



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:39 PM GMT

PDB ID : 1BUV
Title : CRYSTAL STRUCTURE OF THE MT1-MMP-TIMP-2 COMPLEX
Authors : Fernandez-Catalan, C.; Bode, W.; Huber, R.; Turk, D.; Calvete, J.J.; Lichte, A.; Tschesche, H.; Maskos, K.
Deposited on : 1998-09-07
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

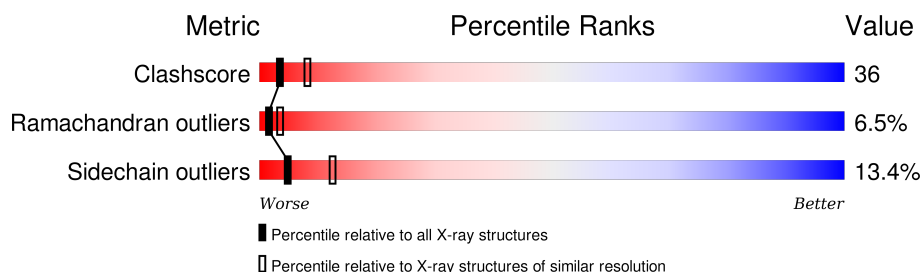
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

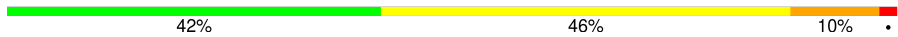
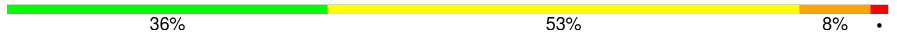
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	M	174	 42% 46% 10% •
2	T	184	 36% 53% 8% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2839 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 PROTEIN (MEMBRANE-TYPE MATRIX METALLOPROTEINASE (CDMT1-MMP)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	174	Total	C	N	O	S	39	0	0
			1403	897	236	266	4			

- Molecule 2 is a protein called PROTEIN (METALLOPROTEINASE INHIBITOR (TIMP-2)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	184	Total	C	N	O	S	6	0	0
			1432	905	247	263	17			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	2	Total	Ca	0	0
			2	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

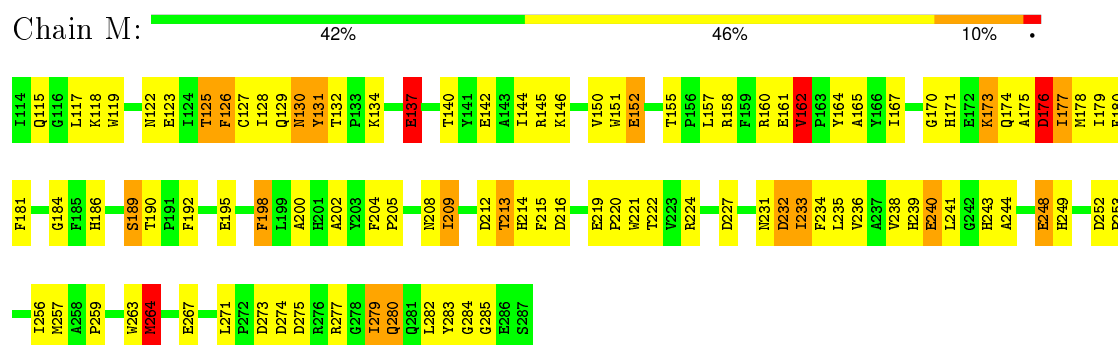
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	2	Total	Zn	0	0
			2	2		

3 Residue-property plots

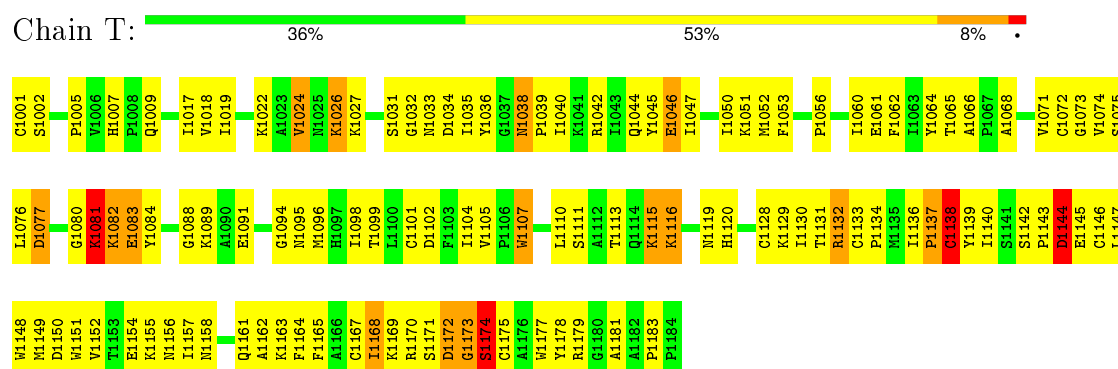
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (MEMBRANE-TYPE MATRIX METALLOPROTEINASE (CDMT1-MMP))



