.59
1:A:726:ALA:HB1	1:A:738:ASN:ND2	2.17	0.59
2:B:271:VAL:HG11	2:B:279:ILE:HD12	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:SER:HB2	2:B:493:VAL:HG21	1.84	0.59
2:B:831:PRO:O	2:B:833:TYR:N	2.36	0.59
1:A:498:LEU:O	1:A:502:VAL:HB	2.01	0.59
2:B:654:ILE:HD13	2:B:733:LEU:HG	1.85	0.59
1:A:660:GLN:O	1:A:661:GLU:HB2	2.01	0.59
2:B:694:VAL:HG22	2:B:756:PRO:HG2	1.85	0.59
1:A:1085:LEU:HD13	1:A:1162:THR:HG22	1.85	0.58
1:A:66:TYR:HE1	1:A:107:ASP:HB3	1.68	0.58
2:B:151:LEU:O	2:B:155:VAL:HG23	2.03	0.58
1:A:86:ALA:O	1:A:90:ILE:HG13	2.03	0.58
2:B:914:VAL:HG12	2:B:915:SER:N	2.18	0.58
1:A:434:GLU:HG2	1:A:437:ARG:HH21	1.68	0.58
1:A:853:ILE:HG12	1:A:917:VAL:CG2	2.34	0.58
1:A:594:LEU:HD21	1:A:604:LEU:HD23	1.85	0.58
2:B:398:GLU:O	2:B:402:ARG:HG3	2.04	0.58
1:A:123:ASN:HB3	1:A:125:LYS:HB2	1.86	0.58
1:A:211:PRO:HG3	1:A:267:VAL:HG13	1.85	0.58
1:A:1011:LYS:O	1:A:1069:ALA:HB2	2.04	0.58
1:A:375:TRP:CE3	1:A:378:VAL:HG21	2.39	0.57
2:B:111:CYS:HB3	2:B:134:ILE:HG13	1.86	0.57
1:A:563:VAL:O	1:A:563:VAL:HG23	2.04	0.57
1:A:814:THR:O	1:A:818:ARG:HB2	2.04	0.57
1:A:397:LYS:HE3	1:A:412:LYS:HE2	1.86	0.57
1:A:484:PHE:O	1:A:519:VAL:HG11	2.04	0.57
2:B:1025:LEU:O	2:B:1029:HIS:CD2	2.56	0.57
2:B:654:ILE:HD12	2:B:737:CYS:SG	2.44	0.57
1:A:1136:VAL:CG1	1:A:1198:LEU:HD12	2.34	0.57
2:B:1289:LEU:HD22	2:B:1342:HIS:CE1	2.39	0.57
1:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.86	0.57
1:A:372:VAL:HG22	1:A:432:ILE:CG2	2.35	0.57
1:A:65:ARG:HA	1:A:68:ILE:HD12	1.85	0.57
2:B:1278:ASN:HA	2:B:1281:LYS:HD2	1.87	0.57
1:A:529:LEU:HD22	1:A:533:LYS:HE3	1.87	0.56
1:A:723:ASP:OD2	1:A:724:LYS:HG3	2.04	0.56
1:A:881:LEU:HA	1:A:911:LEU:HD11	1.87	0.56
2:B:1271:ARG:HB3	2:B:1332:ASN:OD1	2.05	0.56
1:A:298:GLN:HB3	1:A:340:ASP:OD2	2.05	0.56
1:A:651:LEU:HD21	1:A:658:PHE:HB2	1.87	0.56
1:A:858:VAL:HG12	1:A:859:SER:N	2.21	0.56
1:A:937:GLY:O	1:A:941:GLU:HG3	2.04	0.56
2:B:1245:LYS:NZ	2:B:1298:ARG:HD2	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:SER:HB2	1:A:61:GLY:O	2.04	0.56
1:A:908:LEU:HD13	1:A:980:LEU:CD2	2.36	0.56
2:B:1162:CYS:HA	2:B:1222:PRO:HD2	1.87	0.56
1:A:635:GLU:HG3	1:A:645:LYS:HE2	1.88	0.56
2:B:790:PHE:O	2:B:794:VAL:HG23	2.05	0.56
1:A:237:PHE:CD2	1:A:268:GLU:HG2	2.41	0.56
1:A:609:TYR:CZ	1:A:613:ARG:HD2	2.40	0.56
1:A:630:LEU:HD13	1:A:704:MET:HE2	1.87	0.56
1:A:199:LEU:HD23	1:A:202:PHE:CE2	2.41	0.56
1:A:300:ASP:O	1:A:303:LYS:N	2.39	0.56
1:A:427:LEU:HD22	1:A:431:LYS:HD2	1.88	0.56
2:B:483:THR:O	2:B:487:VAL:HG23	2.06	0.56
2:B:523:SER:O	2:B:527:ILE:HG13	2.06	0.56
1:A:1071:VAL:HG13	1:A:1076:ALA:CB	2.32	0.56
2:B:1225:THR:HG22	2:B:1226:ARG:H	1.71	0.56
2:B:664:VAL:HG12	2:B:665:ASP:N	2.19	0.56
1:A:1214:ILE:HD11	1:A:1252:LEU:HD13	1.87	0.55
1:A:671:GLN:HG3	1:A:755:TYR:HB2	1.87	0.55
2:B:829:VAL:O	2:B:831:PRO:HD3	2.06	0.55
1:A:120:ARG:HG2	1:A:172:ARG:NH1	2.21	0.55
2:B:454:LEU:HD22	2:B:458:TYR:HE1	1.72	0.55
1:A:729:SER:O	1:A:735:GLY:HA3	2.07	0.55
2:B:1018:LEU:HG	2:B:1022:CYS:SG	2.47	0.55
2:B:781:SER:O	2:B:785:LEU:HD12	2.06	0.55
1:A:1156:SER:HB3	1:A:1220:LYS:HE2	1.87	0.55
1:A:651:LEU:HD11	1:A:658:PHE:CD1	2.42	0.55
1:A:766:LYS:HB2	1:A:766:LYS:NZ	2.22	0.55
2:B:814:LYS:HG2	2:B:962:GLU:OE2	2.07	0.55
1:A:881:LEU:HG	1:A:911:LEU:HD21	1.89	0.55
2:B:1075:GLY:O	2:B:1081:LYS:HG3	2.07	0.54
1:A:732:THR:HG22	1:A:734:VAL:H	1.71	0.54
2:B:812:ARG:O	2:B:816:LEU:HB2	2.07	0.54
1:A:479:LYS:HA	1:A:479:LYS:HE3	1.90	0.54
1:A:64:ARG:O	1:A:68:ILE:HG13	2.07	0.54
1:A:1059:ASP:O	1:A:1060:VAL:HG23	2.08	0.54
1:A:941:GLU:O	1:A:945:VAL:HG23	2.08	0.54
1:A:651:LEU:HD11	1:A:658:PHE:HD1	1.71	0.54
2:B:370:GLU:HB2	2:B:404:LYS:NZ	2.21	0.54
1:A:187:THR:HG22	1:A:188:PRO:HD2	1.89	0.54
1:A:299:GLY:O	1:A:302:SER:OG	2.26	0.54
1:A:580:GLU:HB2	2:B:129:TYR:CG	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1247:LEU:HD11	2:B:1263:LEU:HG	1.90	0.54
1:A:572:SER:HA	1:A:575:SER:HB2	1.90	0.54
2:B:102:THR:CG2	2:B:108:LEU:HD13	2.38	0.54
2:B:1087:SER:O	2:B:1091:VAL:HG23	2.07	0.54
2:B:1139:LEU:O	2:B:1142:LYS:HB2	2.08	0.54
2:B:698:LEU:HB3	2:B:699:PRO:HD3	1.89	0.54
