Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2020 – 09:04 PM BST

PDB ID	:	6TS8
Title	:	Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) double cysteine mutant G177C/A786C.
Authors	:	Roversi, P.; Zitzmann, N.; Ibba, R.; Hensen, M.; Chandran, A.
Deposited on	:	2019-12-20
Resolution	:	4.60 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
https://www.wwpdb.org/validation/2017/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:

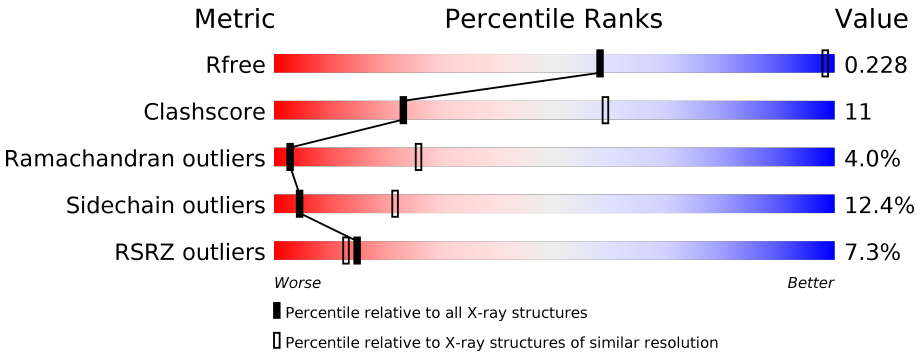
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1382	5%, 58%, 28%, ·, 9%
1	B	1382	9%, 58%, 28%, ·, 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20112 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 UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1254	Total	C	N	O	S	0	0	0
			10056	6439	1711	1879	27			
1	B	1254	Total	C	N	O	S	0	0	0
			10056	6439	1711	1879	27			

There are 4 discrepancies between the modelled and reference sequences:

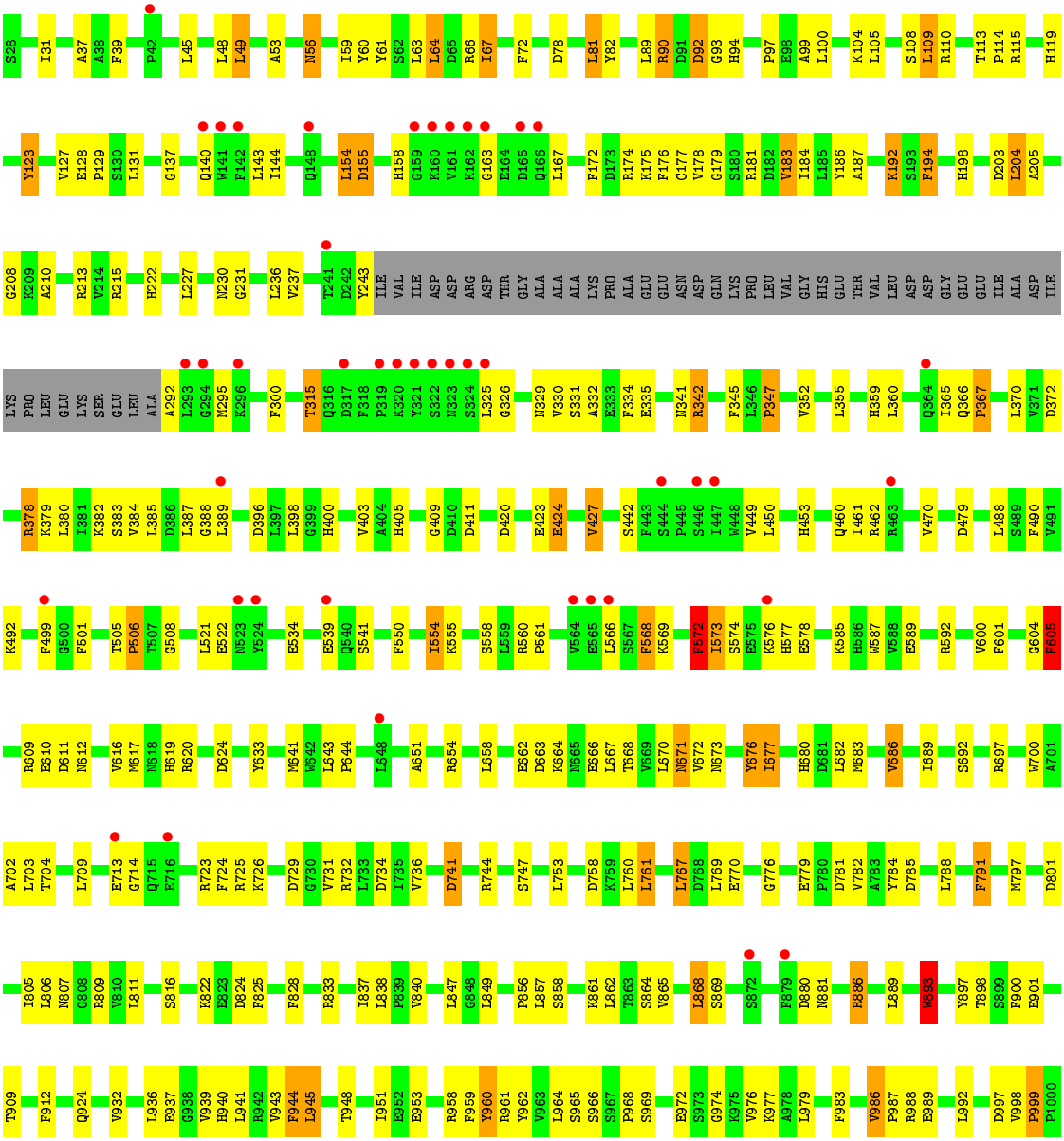
Chain	Residue	Modelled	Actual	Comment	Reference
A	177	CYS	GLY	engineered mutation	UNP G0SB58
A	786	CYS	ALA	engineered mutation	UNP G0SB58
B	177	CYS	GLY	engineered mutation	UNP G0SB58
B	786	CYS	ALA	engineered mutation	UNP G0SB58

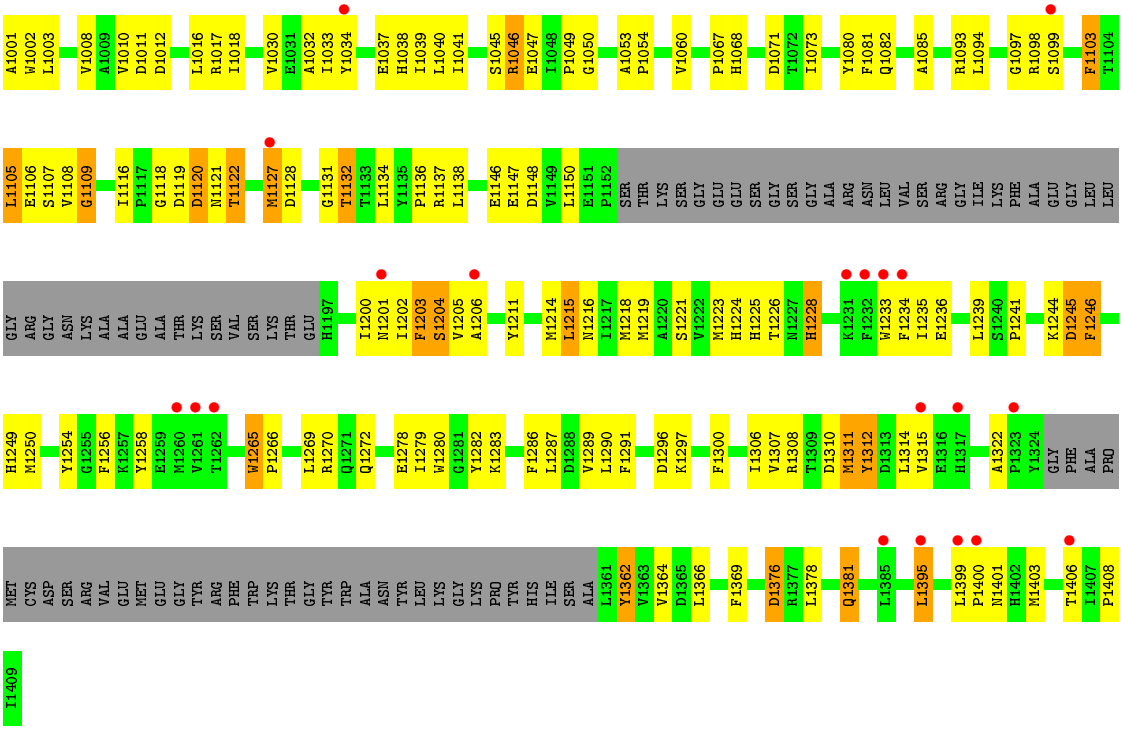
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein

