Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 04:48 PM EST

PDB ID	:	3AGP
Title	:	Structure of viral polymerase form I
Authors	:	Takeshita, D.; Tomita, K.
Deposited on	:	2010-04-06
Resolution	:	2.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

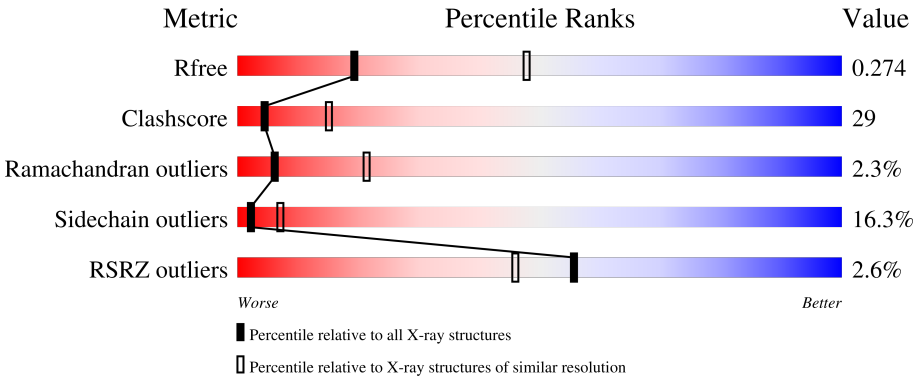
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1289	2% 47% 37% 9% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9311 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 Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1202	9274	5857	1603	1769	45	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	linker	UNP P0A6P3
A	1284	HIS	-	expression tag	UNP Q8LTE0
A	1285	HIS	-	expression tag	UNP Q8LTE0
A	1286	HIS	-	expression tag	UNP Q8LTE0
A	1287	HIS	-	expression tag	UNP Q8LTE0
A	1288	HIS	-	expression tag	UNP Q8LTE0
A	1289	HIS	-	expression tag	UNP Q8LTE0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0

- Molecule 3 is water.

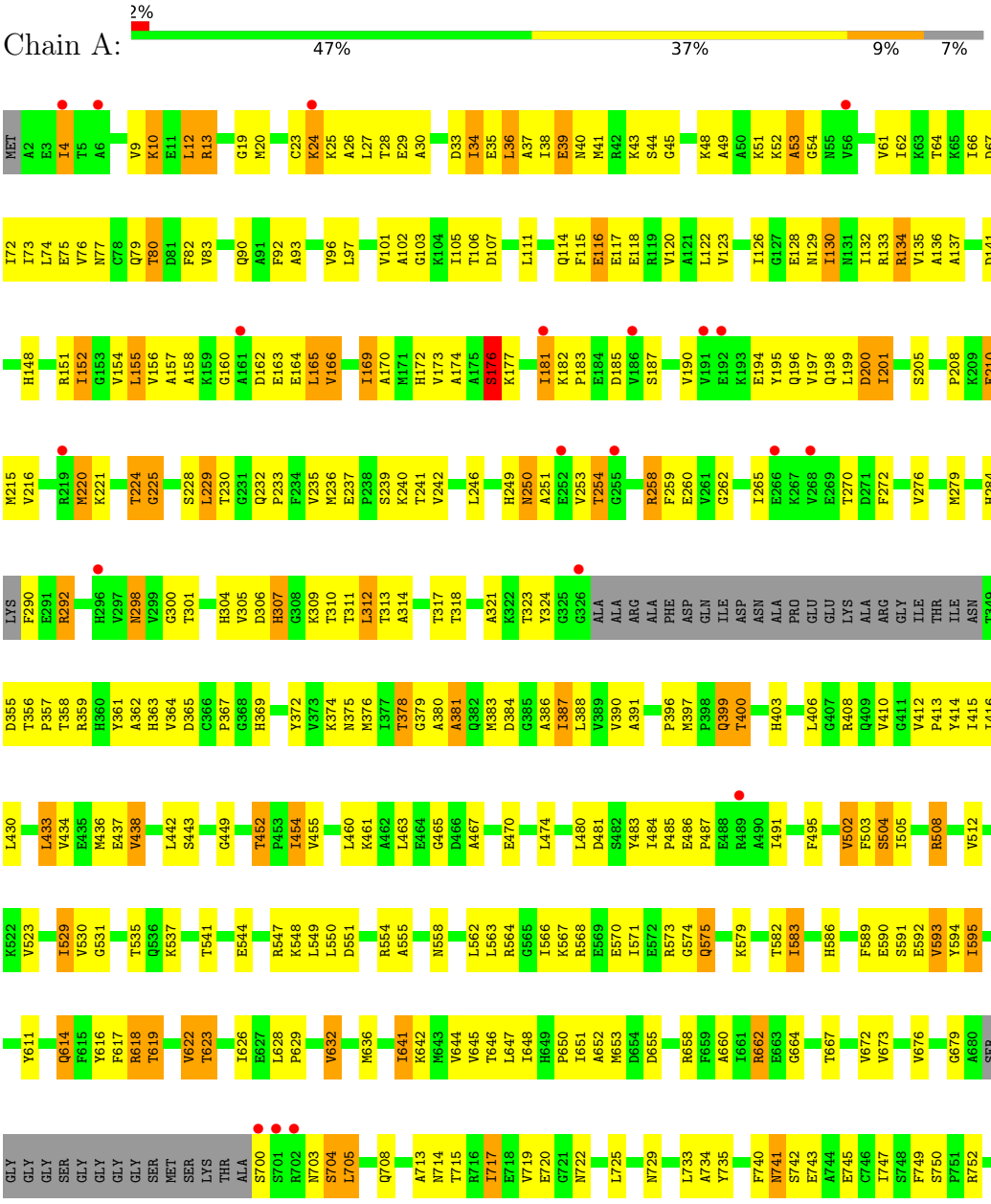
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	36	36	36	0	0

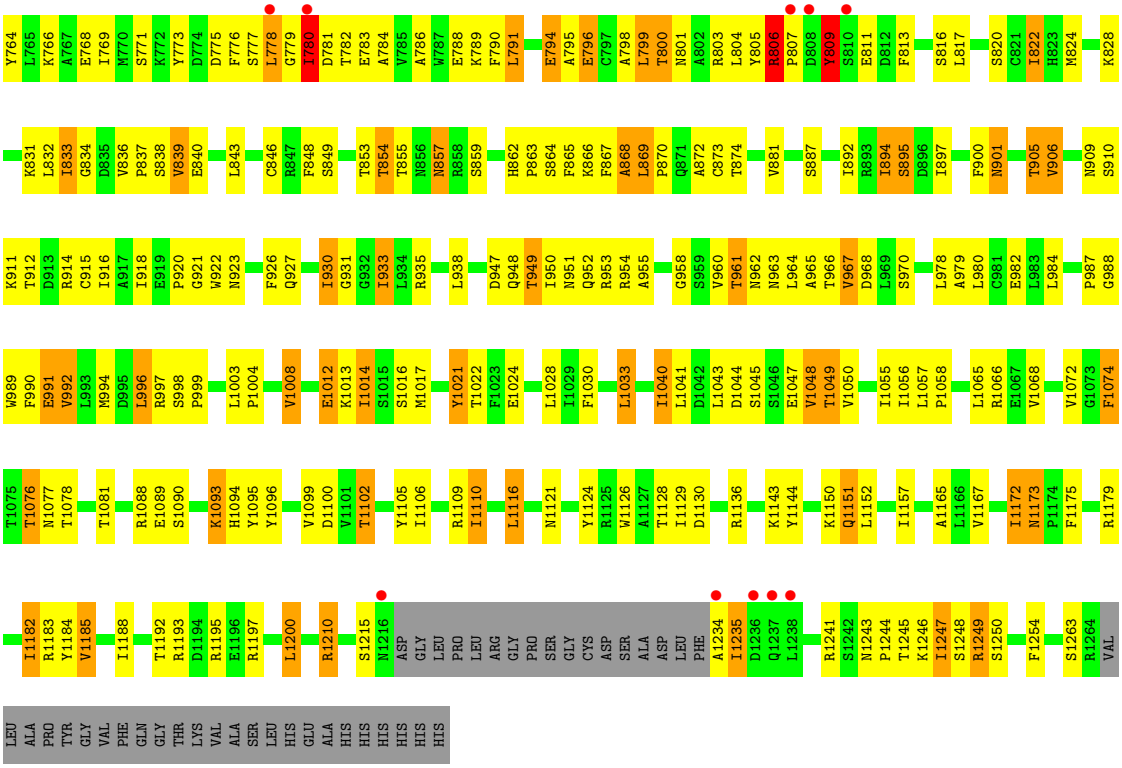
3 Residue-property plots (i)

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: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase

Chain A:




Y764 L765 K766 A767 E768 I769 M770 S771 K772 Y773 D774 D775 F776 S777 L778 G779 I780 D781 T782 E783 A784 V785 A786 W787 E788 K789 F790 L791 E794 A795 E796 C797 A798 L799 T800 N801 A802 R803 L804 Y805 R806 P807 D808 V809 S810 E811 D812 F813 S816 L817 S820 C821 I822 H823 M824 K828
K831 L832 I833 G834 D835 V836 P837 S838 V839 E840 L843 C846 R847 F848 S849 T853 T854 T855 N856 N857 R858 S859 H862 P863 S864 F865 K866 F867 A868 L869 P870 Q871 A872 C873 T874 V881 S887 I892 R893 I894 S895 D896 I897 F900 N901 T905 V906 N909 S910
K911 T912 D913 R914 C915 I916 A917 I918 E919 P920 G921 W922 N923 F926 Q927 I930 G931 G932 I933 L934 R935 L938 D947 Q948 T949 I950 N951 Q952 R953 R954 A955 G958 S959 V960 T961 N962 N963 L964 A965 T966 V967 D968 L969 S970 L978 A979 L980 C981 E982 L983 L984 P987 G988
W989 F990 E991 V992 L993 M994 D995 L996 R997 S998 P999 L1003 P1004 V1008 E1012 K1013 I1014 S1015 S1016 M1017 Y1021 T1022 F1023 E1024 L1028 I1029 F1030 L1033 I1040 L1041 D1042 L1043 D1044 S1045 S1046 E1047 V1048 T1049 V1050 I1055 I1056 L1057 P1058 L1065 R1066 E1067 V1068 V1072 G1073 F1074
T1075 T1076 N1077 T1078 T1081 R1088 E1089 S1090 K1093 H1094 Y1095 Y1096 V1099 D1100 V1101 T1102 Y1105 I1106 R1109 I1110 L1116 N1121 Y1124 R1125 W1126 A1127 T1128 I1129 D1130 R1136 K1143 Y1144 K1150 Q1151 L1152 I1157 A1165 L1166 V1167 I1172 N1173 P1174 F1175 R1179
I1182 R1183 Y1184 V1185 I1188 T1192 R1193 D1194 R1195 E1196 R1197 L1200 R1210 S1215 N1216 ASP GLY LEU PRO LEU ARG GLY PRO SER GLY CYS ASP SER ALA ASP LEU PHE A1234 I1235 D1236 Q1237 L1238 R1241 S1242 N1243 P1244 T1245 K1246 I1247 S1248 R1249 S1250 F1254 S1263 R1264 VAL
LEU ALA PRO TYR GLY VAL PHE GLN GLY THR LYS VAL ALA SER LEU HIS GLU ALA HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	139.50Å 256.43Å 100.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.80 29.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.90-2.80) 98.2 (29.55-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.283 0.210 , 0.274	Depositor DCC
R_{free} test set	2230 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9311	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.39	0/9443	0.56	0/12771

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	9274	0	9256	530	0
2	A	1	0	0	0	0
3	A	36	0	0	3	0
All	All	9311	0	9256	530	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 29.

All (530) 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:491:ILE:HG22	1:A:555:ALA:HB3	1.36	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ASP:OD1	1:A:1102:THR:HG22	1.59	1.02
