



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:48 am BST

PDB ID : 3TEJ  
Title : Crystal structure of a domain fragment involved in peptide natural product biosynthesis  
Authors : Liu, Y.; Zheng, T.; Bruner, S.D.  
Deposited on : 2011-08-15  
Resolution : 1.90 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](mailto: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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

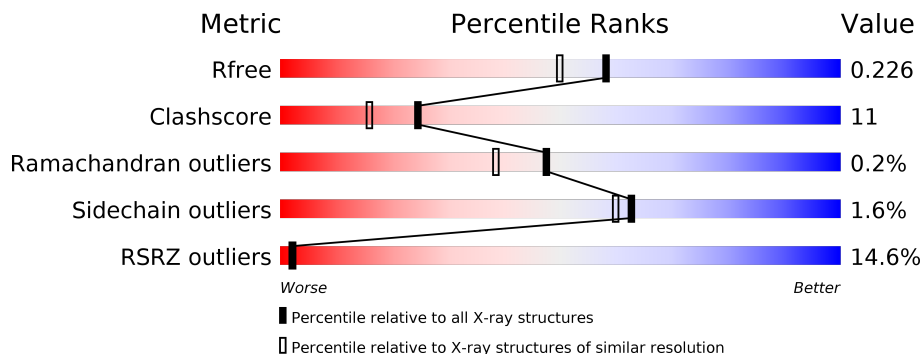
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4855 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 Enterobactin synthase component F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	320	2384	1515	409	450	1	9	0	0	0
1	B	286	2178	1385	377	406	1	9	0	0	0

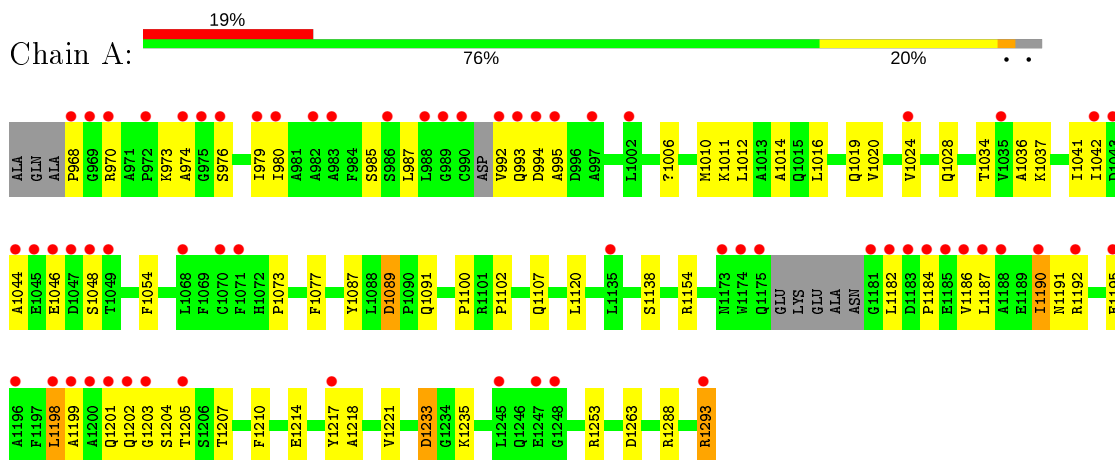
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	161	Total 161	O 161	0	0
2	B	132	Total 132	O 132	0	0