- Molecule 2: PROTEIN (METALLOPROTEINASE INHIBITOR (TIMP-2))



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.65Å 40.10Å 85.68Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75	Depositor
% Data completeness (in resolution range)	97.0 (20.00-2.75)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.189 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2839	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	M	0.58	0/1449	0.80	0/1968
2	T	0.62	1/1467 (0.1%)	0.89	3/1982 (0.2%)
All	All	0.60	1/2916 (0.0%)	0.84	3/3950 (0.1%)

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	M	0	1
2	T	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	1144	ASP	C-N	6.11	1.48	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	1173	GLY	O-C-N	7.32	134.41	122.70
2	T	1174	SER	O-C-N	-6.12	112.92	122.70
2	T	1173	GLY	C-N-CA	5.86	136.36	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	176	ASP	Mainchain
2	T	1174	SER	Mainchain

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	M	1403	0	1284	92	0
2	T	1432	0	1397	115	0
3	M	2	0	0	0	0
4	M	2	0	0	0	0
All	All	2839	0	2681	197	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 36.

All (197) 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:T:1168:ILE:HD11	2:T:1178:TYR:HB2	1.43	0.98
2:T:1133:CYS:HB3	2:T:1152:VAL:HG21	1.44	0.97
1:M:215:PHE:HE1	1:M:236:VAL:HG12	1.29	0.97
1:M:160:ARG:NH2	1:M:162:VAL:HG21	1.80	0.97
2:T:1026:LYS:HB2	2:T:1045:TYR:HD1	1.31	0.95
2:T:1170:ARG:NH2	2:T:1173:GLY:O	2.01	0.93
1:M:130:ASN:HD21	1:M:181:PHE:H	1.15	0.90
1:M:160:ARG:CZ	1:M:162:VAL:HG21	2.00	0.90
2:T:1033:ASN:HA	2:T:1039:PRO:HA	1.54	0.87
1:M:117:LEU:HD12	1:M:204:PHE:HB3	1.59	0.84
1:M:117:LEU:HB2	1:M:205:PRO:HD2	1.59	0.84
2:T:1065:THR:HG21	2:T:1074:VAL:O	1.80	0.81
2:T:1151:TRP:O	2:T:1155:LYS:HD3	1.81	0.81
2:T:1026:LYS:HB2	2:T:1045:TYR:CD1	2.18	0.76
1:M:130:ASN:HD21	1:M:181:PHE:N	1.81	0.76
2:T:1017:ILE:HD13	2:T:1060:ILE:HD11	1.67	0.75
1:M:202:ALA:HB2	1:M:240:GLU:HG3	1.69	0.74
2:T:1052:MET:SD	2:T:1056:PRO:O	2.47	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:127:CYS:SG	1:M:165:ALA:HB2	2.30	0.72
2:T:1115:LYS:HG2	2:T:1116:LYS:N	2.05	0.71
2:T:1138:CYS:O	2:T:1138:CYS:SG	2.48	0.71
2:T:1050:ILE:HG22	2:T:1051:LYS:HG2	1.73	0.70
1:M:151:TRP:CZ3	1:M:279:ILE:HG12	2.26	0.70
1:M:130:ASN:ND2	1:M:181:PHE:H	1.89	0.69
2:T:1072:CYS:HB3	2:T:1099:THR:OG1	1.94	0.68
1:M:215:PHE:CE1	1:M:236:VAL:HG12	2.21	0.68
2:T:1128:CYS:SG	2:T:1169:LYS:HG3	2.34	0.68
1:M:127:CYS:SG	1:M:165:ALA:N	2.67	0.67
2:T:1088:GLY:HA3	2:T:1098:ILE:HD11	1.76	0.67
1:M:142:GLU:CB	1:M:145:ARG:HH21	2.07	0.67
1:M:151:TRP:HZ3	1:M:279:ILE:HG12	1.60	0.67
2:T:1071:VAL:O	2:T:1072:CYS:HB2	1.95	0.67