1:A:133:ARG:HG2	1:A:134:ARG:H	1.25	1.01
1:A:854:THR:HG21	1:A:872:ALA:HB3	1.42	1.01
1:A:806:ARG:H	1:A:807:PRO:HD2	1.31	0.96
1:A:399:GLN:H	1:A:399:GLN:HE21	1.13	0.94
1:A:183:PRO:HD3	1:A:230:THR:HB	1.51	0.93
1:A:467:ALA:HA	1:A:470:GLU:HB2	1.53	0.91
1:A:930:ILE:HD11	1:A:1021:TYR:HB3	1.54	0.89
1:A:961:THR:HG23	1:A:963:ASN:H	1.33	0.89
1:A:930:ILE:HD11	1:A:1021:TYR:CD2	2.07	0.89
1:A:220:MET:O	1:A:224:THR:HG22	1.73	0.88
1:A:558:ASN:HB3	1:A:1210:ARG:HG3	1.57	0.86
1:A:930:ILE:HD11	1:A:1021:TYR:HD2	1.40	0.86
1:A:700:SER:N	1:A:1179:ARG:HG2	1.91	0.86
1:A:947:ASP:OD1	1:A:949:THR:HB	1.75	0.86
1:A:307:HIS:CD2	1:A:391:ALA:H	1.92	0.85
1:A:134:ARG:HH21	1:A:134:ARG:HG3	1.39	0.85
1:A:967:VAL:HG22	1:A:1055:ILE:HB	1.60	0.84
1:A:541:THR:HG21	1:A:564:ARG:HB3	1.59	0.83
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.44	0.82
1:A:224:THR:HG23	1:A:225:GLY:H	1.44	0.82
1:A:800:THR:HG22	1:A:803:ARG:NH1	1.93	0.82
1:A:800:THR:HG22	1:A:803:ARG:HH11	1.44	0.81
1:A:1173:ASN:ND2	1:A:1175:PHE:H	1.79	0.80
1:A:290:PHE:N	1:A:292:ARG:CZ	2.45	0.80
1:A:714:ASN:HD21	1:A:1254:PHE:H	1.30	0.79
1:A:520:ILE:HD11	1:A:554:ARG:HG3	1.63	0.79
1:A:358:THR:HG23	1:A:359:ARG:HG2	1.62	0.78
1:A:806:ARG:H	1:A:807:PRO:CD	1.95	0.78
1:A:198:GLN:HA	1:A:201:ILE:HG12	1.66	0.78
1:A:729:ASN:HD21	1:A:740:PHE:H	1.32	0.78
1:A:752:ARG:H	1:A:763:ASN:HD21	1.32	0.77
1:A:849:SER:HA	1:A:863:PRO:HG3	1.65	0.76
1:A:592:GLU:HG2	1:A:642:LYS:HG2	1.68	0.75
1:A:210:GLU:CD	1:A:210:GLU:H	1.88	0.75
1:A:752:ARG:H	1:A:763:ASN:ND2	1.84	0.75
1:A:103:GLY:O	1:A:105:ILE:HG13	1.86	0.75
1:A:92:PHE:CE1	1:A:132:ILE:HD11	2.21	0.75
1:A:801:ASN:HD22	1:A:1012:GLU:HG3	1.52	0.74
1:A:246:LEU:HD21	1:A:253:VAL:HG13	1.68	0.74
1:A:1129:ILE:O	1:A:1129:ILE:HG22	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ASP:HA	1:A:673:VAL:HG23	1.69	0.73
1:A:790:PHE:HD1	1:A:791:LEU:HD13	1.52	0.73
1:A:356:THR:HG22	1:A:358:THR:H	1.53	0.72
1:A:717:ILE:HD13	1:A:717:ILE:C	2.10	0.72
1:A:854:THR:HG21	1:A:872:ALA:CB	2.20	0.72
1:A:120:VAL:HA	1:A:123:VAL:HG12	1.71	0.72
1:A:133:ARG:HG2	1:A:134:ARG:N	2.03	0.72
1:A:134:ARG:HH21	1:A:134:ARG:CG	2.02	0.71
1:A:923:ASN:O	1:A:927:GLN:HG3	1.90	0.71
1:A:901:ASN:C	1:A:901:ASN:HD22	1.94	0.71
1:A:1110:ILE:HD11	1:A:1116:LEU:HG	1.71	0.71
1:A:544:GLU:HB3	1:A:549:LEU:HG	1.73	0.71
1:A:49:ALA:HB2	1:A:123:VAL:HG11	1.72	0.71
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.73	0.69
1:A:780:ILE:HD13	1:A:780:ILE:H	1.57	0.69
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.75	0.69
1:A:854:THR:HG23	1:A:855:THR:HG23	1.74	0.69
1:A:1143:LYS:HD3	1:A:1144:TYR:CE1	2.28	0.69
1:A:169:ILE:HD11	1:A:229:LEU:HD11	1.75	0.69
1:A:374:LYS:HE3	1:A:594:TYR:CZ	2.28	0.69
1:A:529:ILE:HG12	1:A:529:ILE:O	1.93	0.69
1:A:583:ILE:HG12	1:A:652:ALA:HB1	1.74	0.68
1:A:301:THR:OG1	1:A:309:LYS:HB2	1.92	0.68
1:A:704:SER:O	1:A:708:GLN:HB2	1.93	0.68
1:A:965:ALA:HA	1:A:1088:ARG:NH2	2.08	0.68
1:A:117:GLU:O	1:A:120:VAL:HG22	1.94	0.68
1:A:148:HIS:HB3	1:A:152:ILE:HG22	1.75	0.67
1:A:930:ILE:HD11	1:A:1021:TYR:CB	2.24	0.67
1:A:949:THR:HG23	1:A:953:ARG:NH1	2.10	0.67
1:A:779:GLY:C	1:A:781:ASP:H	1.98	0.67
1:A:618:ARG:NH1	1:A:652:ALA:O	2.28	0.66
1:A:307:HIS:HD2	1:A:391:ALA:H	1.40	0.66
1:A:838:SER:HB2	1:A:840:GLU:HG3	1.77	0.66
1:A:212:ALA:O	1:A:216:VAL:HG23	1.95	0.66
1:A:470:GLU:O	1:A:474:LEU:HD12	1.95	0.65
1:A:502:VAL:HG11	1:A:571:ILE:HB	1.77	0.65
1:A:388:LEU:HB3	1:A:417:VAL:HG22	1.79	0.65
1:A:4:ILE:HD13	1:A:4:ILE:H	1.60	0.65
1:A:72:ILE:HG13	1:A:137:ALA:HB2	1.78	0.65
1:A:298:ASN:HB3	1:A:362:ALA:HB3	1.78	0.65
1:A:92:PHE:HE1	1:A:132:ILE:HD11	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:ASP:H	1:A:1081:THR:HG22	1.62	0.64
1:A:1173:ASN:HD22	1:A:1175:PHE:H	1.46	0.64
1:A:930:ILE:HD13	1:A:931:GLY:H	1.62	0.64
1:A:1151:GLN:HE21	1:A:1151:GLN:H	1.46	0.64
1:A:930:ILE:CD1	1:A:1021:TYR:HD2	2.11	0.64
1:A:1121:ASN:HD21	1:A:1167:VAL:H	1.44	0.64