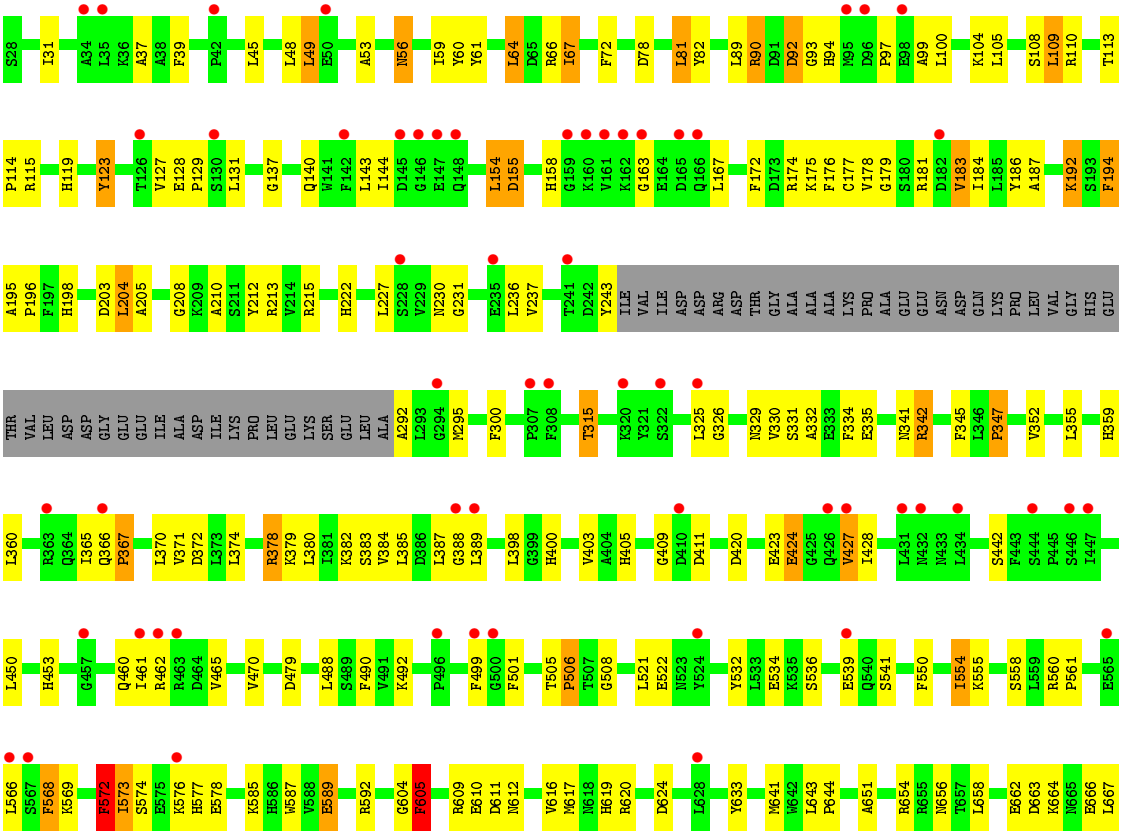
Chain A:

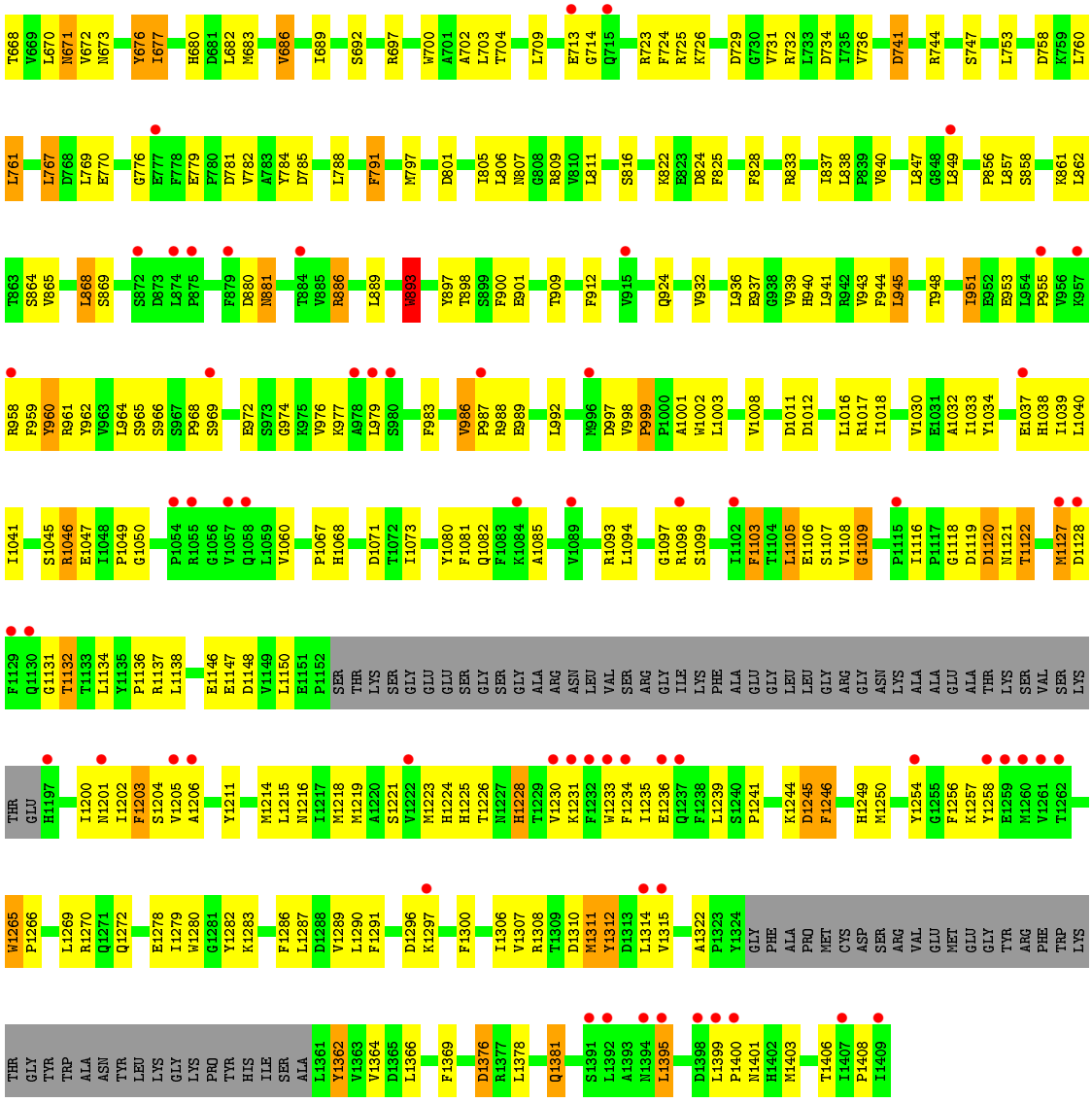




- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain B:




T668 V669 L670 N671 V672 N673 Y676 I677 H680 D681 L682 M683 V686 I689 S692 R697 W700 A701 A702 L703 T704 L709 E713 G714 Q715 R723 F724 R725 K726 D729 G730 V731 R732 L733 D734 I735 V736 D741 R744 S747 L753 D758 K759 L760
L761 L767 D768 L769 E770 G776 E777 F778 E779 F780 D781 V782 A783 Y784 D785 L788 F791 M797 D801 I805 L806 N807 G808 R809 V810 L811 S816 K822 E823 D824 F825 F828 R833 I837 L838 P839 V840 L847 G848 L849 P856 L857 S858 K861 L862
T863 S864 V865 L868 S869 S872 D873 L874 P875 F879 D880 N881 T884 V885 R886 L889 W893 Y897 T898 S899 F900 E901 T909 F912 V915 Q924 V932 L936 E937 G938 V939 H940 L941 R942 V943 F944 L945 T948 I951 E952 E953 L954 P955 V956 K957
R958 F959 Y960 R961 Y962 V963 L964 S965 S966 S967 P968 S969 E972 S973 G974 K975 V976 K977 A978 I979 S980 F983 V986 P987 R988 E989 L992 M996 D997 V998 P999 P1000 A1001 W1002 L1003 V1008 D1011 D1012 L1016 R1017 I1018 V1030 E1031 A1032 I1033 Y1034 E1037 H1038 I1039 L1040
I1041 S1045 R1046 E1047 I1048 P1049 G1050 P1054 R1055 G1056 V1057 Q1058 L1059 V1060 P1067 H1068 D1071 T1072 I1073 Y1080 F1081 Q1082 F1083 K1084 A1085 V1089 R1093 L1094 G1097 R1098 S1099 I1102 F1103 T1104 L1105 E1106 S1107 V1108 G1109 P1115 I1116 P1117 G1118 D1119 D1120 N1121 T1122 M1127 D1128
F1129 Q1130 G1131 T1132 T1133 L1134 Y1135 P1136 R1137 L1138 E1146 E1147 D1148 V1149 L1150 E1151 P1152 SER THR LYS SER GLY GLU GLU SER GLY SER GLY ALA ARG ASN LEU VAL SER ARG GLY ILE LYS PHE ALA GLU GLY LEU LEU GLY ARG GLY ASN LYS ALA ALA GLU GLU ALA THR LYS SER VAL SER LYS
THR GLU H1197 I1200 N1201 I1202 F1203 S1204 V1205 A1206 Y1211 M1214 L1215 N1216 I1217 M1218 M1219 A1220 S1221 V1222 M1223 H1224 H1225 T1226 N1227 H1228 T1229 V1230 K1231 F1232 W1233 F1234 I1235 E1236 Q1237 F1238 L1239 S1240 P1241 K1244 D1245 F1246 H1249 M1250 Y1254 G1255 F1256 K1257 Y1258 E1259 M1260 V1261 T1262
W1265 P1266 L1269 R1270 Q1271 Q1272 E1278 I1279 W1280 G1281 Y1282 K1283 F1286 L1287 D1288 V1289 L1290 F1291 D1296 K1297 F1300 I1306 V1307 R1308 T1309 D1310 M1311 Y1312 D1313 L1314 V1315 A1322 P1323 Y1324 GLY PHE ALA PRO MET CYS ASP SER ARG VAL GLU MET GLU GLY TYR ARG PHE TRP LYS
THR GLY TYR TRP ALA ASN TYR LEU LYS GLY LYS PRO TYR HIS ILE SER ALA L1361 Y1362 V1363 V1364 D1365 L1366 F1369 D1376 R1377 L1378 Q1381 S1391 L1392 A1393 N1394 L1395 D1398 L1399 P1400 N1401 H1402 M1403 T1406 I1407 P1408 I1409

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	139.05Å 139.05Å 176.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	139.04 – 4.60 139.05 – 4.77	Depositor EDS
% Data completeness (in resolution range)	32.1 (139.04-4.60) 36.0 (139.05-4.77)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 4.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.203 , 0.234 0.202 , 0.228	Depositor DCC
R_{free} test set	339 reflections (5.63%)	wwPDB-VP
Wilson B-factor (Å^2)	206.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 500.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.369 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	20112	wwPDB-VP
Average B, all atoms (Å^2)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.64	0/10293	0.77	0/13959
1	B	0.63	0/10293	0.76	0/13959
All	All	0.63	0/20586	0.76	0/27918

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10056	0	9955	226	0
1	B	10056	0	9955	231	0
All	All	20112	0	19910	457	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 11.