1:A:573:ARG:HH11	1:A:573:ARG:HB2	1.72	0.54
1:A:923:GLN:HB3	1:A:924:PRO:HD3	1.90	0.54
2:B:247:PHE:CD2	2:B:260:ILE:HD13	2.43	0.54
1:A:1056:ILE:HG23	1:A:1216:TYR:CD1	2.42	0.53
1:A:300:ASP:O	1:A:304:CYS:N	2.41	0.53
1:A:475:GLN:HG3	1:A:476:ASN:N	2.24	0.53
1:A:783:ILE:O	1:A:787:LYS:HG2	2.08	0.53
2:B:1354:HIS:C	2:B:1356:PRO:HD2	2.29	0.53
2:B:84:HIS:CD2	2:B:85:PRO:HD2	2.42	0.53
1:A:838:MET:O	1:A:842:VAL:HG23	2.08	0.53
2:B:1297:ARG:NH2	2:B:1354:HIS:HA	2.23	0.53
2:B:172:ARG:HG3	2:B:205:LEU:HD11	1.90	0.53
1:A:966:LEU:HD22	1:A:1015:GLN:OE1	2.07	0.53
1:A:75:LEU:HD22	1:A:81:LEU:HD21	1.91	0.53
1:A:533:LYS:HA	1:A:603:MET:HE1	1.89	0.53
1:A:21:LEU:HD13	1:A:64:ARG:HD3	1.89	0.53
2:B:469:GLN:HA	2:B:508:ASN:HD21	1.70	0.53
1:A:244:HIS:CD2	1:A:260:PRO:HB2	2.44	0.53
2:B:1353:LYS:HG3	2:B:1354:HIS:CE1	2.43	0.53
1:A:1249:ILE:O	1:A:1253:VAL:HG23	2.08	0.53
1:A:156:TYR:O	1:A:160:LEU:HB2	2.09	0.53
1:A:328:ASP:O	1:A:332:THR:HG22	2.09	0.53
1:A:77:GLU:OE1	1:A:126:SER:OG	2.22	0.53
2:B:1011:VAL:O	2:B:1014:VAL:HG12	2.09	0.53
2:B:375:HIS:CE1	2:B:409:CYS:SG	3.02	0.53
1:A:298:GLN:C	1:A:301:PRO:HD2	2.30	0.53
2:B:1315:PHE:CZ	2:B:1375:LEU:HD13	2.44	0.53
2:B:735:ARG:HD2	2:B:796:ALA:HB2	1.91	0.53
1:A:69:TYR:O	1:A:73:ILE:HG13	2.09	0.52
2:B:1007:VAL:O	2:B:1011:VAL:HG23	2.09	0.52
1:A:1070:VAL:HG12	1:A:1071:VAL:H	1.74	0.52
1:A:1207:THR:N	1:A:1208:PRO:HD2	2.24	0.52
1:A:456:ILE:HG22	1:A:456:ILE:O	2.08	0.52
1:A:563:VAL:HG12	2:B:167:GLY:O	2.09	0.52
2:B:1266:TRP:CE3	2:B:1266:TRP:HA	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:ASN:OD1	1:A:1083:LEU:HD21	2.09	0.52
2:B:1308:MET:N	2:B:1309:PRO:HD2	2.24	0.52
1:A:865:ASN:OD1	1:A:868:LYS:HB2	2.09	0.52
1:A:46:LEU:O	1:A:50:VAL:HG23	2.09	0.52
1:A:845:THR:O	1:A:849:ILE:HG13	2.09	0.52
2:B:1114:SER:O	2:B:1117:GLN:HG2	2.10	0.52
2:B:293:LEU:O	2:B:293:LEU:HD23	2.10	0.52
2:B:787:PHE:CE1	2:B:820:GLN:HB2	2.44	0.52
1:A:1061:GLU:C	1:A:1062:ILE:HG13	2.29	0.52
1:A:158:ARG:O	1:A:158:ARG:HD3	2.09	0.52
1:A:47:LEU:HD22	1:A:51:LEU:HD11	1.91	0.52
2:B:735:ARG:CD	2:B:796:ALA:HB2	2.40	0.52
1:A:545:ASN:HD22	1:A:549:LEU:HB2	1.75	0.52
2:B:1086:HIS:O	2:B:1090:GLU:HG3	2.10	0.52
2:B:252:LEU:HD23	2:B:252:LEU:H	1.74	0.52
2:B:926:LEU:O	2:B:973:LYS:NZ	2.30	0.52
2:B:106:GLU:HG2	2:B:109:ARG:NH1	2.25	0.52
1:A:245:ARG:HD2	1:A:366:GLU:OE1	2.09	0.52
1:A:227:ARG:HG3	1:A:288:GLU:HG3	1.92	0.52
1:A:641:LEU:O	1:A:643:PRO:HD3	2.09	0.52
2:B:430:CYS:HG	2:B:467:CYS:HG	1.58	0.52
1:A:1198:LEU:HD22	1:A:1201:LEU:HD12	1.91	0.51
1:A:158:ARG:HD3	1:A:158:ARG:C	2.30	0.51
1:A:227:ARG:HG3	1:A:288:GLU:CG	2.40	0.51
2:B:1342:HIS:CD2	2:B:1343:SER:H	2.28	0.51
2:B:647:LEU:HD23	2:B:741:GLN:HG2	1.92	0.51
2:B:1345:ILE:HA	2:B:1351:LEU:HD12	1.92	0.51
2:B:1264:LEU:HG	2:B:1325:LEU:HG	1.92	0.51
1:A:553:PRO:HB2	1:A:558:THR:HG23	1.93	0.51
2:B:206:GLN:O	2:B:210:ILE:HG13	2.10	0.51
2:B:931:PHE:HE1	2:B:973:LYS:HD2	1.75	0.51
1:A:227:ARG:O	1:A:231:ASP:HB2	2.11	0.51
1:A:1072:ASN:H	1:A:1075:THR:HB	1.74	0.51
2:B:1291:VAL:O	2:B:1295:TYR:HD1	1.94	0.51
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.25	0.51
1:A:372:VAL:HG22	1:A:432:ILE:HG21	1.92	0.51
1:A:662:PRO:O	1:A:665:HIS:N	2.40	0.51
1:A:848:LYS:HD3	1:A:858:VAL:HG13	1.92	0.51
2:B:1204:VAL:C	2:B:1207:PRO:HD2	2.31	0.51
2:B:1297:ARG:HH22	2:B:1354:HIS:CD2	2.28	0.51
2:B:149:LYS:HE3	2:B:153:GLU:OE2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:HD2	1:A:351:GLN:OE1	2.10	0.51
1:A:977:GLU:O	1:A:981:LEU:HB2	2.11	0.51
2:B:674:PHE:O	2:B:676:PHE:N	2.39	0.51
1:A:102:GLY:N	1:A:103:PRO:HD2	2.25	0.50
1:A:462:LEU:O	1:A:466:ILE:HG13	2.11	0.50
1:A:540:LEU:HD13	1:A:607:GLY:HA3	1.93	0.50
1:A:938:THR:HG22	1:A:939:GLU:N	2.26	0.50
2:B:55:LEU:HD21	2:B:133:LEU:HD13	1.92	0.50
1:A:755:TYR:CZ	1:A:759:ILE:HD11	2.47	0.50
2:B:1220:THR:O	2:B:1221:PHE:HB3	2.12	0.50
1:A:1150:VAL:HG22	1:A:1167:LEU:HD11	1.93	0.50
1:A:523:ALA:HB3	1:A:535:ALA:HB2	1.92	0.50
1:A:1:MET:O	1:A:5:ILE:HG13	2.11	0.50
1:A:722:LEU:O	1:A:725:SER:OG	2.29	0.50
1:A:129:LEU:O	1:A:133:ILE:HG13	2.12	0.50