2:T:1045:TYR:OH	2:T:1075:SER:HA	1.95	0.66
1:M:200:ALA:O	2:T:1001:CYS:HA	1.96	0.66
2:T:1099:THR:HG23	2:T:1101:CYS:H	1.59	0.65
2:T:1026:LYS:HA	2:T:1045:TYR:HA	1.79	0.65
2:T:1151:TRP:O	2:T:1155:LYS:HA	1.97	0.64
2:T:1161:GLN:HA	2:T:1165:PHE:HD2	1.61	0.64
2:T:1168:ILE:H	2:T:1168:ILE:HD13	1.62	0.63
2:T:1022:LYS:HE2	2:T:1081:LYS:HA	1.80	0.63
2:T:1168:ILE:HD11	2:T:1178:TYR:CB	2.26	0.62
2:T:1142:SER:HB2	2:T:1145:GLU:HB2	1.80	0.62
2:T:1031:SER:OG	2:T:1032:GLY:N	2.33	0.62
2:T:1034:ASP:OD1	2:T:1040:ILE:HG12	1.99	0.62
2:T:1168:ILE:CD1	2:T:1178:TYR:HB2	2.26	0.61
2:T:1089:LYS:O	2:T:1096:MET:HB2	2.00	0.61
2:T:1169:LYS:HA	2:T:1174:SER:O	2.01	0.61
2:T:1060:ILE:HA	2:T:1094:GLY:O	2.01	0.61
2:T:1181:ALA:O	2:T:1183:PRO:HD3	2.02	0.60
1:M:129:GLN:HB2	1:M:180:PHE:HB3	1.83	0.60
1:M:142:GLU:HA	1:M:145:ARG:HE	1.67	0.60
2:T:1170:ARG:NH1	2:T:1172:ASP:HB2	2.17	0.60
1:M:221:TRP:HH2	1:M:236:VAL:HG11	1.67	0.59
2:T:1007:HIS:HE1	2:T:1161:GLN:O	1.85	0.59
1:M:198:PHE:CB	2:T:1101:CYS:SG	2.90	0.59
1:M:142:GLU:HA	1:M:145:ARG:HH21	1.68	0.59
1:M:132:THR:HG22	1:M:140:THR:OG1	2.03	0.59
1:M:234:PHE:O	1:M:238:VAL:HG23	2.04	0.58
1:M:160:ARG:CZ	1:M:162:VAL:CG2	2.79	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:129:GLN:HA	1:M:165:ALA:HB3	1.85	0.58
2:T:1116:LYS:O	2:T:1120:HIS:HB2	2.04	0.57
1:M:126:PHE:HE1	1:M:128:ILE:HG13	1.69	0.57
2:T:1147:LEU:HB3	2:T:1149:MET:HE1	1.85	0.57
1:M:146:LYS:O	1:M:150:VAL:HG23	2.05	0.56
1:M:176:ASP:O	1:M:177:ILE:HG13	2.05	0.56
2:T:1033:ASN:CA	2:T:1039:PRO:HA	2.31	0.56
1:M:151:TRP:HZ2	1:M:238:VAL:O	1.87	0.56
2:T:1007:HIS:CE1	2:T:1162:ALA:HA	2.41	0.56
2:T:1147:LEU:HB3	2:T:1149:MET:CE	2.36	0.56
2:T:1154:GLU:HG3	2:T:1156:ASN:OD1	2.06	0.55
1:M:198:PHE:CD2	2:T:1072:CYS:SG	3.00	0.54
1:M:224:ARG:HH11	1:M:224:ARG:HG2	1.73	0.54
1:M:142:GLU:CA	1:M:145:ARG:HH21	2.20	0.54
2:T:1165:PHE:CE1	2:T:1179:ARG:HB2	2.42	0.54
1:M:179:ILE:HG12	1:M:213:THR:HG23	1.89	0.54
1:M:152:GLU:HG2	1:M:157:LEU:O	2.08	0.54
1:M:115:GLN:O	1:M:248:GLU:HB3	2.08	0.54
2:T:1050:ILE:O	2:T:1051:LYS:HD3	2.08	0.53
2:T:1047:ILE:HG13	2:T:1061:GLU:HA	1.89	0.53
1:M:131:TYR:CD1	1:M:131:TYR:N	2.77	0.53
2:T:1143:PRO:O	2:T:1144:ASP:HB2	2.09	0.53
1:M:198:PHE:HA	2:T:1101:CYS:SG	2.49	0.52
2:T:1164:PHE:O	2:T:1179:ARG:HG3	2.09	0.52
2:T:1068:ALA:HB3	2:T:1071:VAL:HG23	1.92	0.52
1:M:213:THR:HG21	1:M:241:LEU:HD23	1.92	0.52
2:T:1009:GLN:HE22	2:T:1167:CYS:H	1.58	0.51
2:T:1066:ALA:O	2:T:1073:GLY:HA3	2.11	0.51
1:M:127:CYS:HB2	1:M:175:ALA:HB3	1.91	0.51
1:M:126:PHE:CZ	1:M:161:GLU:HG2	2.46	0.51
1:M:222:THR:HG21	1:M:227:ASP:O	2.10	0.51
2:T:1017:ILE:HG21	2:T:1060:ILE:CD1	2.40	0.50
2:T:1138:CYS:C	2:T:1140:ILE:H	2.15	0.50
2:T:1168:ILE:N	2:T:1168:ILE:HD13	2.25	0.50