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.79	0.63
1:A:1049:THR:HG22	1:A:1056:ILE:HB	1.78	0.63
1:A:130:ILE:O	1:A:130:ILE:HG12	1.96	0.63
1:A:775:ASP:OD2	1:A:1109:ARG:HD3	1.98	0.63
1:A:442:LEU:HD12	1:A:452:THR:HG21	1.81	0.63
1:A:356:THR:HG21	1:A:481:ASP:OD1	1.97	0.63
1:A:965:ALA:HA	1:A:1088:ARG:HH21	1.61	0.63
1:A:1157:ILE:HG12	1:A:1165:ALA:HB3	1.79	0.63
1:A:1157:ILE:HG22	1:A:1185:VAL:HG11	1.81	0.63
1:A:764:TYR:OH	1:A:1094:HIS:HD2	1.81	0.63
1:A:784:ALA:O	1:A:788:GLU:HG3	1.99	0.63
1:A:853:THR:HG23	1:A:866:LYS:HE2	1.80	0.63
1:A:276:VAL:HG11	1:A:352:VAL:HG11	1.80	0.63
1:A:801:ASN:ND2	1:A:1012:GLU:HG3	2.13	0.62
1:A:906:VAL:HG13	1:A:914:ARG:HB3	1.80	0.62
1:A:662:ARG:HD2	1:A:667:THR:HG22	1.81	0.62
1:A:741:ASN:HD22	1:A:742:SER:H	1.47	0.62
1:A:132:ILE:HD12	1:A:132:ILE:H	1.64	0.62
1:A:626:ILE:HG22	1:A:645:VAL:HG22	1.82	0.62
1:A:502:VAL:HG13	1:A:512:VAL:HG12	1.82	0.62
1:A:521:ILE:HG23	1:A:521:ILE:O	1.99	0.62
1:A:930:ILE:CD1	1:A:1021:TYR:HB3	2.27	0.62
1:A:148:HIS:HB3	1:A:152:ILE:CG2	2.29	0.61
1:A:1110:ILE:HD12	1:A:1116:LEU:HA	1.82	0.61
1:A:442:LEU:CD1	1:A:452:THR:HG21	2.30	0.61
1:A:704:SER:HB3	3:A:2003:HOH:O	2.01	0.61
1:A:304:HIS:ND1	1:A:397:MET:HG3	2.15	0.61
1:A:848:PHE:HE1	1:A:921:GLY:O	1.84	0.61
1:A:272:PHE:CZ	1:A:313:THR:HG21	2.36	0.60
1:A:1173:ASN:HD22	1:A:1173:ASN:C	2.03	0.60
1:A:529:ILE:HD12	1:A:571:ILE:HG12	1.84	0.60
1:A:717:ILE:HD13	1:A:717:ILE:O	2.01	0.60
1:A:12:LEU:HD22	1:A:27:LEU:HD13	1.83	0.60
1:A:166:VAL:HA	1:A:169:ILE:HG23	1.84	0.60
1:A:62:ILE:HG12	1:A:75:GLU:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:ASN:HB2	1:A:1244:PRO:HD2	1.84	0.59
1:A:980:LEU:HD22	1:A:1072:VAL:HB	1.84	0.59
1:A:743:GLU:HB2	1:A:778:LEU:HD22	1.83	0.59
1:A:304:HIS:HD2	1:A:306:ASP:H	1.50	0.59
1:A:41:MET:HA	1:A:44:SER:OG	2.02	0.59
1:A:399:GLN:HE21	1:A:399:GLN:N	1.92	0.59
1:A:622:VAL:HG22	1:A:647:LEU:HD22	1.83	0.59
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.31	0.59
1:A:839:VAL:HG12	1:A:843:LEU:HD23	1.84	0.59
1:A:862:HIS:HD2	1:A:864:SER:H	1.51	0.58
1:A:790:PHE:CD1	1:A:791:LEU:HD13	2.35	0.58
1:A:549:LEU:HD23	1:A:550:LEU:N	2.18	0.58
1:A:25:LYS:O	1:A:28:THR:HG22	2.03	0.58
1:A:356:THR:HG23	1:A:357:PRO:HD2	1.86	0.58
1:A:967:VAL:HA	1:A:1081:THR:HG22	1.84	0.58
1:A:158:ALA:HB2	1:A:253:VAL:HG12	1.86	0.58
1:A:1047:GLU:HB3	1:A:1058:PRO:HD3	1.85	0.58
1:A:187:SER:HB3	1:A:190:VAL:CG1	2.34	0.58
1:A:817:LEU:HG	1:A:1068:VAL:HG23	1.86	0.58
1:A:111:LEU:HD23	1:A:111:LEU:H	1.68	0.58
1:A:224:THR:HG23	1:A:225:GLY:N	2.17	0.58
1:A:806:ARG:N	1:A:807:PRO:HD2	2.13	0.58
1:A:833:ILE:HG23	1:A:989:TRP:CE2	2.39	0.58
1:A:309:LYS:HE3	1:A:365:ASP:OD2	2.04	0.58
1:A:589:PHE:CD1	1:A:673:VAL:HG12	2.39	0.58
1:A:629:PRO:HG2	1:A:632:VAL:CG1	2.34	0.58
1:A:52:LYS:O	1:A:54:GLY:N	2.37	0.57
1:A:764:TYR:OH	1:A:1094:HIS:CD2	2.56	0.57
1:A:1093:LYS:HB3	1:A:1095:TYR:CE2	2.39	0.57
1:A:857:ASN:H	1:A:857:ASN:ND2	2.02	0.57
1:A:982:GLU:HB3	1:A:990:PHE:CE1	2.40	0.57
1:A:75:GLU:O	1:A:75:GLU:HG3	2.05	0.57
1:A:162:ASP:O	1:A:166:VAL:HG22	2.04	0.57
1:A:798:ALA:HA	1:A:1012:GLU:HG2	1.86	0.57
1:A:132:ILE:HD12	1:A:132:ILE:N	2.19	0.56
1:A:1100:ASP:OD1	1:A:1102:THR:CG2	2.45	0.56
1:A:700:SER:O	1:A:1179:ARG:HD2	2.05	0.56
1:A:38:ILE:HD12	1:A:39:GLU:N	2.20	0.56
1:A:73:ILE:HB	1:A:155:LEU:HD22	1.87	0.56
1:A:836:VAL:CG2	1:A:837:PRO:HD2	2.34	0.56
1:A:988:GLY:O	1:A:992:VAL:HG12	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:HG3	1:A:430:LEU:HD11	1.86	0.56
1:A:182:LYS:HG2	1:A:185:ASP:OD2	2.05	0.56
1:A:614:GLN:HE22	1:A:664:GLY:H	1.54	0.56
1:A:80:THR:HG23	1:A:82:PHE:H	1.69	0.56
1:A:700:SER:N	1:A:1179:ARG:CG	2.67	0.56
1:A:722:ASN:HB3	1:A:725:LEU:HB3	1.87	0.55
1:A:729:ASN:ND2	1:A:740:PHE:H	2.03	0.55
1:A:156:VAL:HG12	1:A:166:VAL:HG12	1.87	0.55
1:A:163:GLU:CD	1:A:163:GLU:H	2.09	0.55
1:A:187:SER:HB3	1:A:190:VAL:HG12	1.88	0.55
1:A:134:ARG:NH2	1:A:259:PHE:CD2	2.75	0.55
1:A:262:GLY:HA2	1:A:265:ILE:HD12	1.89	0.55