1:A:634:TYR:CG	1:A:704:MET:HE3	2.47	0.50
1:A:671:GLN:CG	1:A:755:TYR:HB2	2.40	0.50
1:A:617:GLN:HG2	2:B:128:PHE:N	2.27	0.50
2:B:531:PHE:CE2	2:B:557:ILE:HD13	2.46	0.50
2:B:916:LEU:O	2:B:919:TYR:CD2	2.51	0.50
2:B:1149:LYS:O	2:B:1153:LEU:HG	2.12	0.50
2:B:791:ARG:HH12	2:B:965:PHE:HZ	1.58	0.50
1:A:1131:ILE:O	1:A:1135:ILE:HG13	2.10	0.50
1:A:1139:LEU:O	1:A:1143:VAL:HG23	2.11	0.50
1:A:927:GLN:HG2	1:A:947:VAL:HG22	1.93	0.50
1:A:1105:SER:O	1:A:1106:ALA:C	2.50	0.50
1:A:848:LYS:HZ1	1:A:859:SER:HB2	1.77	0.50
2:B:800:GLN:CB	2:B:805:MET:HG2	2.40	0.50
2:B:84:HIS:CG	2:B:85:PRO:HD2	2.46	0.50
2:B:55:LEU:HD23	2:B:133:LEU:HD13	1.93	0.49
2:B:753:LEU:HD21	2:B:808:LYS:HB3	1.93	0.49
2:B:786:THR:HG22	2:B:819:LEU:HD11	1.93	0.49
2:B:974:LEU:HD11	2:B:1014:VAL:HG21	1.94	0.49
1:A:492:LEU:HD22	1:A:533:LYS:HG2	1.94	0.49
2:B:1100:GLU:HB2	2:B:1103:GLN:HG2	1.94	0.49
2:B:1286:TYR:N	2:B:1287:PRO:HD2	2.27	0.49
2:B:287:VAL:HG13	2:B:292:SER:HB3	1.93	0.49
2:B:370:GLU:HB2	2:B:404:LYS:HZ1	1.77	0.49
2:B:503:SER:O	2:B:506:ARG:HG3	2.13	0.49
2:B:1123:VAL:CG1	2:B:1128:CYS:HB2	2.33	0.49
2:B:287:VAL:O	2:B:287:VAL:CG1	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HA	1:A:46:LEU:HB2	1.94	0.49
1:A:709:THR:HA	1:A:752:LEU:HD13	1.94	0.49
1:A:919:LEU:O	1:A:923:GLN:HB2	2.11	0.49
2:B:87:TYR:O	2:B:90:VAL:HG12	2.11	0.49
1:A:927:GLN:HG2	1:A:947:VAL:CG2	2.42	0.49
1:A:547:LYS:HE3	1:A:615:ASN:HA	1.95	0.49
1:A:1009:ILE:HG22	1:A:1024:LEU:HD11	1.94	0.49
1:A:946:THR:HG22	1:A:947:VAL:N	2.27	0.49
2:B:738:VAL:HG13	2:B:742:HIS:ND1	2.28	0.49
1:A:1156:SER:HB3	1:A:1220:LYS:CE	2.43	0.49
1:A:848:LYS:NZ	1:A:859:SER:HB2	2.28	0.49
2:B:1062:LYS:O	2:B:1066:VAL:HG23	2.12	0.49
2:B:535:SER:OG	2:B:582:ILE:HD12	2.12	0.49
1:A:284:GLU:HG3	1:A:287:ARG:HH12	1.77	0.49
1:A:558:THR:HB	1:A:563:VAL:CG2	2.42	0.49
2:B:963:LEU:HD11	2:B:1025:LEU:HD13	1.94	0.49
1:A:195:VAL:HG13	1:A:217:LEU:HD21	1.95	0.48
1:A:70:SER:O	1:A:74:GLN:HG3	2.13	0.48
1:A:937:GLY:O	1:A:941:GLU:CG	2.61	0.48
2:B:1149:LYS:N	2:B:1149:LYS:HD2	2.28	0.48
2:B:402:ARG:NH2	2:B:443:SER:HB3	2.28	0.48
2:B:969:ASP:OD1	2:B:973:LYS:HE3	2.12	0.48
1:A:158:ARG:NH1	1:A:162:ASP:HB2	2.27	0.48
1:A:24:LEU:C	1:A:26:ASP:H	2.16	0.48
2:B:1022:CYS:O	2:B:1026:GLU:N	2.30	0.48
2:B:1343:SER:O	2:B:1346:ARG:HB2	2.12	0.48
2:B:821:GLY:O	2:B:825:LYS:HG3	2.13	0.48
2:B:611:LEU:HD23	2:B:611:LEU:O	2.13	0.48
1:A:472:LEU:O	1:A:475:GLN:HG2	2.14	0.48
2:B:929:GLU:O	2:B:932:SER:OG	2.24	0.48
1:A:1156:SER:HB3	1:A:1220:LYS:NZ	2.29	0.48
2:B:1033:GLN:HB2	2:B:1122:SER:HB2	1.94	0.48
2:B:222:HIS:ND1	2:B:250:LEU:HD22	2.29	0.48
1:A:1103:LYS:CG	1:A:1180:TYR:HD1	2.21	0.48
1:A:644:LEU:HD21	1:A:708:ILE:HD13	1.96	0.48
1:A:853:ILE:HG12	1:A:917:VAL:HG22	1.95	0.48
2:B:1343:SER:HA	2:B:1346:ARG:HD3	1.96	0.48
2:B:150:MET:O	2:B:153:GLU:HB2	2.13	0.48
2:B:198:ILE:HD13	2:B:210:ILE:HG12	1.94	0.48
2:B:421:THR:HB	2:B:422:HIS:CD2	2.49	0.48
1:A:199:LEU:HA	1:A:202:PHE:CD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:VAL:HG12	2:B:167:GLY:C	2.34	0.48
1:A:666:LEU:O	1:A:670:ILE:HG13	2.14	0.48
1:A:747:GLY:O	1:A:751:VAL:HG23	2.14	0.48
1:A:755:TYR:CE2	1:A:759:ILE:HD11	2.49	0.48
1:A:962:LEU:HB2	1:A:981:LEU:HD13	1.95	0.48
2:B:1233:PHE:CD2	2:B:1277:LEU:HD11	2.48	0.48
2:B:1342:HIS:CD2	2:B:1343:SER:N	2.82	0.48
2:B:241:VAL:HB	2:B:242:PRO:HD3	1.95	0.48
2:B:257:LEU:HA	2:B:260:ILE:HD12	1.95	0.48
2:B:784:PHE:CD1	2:B:823:LEU:HD11	2.46	0.48
1:A:1071:VAL:H	1:A:1075:THR:HG21	1.77	0.48
2:B:1158:LYS:HG3	2:B:1187:TYR:CE1	2.49	0.48
2:B:732:ARG:HD2	2:B:792:GLU:OE2	2.14	0.48
2:B:133:LEU:HD12	2:B:137:LEU:HD13	1.95	0.48
2:B:388:SER:OG	2:B:429:ILE:HG23	2.14	0.48
1:A:165:CYS:HB3	1:A:197:LYS:HG3	1.95	0.48
1:A:502:VAL:HG13	1:A:502:VAL:O	2.13	0.48
1:A:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
2:B:1277:LEU:HB3	2:B:1288:VAL:HG13	1.95	0.48
1:A:851:GLN:O	1:A:851:GLN:HG2	2.14	0.47
1:A:580:GLU:HB2	2:B:129:TYR:CD2	2.49	0.47
2:B:287:VAL:HG13	2:B:292:SER:CB	2.44	0.47
2:B:362:TRP:CE2	2:B:382:MET:HG2	2.47	0.47
1:A:816:LEU:HB3	1:A:838:MET:HE1	1.95	0.47