All (457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:GLY:H	1:A:1136:PRO:HA	1.12	1.11
1:B:1109:GLY:H	1:B:1136:PRO:HA	1.12	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LYS:HA	1:A:385:LEU:HG	1.51	0.93
1:B:382:LYS:HA	1:B:385:LEU:HG	1.51	0.92
1:B:833:ARG:HA	1:B:837:ILE:HB	1.55	0.87
1:A:833:ARG:HA	1:A:837:ILE:HB	1.55	0.85
1:B:704:THR:HB	1:B:805:ILE:HB	1.59	0.85
1:A:704:THR:HB	1:A:805:ILE:HB	1.59	0.84
1:A:123:TYR:HA	1:A:127:VAL:HB	1.60	0.83
1:B:345:PHE:HB3	1:B:893:TRP:NE1	1.94	0.82
1:A:345:PHE:HB3	1:A:893:TRP:NE1	1.95	0.82
1:A:342:ARG:HG2	1:A:347:PRO:HA	1.63	0.81
1:B:123:TYR:HA	1:B:127:VAL:HB	1.60	0.81
1:B:342:ARG:HG2	1:B:347:PRO:HA	1.64	0.80
1:A:901:GLU:OE1	1:A:940:HIS:NE2	2.16	0.78
1:A:676:TYR:HA	1:A:683:MET:HG3	1.68	0.75
1:B:676:TYR:HA	1:B:683:MET:HG3	1.67	0.75
1:A:932:VAL:HG21	1:A:964:LEU:HB3	1.69	0.74
1:B:932:VAL:HG21	1:B:964:LEU:HB3	1.69	0.73
1:A:671:ASN:HA	1:A:864:SER:HB3	1.72	0.72
1:B:1109:GLY:N	1:B:1136:PRO:HA	1.97	0.72
1:A:31:ILE:HA	1:A:1030:VAL:HB	1.72	0.72
1:A:1109:GLY:N	1:A:1136:PRO:HA	1.97	0.71
1:B:671:ASN:HA	1:B:864:SER:HB3	1.71	0.71
1:B:384:VAL:HA	1:B:387:LEU:HG	1.73	0.71
1:B:901:GLU:OE1	1:B:940:HIS:NE2	2.16	0.70
1:A:61:TYR:OH	1:A:174:ARG:O	2.08	0.70
1:B:61:TYR:OH	1:B:174:ARG:O	2.08	0.70
1:A:384:VAL:HA	1:A:387:LEU:HG	1.73	0.70
1:B:31:ILE:HA	1:B:1030:VAL:HB	1.73	0.70
1:B:115:ARG:HA	1:B:1127:MET:HB2	1.73	0.69
1:A:342:ARG:CG	1:A:347:PRO:HA	2.23	0.69
1:A:115:ARG:HA	1:A:1127:MET:HB2	1.75	0.68
1:B:64:LEU:HD23	1:B:198:HIS:CE1	2.29	0.68
1:A:64:LEU:HD23	1:A:198:HIS:CE1	2.28	0.67
1:B:342:ARG:CG	1:B:347:PRO:HA	2.23	0.67
1:B:1201:ASN:HB3	1:B:1233:TRP:HE1	1.59	0.67
1:A:1201:ASN:HB3	1:A:1233:TRP:HE1	1.60	0.66
1:B:1225:HIS:CD2	1:B:1308:ARG:HA	2.30	0.66
1:B:898:THR:HB	1:B:945:LEU:HB3	1.78	0.66
1:B:1109:GLY:H	1:B:1136:PRO:CA	2.01	0.66
1:A:988:ARG:HA	1:A:1018:ILE:HB	1.78	0.66
1:A:898:THR:HB	1:A:945:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:ARG:HA	1:B:1018:ILE:HB	1.78	0.65
1:A:1225:HIS:CD2	1:A:1308:ARG:HA	2.31	0.65
1:B:658:LEU:HB3	1:B:811:LEU:HB3	1.79	0.65
1:A:236:LEU:HB3	1:A:992:LEU:HB3	1.79	0.65
1:A:78:ASP:HB2	1:A:974:GLY:O	1.97	0.65
1:A:398:LEU:HB3	1:A:886:ARG:HD3	1.79	0.65
1:B:236:LEU:HB3	1:B:992:LEU:HB3	1.79	0.64
1:B:378:ARG:HE	1:B:909:THR:HG21	1.62	0.64
1:A:378:ARG:HE	1:A:909:THR:HG21	1.61	0.64
1:B:78:ASP:HB2	1:B:974:GLY:O	1.97	0.64
1:B:105:LEU:HD12	1:B:966:SER:HA	1.79	0.64
1:B:398:LEU:HB3	1:B:886:ARG:HD3	1.79	0.64
1:A:658:LEU:HB3	1:A:811:LEU:HB3	1.79	0.64
1:A:858:SER:O	1:A:862:LEU:HG	1.98	0.64
1:B:858:SER:O	1:B:862:LEU:HG	1.98	0.63
1:A:105:LEU:HD12	1:A:966:SER:HA	1.79	0.63
1:A:192:LYS:HE2	1:A:192:LYS:HA	1.81	0.62
1:A:411:ASP:HA	1:A:664:LYS:HB3	1.80	0.62
1:B:411:ASP:HA	1:B:664:LYS:HB3	1.80	0.62
1:B:1311:MET:HA	1:B:1314:LEU:HD13	1.81	0.61
1:B:192:LYS:HA	1:B:192:LYS:HE2	1.81	0.61
1:A:1311:MET:HA	1:A:1314:LEU:HD13	1.83	0.61
1:B:140:GLN:HG3	1:B:187:ALA:HA	1.83	0.61
1:A:341:ASN:O	1:A:893:TRP:NE1	2.33	0.60
1:A:1109:GLY:H	1:A:1136:PRO:CA	2.01	0.60
1:B:341:ASN:O	1:B:893:TRP:NE1	2.33	0.60
1:A:686:VAL:HG11	1:A:736:VAL:HG22	1.84	0.60
1:A:237:VAL:O	1:A:992:LEU:HA	2.02	0.60
1:A:352:VAL:HG13	1:A:359:HIS:HD2	1.67	0.59
1:A:689:ILE:HG21	1:A:761:LEU:HD21	1.85	0.59
1:B:1322:ALA:HA	1:B:1408:PRO:HB2	1.85	0.59
1:B:366:GLN:HB2	1:B:367:PRO:HD2	1.83	0.59
1:B:686:VAL:HG11	1:B:736:VAL:HG22	1.84	0.59
1:A:140:GLN:HG3	1:A:187:ALA:HA	1.83	0.59
1:A:56:ASN:HB3	1:A:59:ILE:HB	1.83	0.59
1:B:689:ILE:HG21	1:B:761:LEU:HD21	1.85	0.59
1:A:366:GLN:HB2	1:A:367:PRO:HD2	1.84	0.59
1:B:237:VAL:O	1:B:992:LEU:HA	2.02	0.58
1:B:1205:VAL:HG11	1:B:1283:LYS:HE2	1.85	0.58
1:B:352:VAL:HG13	1:B:359:HIS:HD2	1.68	0.58
1:A:450:LEU:HD11	1:A:461:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1322:ALA:HA	1:A:1408:PRO:HB2	1.84	0.58
1:A:236:LEU:HB2	1:A:959:PHE:HB2	1.86	0.58
1:B:833:ARG:HG3	1:B:838:LEU:HG	1.86	0.58
1:A:676:TYR:OH	1:A:704:THR:OG1	2.18	0.58
1:B:1039:ILE:O	1:B:1085:ALA:O	2.22	0.57
1:B:236:LEU:HB2	1:B:959:PHE:HB2	1.86	0.57
1:A:1039:ILE:O	1:A:1085:ALA:O	2.21	0.57
1:B:450:LEU:HD11	1:B:461:ILE:HD13	1.87	0.57
1:A:411:ASP:HA	1:A:664:LYS:CB	2.35	0.57
1:B:179:GLY:HA3	1:B:210:ALA:HA	1.86	0.57
1:B:360:LEU:HB2	1:B:365:ILE:HD11	1.87	0.57
1:B:725:ARG:HD3	1:B:731:VAL:HB	1.86	0.57
1:A:179:GLY:HA3	1:A:210:ALA:HA	1.86	0.57
1:B:411:ASP:HA	1:B:664:LYS:CB	2.35	0.57
1:A:1223:MET:HG3	1:A:1256:PHE:HB3	1.87	0.57
1:A:725:ARG:HD3	1:A:731:VAL:HB	1.86	0.56
1:B:56:ASN:HB3	1:B:59:ILE:HB	1.85	0.56
1:B:1296:ASP:HA	1:B:1366:LEU:HB2	1.88	0.56
1:B:1108:VAL:HA	1:B:1136:PRO:HB3	1.87	0.56
1:A:360:LEU:HB2	1:A:365:ILE:HD11	1.87	0.56
1:A:822:LYS:HA	1:A:825:PHE:HD2	1.71	0.56
1:B:49:LEU:HD11	1:B:64:LEU:HD12	1.88	0.56
1:B:379:LYS:O	1:B:383:SER:OG	2.23	0.56
1:A:1205:VAL:HG11	1:A:1283:LYS:HE2	1.88	0.56
1:A:1272:GLN:HB2	1:A:1278:GLU:HG3	1.88	0.56
1:A:833:ARG:HG3	1:A:838:LEU:HG	1.87	0.56
1:B:676:TYR:OH	1:B:704:THR:OG1	2.18	0.56
1:A:1011:ASP:OD2	1:A:1030:VAL:HG13	2.06	0.55
1:B:1011:ASP:OD2	1:B:1030:VAL:HG13	2.06	0.55
1:B:1223:MET:HG3	1:B:1256:PHE:HB3	1.87	0.55
1:B:1272:GLN:HB2	1:B:1278:GLU:HG3	1.88	0.55
1:A:379:LYS:O	1:A:383:SER:OG	2.23	0.55
1:B:366:GLN:HB2	1:B:367:PRO:CD	2.37	0.55
1:B:822:LYS:HA	1:B:825:PHE:HD2	1.70	0.55
1:A:1080:TYR:CE2	1:A:1266:PRO:HG3	2.42	0.55
1:B:1041:ILE:HD11	1:B:1085:ALA:HB3	1.88	0.55
1:A:1041:ILE:HD11	1:A:1085:ALA:HB3	1.89	0.55
1:A:315:THR:HG23	1:A:924:GLN:HB3	1.88	0.55
1:A:380:LEU:HG	1:A:865:VAL:HG13	1.88	0.55
1:B:315:THR:HG23	1:B:924:GLN:HB3	1.88	0.55
1:B:1003:LEU:HB2	1:B:1038:HIS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1283:LYS:O	1:B:1287:LEU:HG	2.07	0.55
1:A:470:VAL:O	1:A:501:PHE:HB2	2.07	0.55
1:A:366:GLN:HB2	1:A:367:PRO:CD	2.37	0.55
1:B:1362:TYR:C	1:B:1362:TYR:CD1	2.81	0.55
1:A:1296:ASP:HA	1:A:1366:LEU:HB2	1.89	0.54
1:A:1362:TYR:C	1:A:1362:TYR:CD1	2.81	0.54
1:B:1235:ILE:O	1:B:1239:LEU:HG	2.08	0.54
1:A:1362:TYR:C	1:A:1362:TYR:HD1	2.10	0.54
1:B:807:ASN:O	1:B:864:SER:OG	2.26	0.54
1:A:1108:VAL:HA	1:A:1136:PRO:HB3	1.87	0.54
1:A:49:LEU:HD11	1:A:64:LEU:HD12	1.89	0.54
1:B:1362:TYR:C	1:B:1362:TYR:HD1	2.10	0.54
1:B:380:LEU:HG	1:B:865:VAL:HG13	1.88	0.54
1:B:1080:TYR:CE2	1:B:1266:PRO:HG3	2.42	0.54
1:A:144:ILE:HG13	1:A:183:VAL:HB	1.89	0.53
1:A:325:LEU:HA	1:A:330:VAL:HG21	1.89	0.53
1:B:355:LEU:HB2	1:B:360:LEU:HD11	1.89	0.53
1:B:355:LEU:HD13	1:B:912:PHE:CZ	2.44	0.53
1:A:1235:ILE:O	1:A:1239:LEU:HG	2.08	0.53
1:A:1283:LYS:O	1:A:1287:LEU:HG	2.07	0.53
1:B:470:VAL:O	1:B:501:PHE:HB2	2.08	0.53
1:A:1107:SER:HB3	1:A:1120:ASP:HA	1.91	0.53
1:A:355:LEU:HB2	1:A:360:LEU:HD11	1.89	0.53
1:A:89:LEU:HA	1:A:94:HIS:CD2	2.43	0.53
1:A:807:ASN:O	1:A:864:SER:OG	2.26	0.53
1:B:89:LEU:HA	1:B:94:HIS:CD2	2.43	0.53
1:B:144:ILE:HG13	1:B:183:VAL:HB	1.91	0.53
1:B:869:SER:HB2	1:B:886:ARG:HD2	1.90	0.53
1:A:1003:LEU:HB2	1:A:1038:HIS:HB2	1.90	0.53