1:A:1243:ASN:CB	1:A:1244:PRO:HD2	2.36	0.55
1:A:384:ASP:O	1:A:413:PRO:HG2	2.06	0.55
1:A:356:THR:HG22	1:A:358:THR:HG22	1.89	0.55
1:A:900:PHE:CE2	1:A:1008:VAL:HG12	2.42	0.55
1:A:79:GLN:NE2	1:A:129:ASN:H	2.04	0.55
1:A:504:SER:HB2	1:A:568:ARG:HG2	1.89	0.55
1:A:1121:ASN:ND2	1:A:1167:VAL:H	2.04	0.55
1:A:741:ASN:HD22	1:A:742:SER:N	2.05	0.55
1:A:33:ASP:OD1	1:A:36:LEU:HB2	2.06	0.54
1:A:229:LEU:CD2	1:A:242:VAL:HG11	2.37	0.54
1:A:423:ASP:OD2	1:A:461:LYS:HE2	2.07	0.54
1:A:961:THR:CG2	1:A:963:ASN:H	2.13	0.54
1:A:961:THR:HG23	1:A:963:ASN:N	2.15	0.54
1:A:798:ALA:CA	1:A:1012:GLU:HG2	2.37	0.54
1:A:930:ILE:CD1	1:A:1021:TYR:CD2	2.88	0.54
1:A:508:ARG:HD3	1:A:562:LEU:HD21	1.89	0.54
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.42	0.54
1:A:558:ASN:HB3	1:A:1210:ARG:CG	2.33	0.54
1:A:4:ILE:HD13	1:A:4:ILE:N	2.22	0.54
1:A:617:PHE:O	1:A:618:ARG:HG2	2.06	0.54
1:A:1110:ILE:CD1	1:A:1116:LEU:HA	2.37	0.54
1:A:221:LYS:O	1:A:224:THR:HG23	2.08	0.53
1:A:734:ALA:HB1	1:A:1136:ARG:O	2.07	0.53
1:A:794:GLU:HA	1:A:794:GLU:OE1	2.07	0.53
1:A:1245:THR:O	1:A:1246:LYS:HD3	2.08	0.53
1:A:66:ILE:O	1:A:66:ILE:HD12	2.09	0.53
1:A:1017:MET:HA	1:A:1022:THR:HG21	1.89	0.53
1:A:417:VAL:HG12	1:A:454:ILE:HG23	1.91	0.53
1:A:574:GLY:HA2	1:A:619:THR:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ILE:HG22	1:A:771:SER:HA	1.91	0.53
1:A:805:TYR:O	1:A:806:ARG:HB3	2.09	0.53
1:A:128:GLU:O	1:A:130:ILE:HG22	2.09	0.53
1:A:396:PRO:HG3	1:A:437:GLU:HB3	1.90	0.53
1:A:951:ASN:OD1	1:A:1049:THR:HG23	2.09	0.52
1:A:954:ARG:HH11	1:A:1049:THR:CG2	2.22	0.52
1:A:1096:TYR:O	1:A:1099:VAL:HG22	2.09	0.52
1:A:1247:ILE:HD13	1:A:1247:ILE:N	2.24	0.52
1:A:80:THR:HG22	1:A:83:VAL:H	1.74	0.52
1:A:92:PHE:CZ	1:A:132:ILE:HD11	2.43	0.52
1:A:801:ASN:HA	1:A:979:ALA:HB2	1.90	0.52
1:A:930:ILE:HA	1:A:933:ILE:HG23	1.91	0.52
1:A:187:SER:O	1:A:190:VAL:HG12	2.10	0.52
1:A:658:ARG:HG3	1:A:658:ARG:HH11	1.74	0.52
1:A:1057:LEU:HD23	1:A:1057:LEU:H	1.74	0.52
1:A:1173:ASN:HD22	1:A:1175:PHE:N	2.07	0.52
1:A:92:PHE:HB2	1:A:122:LEU:HD11	1.92	0.52
1:A:590:GLU:HB3	1:A:644:VAL:HG22	1.92	0.52
1:A:1193:ARG:HD2	1:A:1249:ARG:HH11	1.72	0.52
1:A:375:ASN:HA	1:A:378:THR:HG22	1.92	0.52
1:A:12:LEU:HG	1:A:13:ARG:N	2.25	0.51
1:A:593:VAL:HG22	1:A:641:ILE:HG22	1.92	0.51
1:A:1173:ASN:ND2	1:A:1175:PHE:N	2.53	0.51
1:A:369:HIS:NE2	1:A:406:LEU:HD23	2.25	0.51
1:A:48:LYS:O	1:A:51:LYS:HB3	2.11	0.51
1:A:566:ILE:HD11	1:A:570:GLU:HB2	1.92	0.51
1:A:676:VAL:HG23	1:A:676:VAL:O	2.10	0.51
1:A:1024:GLU:OE1	1:A:1024:GLU:N	2.40	0.51
1:A:593:VAL:HG22	1:A:641:ILE:CG2	2.40	0.51
1:A:806:ARG:N	1:A:807:PRO:CD	2.68	0.51
1:A:853:THR:CG2	1:A:866:LYS:HE2	2.40	0.51
1:A:20:MET:HE3	1:A:20:MET:HA	1.92	0.51
1:A:412:VAL:HG13	1:A:412:VAL:O	2.11	0.51
1:A:541:THR:CG2	1:A:564:ARG:HB3	2.36	0.51
1:A:987:PRO:HD2	3:A:2007:HOH:O	2.09	0.51
1:A:1182:ILE:HG13	1:A:1184:TYR:CE2	2.45	0.51
1:A:304:HIS:CD2	1:A:305:VAL:N	2.79	0.51
1:A:310:THR:O	1:A:313:THR:HG22	2.10	0.51
1:A:930:ILE:HD11	1:A:1021:TYR:CG	2.44	0.51
1:A:30:ALA:HB1	1:A:36:LEU:HD13	1.93	0.51
1:A:948:GLN:HG2	3:A:2017:HOH:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:HB	1:A:260:GLU:HG3	1.93	0.51
1:A:1045:SER:O	1:A:1048:VAL:HG13	2.10	0.51
1:A:369:HIS:CD2	1:A:406:LEU:HD23	2.46	0.50
1:A:379:GLY:HA2	1:A:658:ARG:HH21	1.75	0.50
1:A:416:ILE:HD12	1:A:480:LEU:HD12	1.92	0.50
1:A:897:ILE:HG12	1:A:897:ILE:O	2.10	0.50
1:A:741:ASN:HD21	1:A:745:GLU:HB2	1.76	0.50
1:A:809:TYR:C	1:A:811:GLU:H	2.13	0.50
1:A:839:VAL:HG12	1:A:843:LEU:CD2	2.41	0.50
1:A:169:ILE:O	1:A:173:VAL:HG23	2.11	0.50
1:A:591:SER:HB2	1:A:672:VAL:O	2.11	0.50
1:A:1030:PHE:HE2	1:A:1074:PHE:CE1	2.30	0.50
1:A:148:HIS:NE2	1:A:636:MET:HG3	2.26	0.50
1:A:158:ALA:HA	1:A:253:VAL:HA	1.94	0.50
1:A:279:MET:SD	1:A:311:THR:HG22	2.52	0.50
1:A:558:ASN:HD22	1:A:1210:ARG:HH21	1.60	0.50
1:A:862:HIS:CD2	1:A:864:SER:H	2.29	0.50
1:A:246:LEU:O	1:A:249:HIS:O	2.29	0.50
1:A:949:THR:CG2	1:A:953:ARG:NH1	2.75	0.50