2:B:814:LYS:HG2	2:B:962:GLU:CD	2.34	0.47
1:A:1075:THR:HG22	1:A:1080:VAL:HG23	1.95	0.47
1:A:124:GLY:O	1:A:127:LEU:N	2.45	0.47
1:A:716:GLU:O	1:A:718:GLU:N	2.44	0.47
2:B:138:LEU:HA	2:B:138:LEU:HD12	1.75	0.47
2:B:680:ALA:HB2	2:B:758:PHE:CE2	2.49	0.47
1:A:131:PRO:HB3	1:A:183:ASP:HB2	1.96	0.47
1:A:641:LEU:HG	1:A:715:SER:CB	2.44	0.47
2:B:1120:HIS:CG	2:B:1121:HIS:N	2.81	0.47
1:A:629:GLN:NE2	1:A:661:GLU:OE2	2.47	0.47
1:A:834:SER:OG	1:A:835:GLY:N	2.47	0.47
2:B:305:VAL:O	2:B:306:GLN:HG3	2.13	0.47
1:A:284:GLU:HG3	1:A:287:ARG:NH1	2.29	0.47
2:B:1149:LYS:H	2:B:1149:LYS:HD2	1.79	0.47
2:B:1263:LEU:HD13	2:B:1307:CYS:SG	2.54	0.47
2:B:1355:VAL:N	2:B:1356:PRO:HD2	2.30	0.47
2:B:545:THR:HG22	2:B:546:SER:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HG23	1:A:14:THR:N	2.29	0.47
1:A:316:LEU:HD22	1:A:322:PHE:HB2	1.96	0.47
2:B:459:ALA:O	2:B:463:PHE:HB2	2.14	0.47
2:B:830:ILE:CG2	2:B:830:ILE:O	2.63	0.47
2:B:472:VAL:O	2:B:476:VAL:HG23	2.14	0.47
1:A:1077:ALA:CB	1:A:1078:PRO:HD3	2.40	0.47
1:A:1076:ALA:HA	1:A:1080:VAL:HB	1.96	0.47
1:A:695:GLU:HA	1:A:698:TYR:HE2	1.78	0.47
2:B:1173:ASN:HB2	2:B:1174:PRO:HD2	1.96	0.47
2:B:1350:ARG:O	2:B:1353:LYS:HG2	2.14	0.47
2:B:170:MET:O	2:B:174:ILE:HG13	2.15	0.47
2:B:433:ILE:HG23	2:B:455:LEU:HD22	1.96	0.47
1:A:218:LEU:HD11	1:A:275:ILE:HG22	1.96	0.47
1:A:377:HIS:HD2	1:A:378:VAL:HG23	1.80	0.47
2:B:189:ASP:O	2:B:193:GLN:HG3	2.15	0.47
1:A:24:LEU:O	1:A:26:ASP:N	2.47	0.47
1:A:215:TYR:HB2	1:A:274:HIS:ND1	2.30	0.47
1:A:337:SER:OG	1:A:359:CYS:HB2	2.15	0.47
1:A:580:GLU:HB2	2:B:129:TYR:CD1	2.50	0.47
1:A:641:LEU:HD23	1:A:719:ASP:OD2	2.14	0.47
1:A:959:GLN:HB2	1:A:1005:TRP:CH2	2.50	0.46
2:B:1105:LEU:O	2:B:1109:VAL:HG23	2.15	0.46
2:B:1184:LEU:HD13	2:B:1232:PHE:HA	1.98	0.46
2:B:1233:PHE:HZ	2:B:1273:PHE:HB3	1.73	0.46
1:A:486:TYR:CE1	2:B:354:TYR:HD1	2.32	0.46
2:B:462:PHE:O	2:B:463:PHE:CD2	2.69	0.46
2:B:686:GLU:OE2	2:B:808:LYS:HE2	2.14	0.46
1:A:121:LEU:C	1:A:123:ASN:N	2.64	0.46
1:A:217:LEU:HD22	1:A:229:VAL:HG13	1.98	0.46
1:A:558:THR:O	1:A:563:VAL:HG22	2.15	0.46
1:A:814:THR:OG1	1:A:879:VAL:HG21	2.15	0.46
1:A:948:THR:HG23	1:A:992:LEU:HA	1.97	0.46
2:B:410:ILE:HG22	2:B:451:PHE:CE1	2.50	0.46
1:A:131:PRO:HA	1:A:184:VAL:HG22	1.96	0.46
1:A:4:LYS:O	1:A:8:LEU:HG	2.14	0.46
2:B:222:HIS:HB2	2:B:251:ARG:HG2	1.97	0.46
2:B:382:MET:O	2:B:386:ILE:HG13	2.16	0.46
1:A:154:GLU:O	1:A:157:LYS:HB3	2.16	0.46
2:B:1206:VAL:N	2:B:1207:PRO:CD	2.75	0.46
2:B:1257:GLN:O	2:B:1261:GLU:HG3	2.16	0.46
1:A:613:ARG:HG2	1:A:676:TRP:CE3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:695:ILE:HB	2:B:757:LEU:CD2	2.45	0.46
1:A:1014:SER:HB2	1:A:1072:ASN:ND2	2.30	0.46
1:A:597:GLN:HG2	1:A:597:GLN:H	1.34	0.46
1:A:835:GLY:CA	1:A:838:MET:HB2	2.46	0.46
2:B:1342:HIS:CG	2:B:1343:SER:N	2.83	0.46
2:B:816:LEU:HD12	2:B:816:LEU:HA	1.81	0.46
1:A:275:ILE:CD1	1:A:312:LEU:HD11	2.42	0.46
1:A:448:VAL:O	1:A:456:ILE:HD13	2.16	0.46
2:B:752:LEU:HA	2:B:755:CYS:SG	2.56	0.46
1:A:41:ARG:N	1:A:41:ARG:HD3	2.31	0.46
2:B:375:HIS:NE2	2:B:409:CYS:SG	2.88	0.46
1:A:1075:THR:HG22	1:A:1080:VAL:CG2	2.45	0.46
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.51	0.46
2:B:1277:LEU:HD13	2:B:1288:VAL:O	2.15	0.46
2:B:401:LEU:O	2:B:405:ILE:HG13	2.15	0.46
1:A:118:GLU:O	1:A:119:ASP:OD1	2.33	0.46
2:B:1229:PHE:CZ	2:B:1280:MET:HG3	2.51	0.46
2:B:1350:ARG:HA	2:B:1353:LYS:HE2	1.97	0.46
2:B:427:LYS:HA	2:B:463:PHE:CE1	2.51	0.46
1:A:112:PHE:O	1:A:116:VAL:HG23	2.16	0.45
1:A:764:LYS:HA	1:A:827:SER:HB2	1.97	0.45
2:B:1326:LEU:HA	2:B:1329:LEU:HD12	1.97	0.45
1:A:754:GLU:OE1	1:A:808:PHE:CB	2.64	0.45
1:A:908:LEU:HD11	1:A:981:LEU:HG	1.99	0.45
2:B:581:GLY:CA	2:B:636:LEU:HD13	2.45	0.45
2:B:1324:SER:HB3	2:B:1385:GLY:HA2	1.97	0.45
1:A:114:GLY:HA2	1:A:117:ARG:NH1	2.31	0.45
1:A:271:VAL:O	1:A:275:ILE:HG23	2.17	0.45
1:A:322:PHE:O	1:A:326:VAL:HG23	2.17	0.45
1:A:545:ASN:O	1:A:549:LEU:HB3	2.16	0.45
1:A:78:SER:OG	1:A:79:GLY:N	2.48	0.45
2:B:1265:TYR:HA	2:B:1268:MET:HB2	1.99	0.45
2:B:695:ILE:HB	2:B:757:LEU:HD23	1.99	0.45