1:A:610:GLU:O	1:A:1050:GLY:HA2	2.09	0.52
1:A:741:ASP:HB2	1:A:744:ARG:HB2	1.89	0.52
1:B:998:VAL:O	1:B:999:PRO:O	2.27	0.52
1:B:113:THR:N	1:B:114:PRO:HD2	2.25	0.52
1:A:869:SER:HB2	1:A:886:ARG:HD2	1.90	0.52
1:B:292:ALA:HA	1:B:295:MET:SD	2.50	0.52
1:A:113:THR:N	1:A:114:PRO:HD2	2.25	0.52
1:A:747:SER:HB3	1:A:784:TYR:HB3	1.92	0.52
1:B:960:TYR:O	1:B:961:ARG:HG2	2.10	0.52
1:A:355:LEU:HD13	1:A:912:PHE:CZ	2.43	0.52
1:B:325:LEU:HA	1:B:330:VAL:HG21	1.90	0.52
1:A:1221:SER:HB2	1:A:1306:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:CYS:HB3	1:A:205:ALA:HB1	1.91	0.52
1:B:345:PHE:HB3	1:B:893:TRP:CE2	2.45	0.52
1:B:741:ASP:HB2	1:B:744:ARG:HB2	1.90	0.52
1:A:960:TYR:O	1:A:961:ARG:HG2	2.10	0.52
1:A:998:VAL:O	1:A:999:PRO:O	2.27	0.52
1:B:610:GLU:O	1:B:1050:GLY:HA2	2.10	0.52
1:B:1107:SER:HB3	1:B:1120:ASP:HA	1.91	0.52
1:B:572:PHE:HA	1:B:577:HIS:ND1	2.25	0.51
1:B:1108:VAL:HB	1:B:1122:THR:HA	1.92	0.51
1:A:998:VAL:CG2	1:A:999:PRO:HD2	2.41	0.51
1:B:1221:SER:HB2	1:B:1306:ILE:HG23	1.92	0.51
1:A:292:ALA:HA	1:A:295:MET:SD	2.51	0.51
1:A:572:PHE:HA	1:A:577:HIS:ND1	2.26	0.51
1:B:1216:ASN:HA	1:B:1219:MET:SD	2.51	0.51
1:B:858:SER:HA	1:B:861:LYS:HD2	1.92	0.51
1:A:1108:VAL:HB	1:A:1122:THR:HA	1.93	0.51
1:A:1228:HIS:NE2	1:A:1310:ASP:OD1	2.44	0.51
1:A:858:SER:HA	1:A:861:LYS:HD2	1.92	0.50
1:B:747:SER:HB3	1:B:784:TYR:HB3	1.93	0.50
1:B:177:CYS:HB3	1:B:205:ALA:HB1	1.92	0.50
1:B:1200:ILE:CD1	1:B:1228:HIS:CD2	2.95	0.50
1:B:1226:THR:OG1	1:B:1228:HIS:CD2	2.65	0.50
1:B:998:VAL:CG2	1:B:999:PRO:HD2	2.41	0.50
1:B:1228:HIS:NE2	1:B:1310:ASP:OD1	2.44	0.50
1:A:1226:THR:OG1	1:A:1228:HIS:CD2	2.65	0.50
1:A:1216:ASN:HA	1:A:1219:MET:SD	2.51	0.50
1:A:345:PHE:HB3	1:A:893:TRP:CE2	2.45	0.50
1:B:208:GLY:HA3	1:B:782:VAL:HB	1.94	0.49
1:A:352:VAL:HG13	1:A:359:HIS:CD2	2.47	0.49
1:B:352:VAL:HG13	1:B:359:HIS:CD2	2.46	0.49
1:B:989:GLU:HA	1:B:1017:ARG:HG2	1.95	0.49
1:A:208:GLY:HA3	1:A:782:VAL:HB	1.94	0.49
1:A:387:LEU:HD21	1:A:861:LYS:HD3	1.95	0.49
1:A:560:ARG:N	1:A:561:PRO:HD3	2.28	0.49
1:B:1080:TYR:OH	1:B:1082:GLN:NE2	2.42	0.49
1:B:1282:TYR:O	1:B:1286:PHE:O	2.31	0.49
1:B:108:SER:OG	1:B:965:SER:O	2.21	0.49
1:B:1108:VAL:HG13	1:B:1136:PRO:HG3	1.95	0.49
1:A:1200:ILE:CD1	1:A:1228:HIS:CD2	2.95	0.49
1:B:1099:SER:O	1:B:1103:PHE:O	2.30	0.49
1:B:1307:VAL:HG11	1:B:1311:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:GLY:O	1:A:605:PHE:O	2.32	0.48
1:A:811:LEU:HD11	1:A:828:PHE:CE2	2.48	0.48
1:B:560:ARG:N	1:B:561:PRO:HD3	2.29	0.48
1:B:697:ARG:HA	1:B:700:TRP:CE3	2.48	0.48
1:B:811:LEU:HD11	1:B:828:PHE:CE2	2.48	0.48
1:A:1099:SER:O	1:A:1103:PHE:O	2.30	0.48
1:A:1282:TYR:O	1:A:1286:PHE:O	2.31	0.48
1:B:387:LEU:HD21	1:B:861:LYS:HD3	1.96	0.48
1:B:92:ASP:OD1	1:B:92:ASP:N	2.46	0.48
1:B:105:LEU:HD11	1:B:932:VAL:HG12	1.96	0.48
1:A:1047:GLU:HA	1:A:1138:LEU:O	2.14	0.48
1:B:1239:LEU:HB2	1:B:1244:LYS:HE3	1.96	0.48
1:A:366:GLN:O	1:A:370:LEU:HB2	2.14	0.48
1:A:53:ALA:HB1	1:A:60:TYR:HA	1.95	0.48
1:B:1030:VAL:HG12	1:B:1032:ALA:H	1.79	0.48
1:B:53:ALA:HB1	1:B:60:TYR:HA	1.96	0.48
1:A:1030:VAL:HG12	1:A:1032:ALA:H	1.79	0.48
1:A:1239:LEU:HB2	1:A:1244:LYS:HE3	1.96	0.48
1:A:92:ASP:OD1	1:A:92:ASP:N	2.46	0.48
1:B:1047:GLU:HA	1:B:1138:LEU:O	2.14	0.48
1:B:366:GLN:O	1:B:370:LEU:HB2	2.14	0.48
1:A:989:GLU:HA	1:A:1017:ARG:HG2	1.95	0.48
1:B:1040:LEU:O	1:B:1131:GLY:HA2	2.14	0.48
1:B:724:PHE:HA	1:B:822:LYS:HE2	1.95	0.48
1:A:1073:ILE:HG12	1:A:1289:VAL:HG12	1.96	0.47
1:A:724:PHE:HA	1:A:822:LYS:HE2	1.95	0.47
1:B:604:GLY:O	1:B:605:PHE:O	2.31	0.47
1:B:1280:TRP:HB3	1:B:1395:LEU:HG	1.95	0.47
1:B:97:PRO:O	1:B:937:GLU:OE1	2.33	0.47
1:A:724:PHE:HA	1:A:822:LYS:CE	2.44	0.47
1:B:724:PHE:HA	1:B:822:LYS:CE	2.44	0.47
1:B:1073:ILE:HG12	1:B:1289:VAL:HG12	1.97	0.47
1:B:791:PHE:CZ	1:B:797:MET:SD	3.07	0.47
1:A:1108:VAL:HG13	1:A:1136:PRO:HG3	1.96	0.47
1:A:1376:ASP:OD1	1:A:1376:ASP:N	2.47	0.47
1:A:1307:VAL:HG11	1:A:1311:MET:SD	2.54	0.47
1:B:703:LEU:HD12	1:B:806:LEU:HB2	1.97	0.47
1:B:1376:ASP:OD1	1:B:1376:ASP:N	2.47	0.47
1:A:176:PHE:CD2	1:A:205:ALA:HB3	2.50	0.47
1:A:697:ARG:HA	1:A:700:TRP:CE3	2.49	0.47
1:B:176:PHE:CD2	1:B:205:ALA:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:LEU:N	1:B:644:PRO:HD2	2.30	0.47
1:A:1280:TRP:HB3	1:A:1395:LEU:HG	1.95	0.46
1:A:791:PHE:CZ	1:A:797:MET:SD	3.08	0.46
1:A:97:PRO:O	1:A:937:GLU:OE1	2.33	0.46
1:A:1040:LEU:O	1:A:1131:GLY:HA2	2.14	0.46
1:A:986:VAL:HG22	1:A:987:PRO:HD2	1.97	0.46
1:A:167:LEU:HA	1:A:184:ILE:HD11	1.96	0.46
1:A:643:LEU:N	1:A:644:PRO:HD2	2.30	0.46
1:A:1001:ALA:HB1	1:A:1040:LEU:HB2	1.97	0.46
1:B:1001:ALA:HB1	1:B:1040:LEU:HB2	1.97	0.46
1:B:186:TYR:HE1	1:B:215:ARG:HD2	1.81	0.46
1:B:723:ARG:HA	1:B:726:LYS:HE3	1.97	0.46
1:A:105:LEU:HD11	1:A:932:VAL:HG12	1.96	0.46
1:A:1134:LEU:C	1:A:1136:PRO:HD3	2.36	0.46
1:A:767:LEU:HA	1:A:770:GLU:HG2	1.97	0.46
1:A:713:GLU:HB3	1:A:816:SER:HA	1.98	0.46
1:B:713:GLU:HB3	1:B:816:SER:HA	1.98	0.46
1:B:104:LYS:HB3	1:B:968:PRO:HD3	1.98	0.46
1:B:1134:LEU:C	1:B:1136:PRO:HD3	2.36	0.46
1:B:1201:ASN:O	1:B:1202:ILE:HG13	2.16	0.46
1:B:167:LEU:HA	1:B:184:ILE:HD11	1.96	0.46
1:A:1200:ILE:HD11	1:A:1312:TYR:HD1	1.81	0.45
1:A:723:ARG:HA	1:A:726:LYS:HE3	1.97	0.45
1:B:560:ARG:N	1:B:561:PRO:CD	2.80	0.45
1:A:1046:ARG:HE	1:A:1137:ARG:HG2	1.80	0.45
1:A:969:SER:HB2	1:A:977:LYS:HD3	1.98	0.45
1:B:1046:ARG:HE	1:B:1137:ARG:HG2	1.80	0.45
1:B:961:ARG:HG2	1:B:983:PHE:CE2	2.52	0.45
1:A:1080:TYR:OH	1:A:1082:GLN:NE2	2.42	0.45
1:A:186:TYR:HE1	1:A:215:ARG:HD2	1.81	0.45
1:A:702:ALA:HA	1:A:732:ARG:HB3	1.99	0.45
1:A:1201:ASN:O	1:A:1202:ILE:HG13	2.16	0.45
1:A:119:HIS:NE2	1:A:172:PHE:CD1	2.85	0.45
1:A:573:ILE:HG22	1:A:574:SER:H	1.81	0.45
1:A:45:LEU:HD12	1:A:81:LEU:HD21	1.99	0.45
1:A:998:VAL:HG21	1:A:1002:TRP:CE3	2.52	0.45
1:B:767:LEU:HA	1:B:770:GLU:HG2	1.98	0.45
1:A:1241:PRO:O	1:A:1245:ASP:OD1	2.35	0.45
1:A:900:PHE:CZ	1:A:943:VAL:HB	2.52	0.45
1:A:108:SER:OG	1:A:965:SER:O	2.21	0.45
1:B:66:ARG:HB2	1:B:72:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:VAL:HG22	1:B:987:PRO:HD2	1.99	0.45
1:B:998:VAL:HG21	1:B:1002:TRP:CE3	2.52	0.45
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.52	0.45
1:B:1008:VAL:HB	1:B:1033:ILE:HB	1.99	0.45
1:B:900:PHE:CZ	1:B:943:VAL:HB	2.52	0.45
1:A:560:ARG:N	1:A:561:PRO:CD	2.80	0.45
1:A:66:ARG:HB2	1:A:72:PHE:CE2	2.52	0.45
1:B:119:HIS:NE2	1:B:172:PHE:CD1	2.85	0.45
1:B:382:LYS:HG2	1:B:385:LEU:HD21	1.98	0.45
1:B:45:LEU:HD12	1:B:81:LEU:HD21	1.99	0.45
1:A:104:LYS:HB3	1:A:968:PRO:HD3	1.99	0.45
1:A:616:VAL:HA	1:A:619:HIS:CD2	2.52	0.45
1:B:1241:PRO:O	1:B:1245:ASP:OD1	2.35	0.44
1:B:573:ILE:HG22	1:B:574:SER:H	1.81	0.44
1:B:969:SER:HB2	1:B:977:LYS:HD3	1.98	0.44
1:A:382:LYS:HG2	1:A:385:LEU:HD21	1.98	0.44
1:B:702:ALA:HA	1:B:732:ARG:HB3	2.00	0.44
1:A:703:LEU:HD12	1:A:806:LEU:HB2	1.98	0.44
1:A:732:ARG:HB2	1:A:856:PRO:HG2	1.99	0.44