1:M:198:PHE:CA	2:T:1101:CYS:SG	3.00	0.50
2:T:1158:ASN:OD1	2:T:1163:LYS:HG2	2.11	0.50
2:T:1072:CYS:HB3	2:T:1099:THR:HG1	1.77	0.50
2:T:1151:TRP:CZ3	2:T:1157:ILE:HG23	2.47	0.49
1:M:173:LYS:HA	1:M:178:MET:HE1	1.94	0.49
1:M:209:ILE:N	2:T:1036:TYR:CD2	2.80	0.49
2:T:1060:ILE:HG23	2:T:1095:ASN:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:134:LYS:HE3	1:M:219:GLU:O	2.11	0.49
1:M:280:GLN:HA	1:M:284:GLY:HA3	1.95	0.49
1:M:127:CYS:SG	1:M:165:ALA:CB	3.00	0.49
1:M:115:GLN:HB3	1:M:248:GLU:HG3	1.94	0.49
2:T:1017:ILE:HD13	2:T:1060:ILE:CD1	2.42	0.48
1:M:240:GLU:O	1:M:243:HIS:HB2	2.13	0.48
1:M:140:THR:HA	1:M:233:ILE:CD1	2.43	0.48
2:T:1098:ILE:CG1	2:T:1104:ILE:HD11	2.43	0.48
2:T:1026:LYS:CB	2:T:1045:TYR:HD1	2.14	0.48
1:M:119:TRP:NE1	1:M:244:ALA:O	2.46	0.48
2:T:1005:PRO:HB3	2:T:1157:ILE:HG22	1.95	0.48
2:T:1133:CYS:O	2:T:1152:VAL:HG22	2.13	0.47
2:T:1019:ILE:HG22	2:T:1052:MET:HA	1.96	0.47
2:T:1098:ILE:HG13	2:T:1104:ILE:HD11	1.97	0.47
1:M:249:HIS:CG	1:M:259:PRO:HD3	2.49	0.47
1:M:118:LYS:NZ	1:M:282:LEU:O	2.48	0.47
2:T:1105:VAL:HG21	2:T:1110:LEU:HD13	1.96	0.47
1:M:160:ARG:HB3	1:M:162:VAL:HG23	1.97	0.47
2:T:1099:THR:N	2:T:1102:ASP:OD2	2.46	0.47
2:T:1161:GLN:HA	2:T:1165:PHE:CD2	2.47	0.46
1:M:222:THR:HB	1:M:227:ASP:HB3	1.98	0.46
2:T:1066:ALA:HB3	2:T:1073:GLY:CA	2.46	0.46
1:M:222:THR:O	1:M:232:ASP:HA	2.16	0.46
1:M:155:THR:HG21	1:M:279:ILE:CG2	2.46	0.46
1:M:252:ASP:OD1	1:M:253:PRO:HD2	2.15	0.46
2:T:1018:VAL:HG12	2:T:1053:PHE:HB2	1.98	0.46
2:T:1131:THR:HB	2:T:1147:LEU:HD23	1.98	0.46
2:T:1005:PRO:O	2:T:1148:TRP:HZ3	2.00	0.45
2:T:1088:GLY:HA3	2:T:1098:ILE:CD1	2.44	0.45
1:M:248:GLU:CD	1:M:248:GLU:H	2.19	0.45
1:M:221:TRP:CH2	1:M:236:VAL:HG11	2.48	0.45
1:M:180:PHE:CE2	1:M:214:HIS:CD2	3.04	0.45
2:T:1136:ILE:HA	2:T:1137:PRO:C	2.37	0.45
1:M:131:TYR:HB3	1:M:137:GLU:HA	1.98	0.45
2:T:1007:HIS:HD2	2:T:1009:GLN:H	1.63	0.45
1:M:189:SER:O	2:T:1042:ARG:NH2	2.50	0.45
1:M:273:ASP:C	1:M:275:ASP:H	2.20	0.45
1:M:152:GLU:OE2	1:M:158:ARG:HA	2.17	0.45
2:T:1132:ARG:NH1	2:T:1134:PRO:HB3	2.32	0.45
2:T:1083:GLU:OE1	2:T:1107:TRP:HB3	2.17	0.45
1:M:160:ARG:NH2	1:M:162:VAL:CG2	2.67	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:190:THR:CG2	2:T:1066:ALA:HB2	2.47	0.45
2:T:1080:GLY:C	2:T:1082:LYS:H	2.19	0.45
2:T:1146:CYS:HB3	2:T:1177:TRP:CE2	2.51	0.44
1:M:151:TRP:CE3	1:M:279:ILE:HG12	2.52	0.44
2:T:1170:ARG:HG2	2:T:1171:SER:H	1.83	0.44
2:T:1091:GLU:CB	2:T:1096:MET:HA	2.48	0.44
1:M:186:HIS:CE1	1:M:192:PHE:CE2	3.05	0.44
1:M:140:THR:HA	1:M:233:ILE:HD11	2.00	0.44
2:T:1091:GLU:HB2	2:T:1096:MET:HA	2.00	0.44
1:M:140:THR:O	1:M:144:ILE:HG12	2.18	0.44
1:M:130:ASN:C	1:M:130:ASN:HD22	2.20	0.43
2:T:1022:LYS:CE	2:T:1081:LYS:HA	2.47	0.43