1:A:1046:SER:HB3	1:A:1145:PHE:CD1	2.52	0.45
1:A:620:SER:O	1:A:624:GLN:HB2	2.16	0.45
2:B:1240:LEU:O	2:B:1244:VAL:HG23	2.17	0.45
2:B:1236:MET:HB3	2:B:1273:PHE:CZ	2.51	0.45
2:B:1300:VAL:HG13	2:B:1365:LEU:HD12	1.99	0.45
1:A:819:ASP:HB3	1:A:820:SER:H	1.52	0.45
2:B:1277:LEU:CD1	2:B:1288:VAL:HG13	2.43	0.45
2:B:265:MET:HE3	2:B:283:LEU:HD22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:SER:O	2:B:449:ILE:HD11	2.17	0.45
2:B:541:GLN:O	2:B:542:GLN:HG3	2.17	0.45
2:B:976:ASN:OD1	2:B:1003:HIS:CE1	2.69	0.45
1:A:1146:PHE:O	1:A:1150:VAL:HG23	2.17	0.45
2:B:1281:LYS:HA	2:B:1284:ASP:O	2.17	0.45
2:B:1342:HIS:CE1	2:B:1344:LYS:H	2.35	0.45
2:B:1361:SER:HA	2:B:1364:LEU:HD12	1.99	0.45
1:A:1200:LYS:HB2	1:A:1277:HIS:HB3	1.98	0.45
2:B:605:ARG:HG2	2:B:646:THR:HG23	1.99	0.45
1:A:1078:PRO:O	1:A:1082:LEU:HG	2.17	0.45
2:B:1278:ASN:O	2:B:1281:LYS:HD3	2.17	0.45
1:A:1050:HIS:ND1	1:A:1148:GLU:OE1	2.50	0.44
1:A:1261:LYS:O	1:A:1264:ILE:HB	2.17	0.44
2:B:1285:SER:OG	2:B:1288:VAL:HB	2.18	0.44
1:A:1071:VAL:HG12	1:A:1071:VAL:O	2.16	0.44
1:A:221:SER:HB3	1:A:229:VAL:HG21	1.98	0.44
1:A:290:LEU:O	1:A:294:LYS:HG2	2.17	0.44
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.99	0.44
2:B:252:LEU:HD11	2:B:257:LEU:HD13	1.99	0.44
2:B:565:VAL:HB	2:B:568:TYR:HD1	1.83	0.44
2:B:604:GLN:O	2:B:608:VAL:HG23	2.18	0.44
2:B:570:LEU:HD12	2:B:628:LEU:HD22	1.99	0.44
2:B:674:PHE:C	2:B:676:PHE:H	2.20	0.44
1:A:1059:ASP:O	1:A:1060:VAL:CG2	2.65	0.44
1:A:1021:CYS:SG	1:A:1075:THR:HG23	2.58	0.44
1:A:1154:LEU:CD1	1:A:1163:LEU:HD12	2.47	0.44
1:A:1140:GLY:HA3	1:A:1198:LEU:HD13	2.00	0.44
2:B:763:GLU:HA	2:B:822:ILE:HD13	2.00	0.44
2:B:925:GLU:CD	2:B:925:GLU:N	2.68	0.44
1:A:1084:VAL:CG1	1:A:1145:PHE:HE1	2.31	0.44
1:A:428:GLU:HA	1:A:431:LYS:HD3	1.99	0.44
1:A:787:LYS:O	1:A:788:ALA:HB3	2.18	0.44
2:B:626:SER:OG	2:B:726:CYS:SG	2.75	0.44
2:B:820:GLN:HE22	2:B:920:ARG:HH12	1.65	0.44
2:B:341:ILE:HD11	2:B:422:HIS:CE1	2.53	0.44
2:B:967:LEU:HB3	2:B:1062:LYS:HB3	1.99	0.44
1:A:1249:ILE:HG13	1:A:1249:ILE:H	1.47	0.44
1:A:661:GLU:HA	1:A:662:PRO:HD3	1.68	0.44
1:A:670:ILE:O	1:A:674:LEU:HB2	2.18	0.44
2:B:1116:LEU:HA	2:B:1119:PHE:HD1	1.83	0.44
2:B:1266:TRP:HA	2:B:1266:TRP:HE3	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1349:THR:O	2:B:1351:LEU:N	2.51	0.44
1:A:858:VAL:CG1	1:A:859:SER:N	2.81	0.44
2:B:1331:LEU:HD12	2:B:1334:ARG:HD2	2.00	0.44
2:B:1281:LYS:HE3	2:B:1342:HIS:HE2	1.83	0.44
2:B:557:ILE:HA	2:B:557:ILE:HD12	1.85	0.44
1:A:466:ILE:HG22	1:A:474:LEU:HD11	1.99	0.44
1:A:816:LEU:HD13	1:A:838:MET:HE1	1.99	0.44
2:B:1277:LEU:HD22	2:B:1288:VAL:HG13	1.99	0.44
2:B:1323:LEU:O	2:B:1327:GLN:HG3	2.17	0.44
1:A:293:LEU:HD13	1:A:313:LEU:HD11	2.00	0.43
2:B:352:ILE:HG22	2:B:358:ILE:HG22	2.00	0.43
2:B:415:LEU:HD23	2:B:454:LEU:HB3	2.00	0.43
2:B:574:ILE:HA	2:B:632:GLU:HG2	2.00	0.43
1:A:973:PHE:CE2	1:A:1015:GLN:HG2	2.51	0.43
1:A:1164:LEU:HD22	1:A:1252:LEU:HD12	2.00	0.43
1:A:90:ILE:CD1	1:A:125:LYS:HB3	2.48	0.43
1:A:275:ILE:HD11	1:A:312:LEU:HD21	2.00	0.43
1:A:798:LYS:N	1:A:801:ASP:OD1	2.51	0.43
2:B:684:LEU:C	2:B:686:GLU:H	2.20	0.43
1:A:654:GLY:O	1:A:655:SER:OG	2.31	0.43
2:B:1162:CYS:O	2:B:1222:PRO:HD2	2.18	0.43
2:B:258:SER:HA	2:B:261:ARG:NH1	2.30	0.43
2:B:444:GLN:CD	2:B:444:GLN:H	2.20	0.43
2:B:87:TYR:N	2:B:88:PRO:CD	2.81	0.43
1:A:297:GLN:O	1:A:301:PRO:HD3	2.18	0.43
2:B:1049:THR:HA	2:B:1052:GLU:HB2	2.00	0.43
2:B:1359:LYS:O	2:B:1363:GLU:HG3	2.19	0.43
2:B:257:LEU:HD12	2:B:260:ILE:HD12	1.99	0.43
2:B:931:PHE:CE1	2:B:973:LYS:HD2	2.53	0.43
1:A:1139:LEU:HA	1:A:1142:LEU:CD2	2.49	0.43
1:A:15:ASP:O	1:A:19:GLU:HB2	2.18	0.43
1:A:396:LYS:HE2	1:A:396:LYS:HB3	1.76	0.43
1:A:451:ARG:HB3	1:A:456:ILE:HD11	2.00	0.43
2:B:1101:GLN:H	2:B:1101:GLN:HG2	1.55	0.43
2:B:366:ILE:HD13	2:B:383:LEU:HG	2.00	0.43
1:A:1070:VAL:O	1:A:1071:VAL:CB	2.62	0.43
1:A:12:LYS:HB2	1:A:16:LYS:NZ	2.34	0.43
1:A:300:ASP:N	1:A:301:PRO:HD2	2.33	0.43
2:B:155:VAL:N	2:B:156:PRO:CD	2.79	0.43
1:A:151:LEU:HB2	1:A:156:TYR:CE1	2.54	0.43
1:A:225:SER:O	1:A:229:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:VAL:O	2:B:479:VAL:HB	2.19	0.43
