Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:47 PM 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

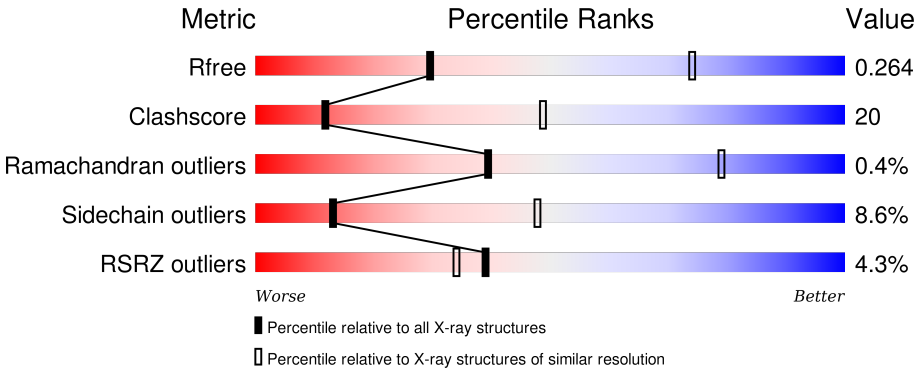
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (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 <=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	4% 54% 35% • 8%
2	B	1323	3% 50% 33% • 13%

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

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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

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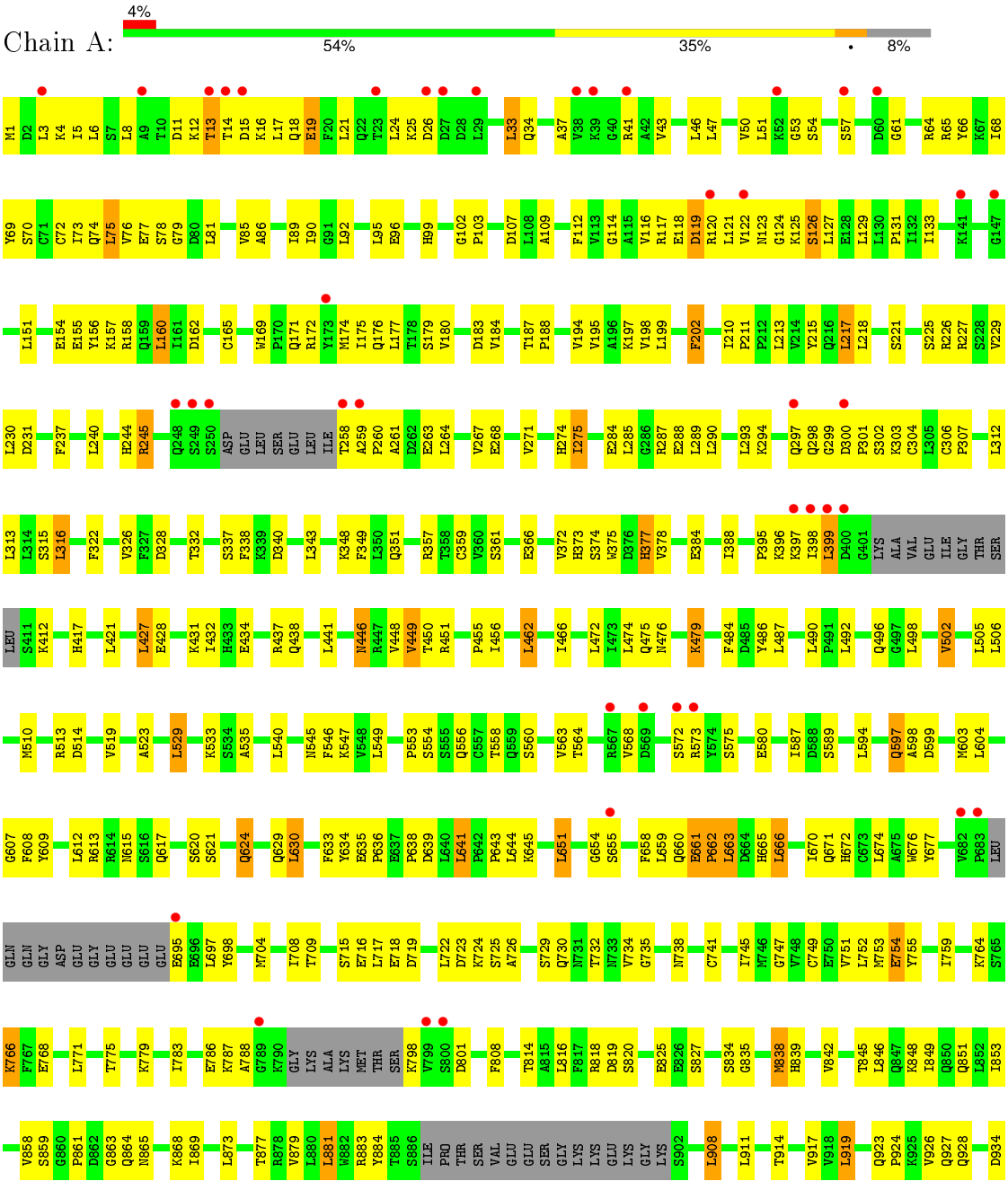
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	GLU	DELETION	UNP Q80V62
B	?	-	SER	DELETION	UNP Q80V62
B	?	-	THR	DELETION	UNP Q80V62
B	?	-	GLY	DELETION	UNP Q80V62
B	?	-	LYS	DELETION	UNP Q80V62
B	?	-	GLU	DELETION	UNP Q80V62
B	?	-	GLY	DELETION	UNP Q80V62

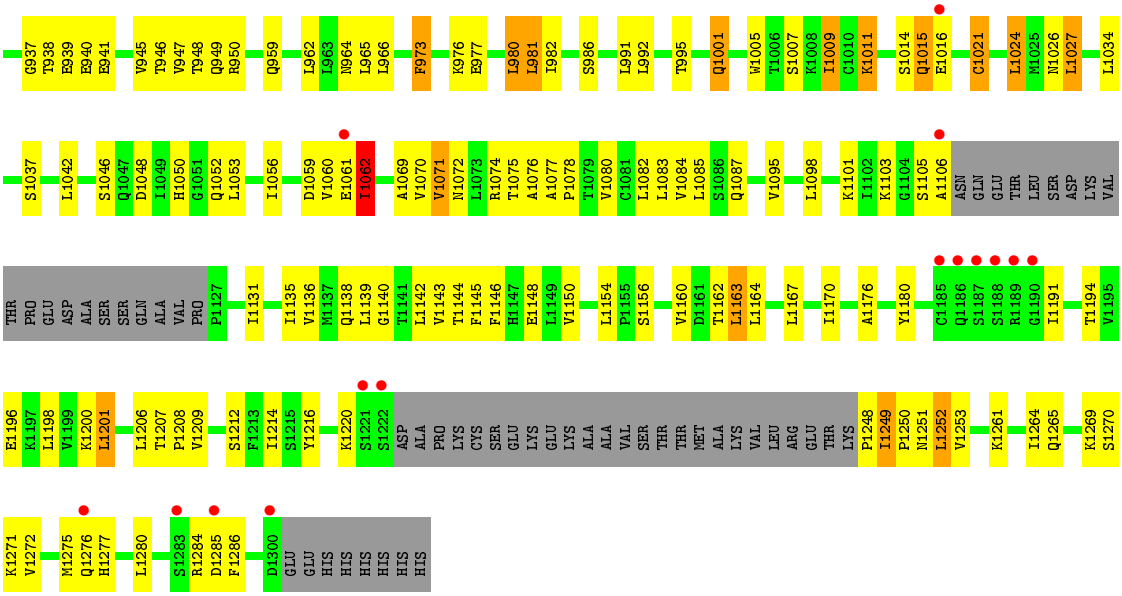
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