1:B:128:GLU:N	1:B:129:PRO:HD2	2.33	0.44
1:B:732:ARG:HB2	1:B:856:PRO:HG2	1.99	0.44
1:A:1008:VAL:HB	1:A:1033:ILE:HB	2.00	0.44
1:B:89:LEU:HA	1:B:94:HIS:HB2	1.99	0.44
1:A:1265:TRP:HE1	1:A:1269:LEU:HG	1.83	0.44
1:A:110:ARG:CZ	1:A:976:VAL:HG11	2.48	0.44
1:B:1378:LEU:HA	1:B:1381:GLN:HB2	2.00	0.44
1:B:589:GLU:HA	1:B:589:GLU:OE1	2.17	0.44
1:A:554:ILE:HG21	1:A:568:PHE:CE1	2.53	0.44
1:A:89:LEU:HA	1:A:94:HIS:HB2	1.99	0.44
1:B:110:ARG:CZ	1:B:976:VAL:HG11	2.48	0.44
1:B:1200:ILE:HD11	1:B:1312:TYR:HD1	1.82	0.44
1:A:1081:PHE:HZ	1:A:1134:LEU:HB2	1.82	0.44
1:A:128:GLU:N	1:A:129:PRO:HD2	2.33	0.44
1:A:1297:LYS:HD2	1:A:1315:VAL:HG13	1.99	0.43
1:A:1399:LEU:N	1:A:1400:PRO:HD2	2.32	0.43
1:B:1081:PHE:HZ	1:B:1134:LEU:HB2	1.82	0.43
1:B:1399:LEU:N	1:B:1400:PRO:HD2	2.32	0.43
1:B:616:VAL:HA	1:B:619:HIS:CD2	2.52	0.43
1:A:380:LEU:HD13	1:A:868:LEU:HD22	2.00	0.43
1:B:1148:ASP:O	1:B:1148:ASP:OD1	2.36	0.43
1:B:1205:VAL:HG21	1:B:1279:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1297:LYS:HD2	1:B:1315:VAL:HG13	1.99	0.43
1:B:144:ILE:HD13	1:B:154:LEU:HD21	2.01	0.43
1:B:90:ARG:HG3	1:B:100:LEU:HD11	2.00	0.43
1:A:144:ILE:HD13	1:A:154:LEU:HD21	2.00	0.43
1:B:572:PHE:CD1	1:B:572:PHE:N	2.86	0.43
1:B:380:LEU:HD13	1:B:868:LEU:HD22	2.01	0.43
1:A:208:GLY:HA3	1:A:782:VAL:CG1	2.49	0.43
1:A:572:PHE:CD1	1:A:572:PHE:N	2.87	0.43
1:B:532:TYR:O	1:B:536:SER:N	2.47	0.43
1:B:37:ALA:HB3	1:B:227:LEU:HB3	2.01	0.43
1:A:67:ILE:HB	1:A:194:PHE:HZ	1.84	0.43
1:B:97:PRO:HA	1:B:100:LEU:HG	1.99	0.43
1:B:53:ALA:HB2	1:B:59:ILE:HG22	2.00	0.43
1:A:1105:LEU:HD12	1:A:1105:LEU:O	2.19	0.43
1:B:154:LEU:O	1:B:155:ASP:CG	2.57	0.43
1:B:654:ARG:NH1	1:B:824:ASP:OD2	2.52	0.43
1:A:505:THR:N	1:A:506:PRO:HD3	2.34	0.43
1:B:554:ILE:HG21	1:B:568:PHE:CE1	2.54	0.43
1:A:1148:ASP:O	1:A:1148:ASP:OD1	2.36	0.43
1:A:154:LEU:O	1:A:155:ASP:CG	2.56	0.43
1:A:37:ALA:HB3	1:A:227:LEU:HB3	2.00	0.42
1:B:1265:TRP:HE1	1:B:1269:LEU:HG	1.83	0.42
1:B:505:THR:N	1:B:506:PRO:HD3	2.34	0.42
1:A:1378:LEU:HA	1:A:1381:GLN:HB2	2.00	0.42
1:A:654:ARG:NH1	1:A:824:ASP:OD2	2.52	0.42
1:B:1119:ASP:C	1:B:1121:ASN:H	2.23	0.42
1:B:673:ASN:OD1	1:B:677:ILE:HD12	2.20	0.42
1:A:97:PRO:HA	1:A:100:LEU:HG	2.00	0.42
1:A:1060:VAL:HB	1:A:1093:ARG:HG2	2.00	0.42
1:A:53:ALA:HB2	1:A:59:ILE:HG22	2.01	0.42
1:A:998:VAL:O	1:A:999:PRO:C	2.58	0.42
1:B:67:ILE:HB	1:B:194:PHE:HZ	1.84	0.42
1:B:208:GLY:HA3	1:B:782:VAL:CG1	2.49	0.42
1:B:936:LEU:HB2	1:B:939:VAL:HG21	2.02	0.42
1:B:998:VAL:O	1:B:999:PRO:C	2.58	0.42
1:A:90:ARG:HG3	1:A:100:LEU:HD11	2.01	0.42
1:B:682:LEU:HD13	1:B:788:LEU:HB2	2.01	0.42
1:A:1116:ILE:HG22	1:A:1118:GLY:H	1.85	0.42
1:A:1403:MET:HB3	1:A:1406:THR:OG1	2.20	0.42
1:A:1203:PHE:CD2	1:A:1300:PHE:HB2	2.55	0.42
1:A:682:LEU:HD22	1:A:788:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1103:PHE:CD1	1:B:1138:LEU:HD22	2.55	0.42
1:B:1206:ALA:HB3	1:B:1239:LEU:CD2	2.50	0.42
1:B:747:SER:HB2	1:B:781:ASP:HB3	2.02	0.42
1:B:389:LEU:HG	1:B:849:LEU:HD22	2.01	0.42
1:A:1119:ASP:C	1:A:1121:ASN:H	2.23	0.42
1:A:747:SER:HB2	1:A:781:ASP:HB3	2.01	0.42
1:B:1060:VAL:HB	1:B:1093:ARG:HG2	2.00	0.42
1:B:143:LEU:HD23	1:B:184:ILE:HD12	2.02	0.42
1:B:332:ALA:HB1	1:B:334:PHE:CE2	2.55	0.42
1:A:204:LEU:HG	1:A:210:ALA:HB3	2.02	0.42
1:A:689:ILE:HD11	1:A:760:LEU:HD13	2.02	0.42
1:B:1116:ILE:HG22	1:B:1118:GLY:H	1.84	0.42
1:B:335:GLU:HB3	1:B:897:TYR:HB3	2.02	0.42
1:A:109:LEU:HA	1:A:230:ASN:HD21	1.85	0.41
1:B:371:VAL:HA	1:B:374:LEU:HG	2.02	0.41
1:A:1205:VAL:HG21	1:A:1279:ILE:HG23	2.02	0.41
1:A:490:PHE:HB3	1:A:499:PHE:CE2	2.56	0.41
1:B:109:LEU:HA	1:B:230:ASN:HD21	1.85	0.41
1:A:403:VAL:C	1:A:405:HIS:H	2.24	0.41
1:B:1105:LEU:HD12	1:B:1105:LEU:O	2.20	0.41
1:B:427:VAL:HG21	1:B:587:TRP:HB3	2.01	0.41
1:B:572:PHE:HD1	1:B:572:PHE:N	2.18	0.41
1:A:589:GLU:OE1	1:A:589:GLU:HA	2.19	0.41
1:B:1403:MET:HB3	1:B:1406:THR:OG1	2.20	0.41
1:B:204:LEU:HG	1:B:210:ALA:HB3	2.02	0.41
1:B:403:VAL:C	1:B:405:HIS:H	2.24	0.41
1:B:423:GLU:O	1:B:424:GLU:HB2	2.20	0.41
1:B:400:HIS:HE2	1:B:847:LEU:HD13	1.86	0.41
1:A:1204:SER:HB3	1:A:1215:LEU:HD12	2.03	0.41
1:B:1250:MET:HG3	1:B:1256:PHE:CZ	2.56	0.41
1:B:1203:PHE:CD2	1:B:1300:PHE:HB2	2.55	0.41
1:B:951:ILE:HG21	1:B:955:PRO:HG3	2.01	0.41
1:A:1103:PHE:CD1	1:A:1138:LEU:HD22	2.55	0.41
1:A:1107:SER:CB	1:A:1120:ASP:HA	2.50	0.41
1:A:1206:ALA:HB3	1:A:1239:LEU:CD2	2.50	0.41
1:A:1378:LEU:HD22	1:A:1399:LEU:HD23	2.02	0.41
1:A:423:GLU:O	1:A:424:GLU:HB2	2.21	0.41
1:B:39:PHE:CE2	1:B:227:LEU:HD22	2.56	0.41
1:B:682:LEU:HD22	1:B:788:LEU:HA	2.01	0.41
1:A:1201:ASN:HB3	1:A:1233:TRP:NE1	2.33	0.41
1:A:342:ARG:HG2	1:A:347:PRO:CA	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CE2	1:A:227:LEU:HD22	2.55	0.41
1:A:488:LEU:O	1:A:492:LYS:HB2	2.21	0.41
1:B:176:PHE:HB3	1:B:212:TYR:HB3	2.02	0.41
1:B:490:PHE:HB3	1:B:499:PHE:CE2	2.55	0.41
1:B:231:GLY:HA2	1:B:964:LEU:CD1	2.50	0.41
1:A:682:LEU:HD13	1:A:788:LEU:HB2	2.01	0.41
1:A:335:GLU:HB3	1:A:897:TYR:HB3	2.02	0.41
1:A:231:GLY:HA2	1:A:964:LEU:CD1	2.51	0.41
1:B:1200:ILE:O	1:B:1230:VAL:HA	2.21	0.41
1:B:1399:LEU:N	1:B:1400:PRO:CD	2.84	0.41
1:A:673:ASN:OD1	1:A:677:ILE:HD12	2.20	0.41
1:B:1132:THR:O	1:B:1134:LEU:HG	2.21	0.41
1:B:195:ALA:HB3	1:B:196:PRO:HD3	2.03	0.41
1:A:427:VAL:HG21	1:A:587:TRP:HB3	2.02	0.41
1:A:554:ILE:O	1:A:558:SER:HB2	2.21	0.41
1:A:893:TRP:HB3	1:A:944:PHE:CZ	2.56	0.41
1:B:998:VAL:HG22	1:B:999:PRO:HD2	2.02	0.41
1:A:936:LEU:HB2	1:A:939:VAL:HG21	2.02	0.41
1:B:465:VAL:HG22	1:B:643:LEU:HD13	2.03	0.41
1:B:488:LEU:O	1:B:492:LYS:HB2	2.21	0.41
1:A:143:LEU:HD23	1:A:184:ILE:HD12	2.02	0.40
1:A:572:PHE:HD1	1:A:572:PHE:N	2.18	0.40
1:B:427:VAL:HG13	1:B:428:ILE:H	1.86	0.40
1:A:961:ARG:HG2	1:A:983:PHE:CZ	2.56	0.40
1:B:1246:PHE:HA	1:B:1249:HIS:ND1	2.36	0.40
1:A:1246:PHE:HA	1:A:1249:HIS:ND1	2.36	0.40
1:A:332:ALA:HB1	1:A:334:PHE:CE2	2.56	0.40
1:A:420:ASP:HA	1:A:423:GLU:OE1	2.21	0.40
1:B:1201:ASN:CB	1:B:1233:TRP:HE1	2.30	0.40
1:B:1378:LEU:HD22	1:B:1399:LEU:HD23	2.02	0.40
1:B:420:ASP:HA	1:B:423:GLU:OE1	2.21	0.40
1:B:689:ILE:HD11	1:B:760:LEU:HD13	2.02	0.40
1:B:961:ARG:HG2	1:B:983:PHE:CZ	2.56	0.40
1:A:1053:ALA:HA	1:A:1054:PRO:HD3	1.92	0.40
1:A:1132:THR:O	1:A:1134:LEU:HG	2.21	0.40
1:A:1250:MET:HG3	1:A:1256:PHE:CZ	2.56	0.40
1:A:389:LEU:HG	1:A:849:LEU:HD22	2.02	0.40
1:A:600:VAL:HG12	1:A:601:PHE:N	2.36	0.40
1:B:382:LYS:HA	1:B:385:LEU:CG	2.37	0.40
1:A:449:VAL:HB	1:A:461:ILE:HD12	2.04	0.40
1:A:53:ALA:HB2	1:A:63:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:HIS:HE2	1:A:847:LEU:HD13	1.86	0.40
1:B:1201:ASN:HB3	1:B:1233:TRP:NE1	2.33	0.40
1:B:1231:LYS:HE3	1:B:1257:LYS:HD2	2.03	0.40
1:B:554:ILE:O	1:B:558:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1246/1382 (90%)	988 (79%)	208 (17%)	50 (4%)	3 26
1	B	1246/1382 (90%)	989 (79%)	207 (17%)	50 (4%)	3 26
All	All	2492/2764 (90%)	1977 (79%)	415 (17%)	100 (4%)	3 26