2:B:753:LEU:HD21	2:B:808:LYS:CB	2.49	0.43
1:A:1042:LEU:HD21	1:A:1087:GLN:HB3	2.01	0.43
1:A:285:LEU:O	1:A:285:LEU:HD23	2.18	0.43
1:A:941:GLU:O	1:A:945:VAL:N	2.51	0.43
2:B:252:LEU:N	2:B:252:LEU:HD23	2.34	0.43
2:B:665:ASP:CA	2:B:692:GLY:O	2.63	0.43
1:A:1048:ASP:CB	1:A:1071:VAL:HG11	2.44	0.43
2:B:573:ILE:O	2:B:577:VAL:HG23	2.19	0.43
2:B:701:PHE:HE2	2:B:778:LEU:HD23	1.84	0.43
2:B:974:LEU:HD12	2:B:1066:VAL:HG13	2.01	0.43
1:A:1016:GLU:HB3	1:A:1074:ARG:HD3	2.00	0.43
1:A:194:VAL:O	1:A:198:VAL:HG23	2.19	0.43
1:A:428:GLU:O	1:A:432:ILE:HG12	2.18	0.43
1:A:514:ASP:OD1	1:A:554:SER:HB2	2.19	0.43
1:A:620:SER:HB3	2:B:128:PHE:HE1	1.83	0.43
1:A:749:CYS:O	1:A:753:MET:HB2	2.19	0.43
1:A:1103:LYS:HG2	1:A:1180:TYR:CD1	2.41	0.42
1:A:230:LEU:HD22	1:A:289:LEU:HD13	2.01	0.42
1:A:636:PRO:O	1:A:638:PRO:HD3	2.19	0.42
1:A:638:PRO:O	1:A:639:ASP:HB2	2.18	0.42
2:B:1277:LEU:HD12	2:B:1292:CYS:SG	2.59	0.42
2:B:787:PHE:O	2:B:791:ARG:HB2	2.19	0.42
2:B:914:VAL:HG22	2:B:922:PHE:HE1	1.81	0.42
2:B:928:ILE:HG13	2:B:928:ILE:H	1.62	0.42
1:A:487:LEU:HD12	1:A:498:LEU:HD23	2.01	0.42
1:A:884:TYR:CE1	1:A:908:LEU:HG	2.54	0.42
2:B:1286:TYR:HB2	2:B:1287:PRO:HD3	2.01	0.42
2:B:1245:LYS:HZ3	2:B:1298:ARG:HD2	1.84	0.42
1:A:316:LEU:HD23	1:A:316:LEU:O	2.19	0.42
1:A:475:GLN:HA	1:A:505:LEU:HD22	2.01	0.42
1:A:72:CYS:O	1:A:76:VAL:HG23	2.18	0.42
2:B:1000:SER:O	2:B:1004:GLN:HG2	2.20	0.42
2:B:1384:LEU:HD23	2:B:1384:LEU:O	2.20	0.42
2:B:296:ILE:HD12	2:B:361:ALA:CB	2.45	0.42
2:B:549:ILE:HG22	2:B:553:MET:CE	2.49	0.42
1:A:187:THR:CG2	1:A:188:PRO:HD2	2.49	0.42
2:B:271:VAL:HG12	2:B:272:ARG:O	2.19	0.42
2:B:1345:ILE:O	2:B:1345:ILE:CG2	2.68	0.42
1:A:1007:SER:O	1:A:1011:LYS:HB2	2.20	0.42
2:B:1375:LEU:O	2:B:1376:ASN:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:513:LYS:HE2	2:B:513:LYS:HB3	1.74	0.42
2:B:749:ILE:O	2:B:749:ILE:HG22	2.18	0.42
1:A:1150:VAL:CG1	1:A:1209:VAL:HG12	2.49	0.42
1:A:1248:PRO:HG2	1:A:1249:ILE:H	1.85	0.42
1:A:176:GLN:HA	1:A:179:SER:OG	2.19	0.42
2:B:1228:THR:O	2:B:1232:PHE:HD1	2.02	0.42
2:B:1019:THR:C	2:B:1021:MET:H	2.22	0.42
2:B:1345:ILE:O	2:B:1345:ILE:HG22	2.20	0.42
2:B:633:PHE:HB3	2:B:733:LEU:HD13	2.01	0.42
2:B:742:HIS:O	2:B:743:ASP:CB	2.65	0.42
1:A:446:ASN:O	1:A:450:THR:HG22	2.20	0.42
2:B:213:LEU:HD22	2:B:217:LEU:HD11	2.01	0.42
2:B:664:VAL:HG12	2:B:665:ASP:H	1.84	0.42
1:A:1001:GLN:HE21	1:A:1001:GLN:HB3	1.60	0.41
2:B:1090:GLU:O	2:B:1093:SER:OG	2.27	0.41
2:B:762:LEU:HD13	2:B:783:THR:HA	2.01	0.41
1:A:372:VAL:HG12	1:A:372:VAL:O	2.20	0.41
1:A:919:LEU:HD11	1:A:991:LEU:HD21	2.01	0.41
2:B:638:GLN:HB3	2:B:736:LEU:CD1	2.48	0.41
1:A:672:HIS:CD2	1:A:861:PRO:HG2	2.56	0.41
1:A:945:VAL:HG11	1:A:950:ARG:NE	2.35	0.41
2:B:1294:LYS:HG3	2:B:1354:HIS:CD2	2.55	0.41
2:B:149:LYS:O	2:B:153:GLU:HG3	2.20	0.41
2:B:541:GLN:C	2:B:542:GLN:HG3	2.41	0.41
2:B:666:PHE:O	2:B:667:CYS:C	2.55	0.41
2:B:1014:VAL:HG22	2:B:1014:VAL:O	2.20	0.41
2:B:1374:VAL:O	2:B:1375:LEU:HG	2.21	0.41
1:A:1098:LEU:HD22	1:A:1131:ILE:CG2	2.50	0.41
1:A:573:ARG:NH1	1:A:573:ARG:HB2	2.35	0.41
2:B:1221:PHE:N	2:B:1222:PRO:HD3	2.35	0.41
2:B:429:ILE:O	2:B:433:ILE:HG13	2.21	0.41
2:B:791:ARG:NH1	2:B:965:PHE:HZ	2.18	0.41
1:A:1052:GLN:HG3	1:A:1071:VAL:HG12	2.01	0.41
2:B:1284:ASP:O	2:B:1285:SER:HB3	2.20	0.41
1:A:1011:LYS:O	1:A:1069:ALA:CB	2.67	0.41
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.21	0.41
1:A:154:GLU:HG3	1:A:155:GLU:N	2.36	0.41
1:A:315:SER:OG	1:A:377:HIS:HB2	2.21	0.41
1:A:787:LYS:HD3	1:A:787:LYS:HA	1.76	0.41
2:B:1204:VAL:O	2:B:1207:PRO:CG	2.68	0.41
2:B:968:GLU:O	2:B:972:GLN:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:LYS:HD3	1:A:1277:HIS:CE1	2.55	0.41
1:A:462:LEU:HD22	1:A:466:ILE:HD11	2.03	0.41
1:A:863:GLY:O	1:A:869:ILE:HD11	2.20	0.41
1:A:90:ILE:HD13	1:A:125:LYS:HB3	2.01	0.41
2:B:112:LEU:HD23	2:B:134:ILE:HD12	2.03	0.41
2:B:287:VAL:O	2:B:289:ASP:O	2.39	0.41
2:B:45:VAL:HG21	2:B:93:GLU:CG	2.50	0.41
2:B:469:GLN:HG3	2:B:508:ASN:HD21	1.86	0.41
2:B:532:CYS:HA	2:B:582:ILE:HD11	2.02	0.41