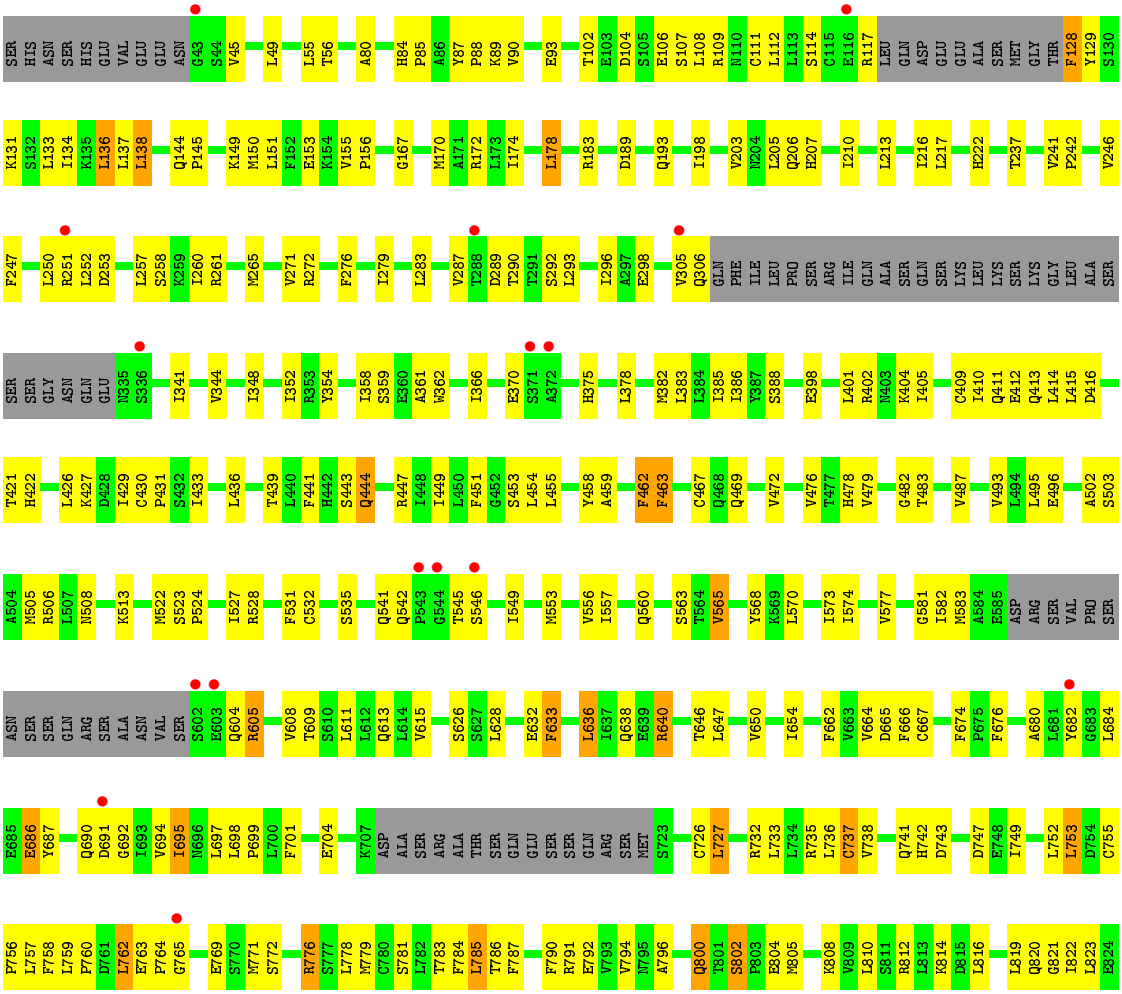
Chain A:

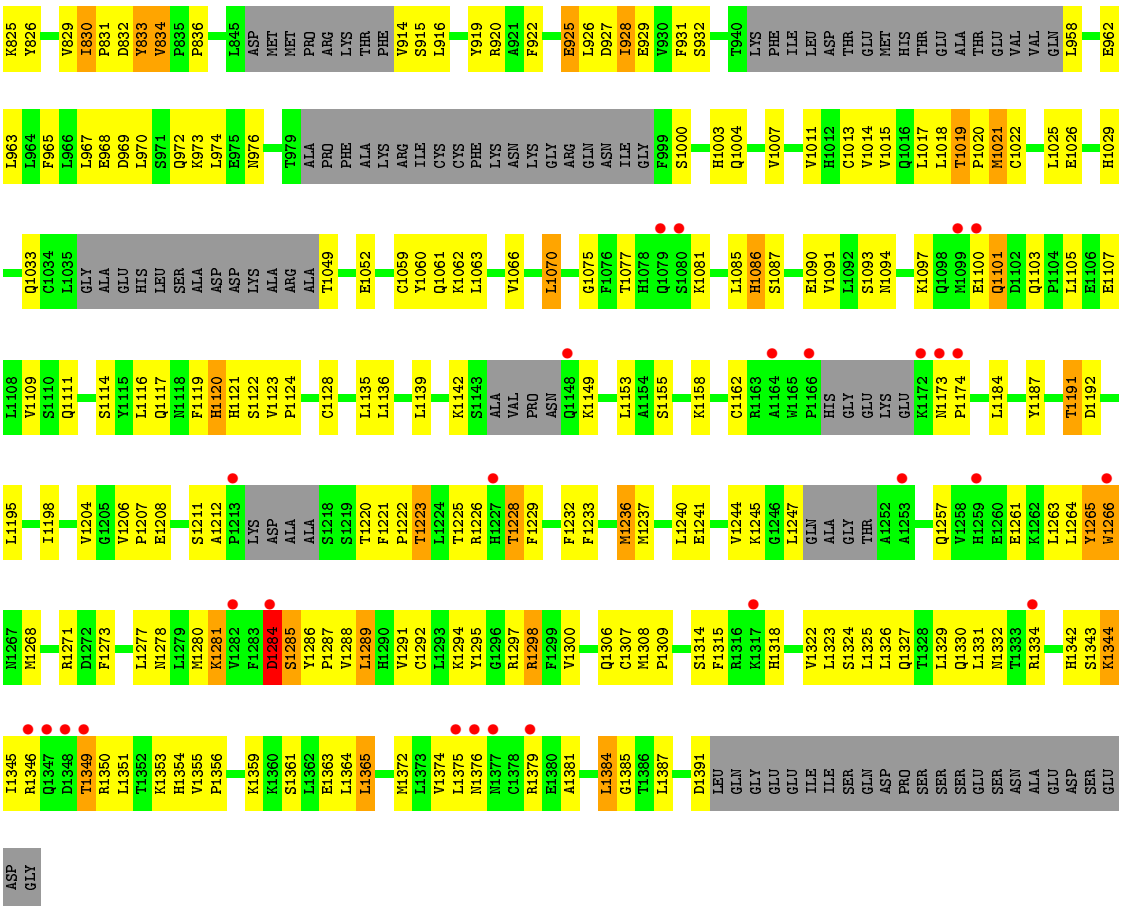




• Molecule 2: Fanconi anemia group D2 protein homolog

Chain B:




K825 Y826 V829 I830 P831 D832 Y833 V834 P835 P836 L845 ASP MET MET PRO ARG LYS THR PHE V914 S915 L916 Y919 R920 A921 F922 E925 L926 D927 I928 E929 V930 F931 S932 T940 LYS PHE ILE LEU ASP THR GLU MET HIS THR GLU ALA THR GLU VAL VAL GLN L958 E962
L963 L964 F965 L966 L967 E968 D969 L970 S971 Q972 K973 L974 E975 N976 T979 ALA PRO PHE ALA LYS ARG ILE CYS CYS PHE LYS ASN LYS GLY ARG GLN ASN ILE GLY F999 S1000 H1003 Q1004 V1007 V1011 H1012 C1013 V1014 V1015 Q1016 L1017 L1018 T1019 P1020 M1021 C1022 L1025 E1026 H1029
Q1033 C1034 L1035 GLY ALA GLU HIS LEU SER ALA ASP ASP LYS ALA ARG ALA T1049 E1052 C1059 Y1060 Q1061 K1062 L1063 V1066 L1070 G1075 F1076 T1077 H1078 Q1079 S1080 K1081 L1085 H1086 S1087 E1090 V1091 L1092 S1093 N1094 K1097 Q1098 M1099 E1100 Q1101 D1102 Q1103 P1104 L1105 E1106 E1107
L1108 V1109 S1110 Q1111 S1114 Y1115 L1116 Q1117 N1118 F1119 H1120 H1121 S1122 V1123 P1124 C1128 L1135 L1136 L1139 K1142 S1143 ALA VAL PRO ASN Q1148 K1149 L1153 A1154 S1155 K1158 C1162 R1163 A1164 W1165 P1166 HIS GLY GLU LYS GLU K1172 N1173 P1174 L1184 Y1187 T1191 D1192
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 E1261 K1262 L1263 L1264 Y1265 W1266
N1267 M1268 R1271 D1272 F1273 L1277 N1278 L1279 M1280 K1281 V1282 F1283 D1284 S1285 Y1286 P1287 V1288 L1289 H1290 V1291 C1292 L1293 K1294 Y1295 G1296 R1297 R1298 F1299 V1300 Q1306 C1307 M1308 P1309 S1314 F1315 R1316 K1317 H1318 V1322 L1323 S1324 L1325 L1326 Q1327 T1328 L1329 Q1330 L1331 N1332 T1333 R1334 H1342 S1343 K1344
I1345 R1346 Q1347 D1348 T1349 R1350 L1351 T1352 K1353 H1354 V1355 P1356 K1359 K1360 S1361 L1362 E1363 L1364 L1365 M1372 L1373 V1374 L1375 N1376 N1377 C1378 R1379 E1380 A1381 L1384 G1385 T1386 L1387 D1391 LEU GLN GLY GLU GLU ILE ILE SER GLN ASP PRO SER SER SER GLU SER ASN ALA GLU ASP SER GLU
ASP GLY

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 42934 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	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

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:776:ARG:HH21	2:B:779:MET:HG3	1.53	0.74
2:B:523:SER:HB2	2:B:524:PRO:HD2	1.69	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
2:B:735:ARG:HD2	2:B:796:ALA:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ILE:HG22	1:A:752:LEU:HD11	1.71	0.72
1:A:1142:LEU:HA	1:A:1145:PHE:HB3	1.71	0.72
2:B:1223:THR:HG22	2:B:1228:THR:HG21	1.70	0.72
2:B:1277:LEU:HA	2:B:1280:MET:HB2	1.70	0.72
1:A:818:ARG:NH1	1:A:825:GLU:OE1	2.22	0.72
1:A:202:PHE:CE1	1:A:210:ILE:HG23	2.25	0.72
2:B:1206:VAL:N	2:B:1207:PRO:HD2	2.04	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:636:LEU:O	2:B:636:LEU:HD12	1.92	0.69
2:B:258:SER:HA	2:B:261:ARG:HH11	1.55	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:662:PRO:HB2	1:A:665:HIS:HB2	1.75	0.68
1:A:641:LEU:HG	1:A:715:SER:HB3	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
2:B:155:VAL:N	2:B:156:PRO:HD2	2.08	0.68
1:A:449:VAL:HA	1:A:490:LEU:HD21	1.75	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