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
1	A	424	GLU
1	A	427	VAL
1	A	506	PRO
1	A	541	SER
1	A	592	ARG
1	A	605	PHE
1	A	651	ALA
1	A	880	ASP
1	A	972	GLU
1	A	999	PRO
1	A	1067	PRO
1	A	1236	GLU
1	B	155	ASP

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Mol	Chain	Res	Type
1	B	424	GLU
1	B	427	VAL
1	B	506	PRO
1	B	541	SER
1	B	592	ARG
1	B	605	PHE
1	B	651	ALA
1	B	880	ASP
1	B	999	PRO
1	B	1067	PRO
1	B	1236	GLU
1	A	163	GLY
1	A	329	ASN
1	A	331	SER
1	A	367	PRO
1	A	508	GLY
1	A	572	PHE
1	A	578	GLU
1	A	881	ASN
1	A	1146	GLU
1	B	163	GLY
1	B	329	ASN
1	B	331	SER
1	B	367	PRO
1	B	508	GLY
1	B	572	PHE
1	B	578	GLU
1	B	881	ASN
1	B	972	GLU
1	B	1146	GLU
1	A	99	ALA
1	A	131	LEU
1	A	347	PRO
1	A	569	LYS
1	A	611	ASP
1	A	666	GLU
1	A	714	GLY
1	A	776	GLY
1	A	857	LEU
1	A	893	TRP
1	B	99	ALA
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	347	PRO
1	B	569	LYS
1	B	611	ASP
1	B	666	GLU
1	B	714	GLY
1	B	776	GLY
1	B	857	LEU
1	B	893	TRP
1	A	154	LEU
1	A	566	LEU
1	A	671	ASN
1	A	677	ILE
1	A	692	SER
1	A	1049	PRO
1	A	1097	GLY
1	A	1109	GLY
1	A	1270	ARG
1	B	154	LEU
1	B	566	LEU
1	B	671	ASN
1	B	677	ILE
1	B	692	SER
1	B	1049	PRO
1	B	1097	GLY
1	B	1109	GLY
1	B	1270	ARG
1	A	1127	MET
1	B	568	PHE
1	B	1311	MET
1	A	137	GLY
1	A	568	PHE
1	A	1098	ARG
1	A	1311	MET
1	B	137	GLY
1	B	1098	ARG
1	B	1127	MET
1	A	93	GLY
1	A	388	GLY
1	A	409	GLY
1	B	388	GLY
1	B	409	GLY
1	A	326	GLY

