



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:14 AM UTC

PDB ID : 3TEJ / pdb_00003tej
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

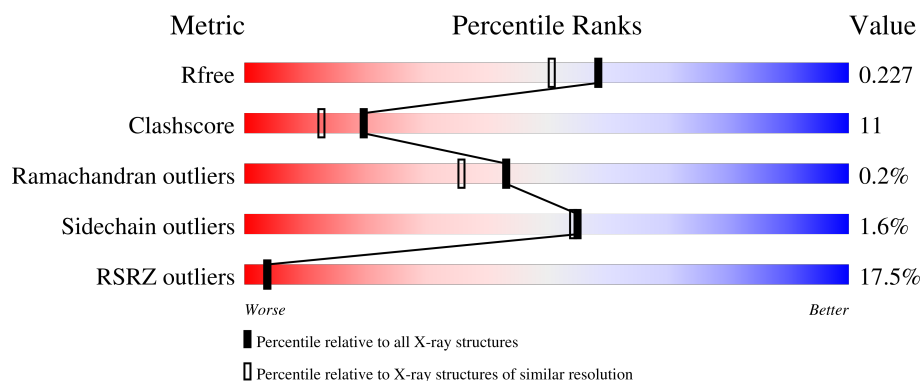
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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 $\leq 5\%$. 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	23% 74% 20% .
1	B	329	9% 69% 16% . 13%

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
1	A	320	Total	C	N	O	P	S	0	0	0
			2384	1515	409	450	1	9			
1	B	286	Total	C	N	O	P	S	0	0	0
			2178	1385	377	406	1	9			

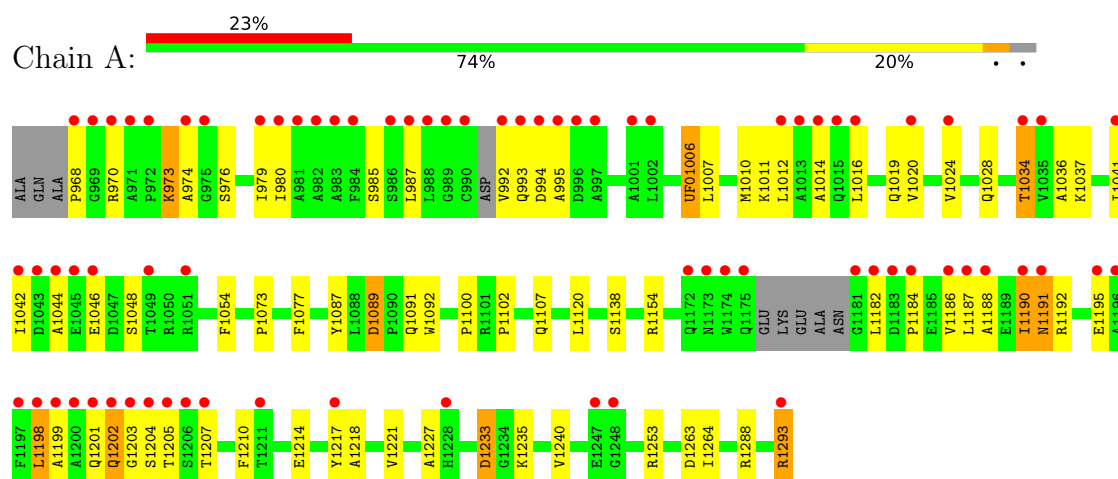
- Molecule 2 is water.