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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:85:VAL:O	1:A:89:ILE:HG13	1.96	0.65
1:A:349:PHE:CZ	1:A:1138:GLN:HG3	2.32	0.65
2:B:545:THR:HG22	2:B:546:SER:H	1.61	0.65
2:B:1061:GLN:HG3	2:B:1128:CYS:SG	2.37	0.65
1:A:1270:SER:OG	1:A:1271:LYS:N	2.28	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:826:TYR:O	2:B:830:ILE:HG22	1.96	0.65
2:B:412:GLU:HG2	2:B:454:LEU:HD11	1.79	0.65
2:B:784:PHE:HD1	2:B:823:LEU:HD11	1.62	0.65
2:B:583:MET:HG3	2:B:608:VAL:HG22	1.77	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
2:B:914:VAL:HG22	2:B:922:PHE:CE1	2.33	0.63
2:B:1020:PRO:O	2:B:1021:MET:HE3	1.98	0.63
1:A:633:PHE:HB3	1:A:663:LEU:HD11	1.79	0.63
2:B:131:LYS:HG3	2:B:136:LEU:HD22	1.80	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
2:B:830:ILE:HD13	2:B:834:VAL:HG22	1.81	0.63
2:B:454:LEU:O	2:B:458:TYR:HD1	1.82	0.63
1:A:127:LEU:HB3	1:A:180:VAL:HG21	1.79	0.63
2:B:735:ARG:HD2	2:B:796:ALA:CA	2.28	0.63
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
1:A:109:ALA:HB2	1:A:133:ILE:HG21	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1280:LEU:H	1:A:1280:LEU:HD23	1.64	0.62
2:B:528:ARG:HH22	2:B:1000:SER:HB2	1.65	0.62
1:A:21:LEU:O	1:A:64:ARG:NH2	2.33	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
2:B:963:LEU:HD23	2:B:1059:CYS:SG	2.41	0.61
2:B:1085:LEU:HD11	2:B:1142:LYS:HE3	1.82	0.61
1:A:33:LEU:HA	1:A:75:LEU:HD11	1.83	0.61
2:B:830:ILE:O	2:B:830:ILE:HG23	2.01	0.61
2:B:502:ALA:O	2:B:506:ARG:HG2	2.00	0.61
1:A:66:TYR:CE1	1:A:107:ASP:HB3	2.35	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
2:B:779:MET:HB3	2:B:826:TYR:CZ	2.37	0.60
1:A:816:LEU:HD13	1:A:838:MET:CE	2.32	0.60
1:A:395:PRO:HB3	1:A:398:ILE:HD12	1.83	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
2:B:640:ARG:H	2:B:640:ARG:HD2	1.68	0.59
1:A:908:LEU:HD13	1:A:980:LEU:HD21	1.83	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
2:B:772:SER:HA	2:B:776:ARG:HD2	1.84	0.59
2:B:430:CYS:HB3	2:B:431:PRO:HD3	1.83	0.59
1:A:226:ARG:HB2	1:A:288:GLU:HG2	1.84	0.59
1:A:838:MET:HA	1:A:838:MET:CE	2.33	0.59
1:A:754:GLU:OE1	1:A:808:PHE:HB2	2.02	0.59
1:A:510:MET:HA	1:A:513:ARG:NH1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:PRO:O	2:B:833:TYR:N	2.36	0.59
2:B:453:SER:HB2	2:B:493:VAL:HG21	1.84	0.59
2:B:654:ILE:HD13	2:B:733:LEU:HG	1.85	0.59
1:A:498:LEU:O	1:A:502:VAL:HB	2.01	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:66:TYR:HE1	1:A:107:ASP:HB3	1.68	0.58
1:A:1085:LEU:HD13	1:A:1162:THR:HG22	1.85	0.58
2:B:151:LEU:O	2:B:155:VAL:HG23	2.03	0.58
2:B:914:VAL:HG12	2:B:915:SER:N	2.18	0.58
1:A:86:ALA:O	1:A:90:ILE:HG13	2.03	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:211:PRO:HG3	1:A:267:VAL:HG13	1.85	0.58
1:A:123:ASN:HB3	1:A:125:LYS:HB2	1.86	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:814:THR:O	1:A:818:ARG:HB2	2.04	0.57
1:A:563:VAL:O	1:A:563:VAL:HG23	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: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
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:372:VAL:HG22	1:A:432:ILE:CG2	2.35	0.57
1:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.86	0.57
2:B:1278:ASN:HA	2:B:1281:LYS:HD2	1.87	0.57
1:A:65:ARG:HA	1:A:68:ILE:HD12	1.85	0.57
2:B:1271:ARG:HB3	2:B:1332:ASN:OD1	2.05	0.56
1:A:723:ASP:OD2	1:A:724:LYS:HG3	2.04	0.56
1:A:529:LEU:HD22	1:A:533:LYS:HE3	1.87	0.56
1:A:881:LEU:HA	1:A:911:LEU:HD11	1.87	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:908:LEU:HD13	1:A:980:LEU:CD2	2.36	0.56
1:A:937:GLY:O	1:A:941:GLU:HG3	2.04	0.56
1:A:858:VAL:HG12	1:A:859:SER:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1245:LYS:NZ	2:B:1298:ARG:HD2	2.21	0.56
1:A:54:SER:HB2	1:A:61:GLY:O	2.04	0.56
2:B:1162:CYS:HA	2:B:1222:PRO:HD2	1.87	0.56
2:B:790:PHE:O	2:B:794:VAL:HG23	2.05	0.56
1:A:635:GLU:HG3	1:A:645:LYS:HE2	1.88	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
2:B:523:SER:O	2:B:527:ILE:HG13	2.06	0.56
1:A:427:LEU:HD22	1:A:431:LYS:HD2	1.88	0.56
1:A:300:ASP:O	1:A:303:LYS:N	2.39	0.56
2:B:483:THR:O	2:B:487:VAL:HG23	2.06	0.56
1:A:1071:VAL:HG13	1:A:1076:ALA:CB	2.32	0.56
2:B:664:VAL:HG12	2:B:665:ASP:N	2.19	0.56
2:B:1225:THR:HG22	2:B:1226:ARG:H	1.71	0.56
2:B:829:VAL:O	2:B:831:PRO:HD3	2.06	0.55
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:454:LEU:HD22	2:B:458:TYR:HE1	1.72	0.55
1:A:120:ARG:HG2	1:A:172:ARG:NH1	2.21	0.55
2:B:1018:LEU:HG	2:B:1022:CYS:SG	2.47	0.55
1:A:729:SER:O	1:A:735:GLY:HA3	2.07	0.55
2:B:781:SER:O	2:B:785:LEU:HD12	2.06	0.55
1:A:651:LEU:HD11	1:A:658:PHE:CD1	2.42	0.55
1:A:1156:SER:HB3	1:A:1220:LYS:HE2	1.87	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:64:ARG:O	1:A:68:ILE:HG13	2.07	0.54
1:A:479:LYS:HA	1:A:479:LYS:HE3	1.90	0.54
1:A:941:GLU:O	1:A:945:VAL:HG23	2.08	0.54
1:A:1059:ASP:O	1:A:1060: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:299:GLY:O	1:A:302:SER:OG	2.26	0.54
1:A:187:THR:HG22	1:A:188:PRO:HD2	1.89	0.54
1:A:580:GLU:HB2	2:B:129:TYR:CG	2.42	0.54

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

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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
2:B:787:PHE:CE1	2:B:820:GLN:HB2	2.44	0.52
1:A:845:THR:O	1:A:849:ILE:HG13	2.09	0.52
2:B:293:LEU:O	2:B:293:LEU:HD23	2.10	0.52
2:B:1114:SER:O	2:B:1117:GLN:HG2	2.10	0.52
2:B:735:ARG:CD	2:B:796:ALA:HB2	2.40	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:1086:HIS:O	2:B:1090:GLU:HG3	2.10	0.52
2:B:252:LEU:H	2:B:252:LEU:HD23	1.74	0.52
2:B:926:LEU:O	2:B:973:LYS:NZ	2.30	0.52
1:A:545:ASN:HD22	1:A:549:LEU:HB2	1.75	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: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:227:ARG:HG3	1:A:288:GLU:HG3	1.92	0.52
1:A:1198:LEU:HD22	1:A:1201:LEU:HD12	1.91	0.51
1:A:227:ARG:HG3	1:A:288:GLU:CG	2.40	0.51
1:A:158:ARG:HD3	1:A:158:ARG:C	2.30	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
2:B:206:GLN:O	2:B:210:ILE:HG13	2.10	0.51
1:A:553:PRO:HB2	1:A:558:THR:HG23	1.93	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
2:B:1204:VAL:C	2:B:1207:PRO:HD2	2.31	0.51
1:A:662:PRO:O	1:A:665:HIS:N	2.40	0.51
1:A:372:VAL:HG22	1:A:432:ILE:HG21	1.92	0.51
1:A:848:LYS:HD3	1:A:858:VAL:HG13	1.92	0.51
2:B:1297:ARG:HH22	2:B:1354:HIS:CD2	2.28	0.51
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.25	0.51
2:B:149:LYS:HE3	2:B:153:GLU:OE2	2.11	0.51