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Mol	Chain	Res	Type
1	B	93	GLY
1	B	326	GLY

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	1097/1197 (92%)	961 (88%)	136 (12%)	4	21
1	B	1097/1197 (92%)	960 (88%)	137 (12%)	4	21
All	All	2194/2394 (92%)	1921 (88%)	273 (12%)	4	21

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	49	LEU
1	A	56	ASN
1	A	64	LEU
1	A	67	ILE
1	A	81	LEU
1	A	82	TYR
1	A	90	ARG
1	A	92	ASP
1	A	109	LEU
1	A	123	TYR
1	A	158	HIS
1	A	175	LYS
1	A	178	VAL
1	A	181	ARG
1	A	183	VAL
1	A	192	LYS
1	A	194	PHE
1	A	203	ASP
1	A	204	LEU
1	A	213	ARG

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Mol	Chain	Res	Type
1	A	222	HIS
1	A	243	TYR
1	A	300	PHE
1	A	315	THR
1	A	342	ARG
1	A	372	ASP
1	A	378	ARG
1	A	396	ASP
1	A	442	SER
1	A	453	HIS
1	A	460	GLN
1	A	462	ARG
1	A	479	ASP
1	A	521	LEU
1	A	522	GLU
1	A	534	GLU
1	A	539	GLU
1	A	550	PHE
1	A	554	ILE
1	A	555	LYS
1	A	572	PHE
1	A	573	ILE
1	A	576	LYS
1	A	585	LYS
1	A	605	PHE
1	A	609	ARG
1	A	612	ASN
1	A	617	MET
1	A	620	ARG
1	A	624	ASP
1	A	633	TYR
1	A	641	MET
1	A	662	GLU
1	A	663	ASP
1	A	667	LEU
1	A	668	THR
1	A	670	LEU
1	A	672	VAL
1	A	676	TYR
1	A	680	HIS
1	A	686	VAL
1	A	709	LEU

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Mol	Chain	Res	Type
1	A	729	ASP
1	A	734	ASP
1	A	741	ASP
1	A	753	LEU
1	A	758	ASP
1	A	761	LEU
1	A	767	LEU
1	A	769	LEU
1	A	779	GLU
1	A	785	ASP
1	A	791	PHE
1	A	801	ASP
1	A	809	ARG
1	A	840	VAL
1	A	868	LEU
1	A	886	ARG
1	A	889	LEU
1	A	893	TRP
1	A	941	LEU
1	A	944	PHE
1	A	945	LEU
1	A	948	THR
1	A	951	ILE
1	A	953	GLU
1	A	958	ARG
1	A	960	TYR
1	A	962	TYR
1	A	979	LEU
1	A	986	VAL
1	A	997	ASP
1	A	1010	VAL
1	A	1012	ASP
1	A	1016	LEU
1	A	1034	TYR
1	A	1037	GLU
1	A	1045	SER
1	A	1046	ARG
1	A	1068	HIS
1	A	1071	ASP
1	A	1094	LEU
1	A	1103	PHE
1	A	1105	LEU

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Mol	Chain	Res	Type
1	A	1106	GLU
1	A	1120	ASP
1	A	1122	THR
1	A	1128	ASP
1	A	1132	THR
1	A	1147	GLU
1	A	1150	LEU
1	A	1203	PHE
1	A	1204	SER
1	A	1211	TYR
1	A	1214	MET
1	A	1215	LEU
1	A	1218	MET
1	A	1224	HIS
1	A	1228	HIS
1	A	1234	PHE
1	A	1245	ASP
1	A	1246	PHE
1	A	1254	TYR
1	A	1258	TYR
1	A	1265	TRP
1	A	1290	LEU
1	A	1291	PHE
1	A	1312	TYR
1	A	1362	TYR
1	A	1364	VAL
1	A	1369	PHE
1	A	1376	ASP
1	A	1381	GLN
1	A	1395	LEU
1	A	1401	ASN
1	B	48	LEU
1	B	49	LEU
1	B	56	ASN
1	B	64	LEU
1	B	67	ILE
1	B	81	LEU
1	B	82	TYR
1	B	90	ARG
1	B	92	ASP
1	B	109	LEU
1	B	123	TYR

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Mol	Chain	Res	Type
1	B	158	HIS
1	B	175	LYS
1	B	178	VAL
1	B	181	ARG
1	B	183	VAL
1	B	192	LYS
1	B	194	PHE
1	B	203	ASP
1	B	204	LEU
1	B	213	ARG
1	B	222	HIS
1	B	243	TYR
1	B	300	PHE
1	B	315	THR
1	B	342	ARG
1	B	372	ASP
1	B	378	ARG
1	B	442	SER
1	B	453	HIS
1	B	460	GLN
1	B	462	ARG
1	B	479	ASP
1	B	521	LEU
1	B	522	GLU
1	B	534	GLU
1	B	539	GLU
1	B	550	PHE
1	B	554	ILE
1	B	555	LYS
1	B	572	PHE
1	B	573	ILE
1	B	576	LYS
1	B	585	LYS
1	B	589	GLU
1	B	605	PHE
1	B	609	ARG
1	B	612	ASN
1	B	617	MET
1	B	620	ARG
1	B	624	ASP
1	B	633	TYR
1	B	641	MET