2:B:88:PRO:HB2	2:B:89:LYS:HD2	2.03	0.41
2:B:914:VAL:CG1	2:B:915:SER:N	2.82	0.41
1:A:348:LYS:HD3	1:A:1034:LEU:O	2.20	0.41
2:B:1198:ILE:HG12	2:B:1236:MET:CE	2.51	0.41
2:B:1277:LEU:HD22	2:B:1288:VAL:CG1	2.51	0.41
2:B:222:HIS:CD2	2:B:251:ARG:HG2	2.56	0.41
2:B:556:VAL:O	2:B:560:GLN:HG2	2.20	0.41
2:B:609:THR:O	2:B:613:GLN:HG2	2.20	0.41
2:B:787:PHE:HA	2:B:819:LEU:HD13	2.02	0.41
1:A:608:PHE:HD2	1:A:608:PHE:HA	1.81	0.41
1:A:818:ARG:O	1:A:819:ASP:HB2	2.21	0.41
1:A:92:LEU:HA	1:A:95:LEU:HB2	2.02	0.41
2:B:1123:VAL:HA	2:B:1124:PRO:HD3	1.76	0.41
2:B:117:ARG:HA	2:B:117:ARG:HD2	1.93	0.41
2:B:1211:SER:OG	2:B:1212:ALA:N	2.53	0.41
2:B:1229:PHE:HE2	2:B:1277:LEU:HD21	1.86	0.41
2:B:150:MET:HA	2:B:153:GLU:OE1	2.21	0.41
2:B:413:GLN:HG3	2:B:414:LEU:N	2.35	0.41
1:A:651:LEU:CD2	1:A:658:PHE:HB2	2.49	0.41
1:A:741:CYS:O	1:A:745:ILE:HG13	2.20	0.41
1:A:923:GLN:HA	1:A:926:VAL:HG23	2.03	0.41
2:B:1155:SER:HA	2:B:1158:LYS:HB2	2.02	0.41
2:B:1306:GLN:O	2:B:1309:PRO:HG2	2.21	0.41
2:B:296:ILE:HD11	2:B:358:ILE:HG23	2.02	0.41
2:B:401:LEU:HD12	2:B:401:LEU:HA	1.96	0.41
1:A:1070:VAL:HG12	1:A:1071:VAL:N	2.34	0.40
1:A:210:ILE:N	1:A:211:PRO:CD	2.84	0.40
1:A:858:VAL:HG12	1:A:859:SER:H	1.85	0.40
2:B:1245:LYS:HZ1	2:B:1298:ARG:HD2	1.85	0.40
2:B:1323:LEU:HG	2:B:1381:ALA:HB1	2.04	0.40
2:B:144:GLN:HB3	2:B:145:PRO:HD3	2.02	0.40
2:B:237:THR:O	2:B:237:THR:HG22	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:HIS:CD2	2:B:242:PRO:HG3	2.56	0.40
2:B:812:ARG:HD2	2:B:812:ARG:HA	1.69	0.40
1:A:1176:ALA:O	1:A:1180:TYR:N	2.54	0.40
1:A:506:LEU:O	1:A:513:ARG:NH2	2.48	0.40
1:A:779:LYS:O	1:A:783:ILE:HG13	2.21	0.40
2:B:662:PHE:CG	2:B:727:LEU:HD12	2.56	0.40
2:B:763:GLU:CB	2:B:764:PRO:CD	2.87	0.40
1:A:1160:VAL:O	1:A:1164:LEU:HG	2.21	0.40
1:A:169:TRP:N	1:A:169:TRP:CD1	2.90	0.40
1:A:372:VAL:HG22	1:A:432:ILE:HG23	2.02	0.40
1:A:375:TRP:HE3	1:A:378:VAL:HG21	1.83	0.40
1:A:938:THR:HG22	1:A:939:GLU:H	1.86	0.40
2:B:1241:GLU:OE2	2:B:1298:ARG:NH1	2.49	0.40
2:B:1344:LYS:HE3	2:B:1344:LYS:HA	2.03	0.40
2:B:352:ILE:HB	2:B:359:SER:HB3	2.03	0.40
2:B:664:VAL:CG1	2:B:665:ASP:N	2.85	0.40
1:A:986:SER:HB3	1:A:1027:LEU:HD22	2.03	0.40
1:A:357:ARG:HD3	1:A:1101:LYS:NZ	2.37	0.40
2:B:1116:LEU:HB2	2:B:1136:LEU:CD2	2.48	0.40
2:B:1233:PHE:CE1	2:B:1277:LEU:HG	2.56	0.40
2:B:222:HIS:CB	2:B:251:ARG:HG2	2.51	0.40
2:B:478:HIS:O	2:B:482:GLY:HA3	2.21	0.40
2:B:690:GLN:O	2:B:691:ASP:HB2	2.21	0.40
1:A:1191:ILE:HG22	1:A:1196:GLU:HG3	2.03	0.40
1:A:384:GLU:O	1:A:388:ILE:HG13	2.22	0.40
1:A:338:PHE:CD2	1:A:417:HIS:HB3	2.57	0.40
2:B:970:LEU:HD23	2:B:1066:VAL:HG11	2.03	0.40
2:B:1286:TYR:N	2:B:1287:PRO:CD	2.85	0.40
2:B:1326:LEU:O	2:B:1330:GLN:HG3	2.22	0.40
2:B:810:LEU:HD21	2:B:958:LEU:HB2	2.04	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	1190/1308 (91%)	1108 (93%)	75 (6%)	7 (1%)	28	68
2	B	1120/1323 (85%)	1043 (93%)	75 (7%)	2 (0%)	51	84
All	All	2310/2631 (88%)	2151 (93%)	150 (6%)	9 (0%)	38	75

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	568	VAL
2	B	1285	SER
1	A	25	LYS
1	A	717	LEU
2	B	832	ASP
1	A	661	GLU
1	A	662	PRO
1	A	1071	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1093/1188 (92%)	992 (91%)	101 (9%)	11	40
2	B	1030/1193 (86%)	949 (92%)	81 (8%)	14	48
All	All	2123/2381 (89%)	1941 (91%)	182 (9%)	12	44

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	13	THR
1	A	19	GLU
1	A	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	57	SER
1	A	75	LEU
1	A	96	GLU
1	A	99	HIS
1	A	119	ASP
1	A	126	SER
1	A	160	LEU
1	A	171	GLN
1	A	175	ILE
1	A	177	LEU
1	A	202	PHE
1	A	217	LEU
1	A	240	LEU
1	A	245	ARG
1	A	263	GLU
1	A	264	LEU
1	A	275	ILE
1	A	316	LEU
1	A	343	LEU
1	A	377	HIS
1	A	399	LEU
1	A	427	LEU
1	A	438	GLN
1	A	441	LEU
1	A	446	ASN
1	A	449	VAL
1	A	462	LEU
1	A	479	LYS
1	A	496	GLN
1	A	502	VAL
1	A	529	LEU
1	A	546	PHE
1	A	556	GLN
1	A	560	SER
1	A	564	THR
1	A	587	ILE
1	A	589	SER
1	A	597	GLN
1	A	599	ASP
1	A	612	LEU
1	A	621	SER
1	A	624	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	630	LEU
1	A	641	LEU
1	A	651	LEU
1	A	659	LEU
1	A	663	LEU