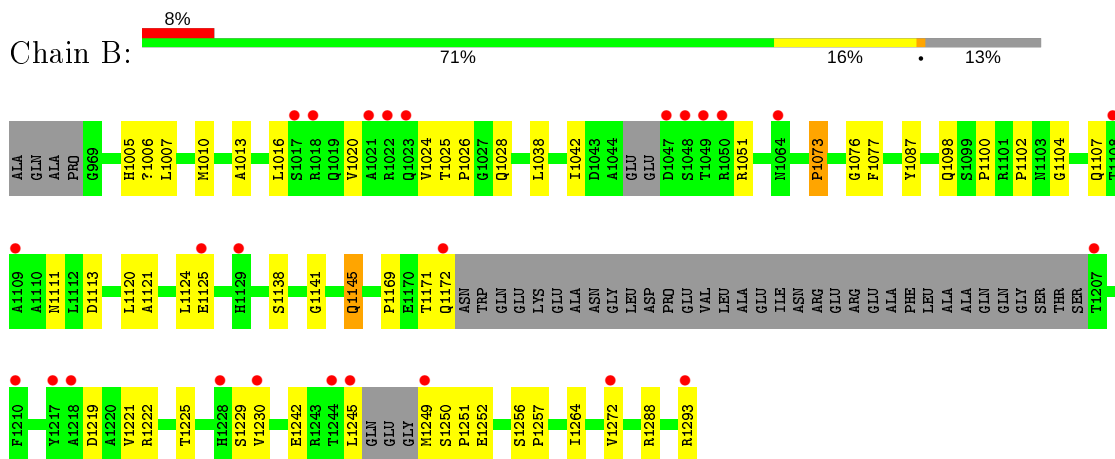
### 3 Residue-property plots [i](#)

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



- Molecule 1: Enterobactin synthase component F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.40Å 90.36Å 97.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.90) 93.1 (29.91-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 1.91Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.227 0.209 , 0.226	Depositor DCC
$R_{free}$ test set	4590 reflections (9.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UF0