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Mol	Chain	Res	Type
1	B	656	ASN
1	B	662	GLU
1	B	663	ASP
1	B	667	LEU
1	B	668	THR
1	B	670	LEU
1	B	672	VAL
1	B	676	TYR
1	B	680	HIS
1	B	686	VAL
1	B	709	LEU
1	B	729	ASP
1	B	734	ASP
1	B	741	ASP
1	B	753	LEU
1	B	758	ASP
1	B	761	LEU
1	B	767	LEU
1	B	769	LEU
1	B	779	GLU
1	B	785	ASP
1	B	791	PHE
1	B	801	ASP
1	B	809	ARG
1	B	840	VAL
1	B	868	LEU
1	B	881	ASN
1	B	886	ARG
1	B	889	LEU
1	B	893	TRP
1	B	941	LEU
1	B	944	PHE
1	B	945	LEU
1	B	948	THR
1	B	951	ILE
1	B	953	GLU
1	B	958	ARG
1	B	960	TYR
1	B	962	TYR
1	B	979	LEU
1	B	986	VAL
1	B	997	ASP

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Mol	Chain	Res	Type
1	B	1012	ASP
1	B	1016	LEU
1	B	1034	TYR
1	B	1037	GLU
1	B	1045	SER
1	B	1046	ARG
1	B	1068	HIS
1	B	1071	ASP
1	B	1094	LEU
1	B	1103	PHE
1	B	1105	LEU
1	B	1106	GLU
1	B	1120	ASP
1	B	1122	THR
1	B	1128	ASP
1	B	1132	THR
1	B	1147	GLU
1	B	1150	LEU
1	B	1203	PHE
1	B	1204	SER
1	B	1211	TYR
1	B	1214	MET
1	B	1215	LEU
1	B	1218	MET
1	B	1224	HIS
1	B	1228	HIS
1	B	1234	PHE
1	B	1245	ASP
1	B	1246	PHE
1	B	1254	TYR
1	B	1258	TYR
1	B	1265	TRP
1	B	1290	LEU
1	B	1291	PHE
1	B	1312	TYR
1	B	1362	TYR
1	B	1364	VAL
1	B	1369	PHE
1	B	1376	ASP
1	B	1381	GLN
1	B	1395	LEU
1	B	1401	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	166	GLN
1	A	198	HIS
1	A	351	ASN
1	A	359	HIS
1	A	366	GLN
1	A	612	ASN
1	A	638	ASN
1	A	656	ASN
1	A	728	ASN
1	A	876	GLN
1	A	881	ASN
1	A	946	ASN
1	A	1038	HIS
1	A	1044	HIS
1	A	1082	GLN
1	A	1225	HIS
1	A	1227	ASN
1	A	1272	GLN
1	A	1397	GLN
1	B	94	HIS
1	B	166	GLN
1	B	198	HIS
1	B	351	ASN
1	B	359	HIS
1	B	366	GLN
1	B	612	ASN
1	B	638	ASN
1	B	656	ASN
1	B	728	ASN
1	B	876	GLN
1	B	881	ASN
1	B	946	ASN
1	B	1038	HIS
1	B	1044	HIS
1	B	1082	GLN
1	B	1225	HIS
1	B	1227	ASN
1	B	1272	GLN
1	B	1397	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	1254/1382 (90%)	0.24	63 (5%) 28 25	73, 141, 251, 333	0
1	B	1254/1382 (90%)	0.50	121 (9%) 8 8	106, 188, 295, 398	0
All	All	2508/2764 (90%)	0.37	184 (7%) 15 13	73, 168, 272, 398	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	LYS	9.3
1	A	565	GLU	7.7
1	B	565	GLU	7.6
1	B	159	GLY	7.2
1	A	160	LYS	6.9
1	B	161	VAL	5.7
1	B	148	GLN	5.6
1	A	322	SER	5.2
1	A	325	LEU	5.0
1	B	1262	THR	5.0
1	B	1260	MET	4.7
1	B	162	LYS	4.4
1	B	1231	LYS	4.3
1	A	162	LYS	4.3
1	A	159	GLY	4.3
1	B	461	ILE	4.3
1	B	979	LEU	4.2
1	B	463	ARG	4.2
1	A	148	GLN	4.2
1	A	161	VAL	4.1
1	B	1399	LEU	4.1
1	A	324	SER	4.0
1	B	1392	LEU	4.0
1	B	1315	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	294	GLY	3.9
1	B	228	SER	3.9
1	B	576	LYS	3.9
1	B	1129	PHE	3.8
1	B	1128	ASP	3.8
1	B	1206	ALA	3.7
1	B	1400	PRO	3.7
1	A	446	SER	3.6
1	A	1260	MET	3.6
1	B	978	ALA	3.6
1	B	1055	ARG	3.6
1	B	713	GLU	3.6
1	A	1262	THR	3.6
1	A	1234	PHE	3.5
1	A	323	ASN	3.5
1	B	426	GLN	3.5
1	B	567	SER	3.4
1	B	166	GLN	3.4
1	B	1261	VAL	3.4
1	A	1231	LYS	3.4
1	B	1394	ASN	3.4
1	B	308	PHE	3.3
1	B	980	SER	3.3
1	B	879	PHE	3.2
1	A	1317	HIS	3.2
1	B	958	ARG	3.2
1	A	317	ASP	3.2
1	B	1197	HIS	3.1
1	B	1233	TRP	3.1
1	A	241	THR	3.1
1	B	165	ASP	3.1
1	B	389	LEU	3.1
1	B	434	LEU	3.1
1	A	142	PHE	3.0
1	B	96	ASP	3.0
1	B	446	SER	3.0
1	B	539	GLU	3.0
1	B	325	LEU	3.0
1	B	34	ALA	3.0
1	B	322	SER	3.0
1	B	1234	PHE	2.9
1	A	1385	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	432	ASN	2.9
1	B	875	PRO	2.9
1	B	410	ASP	2.9
1	A	1233	TRP	2.9
1	B	524	TYR	2.9
1	B	98	GLU	2.9
1	B	147	GLU	2.9
1	B	427	VAL	2.9
1	A	166	GLN	2.9
1	B	462	ARG	2.8
1	B	987	PRO	2.8
1	B	1232	PHE	2.8
1	A	872	SER	2.7
1	A	1201	ASN	2.7
1	B	1057	VAL	2.7
1	B	1127	MET	2.7
1	A	539	GLU	2.7
1	B	126	THR	2.7
1	B	566	LEU	2.7
1	A	42	PRO	2.7
1	B	1230	VAL	2.7
1	B	95	MET	2.7
1	B	1259	GLU	2.7
1	B	42	PRO	2.7
1	B	1058	GLN	2.7
1	A	1323	PRO	2.7
1	A	1261	VAL	2.7
1	A	320	LYS	2.6
1	A	713	GLU	2.6
1	A	566	LEU	2.6
1	B	628	LEU	2.6
1	A	293	LEU	2.6
1	A	319	PRO	2.6
1	B	1084	LYS	2.6
1	B	35	LEU	2.5
1	A	1206	ALA	2.5
1	B	1314	LEU	2.5
1	B	1037	GLU	2.5
1	B	1297	LYS	2.5
1	B	142	PHE	2.5
1	B	849	LEU	2.5
1	B	496	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1054	PRO	2.5
1	B	1205	VAL	2.4
1	B	363	ARG	2.4
1	B	915	VAL	2.4
1	A	447	ILE	2.4
1	A	1232	PHE	2.4
1	B	146	GLY	2.4
1	B	447	ILE	2.4
1	B	872	SER	2.4
1	A	1399	LEU	2.4
1	B	500	GLY	2.4
1	A	165	ASP	2.4
1	B	182	ASP	2.4
1	A	163	GLY	2.4
1	A	1395	LEU	2.4
1	B	1089	VAL	2.4
1	A	648	LEU	2.3
1	B	1130	GLN	2.3
1	A	1406	THR	2.3
1	B	957	LYS	2.3
1	A	1034	TYR	2.3
1	B	1407	ILE	2.3
1	A	523	ASN	2.3
1	B	235	GLU	2.3
1	A	564	VAL	2.3
1	B	444	SER	2.3
1	B	1098	ARG	2.3
1	A	576	LYS	2.3
1	B	1236	GLU	2.3
1	B	294	GLY	2.3
1	B	1254	TYR	2.3
1	A	141	TRP	2.3
1	A	1315	VAL	2.3
1	B	130	SER	2.2
1	A	389	LEU	2.2
1	B	1395	LEU	2.2
1	B	307	PRO	2.2
1	A	444	SER	2.2
1	B	969	SER	2.2
1	B	1237	GLN	2.2
1	B	955	PRO	2.2
1	A	1400	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1099	SER	2.2
1	B	1398	ASP	2.2
1	B	1391	SER	2.2
1	B	996	MET	2.2
1	A	499	PHE	2.2
1	B	320	LYS	2.2
1	B	1409	ILE	2.2
1	A	296	LYS	2.2
1	A	524	TYR	2.2
1	B	884	THR	2.1
1	A	716	GLU	2.1
1	A	1127	MET	2.1
1	B	1258	TYR	2.1
1	B	50	GLU	2.1
1	B	1222	VAL	2.1
1	B	1201	ASN	2.1
1	A	879	PHE	2.1
1	B	874	LEU	2.1
1	B	163	GLY	2.1
1	B	777	GLU	2.1
1	B	366	GLN	2.1
1	B	145	ASP	2.1
1	A	321	TYR	2.1
1	B	499	PHE	2.1
1	B	241	THR	2.1
1	B	1115	PRO	2.1
1	B	457	GLY	2.0
1	B	1102	ILE	2.0
1	A	140	GLN	2.0
1	B	715	GLN	2.0
1	A	463	ARG	2.0
1	B	431	LEU	2.0
1	B	388	GLY	2.0
1	A	364	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.