1:A:586:HIS:HB2	1:A:653:MET:CE	2.42	0.50
1:A:779:GLY:C	1:A:781:ASP:N	2.65	0.50
1:A:892:ILE:HG23	1:A:922:TRP:CZ2	2.47	0.50
1:A:195:TYR:CD1	1:A:195:TYR:C	2.84	0.49
1:A:359:ARG:HD2	1:A:361:TYR:OH	2.12	0.49
1:A:516:VAL:HG13	1:A:555:ALA:HA	1.94	0.49
1:A:579:LYS:O	1:A:582:THR:HB	2.12	0.49
1:A:714:ASN:ND2	1:A:1254:PHE:H	2.06	0.49
1:A:194:GLU:HA	1:A:197:VAL:HG12	1.94	0.49
1:A:399:GLN:H	1:A:399:GLN:NE2	1.96	0.49
1:A:232:GLN:O	1:A:242:VAL:HG23	2.11	0.49
1:A:1110:ILE:HD11	1:A:1116:LEU:CG	2.41	0.49
1:A:165:LEU:O	1:A:169:ILE:HG22	2.12	0.49
1:A:376:MET:HG3	1:A:410:VAL:CG2	2.43	0.49
1:A:796:GLU:O	1:A:800:THR:HG23	2.11	0.49
1:A:900:PHE:HE2	1:A:1008:VAL:HG12	1.77	0.49
1:A:914:ARG:HH22	1:A:1017:MET:CE	2.26	0.49
1:A:930:ILE:HD13	1:A:931:GLY:N	2.28	0.49
1:A:181:ILE:HG22	1:A:185:ASP:OD1	2.12	0.49
1:A:434:VAL:O	1:A:438:VAL:HG12	2.12	0.49
1:A:132:ILE:H	1:A:132:ILE:CD1	2.26	0.49
1:A:1182:ILE:HD12	1:A:1183:ARG:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:HG2	1:A:164:GLU:H	1.76	0.49
1:A:205:SER:O	1:A:757:PRO:HG2	2.13	0.49
1:A:12:LEU:HD11	1:A:23:CYS:SG	2.53	0.49
1:A:276:VAL:HG21	1:A:313:THR:HG23	1.95	0.49
1:A:967:VAL:CG2	1:A:1055:ILE:HB	2.36	0.49
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.60	0.48
1:A:208:PRO:HG2	1:A:211:ILE:HD13	1.94	0.48
1:A:914:ARG:HH12	1:A:1017:MET:HG3	1.78	0.48
1:A:400:THR:HA	1:A:403:HIS:CD2	2.48	0.48
1:A:25:LYS:HG3	1:A:26:ALA:N	2.28	0.48
1:A:356:THR:CG2	1:A:358:THR:HG22	2.43	0.48
1:A:954:ARG:HD3	1:A:1049:THR:HG21	1.95	0.48
1:A:80:THR:HB	1:A:128:GLU:OE1	2.14	0.48
1:A:199:LEU:HD23	1:A:199:LEU:O	2.13	0.48
1:A:126:ILE:O	1:A:304:HIS:HE1	1.96	0.48
1:A:978:LEU:HD23	1:A:1014:ILE:HG12	1.95	0.48
1:A:66:ILE:HG22	1:A:71:GLY:HA3	1.95	0.48
1:A:990:PHE:O	1:A:994:MET:HG2	2.14	0.48
1:A:1055:ILE:C	1:A:1056:ILE:HD12	2.34	0.48
1:A:177:LYS:HG2	1:A:258:ARG:NH2	2.29	0.48
1:A:313:THR:O	1:A:317:THR:HG23	2.13	0.48
1:A:317:THR:HG22	1:A:354:TYR:HD1	1.79	0.48
1:A:10:LYS:HB3	1:A:433:LEU:HD11	1.96	0.48
1:A:163:GLU:HG2	1:A:164:GLU:N	2.29	0.48
1:A:822:ILE:HB	1:A:984:LEU:CD1	2.44	0.48
1:A:64:THR:HG21	1:A:145:SER:HB2	1.96	0.47
1:A:323:THR:O	1:A:324:TYR:CD2	2.67	0.47
1:A:502:VAL:CG1	1:A:512:VAL:HG12	2.42	0.47
1:A:703:ASN:O	1:A:705:LEU:N	2.45	0.47
1:A:365:ASP:C	1:A:367:PRO:HD3	2.34	0.47
1:A:655:ASP:HA	1:A:673:VAL:CG2	2.41	0.47
1:A:783:GLU:OE1	1:A:905:THR:HG21	2.15	0.47
1:A:148:HIS:CE1	1:A:636:MET:HG3	2.50	0.47
1:A:894:ILE:HD11	1:A:897:ILE:HB	1.96	0.47
1:A:966:THR:HG22	1:A:1056:ILE:HG13	1.95	0.47
1:A:160:GLY:O	1:A:251:ALA:HB2	2.15	0.47
1:A:568:ARG:HD2	1:A:568:ARG:O	2.15	0.47
1:A:805:TYR:O	1:A:806:ARG:CB	2.63	0.47
1:A:284:HIS:CE1	1:A:318:THR:HG22	2.49	0.47
1:A:233:PRO:HA	1:A:241:THR:HA	1.97	0.47
1:A:749:PHE:CE2	1:A:766:LYS:HE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:LYS:HD2	1:A:1150:LYS:N	2.30	0.47
1:A:1057:LEU:CD1	1:A:1065:LEU:HD22	2.45	0.46
1:A:795:ALA:O	1:A:799:LEU:HD22	2.14	0.46
1:A:968:ASP:N	1:A:1081:THR:HG22	2.29	0.46
1:A:1021:TYR:CD1	1:A:1021:TYR:C	2.88	0.46
1:A:134:ARG:CG	1:A:134:ARG:NH2	2.67	0.46
1:A:200:ASP:O	1:A:201:ILE:C	2.53	0.46
1:A:520:ILE:CD1	1:A:554:ARG:HG3	2.42	0.46
1:A:833:ILE:HG22	1:A:834:GLY:N	2.29	0.46
1:A:1195:ARG:HB2	1:A:1247:ILE:HG22	1.97	0.46
1:A:1235:ILE:HG22	1:A:1235:ILE:O	2.15	0.46
1:A:45:GLY:HA2	1:A:48:LYS:HD3	1.96	0.46
1:A:523:VAL:HG13	1:A:551:ASP:O	2.16	0.46
1:A:703:ASN:C	1:A:705:LEU:H	2.18	0.46
1:A:909:ASN:HB2	1:A:912:THR:HG22	1.98	0.46
1:A:1150:LYS:HD2	1:A:1150:LYS:H	1.81	0.46
1:A:116:GLU:O	1:A:120:VAL:HG13	2.15	0.46
1:A:318:THR:O	1:A:321:ALA:HB3	2.15	0.46
1:A:909:ASN:HB3	1:A:911:LYS:H	1.81	0.46
1:A:629:PRO:HD3	1:A:642:LYS:O	2.15	0.46
1:A:115:PHE:O	1:A:117:GLU:N	2.48	0.45
1:A:1129:ILE:O	1:A:1129:ILE:CG2	2.58	0.45
1:A:1247:ILE:HG22	1:A:1248:SER:N	2.31	0.45
1:A:629:PRO:HG2	1:A:632:VAL:HG12	1.97	0.45
1:A:735:TYR:CG	1:A:762:ILE:HG13	2.52	0.45
1:A:111:LEU:HA	1:A:114:GLN:HB3	1.98	0.45