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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:462:LEU:O	1:A:466:ILE:HG13	2.11	0.50
1:A:102:GLY:N	1:A:103:PRO:HD2	2.25	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
2:B:1220:THR:O	2:B:1221:PHE:HB3	2.12	0.50
1:A:755:TYR:CZ	1:A:759:ILE:HD11	2.47	0.50
1:A:523:ALA:HB3	1:A:535:ALA:HB2	1.92	0.50
1:A:722:LEU:O	1:A:725:SER:OG	2.29	0.50
1:A:1:MET:O	1:A:5:ILE:HG13	2.11	0.50
1:A:1150:VAL:HG22	1:A:1167:LEU:HD11	1.93	0.50
2:B:916:LEU:O	2:B:919:TYR:CD2	2.51	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:791:ARG:HH12	2:B:965:PHE:HZ	1.58	0.50
2:B:1149:LYS:O	2:B:1153:LEU:HG	2.12	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:1131:ILE:O	1:A:1135:ILE:HG13	2.10	0.50
2:B:800:GLN:CB	2:B:805:MET:HG2	2.40	0.50
1:A:848:LYS:HZ1	1:A:859:SER:HB2	1.77	0.50
2:B:84:HIS:CG	2:B:85:PRO:HD2	2.46	0.50
1:A:1105:SER:O	1:A:1106:ALA:C	2.50	0.50
2:B:55:LEU:HD23	2:B:133:LEU:HD13	1.93	0.49
2:B:974:LEU:HD11	2:B:1014:VAL:HG21	1.94	0.49
2:B:786:THR:HG22	2:B:819:LEU:HD11	1.93	0.49
2:B:753:LEU:HD21	2:B:808:LYS:HB3	1.93	0.49
2:B:503:SER:O	2:B:506:ARG:HG3	2.13	0.49
1:A:492:LEU:HD22	1:A:533:LYS:HG2	1.94	0.49
2:B:370:GLU:HB2	2:B:404:LYS:HZ1	1.77	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:1100:GLU:HB2	2:B:1103:GLN:HG2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:43:VAL:HA	1:A:46:LEU:HB2	1.94	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:946:THR:HG22	1:A:947:VAL:N	2.27	0.49
1:A:1009:ILE:HG22	1:A:1024:LEU:HD11	1.94	0.49
2:B:738:VAL:HG13	2:B:742:HIS:ND1	2.28	0.49
1:A:848:LYS:NZ	1:A:859:SER:HB2	2.28	0.49
1:A:1156:SER:HB3	1:A:1220:LYS:CE	2.43	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
2:B:963:LEU:HD11	2:B:1025:LEU:HD13	1.94	0.49
1:A:558:THR:HB	1:A:563:VAL:CG2	2.42	0.49
1:A:284:GLU:HG3	1:A:287:ARG:HH12	1.77	0.49
2:B:402:ARG:NH2	2:B:443:SER:HB3	2.28	0.48
1:A:937:GLY:O	1:A:941:GLU:CG	2.61	0.48
2:B:969:ASP:OD1	2:B:973:LYS:HE3	2.12	0.48
2:B:1149:LYS:N	2:B:1149:LYS:HD2	2.28	0.48
1:A:70:SER:O	1:A:74:GLN:HG3	2.13	0.48
1:A:195:VAL:HG13	1:A:217:LEU:HD21	1.95	0.48
2:B:1343:SER:O	2:B:1346:ARG:HB2	2.12	0.48
2:B:1022:CYS:O	2:B:1026:GLU:N	2.30	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: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
2:B:1343:SER:HA	2:B:1346:ARG:HD3	1.96	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
2:B:198:ILE:HD13	2:B:210:ILE:HG12	1.94	0.48
1:A:853:ILE:HG12	1:A:917:VAL:HG22	1.95	0.48
2:B:150:MET:O	2:B:153:GLU:HB2	2.13	0.48
2:B:421:THR:HB	2:B:422:HIS:CD2	2.49	0.48
2:B:1233:PHE:CD2	2:B:1277:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1342:HIS:CD2	2:B:1343:SER:N	2.82	0.48
1:A:199:LEU:HA	1:A:202:PHE:CD2	2.49	0.48
1:A:563:VAL:HG12	2:B:167:GLY:C	2.34	0.48
2:B:784:PHE:CD1	2:B:823:LEU:HD11	2.46	0.48
1:A:962:LEU:HB2	1:A:981:LEU:HD13	1.95	0.48
1:A:755:TYR:CE2	1:A:759:ILE:HD11	2.49	0.48
2:B:257:LEU:HA	2:B:260:ILE:HD12	1.95	0.48
2:B:241:VAL:HB	2:B:242:PRO:HD3	1.95	0.48
1:A:747:GLY:O	1:A:751:VAL:HG23	2.14	0.48
1:A:666:LEU:O	1:A:670:ILE:HG13	2.14	0.48
1:A:1071:VAL:H	1:A:1075:THR:HG21	1.77	0.48
2:B:732:ARG:HD2	2:B:792:GLU:OE2	2.14	0.48
2:B:1158:LYS:HG3	2:B:1187:TYR:CE1	2.49	0.48
2:B:388:SER:OG	2:B:429:ILE:HG23	2.14	0.48
2:B:133:LEU:HD12	2:B:137:LEU:HD13	1.95	0.48
2:B:1277:LEU:HB3	2:B:1288:VAL:HG13	1.95	0.48
1:A:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
1:A:502:VAL:HG13	1:A:502:VAL:O	2.13	0.48
1:A:165:CYS:HB3	1:A:197:LYS:HG3	1.95	0.48
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:851:GLN:O	1:A:851:GLN:HG2	2.14	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:641:LEU:HG	1:A:715:SER:CB	2.44	0.47
1:A:131:PRO:HB3	1:A:183:ASP:HB2	1.96	0.47
2:B:1120:HIS:CG	2:B:1121:HIS:N	2.81	0.47
1:A:834:SER:OG	1:A:835:GLY:N	2.47	0.47
1:A:629:GLN:NE2	1:A:661:GLU:OE2	2.47	0.47
2:B:305:VAL:O	2:B:306:GLN:HG3	2.13	0.47
2:B:545:THR:HG22	2:B:546:SER:N	2.28	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:1149:LYS:H	2:B:1149:LYS:HD2	1.79	0.47
1:A:284:GLU:HG3	1:A:287:ARG:NH1	2.29	0.47