2:T:1150:ASP:O	2:T:1154:GLU:HG2	2.18	0.43
2:T:1113:THR:HA	2:T:1116:LYS:HD2	2.00	0.43
1:M:249:HIS:HD2	1:M:257:MET:O	2.01	0.43
2:T:1137:PRO:O	2:T:1139:TYR:N	2.51	0.43
2:T:1130:ILE:HD12	2:T:1130:ILE:C	2.39	0.43
2:T:1169:LYS:HG3	2:T:1175:CYS:SG	2.58	0.43
1:M:131:TYR:CB	1:M:137:GLU:HA	2.48	0.43
2:T:1062:PHE:O	2:T:1095:ASN:HB2	2.19	0.43
1:M:155:THR:HG22	1:M:279:ILE:HB	2.00	0.43
2:T:1005:PRO:HG2	2:T:1151:TRP:CE2	2.54	0.43
2:T:1076:LEU:HD13	2:T:1084:TYR:CE1	2.54	0.43
1:M:180:PHE:CZ	1:M:214:HIS:CD2	3.07	0.42
2:T:1137:PRO:C	2:T:1139:TYR:N	2.73	0.42
2:T:1170:ARG:HG2	2:T:1171:SER:N	2.34	0.42
1:M:208:ASN:HB3	2:T:1036:TYR:CD2	2.54	0.42
1:M:184:GLY:HA2	1:M:192:PHE:O	2.20	0.42
1:M:123:GLU:OE2	1:M:160:ARG:HD2	2.20	0.42
2:T:1148:TRP:CE2	2:T:1150:ASP:HB2	2.55	0.42
2:T:1017:ILE:HG22	2:T:1019:ILE:HG23	2.02	0.42
1:M:129:GLN:HG2	1:M:165:ALA:CB	2.50	0.42
1:M:125:THR:HB	1:M:176:ASP:HB2	2.02	0.42
1:M:151:TRP:CZ2	1:M:238:VAL:O	2.70	0.42
1:M:273:ASP:C	1:M:275:ASP:N	2.72	0.41
1:M:128:ILE:HD11	1:M:144:ILE:HB	2.02	0.41
2:T:1047:ILE:HD11	2:T:1060:ILE:O	2.20	0.41
2:T:1105:VAL:CG2	2:T:1110:LEU:HD13	2.50	0.41
2:T:1044:GLN:NE2	2:T:1064:TYR:OH	2.54	0.41
1:M:157:LEU:HD11	1:M:283:TYR:CD2	2.56	0.41
2:T:1027:LYS:H	2:T:1027:LYS:HG2	1.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:198:PHE:HB3	2:T:1101:CYS:SG	2.60	0.41
1:M:239:HIS:ND1	1:M:256:ILE:O	2.53	0.41
2:T:1024:VAL:HB	2:T:1046:GLU:O	2.21	0.41
2:T:1136:ILE:HG23	2:T:1152:VAL:HG11	2.03	0.41
1:M:283:TYR:C	1:M:285:GLY:H	2.24	0.41
1:M:220:PRO:HG2	1:M:231:ASN:HD22	1.86	0.41
2:T:1170:ARG:NH1	2:T:1173:GLY:H	2.19	0.41
2:T:1129:LYS:O	2:T:1145:GLU:HA	2.21	0.41
1:M:263:TRP:CG	1:M:264:MET:N	2.88	0.41
1:M:202:ALA:HB2	1:M:213:THR:HB	2.03	0.41
2:T:1158:ASN:HA	2:T:1162:ALA:HB3	2.03	0.40
2:T:1032:GLY:O	2:T:1033:ASN:OD1	2.38	0.40
2:T:1099:THR:HG23	2:T:1101:CYS:N	2.32	0.40
1:M:216:ASP:O	1:M:221:TRP:NE1	2.50	0.40
2:T:1034:ASP:HB3	2:T:1035:ILE:H	1.69	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	M	172/174 (99%)	131 (76%)	29 (17%)	12 (7%)	1	3
2	T	182/184 (99%)	140 (77%)	31 (17%)	11 (6%)	2	4
All	All	354/358 (99%)	271 (77%)	60 (17%)	23 (6%)	1	3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	162	VAL
1	M	167	ILE
1	M	173	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	1137	PRO
2	T	1144	ASP
2	T	1174	SER
1	M	174	GLN
1	M	176	ASP
2	T	1038	ASN
2	T	1077	ASP
2	T	1107	TRP
2	T	1138	CYS
1	M	171	HIS
1	M	195	GLU
1	M	209	ILE
1	M	264	MET
1	M	137	GLU
1	M	170	GLY
1	M	177	ILE
2	T	1081	LYS
2	T	1082	LYS
2	T	1172	ASP
2	T	1024	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	143/143 (100%)	117 (82%)	26 (18%)	2	5
2	T	155/155 (100%)	141 (91%)	14 (9%)	12	31
All	All	298/298 (100%)	258 (87%)	40 (13%)	5	12