1:A:361:TYR:CZ	1:A:480:LEU:HB3	2.51	0.45
1:A:914:ARG:HH22	1:A:1017:MET:HE3	1.82	0.45
1:A:73:ILE:HG23	1:A:73:ILE:O	2.17	0.45
1:A:786:ALA:O	1:A:789:LYS:HB2	2.15	0.45
1:A:745:GLU:O	1:A:745:GLU:HG2	2.17	0.45
1:A:36:LEU:HD23	1:A:40:ASN:HD21	1.82	0.45
1:A:43:LYS:C	1:A:45:GLY:H	2.20	0.45
1:A:417:VAL:HB	1:A:454:ILE:HD13	1.97	0.45
1:A:838:SER:HB2	1:A:840:GLU:CG	2.45	0.45
1:A:839:VAL:O	1:A:843:LEU:HD23	2.17	0.45
1:A:1003:LEU:HB3	1:A:1004:PRO:HD2	1.99	0.45
1:A:1173:ASN:ND2	1:A:1173:ASN:C	2.70	0.45
1:A:1183:ARG:NH2	1:A:1183:ARG:HB2	2.31	0.45
1:A:53:ALA:HA	1:A:129:ASN:ND2	2.32	0.45
1:A:304:HIS:CD2	1:A:305:VAL:HG12	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:PRO:O	1:A:651:ILE:HG12	2.16	0.45
1:A:846:CYS:HG	1:A:926:PHE:HD1	1.62	0.45
1:A:920:PRO:O	1:A:923:ASN:HB2	2.17	0.45
1:A:133:ARG:CG	1:A:134:ARG:H	2.12	0.45
1:A:324:TYR:CE2	1:A:357:PRO:HG3	2.52	0.45
1:A:833:ILE:HG21	1:A:833:ILE:HD13	1.66	0.45
1:A:848:PHE:O	1:A:849:SER:HB2	2.17	0.45
1:A:960:VAL:CG2	1:A:961:THR:N	2.78	0.45
1:A:1050:VAL:HG22	1:A:1055:ILE:HA	1.98	0.45
1:A:486:GLU:HA	1:A:487:PRO:HD2	1.83	0.45
1:A:800:THR:O	1:A:804:LEU:HB2	2.16	0.45
1:A:955:ALA:HB2	1:A:1090:SER:HB3	1.98	0.45
1:A:705:LEU:HD22	1:A:705:LEU:HA	1.75	0.44
1:A:749:PHE:CE1	1:A:766:LYS:HG2	2.52	0.44
1:A:773:TYR:HB3	1:A:776:PHE:CE1	2.52	0.44
1:A:1041:LEU:HB2	1:A:1043:LEU:HD12	1.99	0.44
1:A:80:THR:CG2	1:A:82:PHE:H	2.29	0.44
1:A:62:ILE:HG12	1:A:75:GLU:CB	2.46	0.44
1:A:567:LYS:HB2	1:A:570:GLU:HG3	1.99	0.44
1:A:870:PRO:HB2	1:A:895:SER:HB3	1.99	0.44
1:A:67:ASP:O	1:A:69:ASN:N	2.50	0.44
1:A:794:GLU:OE1	1:A:1013:LYS:HD3	2.18	0.44
1:A:1151:GLN:H	1:A:1151:GLN:NE2	2.12	0.44
1:A:386:ALA:HB3	1:A:415:ILE:HG12	1.99	0.44
1:A:622:VAL:HG11	1:A:651:ILE:HG13	1.98	0.44
1:A:848:PHE:HD2	1:A:867:PHE:CZ	2.36	0.44
1:A:4:ILE:H	1:A:4:ILE:CD1	2.29	0.44
1:A:998:SER:HA	1:A:999:PRO:HD2	1.83	0.44
1:A:61:VAL:HG11	1:A:90:GLN:NE2	2.33	0.44
1:A:154:VAL:HG21	1:A:170:ALA:O	2.18	0.44
1:A:616:TYR:HB3	1:A:660:ALA:HB3	1.99	0.44
1:A:768:GLU:HB3	1:A:1105:TYR:CE1	2.52	0.44
1:A:833:ILE:HG23	1:A:989:TRP:NE1	2.33	0.44
1:A:1172:ILE:HD13	1:A:1172:ILE:HA	1.64	0.44
1:A:1234:ALA:O	1:A:1235:ILE:HG12	2.17	0.44
1:A:37:ALA:O	1:A:41:MET:HG3	2.18	0.44
1:A:52:LYS:C	1:A:54:GLY:H	2.21	0.44
1:A:495:PHE:CE2	1:A:521:ILE:HB	2.53	0.44
1:A:508:ARG:HE	1:A:562:LEU:HD11	1.81	0.44
1:A:833:ILE:CG2	1:A:989:TRP:NE1	2.81	0.44
1:A:901:ASN:HB2	1:A:918:ILE:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HA	1:A:387:ILE:HG23	1.99	0.43
1:A:836:VAL:HG22	1:A:837:PRO:CD	2.46	0.43
1:A:958:GLY:HA2	1:A:961:THR:HG22	2.00	0.43
1:A:1234:ALA:C	1:A:1235:ILE:HG12	2.39	0.43
1:A:181:ILE:HD13	1:A:181:ILE:C	2.39	0.43
1:A:460:LEU:O	1:A:463:LEU:HB2	2.18	0.43
1:A:484:ILE:HA	1:A:485:PRO:HD3	1.86	0.43
1:A:573:ARG:NH1	1:A:1241:ARG:HB2	2.33	0.43
1:A:713:ALA:HB2	1:A:1188:ILE:HD12	2.01	0.43
1:A:854:THR:HG23	1:A:855:THR:N	2.34	0.43
1:A:36:LEU:CD2	1:A:40:ASN:HD21	2.32	0.43
1:A:134:ARG:CZ	1:A:259:PHE:CD2	3.02	0.43
1:A:154:VAL:HG12	1:A:258:ARG:HB2	2.00	0.43
1:A:948:GLN:O	1:A:952:GLN:HG3	2.17	0.43
1:A:1247:ILE:N	1:A:1247:ILE:CD1	2.81	0.43
1:A:49:ALA:CB	1:A:123:VAL:HG11	2.44	0.43
1:A:106:THR:HG23	1:A:107:ASP:N	2.33	0.43
1:A:1033:LEU:HD12	1:A:1033:LEU:HA	1.63	0.43
1:A:1183:ARG:HB2	1:A:1183:ARG:HH21	1.84	0.43
1:A:35:GLU:HA	1:A:38:ILE:HG12	2.01	0.43
1:A:115:PHE:O	1:A:118:GLU:N	2.52	0.43
1:A:617:PHE:C	1:A:618:ARG:HG2	2.38	0.43
1:A:846:CYS:SG	1:A:926:PHE:HA	2.59	0.43
1:A:782:THR:HG21	1:A:784:ALA:HB3	2.01	0.43
1:A:790:PHE:HB2	1:A:915:CYS:SG	2.59	0.43
1:A:967:VAL:CA	1:A:1081:THR:HG22	2.46	0.43
1:A:1126:TRP:CD2	1:A:1126:TRP:O	2.72	0.43
1:A:465:GLY:HA2	1:A:470:GLU:OE1	2.19	0.43
1:A:824:MET:HE1	1:A:1040:ILE:HD11	2.00	0.43
1:A:449:GLY:O	1:A:452:THR:HG22	2.18	0.43
1:A:960:VAL:HG22	1:A:961:THR:N	2.33	0.43
1:A:1057:LEU:HD23	1:A:1057:LEU:N	2.32	0.43
1:A:80:THR:CG2	1:A:82:PHE:HB2	2.49	0.43
1:A:181:ILE:HG13	1:A:253:VAL:HG23	2.01	0.43