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	0.33	0/2405	0.61	1/3282 (0.0%)
1	B	0.32	0/2195	0.56	0/2990
All	All	0.32	0/4600	0.59	1/6272 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	968	PRO	N-CA-CB	5.59	110.01	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2384	0	2293	65	0
1	B	2178	0	2131	33	0
2	A	161	0	0	9	0
2	B	132	0	0	2	0
All	All	4855	0	4424	98	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 (98) 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:1011:LYS:HA	1:A:1201:GLN:HG2	1.50	0.93
1:A:1187:LEU:HD23	2:A:257:HOH:O	1.77	0.84
1:B:1249:MET:HG2	1:B:1250:SER:H	1.48	0.78
1:A:1205:THR:HG22	1:A:1205:THR:O	1.83	0.78
1:B:1121:ALA:O	1:B:1125:GLU:HG2	1.87	0.75
1:A:1192:ARG:O	1:A:1195:GLU:HB3	1.88	0.73
1:A:1190:ILE:HD13	1:A:1191:ASN:N	2.04	0.73
1:A:1184:PRO:HB2	1:A:1186:VAL:HG22	1.72	0.71
1:B:1145:GLN:NE2	2:B:20:HOH:O	2.24	0.70
1:A:1186:VAL:O	1:A:1190:ILE:HG23	1.91	0.70
1:A:1089:ASP:OD1	1:A:1288:ARG:HD2	1.92	0.70
1:A:1190:ILE:HD13	1:A:1191:ASN:H	1.58	0.69
1:B:1016:LEU:O	1:B:1020:VAL:HG22	1.95	0.66
1:A:1014:ALA:HB3	1:A:1201:GLN:HG3	1.76	0.66
1:B:1221:VAL:O	1:B:1225:THR:HG23	1.96	0.65
1:A:979:ILE:HG23	1:A:1019:GLN:NE2	2.12	0.64
1:A:1034:THR:HG22	1:A:1036:ALA:N	2.14	0.62
1:A:1233:ASP:CG	1:A:1233:ASP:O	2.37	0.62
1:A:1087:TYR:O	1:A:1288:ARG:HD3	1.99	0.62
1:A:1198:LEU:HD13	1:A:1210:PHE:CE2	2.35	0.62
1:B:1249:MET:HG2	1:B:1250:SER:N	2.12	0.62
1:B:1010:MET:HA	1:B:1026:PRO:HG3	1.82	0.61
1:B:1252:GLU:HG3	1:B:1264:ILE:HD12	1.83	0.60
1:A:1048:SER:HB3	2:A:180:HOH:O	2.01	0.60
1:B:1120:LEU:O	1:B:1124:LEU:HG	2.02	0.60
1:A:1205:THR:CG2	1:A:1205:THR:O	2.50	0.60
1:B:1006:UF0:O1G	1:B:1006:UF0:H1Q	2.00	0.60
1:B:1005:HIS:CE1	1:B:1007:LEU:HB3	2.37	0.59
1:A:1198:LEU:HD23	1:A:1199:ALA:N	2.18	0.58
1:B:1256:SER:HB3	1:B:1257:PRO:HD3	1.85	0.58
1:A:985:SER:HG	1:A:992:VAL:N	2.01	0.57
1:B:1171:THR:O	1:B:1172:GLN:HB3	2.04	0.57
1:A:1198:LEU:HD13	1:A:1210:PHE:HE2	1.70	0.56
1:A:1024:VAL:HG22	1:A:1042:ILE:HD12	1.87	0.56
1:A:1044:ALA:HB2	2:A:262:HOH:O	2.06	0.55
1:A:1006:UF0:H1MA	1:A:1187:LEU:HD11	1.88	0.55
1:A:976:SER:O	1:A:980:ILE:HG12	2.06	0.55
1:B:1102:PRO:O	1:B:1107:GLN:HG2	2.07	0.54
1:B:1251:PRO:HB2	1:B:1264:ILE:HD13	1.90	0.54
1:A:1010:MET:SD	1:A:1198:LEU:HB2	2.48	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:ALA:O	1:A:1034:THR:HG23	2.08	0.53
1:A:1037:LYS:O	1:A:1041:ILE:HG12	2.08	0.53
1:A:1202:GLN:O	1:A:1203:GLY:C	2.46	0.53
1:A:1120:LEU:HD21	1:A:1154:ARG:HE	1.74	0.53
1:A:1184:PRO:HD2	2:A:250:HOH:O	2.09	0.52
1:A:1014:ALA:HB3	1:A:1201:GLN:CG	2.39	0.52
1:A:1006:UF0:H1Q	1:A:1006:UF0:O1G	2.08	0.52
1:A:973:LYS:HG2	1:A:974:ALA:N	2.26	0.51
1:A:973:LYS:NZ	1:A:973:LYS:HB2	2.26	0.50
1:B:1038:LEU:O	1:B:1042:ILE:HD13	2.11	0.50
1:A:1184:PRO:CB	1:A:1186:VAL:HG22	2.40	0.50
1:A:1207:THR:HA	2:A:179:HOH:O	2.11	0.49
1:A:1034:THR:HG22	1:A:1036:ALA:H	1.77	0.49
1:A:1011:LYS:CB	1:A:1201:GLN:HE21	2.26	0.49
1:A:970:ARG:O	1:A:994:ASP:HB2	2.12	0.48
1:B:1138:SER:O	1:B:1141:GLY:N	2.43	0.48
1:A:1089:ASP:HB3	1:A:1091:GLN:OE1	2.13	0.48
1:A:1044:ALA:N	2:A:262:HOH:O	2.46	0.48
1:A:987:LEU:HD12	1:A:1012:LEU:HD13	1.96	0.48
1:B:1073:PRO:HD2	1:B:1077:PHE:O	2.13	0.48
1:A:1184:PRO:CD	2:A:250:HOH:O	2.62	0.47
1:A:1010:MET:SD	1:A:1198:LEU:HD12	2.55	0.47
1:A:993:GLN:H	1:A:993:GLN:CD	2.17	0.47
1:B:1087:TYR:O	1:B:1288:ARG:HD3	2.15	0.46
1:B:1242:GLU:O	1:B:1245:LEU:HB3	2.16	0.46
1:B:1006:UF0:H1NA	1:B:1073:PRO:HB2	1.98	0.45
1:A:1006:UF0:C1U	1:A:1138:SER:OG	2.65	0.45
1:A:1204:SER:O	1:A:1205:THR:HB	2.17	0.45
1:B:1111:ASN:OD1	1:B:1113:ASP:HB2	2.17	0.44
1:A:1102:PRO:HA	1:A:1107:GLN:OE1	2.18	0.44
1:A:1182:LEU:HD21	1:A:1218:ALA:HA	1.98	0.44
1:B:1100:PRO:O	1:B:1104:GLY:HA3	2.18	0.44
1:A:1184:PRO:CG	1:A:1186:VAL:HG22	2.48	0.43
1:B:1169:PRO:HD2	1:B:1229:SER:OG	2.19	0.43
1:A:1210:PHE:O	1:A:1214:GLU:HG2	2.18	0.43
1:A:1253:ARG:HB2	1:A:1253:ARG:HH11	1.83	0.43
1:B:1171:THR:O	1:B:1172:GLN:CB	2.66	0.43
1:A:980:ILE:CD1	1:A:1016:LEU:HD13	2.49	0.43
1:A:1253:ARG:NH1	1:A:1253:ARG:CB	2.82	0.43
1:A:1217:TYR:O	1:A:1221:VAL:HG23	2.18	0.43
1:B:1010:MET:HG2	1:B:1026:PRO:HG2	2.01	0.43