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

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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
2:B:1342:HIS:CG	2:B:1343:SER:N	2.83	0.46
1:A:835:GLY:CA	1:A:838:MET:HB2	2.46	0.46
2:B:816:LEU:HD12	2:B:816:LEU:HA	1.81	0.46
1:A:597:GLN:HG2	1:A:597:GLN:H	1.34	0.46
2:B:752:LEU:HA	2:B:755:CYS:SG	2.56	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:375:HIS:NE2	2:B:409:CYS:SG	2.88	0.46
1:A:41:ARG:N	1:A:41:ARG:HD3	2.31	0.46
1:A:1075:THR:HG22	1:A:1080:VAL:CG2	2.45	0.46
2:B:1277:LEU:HD13	2:B:1288:VAL:O	2.15	0.46
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.51	0.46
2:B:401:LEU:O	2:B:405:ILE:HG13	2.15	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:118:GLU:O	1:A:119:ASP:OD1	2.33	0.46
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:112:PHE:O	1:A:116:VAL:HG23	2.16	0.45
2:B:581:GLY:CA	2:B:636:LEU:HD13	2.45	0.45
1:A:908:LEU:HD11	1:A:981:LEU:HG	1.99	0.45
1:A:754:GLU:OE1	1:A:808:PHE:CB	2.64	0.45
2:B:1324:SER:HB3	2:B:1385:GLY:HA2	1.97	0.45
1:A:271:VAL:O	1:A:275:ILE:HG23	2.17	0.45
1:A:545:ASN:O	1:A:549:LEU:HB3	2.16	0.45
1:A:322:PHE:O	1:A:326:VAL:HG23	2.17	0.45
2:B:695:ILE:HB	2:B:757:LEU:HD23	1.99	0.45
2:B:1265:TYR:HA	2:B:1268:MET:HB2	1.99	0.45
1:A:114:GLY:HA2	1:A:117:ARG:NH1	2.31	0.45
1:A:78:SER:OG	1:A:79:GLY:N	2.48	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
2:B:1277:LEU:CD1	2:B:1288:VAL:HG13	2.43	0.45
1:A:819:ASP:HB3	1:A:820:SER:H	1.52	0.45
2:B:443:SER:O	2:B:449:ILE:HD11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:541:GLN:O	2:B:542:GLN:HG3	2.17	0.45
2:B:265:MET:HE3	2:B:283:LEU:HD22	1.99	0.45
2:B:976:ASN:OD1	2:B:1003:HIS:CE1	2.69	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
1:A:1146:PHE:O	1:A:1150:VAL:HG23	2.17	0.45
2:B:1361:SER:HA	2:B:1364:LEU:HD12	1.99	0.45
2:B:605:ARG:HG2	2:B:646:THR:HG23	1.99	0.45
1:A:1200:LYS:HB2	1:A:1277:HIS:HB3	1.98	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
2:B:1285:SER:OG	2:B:1288:VAL:HB	2.18	0.44
1:A:1261:LYS:O	1:A:1264:ILE:HB	2.17	0.44
1:A:1050:HIS:ND1	1:A:1148:GLU:OE1	2.50	0.44
1:A:1071:VAL:HG12	1:A:1071:VAL:O	2.16	0.44
2:B:604:GLN:O	2:B:608:VAL:HG23	2.18	0.44
2:B:252:LEU:HD11	2:B:257:LEU:HD13	1.99	0.44
2:B:674:PHE:C	2:B:676:PHE:H	2.20	0.44
1:A:221:SER:HB3	1:A:229:VAL:HG21	1.98	0.44
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.99	0.44
2:B:570:LEU:HD12	2:B:628:LEU:HD22	1.99	0.44
1:A:290:LEU:O	1:A:294:LYS:HG2	2.17	0.44
2:B:565:VAL:HB	2:B:568:TYR:HD1	1.83	0.44
1:A:1021:CYS:SG	1:A:1075:THR:HG23	2.58	0.44
2:B:763:GLU:HA	2:B:822:ILE:HD13	2.00	0.44
1:A:1140:GLY:HA3	1:A:1198:LEU:HD13	2.00	0.44
2:B:925:GLU:N	2:B:925:GLU:CD	2.68	0.44
1:A:1059:ASP:O	1:A:1060:VAL:CG2	2.65	0.44
1:A:1154:LEU:CD1	1:A:1163:LEU:HD12	2.47	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:820:GLN:HE22	2:B:920:ARG:HH12	1.65	0.44
2:B:626:SER:OG	2:B:726:CYS:SG	2.75	0.44
2:B:967:LEU:HB3	2:B:1062:LYS:HB3	1.99	0.44
2:B:341:ILE:HD11	2:B:422:HIS:CE1	2.53	0.44
2:B:1266:TRP:HA	2:B:1266:TRP:HE3	1.80	0.44
1:A:661:GLU:HA	1:A:662:PRO:HD3	1.68	0.44
2:B:1116:LEU:HA	2:B:1119:PHE:HD1	1.83	0.44
1:A:1249:ILE:HG13	1:A:1249:ILE:H	1.47	0.44
2:B:1349:THR:O	2:B:1351:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ILE:O	1:A:674:LEU:HB2	2.18	0.44
2:B:1281:LYS:HE3	2:B:1342:HIS:HE2	1.83	0.44
2:B:1331:LEU:HD12	2:B:1334:ARG:HD2	2.00	0.44
1:A:858:VAL:CG1	1:A:859:SER:N	2.81	0.44
2:B:557:ILE:HA	2:B:557:ILE:HD12	1.85	0.44
2:B:1277:LEU:HD22	2:B:1288:VAL:HG13	1.99	0.44
1:A:816:LEU:HD13	1:A:838:MET:HE1	1.99	0.44
1:A:466:ILE:HG22	1:A:474:LEU:HD11	1.99	0.44
2:B:1323:LEU:O	2:B:1327:GLN:HG3	2.17	0.44
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:293:LEU:HD13	1:A:313:LEU:HD11	2.00	0.43
1:A:275:ILE:HD11	1:A:312:LEU:HD21	2.00	0.43
1:A:90:ILE:CD1	1:A:125:LYS:HB3	2.48	0.43
1:A:1164:LEU:HD22	1:A:1252:LEU:HD12	2.00	0.43
1:A:973:PHE:CE2	1:A:1015:GLN:HG2	2.51	0.43
2:B:684:LEU:C	2:B:686:GLU:H	2.20	0.43
1:A:798:LYS:N	1:A:801:ASP:OD1	2.51	0.43
2:B:258:SER:HA	2:B:261:ARG:NH1	2.30	0.43
2:B:1162:CYS:O	2:B:1222:PRO:HD2	2.18	0.43
2:B:87:TYR:N	2:B:88:PRO:CD	2.81	0.43
1:A:654:GLY:O	1:A:655:SER:OG	2.31	0.43
2:B:444:GLN:CD	2:B:444:GLN:H	2.20	0.43
1:A:297:GLN:O	1:A:301:PRO:HD3	2.18	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
2:B:1359:LYS:O	2:B:1363:GLU:HG3	2.19	0.43
2:B:1049:THR:HA	2:B:1052:GLU:HB2	2.00	0.43
1:A:1139:LEU:HA	1:A:1142:LEU:CD2	2.49	0.43
1:A:451:ARG:HB3	1:A:456:ILE:HD11	2.00	0.43
1:A:15:ASP:O	1:A:19:GLU:HB2	2.18	0.43
2:B:366:ILE:HD13	2:B:383:LEU:HG	2.00	0.43
2:B:1101:GLN:H	2:B:1101:GLN:HG2	1.55	0.43
1:A:396:LYS:HE2	1:A:396:LYS:HB3	1.76	0.43
1:A:1070:VAL:O	1:A:1071:VAL:CB	2.62	0.43
2:B:155:VAL:N	2:B:156:PRO:CD	2.79	0.43
1:A:300:ASP:N	1:A:301:PRO:HD2	2.33	0.43
1:A:12:LYS:HB2	1:A:16:LYS:NZ	2.34	0.43
1:A:151:LEU:HB2	1:A:156:TYR:CE1	2.54	0.43
2:B:753:LEU:HD21	2:B:808:LYS:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:O	1:A:229:VAL:HG23	2.19	0.43
2:B:476:VAL:O	2:B:479:VAL:HB	2.19	0.43
2:B:665:ASP:CA	2:B:692:GLY:O	2.63	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
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:1048:ASP:CB	1:A:1071:VAL:HG11	2.44	0.43
2:B:974:LEU:HD12	2:B:1066:VAL:HG13	2.01	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
1:A:428:GLU:O	1:A:432:ILE:HG12	2.18	0.43
1:A:620:SER:HB3	2:B:128:PHE:HE1	1.83	0.43
1:A:514:ASP:OD1	1:A:554:SER:HB2	2.19	0.43