1	A	666	LEU
1	A	677	TYR
1	A	697	LEU
1	A	730	GLN
1	A	754	GLU
1	A	766	LYS
1	A	768	GLU
1	A	771	LEU
1	A	775	THR
1	A	786	GLU
1	A	838	MET
1	A	839	HIS
1	A	846	LEU
1	A	864	GLN
1	A	881	LEU
1	A	883	ARG
1	A	908	LEU
1	A	919	LEU
1	A	928	GLN
1	A	934	ASP
1	A	940	GLU
1	A	949	GLN
1	A	964	ASN
1	A	965	LEU
1	A	973	PHE
1	A	980	LEU
1	A	981	LEU
1	A	982	ILE
1	A	995	THR
1	A	1001	GLN
1	A	1009	ILE
1	A	1011	LYS
1	A	1015	GLN
1	A	1021	CYS
1	A	1024	LEU
1	A	1027	LEU
1	A	1037	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1062	ILE
1	A	1163	LEU
1	A	1170	ILE
1	A	1201	LEU
1	A	1206	LEU
1	A	1212	SER
1	A	1249	ILE
1	A	1251	ASN
1	A	1252	LEU
1	A	1272	VAL
1	A	1275	MET
1	A	1276	GLN
1	A	1284	ARG
2	B	56	THR
2	B	114	SER
2	B	128	PHE
2	B	136	LEU
2	B	138	LEU
2	B	178	LEU
2	B	183	ARG
2	B	253	ASP
2	B	276	PHE
2	B	298	GLU
2	B	378	LEU
2	B	416	ASP
2	B	436	LEU
2	B	439	THR
2	B	441	PHE
2	B	444	GLN
2	B	447	ARG
2	B	462	PHE
2	B	463	PHE
2	B	495	LEU
2	B	496	GLU
2	B	505	MET
2	B	522	MET
2	B	563	SER
2	B	565	VAL
2	B	605	ARG
2	B	633	PHE
2	B	636	LEU
2	B	640	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	650	VAL
2	B	682	TYR
2	B	686	GLU
2	B	687	TYR
2	B	695	ILE
2	B	704	GLU
2	B	727	LEU
2	B	737	CYS
2	B	747	ASP
2	B	753	LEU
2	B	762	LEU
2	B	776	ARG
2	B	785	LEU
2	B	800	GLN
2	B	802	SER
2	B	830	ILE
2	B	833	TYR
2	B	834	VAL
2	B	925	GLU
2	B	927	ASP
2	B	928	ILE
2	B	1013	CYS
2	B	1019	THR
2	B	1021	MET
2	B	1060	TYR
2	B	1070	LEU
2	B	1086	HIS
2	B	1097	LYS
2	B	1101	GLN
2	B	1120	HIS
2	B	1135	LEU
2	B	1191	THR
2	B	1208	GLU
2	B	1223	THR
2	B	1228	THR
2	B	1236	MET
2	B	1237	MET
2	B	1265	TYR
2	B	1266	TRP
2	B	1281	LYS
2	B	1284	ASP
2	B	1289	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1298	ARG
2	B	1314	SER
2	B	1318	HIS
2	B	1344	LYS
2	B	1349	THR
2	B	1365	LEU
2	B	1379	ARG
2	B	1384	LEU
2	B	1387	LEU
2	B	1391	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	545	ASN
1	A	738	ASN
2	B	193	GLN
2	B	236	ASN
2	B	411	GLN
2	B	422	HIS
2	B	508	ASN
2	B	800	GLN
2	B	1003	HIS
2	B	1016	GLN
2	B	1029	HIS
2	B	1086	HIS
2	B	1330	GLN
2	B	1342	HIS
2	B	1354	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	1206/1308 (92%)	-0.13	52 (4%) 36 33	48, 100, 204, 311	0
2	B	1146/1323 (86%)	-0.01	40 (3%) 44 40	74, 127, 192, 236	0
All	All	2352/2631 (89%)	-0.07	92 (3%) 40 36	48, 116, 198, 311	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	LEU	7.1
2	B	543	PRO	7.0
1	A	14	THR	6.8
1	A	397	LYS	6.1
1	A	258	THR	5.8
1	A	13	THR	5.2
1	A	398	ILE	5.0
1	A	248	GLN	5.0
1	A	1189	ARG	4.9
1	A	1186	GLN	4.7
2	B	1348	ASP	4.5
1	A	297	GLN	4.5
1	A	15	ASP	4.1
2	B	546	SER	4.1
1	A	259	ALA	4.0
1	A	683	PRO	4.0
1	A	23	THR	3.8
2	B	1284	ASP	3.8
1	A	38	VAL	3.8
1	A	141	LYS	3.7
1	A	1300	ASP	3.6
1	A	1190	GLY	3.6
2	B	1347	GLN	3.5
2	B	1379	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	249	SER	3.4
1	A	572	SER	3.4
1	A	1187	SER	3.4
2	B	305	VAL	3.3
1	A	26	ASP	3.3
1	A	682	VAL	3.2
2	B	43	GLY	3.2
2	B	1173	ASN	3.1
2	B	603	GLU	3.0
1	A	400	ASP	3.0
2	B	1100	GLU	3.0
1	A	789	GLY	3.0
1	A	567	ARG	3.0
1	A	1222	SER	2.9
2	B	371	SER	2.9
2	B	602	SER	2.9
1	A	27	ASP	2.8
1	A	1106	ALA	2.8
1	A	695	GLU	2.8
2	B	1172	LYS	2.8
1	A	1276	GLN	2.8
1	A	120	ARG	2.8
2	B	1174	PRO	2.8
2	B	1346	ARG	2.8
2	B	1349	THR	2.7
1	A	569	ASP	2.7
1	A	799	VAL	2.7
1	A	57	SER	2.7
1	A	60	ASP	2.6
2	B	1259	HIS	2.6
1	A	122	VAL	2.6
2	B	336	SER	2.5
2	B	1376	ASN	2.5
1	A	250	SER	2.5
2	B	1253	ALA	2.5
1	A	1188	SER	2.5
2	B	1166	PRO	2.4
2	B	682	TYR	2.4
1	A	39	LYS	2.3
2	B	1148	GLN	2.3
2	B	1266	TRP	2.3
2	B	691	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	544	GLY	2.3
2	B	372	ALA	2.3
1	A	1221	SER	2.3
2	B	1282	VAL	2.3
2	B	1377	ASN	2.2
1	A	800	SER	2.2
1	A	147	GLY	2.2
1	A	300	ASP	2.2
1	A	3	LEU	2.2
2	B	1079	GLN	2.2
2	B	1227	HIS	2.2
1	A	573	ARG	2.2
1	A	1283	SER	2.2
2	B	1213	PRO	2.2
2	B	251	ARG	2.1
2	B	1375	LEU	2.1
1	A	1016	GLU	2.1
2	B	1099	MET	2.1
2	B	288	THR	2.1
1	A	655	SER	2.1
2	B	116	GLU	2.1
1	A	41	ARG	2.1
2	B	1080	SER	2.1
2	B	1164	ALA	2.0
1	A	1185	CYS	2.0
1	A	29	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.