1:A:795:ALA:O	1:A:798:ALA:HB3	2.19	0.43
1:A:79:GLN:HG2	1:A:128:GLU:HB3	2.01	0.42
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.71	0.42
1:A:964:LEU:O	1:A:1088:ARG:NH2	2.52	0.42
1:A:169:ILE:CD1	1:A:229:LEU:HD11	2.47	0.42
1:A:220:MET:CE	1:A:220:MET:HA	2.49	0.42
1:A:301:THR:HB	1:A:363:HIS:NE2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:PHE:CZ	1:A:645:VAL:HB	2.54	0.42
1:A:820:SER:O	1:A:824:MET:HE2	2.19	0.42
1:A:996:LEU:HA	1:A:996:LEU:HD12	1.78	0.42
1:A:250:ASN:N	1:A:250:ASN:ND2	2.64	0.42
1:A:874:THR:HG22	1:A:923:ASN:OD1	2.19	0.42
1:A:954:ARG:NH1	1:A:1049:THR:HB	2.34	0.42
1:A:1192:THR:HG22	1:A:1250:SER:HA	2.01	0.42
1:A:35:GLU:HA	1:A:38:ILE:CG1	2.49	0.42
1:A:199:LEU:HA	1:A:216:VAL:HG21	2.01	0.42
1:A:276:VAL:HG23	1:A:314:ALA:HB2	2.02	0.42
1:A:290:PHE:N	1:A:292:ARG:NE	2.68	0.42
1:A:307:HIS:CD2	1:A:391:ALA:N	2.75	0.42
1:A:356:THR:HG21	1:A:481:ASP:CG	2.39	0.42
1:A:505:ILE:HG21	1:A:508:ARG:HD2	2.00	0.42
1:A:824:MET:O	1:A:828:LYS:HG3	2.19	0.42
1:A:77:ASN:O	1:A:130:ILE:HA	2.20	0.42
1:A:595:ILE:HD13	1:A:607:PHE:HE2	1.85	0.42
1:A:623:THR:O	1:A:648:ILE:HG22	2.19	0.42
1:A:135:VAL:HG22	1:A:136:ALA:N	2.35	0.42
1:A:156:VAL:CG1	1:A:166:VAL:HG12	2.48	0.42
1:A:658:ARG:HG3	1:A:658:ARG:NH1	2.34	0.42
1:A:773:TYR:CE2	1:A:775:ASP:HB3	2.55	0.42
1:A:982:GLU:HB3	1:A:990:PHE:CZ	2.54	0.42
1:A:101:VAL:O	1:A:102:ALA:C	2.57	0.41
1:A:502:VAL:O	1:A:1197:ARG:NH1	2.52	0.41
1:A:991:GLU:O	1:A:994:MET:N	2.52	0.41
1:A:1157:ILE:O	1:A:1167:VAL:HA	2.20	0.41
1:A:1200:LEU:HD23	1:A:1200:LEU:HA	1.83	0.41
1:A:172:HIS:O	1:A:176:SER:HB2	2.20	0.41
1:A:869:LEU:H	1:A:869:LEU:HD22	1.84	0.41
1:A:777:SER:O	1:A:779:GLY:N	2.53	0.41
1:A:865:PHE:HA	1:A:868:ALA:HB3	2.01	0.41
1:A:872:ALA:O	1:A:922:TRP:HB2	2.19	0.41
1:A:641:ILE:HD13	1:A:642:LYS:N	2.35	0.41
1:A:93:ALA:HA	1:A:96:VAL:CG1	2.47	0.41
1:A:300:GLY:HA3	1:A:383:MET:SD	2.60	0.41
1:A:503:PHE:CD1	1:A:503:PHE:N	2.88	0.41
1:A:1121:ASN:O	1:A:1124:TYR:HB3	2.21	0.41
1:A:380:ALA:O	1:A:381:ALA:HB2	2.21	0.41
1:A:414:TYR:HB3	1:A:483:TYR:CE2	2.56	0.41
1:A:97:LEU:O	1:A:101:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:HIS:CE1	1:A:406:LEU:HD23	2.55	0.41
1:A:575:GLN:H	1:A:575:GLN:HG2	1.73	0.41
1:A:897:ILE:O	1:A:897:ILE:CG1	2.69	0.41
1:A:323:THR:O	1:A:323:THR:HG22	2.21	0.41
1:A:586:HIS:HB2	1:A:653:MET:HE3	2.03	0.41
1:A:741:ASN:ND2	1:A:742:SER:H	2.15	0.41
1:A:1173:ASN:HD21	1:A:1175:PHE:HB2	1.85	0.41
1:A:9:VAL:HA	1:A:12:LEU:HD23	2.02	0.41
1:A:35:GLU:O	1:A:38:ILE:HG13	2.21	0.41
1:A:641:ILE:HD13	1:A:642:LYS:C	2.42	0.41
1:A:837:PRO:HD3	1:A:989:TRP:CE2	2.56	0.41
1:A:935:ARG:NH2	1:A:1024:GLU:OE2	2.45	0.41
1:A:949:THR:CG2	1:A:953:ARG:HH12	2.32	0.41
1:A:304:HIS:HB3	1:A:307:HIS:CG	2.55	0.41
1:A:30:ALA:HB1	1:A:36:LEU:HB3	2.03	0.40
1:A:66:ILE:HD12	1:A:66:ILE:C	2.41	0.40
1:A:195:TYR:OH	1:A:213:GLU:HG2	2.21	0.40
1:A:224:THR:O	1:A:225:GLY:C	2.60	0.40
1:A:305:VAL:HG13	1:A:306:ASP:N	2.36	0.40
1:A:312:LEU:O	1:A:312:LEU:HD23	2.21	0.40
1:A:949:THR:HG23	1:A:953:ARG:HH12	1.86	0.40
1:A:1057:LEU:HD11	1:A:1065:LEU:HD22	2.03	0.40
1:A:236:MET:HG3	1:A:608:PHE:CZ	2.55	0.40
1:A:1066:ARG:HG2	1:A:1076:THR:HG21	2.03	0.40
1:A:120:VAL:HA	1:A:123:VAL:CG1	2.47	0.40
1:A:157:ALA:C	1:A:254:THR:HG23	2.42	0.40
1:A:174:ALA:O	1:A:258:ARG:NH1	2.53	0.40
1:A:210:GLU:CD	1:A:210:GLU:N	2.66	0.40
1:A:414:TYR:CE1	1:A:485:PRO:HG2	2.57	0.40
1:A:752:ARG:N	1:A:763:ASN:HD21	2.09	0.40
1:A:930:ILE:HD13	1:A:930:ILE:N	2.36	0.40
1:A:37:ALA:HA	1:A:40:ASN:OD1	2.20	0.40
1:A:211:ILE:O	1:A:215:MET:HG3	2.22	0.40
1:A:229:LEU:HD22	1:A:242:VAL:HG11	2.03	0.40
1:A:408:ARG:HD3	1:A:408:ARG:O	2.21	0.40
1:A:521:ILE:O	1:A:521:ILE:CG2	2.68	0.40
1:A:82:PHE:HE1	1:A:406:LEU:HB2	1.86	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	1192/1289 (92%)	1045 (88%)	120 (10%)	27 (2%)	6 21

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ALA
1	A	778	LEU
1	A	806	ARG
1	A	970	SER
1	A	19	GLY