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:ARG:HG2	1:A:1293:ARG:HH11	1.84	0.42
1:A:1046:GLU:HG3	2:A:215:HOH:O	2.18	0.42
1:B:1076:GLY:O	1:B:1098:GLN:HB3	2.19	0.42
1:B:1051:ARG:HH11	1:B:1051:ARG:HG3	1.84	0.42
1:A:1028:GLN:HG2	1:A:1041:ILE:HG21	2.01	0.42
1:B:1013:ALA:HB1	1:B:1024:VAL:O	2.20	0.42
1:B:1272:VAL:O	1:B:1272:VAL:HG22	2.19	0.42
1:B:1219:ASP:HA	1:B:1222:ARG:HG2	2.01	0.42
1:A:1073:PRO:HD2	1:A:1077:PHE:O	2.20	0.41
1:A:1235:LYS:HD2	1:A:1263:ASP:OD2	2.20	0.41
1:B:1025:THR:OG1	1:B:1028:GLN:HG3	2.20	0.41
1:A:1016:LEU:O	1:A:1020:VAL:HG22	2.21	0.41
1:A:1006:UF0:O1W	1:A:1138:SER:HB3	2.20	0.41
1:A:1054:PHE:O	1:A:1100:PRO:HB3	2.20	0.41
1:B:1230:VAL:CG2	2:B:203:HOH:O	2.69	0.40
1:A:1182:LEU:HD23	1:A:1221:VAL:HG21	2.02	0.40
1:A:1190:ILE:HG13	2:A:173:HOH:O	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	313/329 (95%)	301 (96%)	12 (4%)	0	100	100
1	B	277/329 (84%)	270 (98%)	6 (2%)	1 (0%)	34	24
All	All	590/658 (90%)	571 (97%)	18 (3%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1073	PRO

### 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	231/259 (89%)	226 (98%)	5 (2%)	52	47
1	B	218/259 (84%)	216 (99%)	2 (1%)	78	79
All	All	449/518 (87%)	442 (98%)	7 (2%)	62	60

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1089	ASP
1	A	1190	ILE
1	A	1198	LEU
1	A	1233	ASP
1	A	1293	ARG
1	B	1145	GLN
1	B	1293	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1005	HIS
1	A	1019	GLN
1	A	1201	GLN
1	B	1127	GLN
1	B	1145	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	UF0	B	1006	1	26,30,31	0.48	0	33,40,42	1.52	5 (15%)
1	UF0	A	1006	1	26,30,31	0.46	0	33,40,42	1.38	5 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UF0	B	1006	1	-	2/36/40/42	-
1	UF0	A	1006	1	-	1/36/40/42	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1006	UF0	O1Y-CB-CA	5.53	113.52	108.14
1	A	1006	UF0	O1Y-CB-CA	4.17	112.20	108.14
1	B	1006	UF0	C1I-C1H-N1F	-3.43	104.98	111.90
1	A	1006	UF0	C1I-C1H-N1F	-3.41	105.01	111.90
1	B	1006	UF0	C1H-N1F-C1E	2.49	127.02	122.59
1	A	1006	UF0	C1H-N1F-C1E	2.46	126.98	122.59
1	B	1006	UF0	C1N-N1O-C1U	2.25	127.01	122.84
1	B	1006	UF0	C1M-N1K-C1J	2.24	127.00	122.84
1	A	1006	UF0	C1N-N1O-C1U	2.24	126.99	122.84
1	A	1006	UF0	C1M-N1K-C1J	2.23	126.98	122.84