1:A:194:VAL:O	1:A:198:VAL:HG23	2.19	0.43
1:A:749:CYS:O	1:A:753:MET:HB2	2.19	0.43
1:A:1016:GLU:HB3	1:A:1074:ARG:HD3	2.00	0.43
2:B:914:VAL:HG22	2:B:922:PHE:HE1	1.81	0.42
2:B:1277:LEU:HD12	2:B:1292:CYS:SG	2.59	0.42
1:A:1103:LYS:HG2	1:A:1180:TYR:CD1	2.41	0.42
2:B:787:PHE:O	2:B:791:ARG:HB2	2.19	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
1:A:230:LEU:HD22	1:A:289:LEU:HD13	2.01	0.42
2:B:928:ILE:HG13	2:B:928:ILE:H	1.62	0.42
1:A:884:TYR:CE1	1:A:908:LEU:HG	2.54	0.42
1:A:487:LEU:HD12	1:A:498:LEU:HD23	2.01	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
2:B:296:ILE:HD12	2:B:361:ALA:CB	2.45	0.42
2:B:1000:SER:O	2:B:1004:GLN:HG2	2.20	0.42
1:A:475:GLN:HA	1:A:505:LEU:HD22	2.01	0.42
1:A:316:LEU:HD23	1:A:316:LEU:O	2.19	0.42
2:B:549:ILE:HG22	2:B:553:MET:CE	2.49	0.42
1:A:72:CYS:O	1:A:76:VAL:HG23	2.18	0.42
2:B:1384:LEU:HD23	2:B:1384:LEU:O	2.20	0.42
2:B:271:VAL:HG12	2:B:272:ARG:O	2.19	0.42
1:A:187:THR:CG2	1:A:188:PRO:HD2	2.49	0.42
2:B:1345:ILE:O	2:B:1345:ILE:CG2	2.68	0.42
2:B:749:ILE:O	2:B:749:ILE:HG22	2.18	0.42
2:B:1375:LEU:O	2:B:1376:ASN:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:SER:O	1:A:1011:LYS:HB2	2.20	0.42
2:B:513:LYS:HE2	2:B:513:LYS:HB3	1.74	0.42
2:B:1228:THR:O	2:B:1232:PHE:HD1	2.02	0.42
1:A:1248:PRO:HG2	1:A:1249:ILE:H	1.85	0.42
1:A:1150:VAL:CG1	1:A:1209:VAL:HG12	2.49	0.42
1:A:176:GLN:HA	1:A:179:SER:OG	2.19	0.42
2:B:742:HIS:O	2:B:743:ASP:CB	2.65	0.42
2:B:1019:THR:C	2:B:1021:MET:H	2.22	0.42
2:B:633:PHE:HB3	2:B:733:LEU:HD13	2.01	0.42
2:B:1345:ILE:O	2:B:1345:ILE:HG22	2.20	0.42
2:B:664:VAL:HG12	2:B:665:ASP:H	1.84	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:1090:GLU:O	2:B:1093:SER:OG	2.27	0.41
1:A:1001:GLN:HE21	1:A:1001:GLN:HB3	1.60	0.41
2:B:762:LEU:HD13	2:B:783:THR:HA	2.01	0.41
2:B:638:GLN:HB3	2:B:736:LEU:CD1	2.48	0.41
1:A:372:VAL:O	1:A:372:VAL:HG12	2.20	0.41
1:A:919:LEU:HD11	1:A:991:LEU:HD21	2.01	0.41
2:B:666:PHE:O	2:B:667:CYS:C	2.55	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
1:A:672:HIS:CD2	1:A:861:PRO:HG2	2.56	0.41
2:B:1374:VAL:O	2:B:1375:LEU:HG	2.21	0.41
2:B:1014:VAL:HG22	2:B:1014:VAL:O	2.20	0.41
2:B:429:ILE:O	2:B:433:ILE:HG13	2.21	0.41
1:A:1098:LEU:HD22	1:A:1131:ILE:CG2	2.50	0.41
2:B:1221:PHE:N	2:B:1222:PRO:HD3	2.35	0.41
1:A:573:ARG:HB2	1:A:573:ARG:NH1	2.35	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
2:B:1204:VAL:O	2:B:1207:PRO:CG	2.68	0.41
1:A:1011:LYS:O	1:A:1069:ALA:CB	2.67	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
1:A:154:GLU:HG3	1:A:155:GLU:N	2.36	0.41
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.21	0.41
2:B:968:GLU:O	2:B:972:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:914:VAL:CG1	2:B:915:SER:N	2.82	0.41
2:B:469:GLN:HG3	2:B:508:ASN:HD21	1.86	0.41
1:A:90:ILE:HD13	1:A:125:LYS:HB3	2.01	0.41
2:B:45:VAL:HG21	2:B:93:GLU:CG	2.50	0.41
2:B:112:LEU:HD23	2:B:134:ILE:HD12	2.03	0.41
1:A:462:LEU:HD22	1:A:466:ILE:HD11	2.03	0.41
2:B:287:VAL:O	2:B:289:ASP:O	2.39	0.41
2:B:88:PRO:HB2	2:B:89:LYS:HD2	2.03	0.41
2:B:532:CYS:HA	2:B:582:ILE:HD11	2.02	0.41
1:A:1200:LYS:HD3	1:A:1277:HIS:CE1	2.55	0.41
1:A:863:GLY:O	1:A:869:ILE:HD11	2.20	0.41
2:B:1123:VAL:HA	2:B:1124:PRO:HD3	1.76	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:1229:PHE:HE2	2:B:1277:LEU:HD21	1.86	0.41
1:A:818:ARG:O	1:A:819:ASP:HB2	2.21	0.41
1:A:608:PHE:HD2	1:A:608:PHE:HA	1.81	0.41
2:B:787:PHE:HA	2:B:819:LEU:HD13	2.02	0.41
2:B:150:MET:HA	2:B:153:GLU:OE1	2.21	0.41
1:A:348:LYS:HD3	1:A:1034:LEU:O	2.20	0.41
2:B:222:HIS:CD2	2:B:251:ARG:HG2	2.56	0.41
2:B:609:THR:O	2:B:613:GLN:HG2	2.20	0.41
2:B:556:VAL:O	2:B:560:GLN:HG2	2.20	0.41
2:B:413:GLN:HG3	2:B:414:LEU:N	2.35	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
1:A:92:LEU:HA	1:A:95:LEU:HB2	2.02	0.41
2:B:296:ILE:HD11	2:B:358:ILE:HG23	2.02	0.41
1:A:651:LEU:CD2	1:A:658:PHE:HB2	2.49	0.41
1:A:923:GLN:HA	1:A:926:VAL:HG23	2.03	0.41
2:B:1306:GLN:O	2:B:1309:PRO:HG2	2.21	0.41
2:B:1155:SER:HA	2:B:1158:LYS:HB2	2.02	0.41
2:B:401:LEU:HD12	2:B:401:LEU:HA	1.96	0.41
1:A:741:CYS:O	1:A:745:ILE:HG13	2.20	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:812:ARG:HD2	2:B:812:ARG:HA	1.69	0.40
2:B:207:HIS:CD2	2:B:242:PRO:HG3	2.56	0.40
2:B:1323:LEU:HG	2:B:1381:ALA:HB1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:763:GLU:CB	2:B:764:PRO:CD	2.87	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:664:VAL:CG1	2:B:665:ASP:N	2.85	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
1:A:375:TRP:HE3	1:A:378:VAL:HG21	1.83	0.40
1:A:372:VAL:HG22	1:A:432:ILE:HG23	2.02	0.40
2:B:1241:GLU:OE2	2:B:1298:ARG:NH1	2.49	0.40
1:A:1160:VAL:O	1:A:1164:LEU:HG	2.21	0.40
1:A:938:THR:HG22	1:A:939:GLU:H	1.86	0.40
1:A:169:TRP:N	1:A:169:TRP:CD1	2.90	0.40
2:B:1233:PHE:CE1	2:B:1277:LEU:HG	2.56	0.40
2:B:1116:LEU:HB2	2:B:1136:LEU:CD2	2.48	0.40
2:B:222:HIS:CB	2:B:251:ARG:HG2	2.51	0.40
1:A:357:ARG:HD3	1:A:1101:LYS:NZ	2.37	0.40
1:A:986:SER:HB3	1:A:1027:LEU:HD22	2.03	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:338:PHE:CD2	1:A:417:HIS:HB3	2.57	0.40
2:B:1326:LEU:O	2:B:1330:GLN:HG3	2.22	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
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
2:B:810:LEU:HD21	2:B:958:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1190/1308 (91%)	1108 (93%)	75 (6%)	7 (1%)	30 72
2	B	1120/1323 (85%)	1043 (93%)	75 (7%)	2 (0%)	52 87
All	All	2310/2631 (88%)	2151 (93%)	150 (6%)	9 (0%)	39 79