1	A	34	ILE
1	A	68	GLY
1	A	618	ARG
1	A	780	ILE
1	A	809	TYR
1	A	854	THR
1	A	895	SER
1	A	1074	PHE
1	A	116	GLU
1	A	176	SER
1	A	1263	SER
1	A	381	ALA
1	A	547	ARG
1	A	704	SER
1	A	1130	ASP
1	A	813	PHE
1	A	868	ALA
1	A	679	GLY
1	A	201	ILE
1	A	225	GLY
1	A	1235	ILE
1	A	531	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	993/1060 (94%)	831 (84%)	162 (16%)	2 7

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	10	LYS
1	A	12	LEU
1	A	13	ARG
1	A	24	LYS
1	A	29	GLU
1	A	34	ILE
1	A	36	LEU
1	A	39	GLU
1	A	74	LEU
1	A	76	VAL
1	A	80	THR
1	A	130	ILE
1	A	134	ARG
1	A	141	ASP
1	A	143	LEU
1	A	151	ARG
1	A	152	ILE
1	A	155	LEU
1	A	165	LEU
1	A	166	VAL
1	A	169	ILE
1	A	176	SER
1	A	181	ILE
1	A	196	GLN
1	A	200	ASP
1	A	210	GLU
1	A	220	MET
1	A	224	THR
1	A	228	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	229	LEU
1	A	235	VAL
1	A	237	GLU
1	A	239	SER
1	A	240	LYS
1	A	250	ASN
1	A	254	THR
1	A	258	ARG
1	A	270	THR
1	A	286	SER
1	A	292	ARG
1	A	298	ASN
1	A	307	HIS
1	A	312	LEU
1	A	355	ASP
1	A	364	VAL
1	A	378	THR
1	A	387	ILE
1	A	390	VAL
1	A	399	GLN
1	A	400	THR
1	A	433	LEU
1	A	436	MET
1	A	438	VAL
1	A	443	SER
1	A	452	THR
1	A	454	ILE
1	A	455	VAL
1	A	502	VAL
1	A	504	SER
1	A	508	ARG
1	A	520	ILE
1	A	529	ILE
1	A	530	VAL
1	A	535	THR
1	A	537	LYS
1	A	548	LYS
1	A	563	LEU
1	A	575	GLN
1	A	583	ILE
1	A	593	VAL
1	A	595	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	605	THR
1	A	614	GLN
1	A	619	THR
1	A	622	VAL
1	A	623	THR
1	A	628	LEU
1	A	632	VAL
1	A	641	ILE
1	A	646	THR
1	A	662	ARG
1	A	705	LEU
1	A	715	THR
1	A	717	ILE
1	A	719	VAL
1	A	720	GLU
1	A	733	LEU
1	A	741	ASN
1	A	750	SER
1	A	762	ILE
1	A	769	ILE
1	A	780	ILE
1	A	791	LEU
1	A	794	GLU
1	A	796	GLU
1	A	799	LEU
1	A	800	THR
1	A	806	ARG
1	A	809	TYR
1	A	816	SER
1	A	822	ILE
1	A	831	LYS
1	A	832	LEU
1	A	833	ILE
1	A	839	VAL
1	A	857	ASN
1	A	859	SER
1	A	869	LEU
1	A	873	CYS
1	A	881	VAL
1	A	887	SER
1	A	894	ILE
1	A	901	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	905	THR
1	A	906	VAL
1	A	910	SER
1	A	916	ILE
1	A	930	ILE
1	A	933	ILE
1	A	938	LEU
1	A	949	THR
1	A	950	ILE
1	A	961	THR
1	A	962	ASN
1	A	967	VAL
1	A	991	GLU
1	A	992	VAL
1	A	996	LEU
1	A	997	ARG
1	A	1008	VAL
1	A	1012	GLU
1	A	1014	ILE
1	A	1016	SER
1	A	1021	TYR
1	A	1028	LEU
1	A	1033	LEU
1	A	1040	ILE
1	A	1044	ASP
1	A	1048	VAL
1	A	1049	THR
1	A	1076	THR
1	A	1077	ASN
1	A	1078	THR
1	A	1089	GLU
1	A	1093	LYS
1	A	1102	THR
1	A	1106	ILE
1	A	1110	ILE
1	A	1116	LEU
1	A	1128	THR
1	A	1151	GLN
1	A	1152	LEU
1	A	1172	ILE
1	A	1173	ASN
1	A	1182	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1185	VAL
1	A	1200	LEU
1	A	1210	ARG
1	A	1215	SER
1	A	1247	ILE
1	A	1249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	77	ASN
1	A	79	GLN
1	A	114	GLN
1	A	250	ASN
1	A	304	HIS
1	A	307	HIS
1	A	399	GLN
1	A	403	HIS
1	A	536	GLN
1	A	558	ASN
1	A	614	GLN
1	A	714	ASN
1	A	729	ASN
1	A	741	ASN
1	A	763	ASN
1	A	857	ASN
1	A	862	HIS
1	A	871	GLN
1	A	901	ASN
1	A	946	ASN
1	A	948	GLN
1	A	952	GLN
1	A	963	ASN
1	A	1077	ASN
1	A	1094	HIS
1	A	1121	ASN
1	A	1122	ASN
1	A	1151	GLN
1	A	1155	ASN
1	A	1173	ASN
1	A	1178	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1202/1289 (93%)	-0.16	31 (2%) 56 46	35, 75, 124, 148	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	807	PRO	4.4
1	A	1234	ALA	4.3
1	A	701	SER	3.9
1	A	161	ALA	3.8
1	A	810	SER	3.6
1	A	700	SER	3.3
1	A	4	ILE	3.2
1	A	285	MET	3.0
1	A	268	VAL	2.9
1	A	1216	ASN	2.9
1	A	6	ALA	2.8
1	A	780	ILE	2.7
1	A	255	GLY	2.7
1	A	702	ARG	2.7
1	A	24	LYS	2.7
1	A	326	GLY	2.6
1	A	266	GLU	2.6
1	A	489	ARG	2.5
1	A	808	ASP	2.5
1	A	191	VAL	2.5
1	A	296	HIS	2.4
1	A	192	GLU	2.4
1	A	1237	GLN	2.3
1	A	1236	ASP	2.3
1	A	252	GLU	2.2
1	A	778	LEU	2.2
1	A	186	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	56	VAL	2.1
1	A	219	ARG	2.1
1	A	181	ILE	2.0
1	A	1238	LEU	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	2001	1/1	0.97	0.22	82,82,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.