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1006	UF0	O1W-C1U-C1V-O1
1	A	1006	UF0	O1W-C1U-C1V-O1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	B	1006	UF0	C1C-C1B-O1A-P1R

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1006	UF0	2	0
1	A	1006	UF0	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	319/329 (96%)	1.01	62 (19%) <b>1</b>   <b>1</b>	14, 28, 73, 84	0
1	B	285/329 (86%)	0.49	26 (9%) <b>9</b>   <b>10</b>	16, 30, 52, 70	0
All	All	604/658 (91%)	0.77	88 (14%) <b>2</b>   <b>2</b>	14, 29, 66, 84	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1183	ASP	9.6
1	A	1174	TRP	6.5
1	A	1186	VAL	6.5
1	A	1182	LEU	6.1
1	A	1201	GLN	6.1
1	B	1021	ALA	6.0
1	A	1202	GLN	5.9
1	A	1198	LEU	5.7
1	A	975	GLY	5.6
1	A	994	ASP	5.5
1	A	1203	GLY	5.4
1	A	1187	LEU	5.1
1	A	1190	ILE	5.1
1	A	1173	ASN	5.1
1	A	1045	GLU	4.9
1	A	1205	THR	4.7
1	A	1188	ALA	4.7
1	A	1247	GLU	4.7
1	A	993	GLN	4.6
1	B	1049	THR	4.4
1	A	988	LEU	4.3
1	A	997	ALA	4.3
1	B	1129	HIS	4.2
1	A	1048	SER	4.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1047	ASP	4.1
1	A	1046	GLU	4.0
1	A	1044	ALA	4.0
1	A	983	ALA	4.0
1	A	1200	ALA	3.9
1	A	989	GLY	3.9
1	A	1293	ARG	3.9
1	A	979	ILE	3.8
1	A	1248	GLY	3.8
1	A	968	PRO	3.7
1	B	1207	THR	3.7
1	B	1109	ALA	3.7
1	A	972	PRO	3.6
1	B	1217	TYR	3.6
1	B	1050	ARG	3.6
1	B	1293	ARG	3.5
1	A	990	CYS	3.5
1	A	970	ARG	3.4
1	B	1172	GLN	3.4
1	B	1249	MET	3.4
1	A	1175	GLN	3.3
1	A	974	ALA	3.3
1	A	986	SER	3.3
1	A	1185	GLU	3.3
1	A	1181	GLY	3.1
1	A	969	GLY	3.1
1	B	1244	THR	3.0
1	A	980	ILE	3.0
1	B	1228	HIS	2.8
1	B	1018	ARG	2.8
1	A	1135	LEU	2.8
1	A	976	SER	2.8
1	B	1108	THR	2.8
1	A	1217	TYR	2.7
1	B	1245	LEU	2.7
1	A	1035	VAL	2.7
1	A	1043	ASP	2.7
1	B	1017	SER	2.7
1	A	1042	ILE	2.6
1	A	1002	LEU	2.6
1	A	1245	LEU	2.6
1	A	1195	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1199	ALA	2.5
1	B	1064	ASN	2.5
1	B	1023	GLN	2.5
1	B	1272	VAL	2.5
1	B	1210	PHE	2.5
1	A	1184	PRO	2.4
1	A	995	ALA	2.4
1	A	1196	ALA	2.4
1	A	992	VAL	2.4
1	A	1071	PHE	2.3
1	A	1049	THR	2.3
1	B	1218	ALA	2.3
1	B	1022	ARG	2.3
1	B	1047	ASP	2.2
1	B	1230	VAL	2.2
1	A	1024	VAL	2.1
1	B	1125	GLU	2.1
1	A	1192	ARG	2.1
1	A	982	ALA	2.0
1	A	1068	LEU	2.0
1	B	1048	SER	2.0
1	A	1070	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	UF0	B	1006	31/32	0.91	0.16	26,35,42,43	0
1	UF0	A	1006	31/32	0.93	0.13	19,26,36,41	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.