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 (i)

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 43
2	B	1030/1193 (86%)	949 (92%)	81 (8%)	15 52
All	All	2123/2381 (89%)	1941 (91%)	182 (9%)	13 48

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

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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

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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

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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

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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

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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

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, 95^{th} 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%)	-0.11	57 (4%)	35	32	48, 100, 204, 311	0
2	B	1146/1323 (86%)	0.01	43 (3%)	44	39	74, 127, 192, 236	0
All	All	2352/2631 (89%)	-0.05	100 (4%)	39	34	48, 116, 198, 311	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	LEU	7.3
2	B	543	PRO	7.2
1	A	14	THR	7.0
1	A	397	LYS	6.2
1	A	258	THR	6.0
1	A	13	THR	5.4
1	A	398	ILE	5.1
1	A	248	GLN	5.1
1	A	1189	ARG	5.1
1	A	1186	GLN	4.8
2	B	1348	ASP	4.6
1	A	297	GLN	4.6
1	A	15	ASP	4.2
2	B	546	SER	4.2
1	A	259	ALA	4.1
1	A	683	PRO	4.1
1	A	23	THR	4.0
2	B	1284	ASP	3.9
1	A	38	VAL	3.9
1	A	141	LYS	3.8
1	A	1300	ASP	3.7
1	A	1190	GLY	3.7
2	B	1379	ARG	3.6
2	B	1347	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	249	SER	3.5
1	A	572	SER	3.5
1	A	1187	SER	3.5
2	B	305	VAL	3.4
1	A	26	ASP	3.4
1	A	682	VAL	3.3
2	B	43	GLY	3.3
2	B	1173	ASN	3.2
2	B	603	GLU	3.1
1	A	400	ASP	3.1
2	B	1100	GLU	3.1
1	A	567	ARG	3.1
1	A	789	GLY	3.1
1	A	1222	SER	3.0
2	B	371	SER	3.0
2	B	602	SER	3.0
1	A	27	ASP	2.9
1	A	1106	ALA	2.9
1	A	695	GLU	2.9
2	B	1172	LYS	2.9
1	A	120	ARG	2.9
2	B	1346	ARG	2.9
2	B	1174	PRO	2.8
1	A	1276	GLN	2.8
2	B	1349	THR	2.8
1	A	569	ASP	2.8
1	A	799	VAL	2.8
1	A	57	SER	2.8
1	A	60	ASP	2.7
1	A	122	VAL	2.6
2	B	336	SER	2.6
2	B	1259	HIS	2.6
2	B	1376	ASN	2.6
1	A	250	SER	2.6
2	B	1253	ALA	2.6
1	A	1188	SER	2.6
2	B	682	TYR	2.5
2	B	1166	PRO	2.5
1	A	39	LYS	2.4
2	B	1266	TRP	2.4
2	B	691	ASP	2.4
2	B	1148	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	544	GLY	2.4
2	B	372	ALA	2.4
1	A	1221	SER	2.4
2	B	1282	VAL	2.3
1	A	800	SER	2.3
1	A	147	GLY	2.3
2	B	1377	ASN	2.3
1	A	300	ASP	2.3
1	A	3	LEU	2.3
1	A	573	ARG	2.3
2	B	1079	GLN	2.3
2	B	1213	PRO	2.2
1	A	1283	SER	2.2
2	B	251	ARG	2.2
2	B	1227	HIS	2.2
2	B	1375	LEU	2.2
2	B	1099	MET	2.2
1	A	41	ARG	2.2
1	A	1016	GLU	2.2
2	B	288	THR	2.2
1	A	655	SER	2.2
2	B	116	GLU	2.1
2	B	1080	SER	2.1
1	A	1185	CYS	2.1
1	A	173	TYR	2.1
2	B	1164	ALA	2.1
1	A	29	LEU	2.1
1	A	1285	ASP	2.1
2	B	1317	LYS	2.1
2	B	765	GLY	2.1
1	A	9	ALA	2.1
1	A	1061	GLU	2.0
2	B	1334	ARG	2.0
1	A	52	LYS	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.