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	122	ASN
1	M	125	THR
1	M	126	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	130	ASN
1	M	131	TYR
1	M	137	GLU
1	M	152	GLU
1	M	162	VAL
1	M	164	TYR
1	M	176	ASP
1	M	189	SER
1	M	198	PHE
1	M	212	ASP
1	M	213	THR
1	M	232	ASP
1	M	233	ILE
1	M	235	LEU
1	M	240	GLU
1	M	248	GLU
1	M	264	MET
1	M	267	GLU
1	M	271	LEU
1	M	274	ASP
1	M	277	ARG
1	M	279	ILE
1	M	280	GLN
2	T	1002	SER
2	T	1026	LYS
2	T	1038	ASN
2	T	1046	GLU
2	T	1077	ASP
2	T	1081	LYS
2	T	1083	GLU
2	T	1111	SER
2	T	1115	LYS
2	T	1116	LYS
2	T	1119	ASN
2	T	1132	ARG
2	T	1138	CYS
2	T	1168	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	122	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	130	ASN
1	M	201	HIS
1	M	214	HIS
1	M	262	GLN
2	T	1007	HIS
2	T	1009	GLN
2	T	1014	ASN
2	T	1033	ASN
2	T	1044	GLN
2	T	1049	GLN
2	T	1058	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.