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

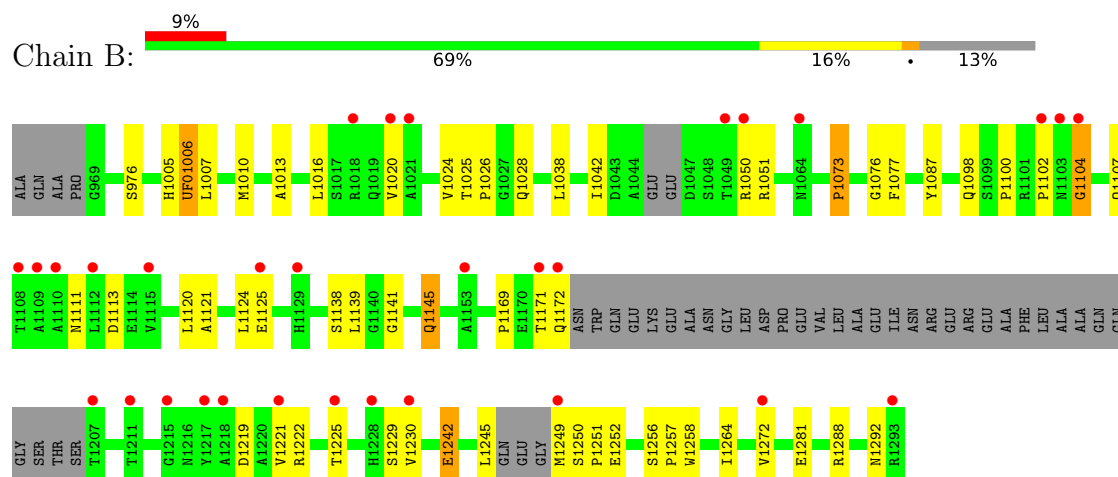
3 Residue-property plots

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: 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, α , β , γ	69.40Å 90.36Å 97.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.90) 93.0 (30.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.227 0.211 , 0.227	Depositor DCC
R_{free} test set	4590 reflections (9.72%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4855	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.39	0/2405	0.94	10/3282 (0.3%)
1	B	0.37	0/2195	0.89	8/2990 (0.3%)
All	All	0.38	0/4600	0.92	18/6272 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1202	GLN	N-CA-C	8.79	122.01	111.02
1	A	968	PRO	N-CA-CB	6.37	110.01	103.00
1	A	1191	ASN	N-CA-C	-5.76	105.08	111.36
1	A	1240	VAL	N-CA-C	5.52	116.25	108.36
1	B	1242	GLU	N-CA-C	5.49	117.27	111.28
1	A	1092	TRP	N-CA-C	5.41	118.36	109.76
1	B	1050	ARG	N-CA-C	-5.37	105.36	112.94
1	B	976	SER	N-CA-C	5.37	117.55	111.11
1	A	1089	ASP	CA-C-N	5.37	125.44	119.32
1	A	1089	ASP	C-N-CA	5.37	125.44	119.32
1	A	1188	ALA	N-CA-C	-5.28	107.01	113.50
1	B	1281	GLU	N-CA-C	-5.24	105.99	112.38
1	A	1264	ILE	N-CA-C	5.23	115.84	108.36
1	B	1104	GLY	CA-C-N	5.11	125.14	119.32
1	B	1104	GLY	C-N-CA	5.11	125.14	119.32
1	B	1292	ASN	N-CA-C	5.09	117.26	109.62
1	B	1258	TRP	N-CA-C	5.07	120.09	113.30
1	A	1227	ALA	N-CA-C	5.01	117.73	109.76

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	2384	0	2293	69	0
1	B	2178	0	2131	34	0
2	A	161	0	0	9	0
2	B	132	0	0	2	0
All	All	4855	0	4424	103	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 (103) 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:A:1007:LEU:HA	1:A:1010:MET:HE3	1.60	0.81
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:1089:ASP:OD1	1:A:1288:ARG:HD2	1.92	0.70
1:A:1186:VAL:O	1:A:1190:ILE:HG23	1.91	0.70
1:A:1190:ILE:HD13	1:A:1191:ASN:H	1.58	0.69
1:A:1233:ASP:O	1:A:1233:ASP:CG	2.37	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:1205:THR:CG2	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:A:1202:GLN:O	1:A:1203:GLY:C	2.46	0.58
1:B:1256:SER:HB3	1:B:1257:PRO:HD3	1.85	0.58
1:B:1171:THR:O	1:B:1172:GLN:HB3	2.04	0.57
1:A:985:SER:HG	1:A:992:VAL:N	2.02	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:995:ALA:O	1:A:1034:THR:HG23	2.08	0.53
1:A:1010:MET:SD	1:A:1198:LEU:HB2	2.48	0.53
1:A:1037:LYS:O	1:A:1041:ILE:HG12	2.08	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:O1G	1:A:1006:UF0:H1Q	2.08	0.52
1:A:993:GLN:H	1:A:993:GLN:CD	2.17	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:993:GLN:CD	1:A:993:GLN:N	2.75	0.44
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:A:1293:ARG:HD2	1:A:1293:ARG:C	2.43	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:HH11	1:A:1253:ARG:HB2	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:CB	1:A:1253:ARG:NH1	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
1:A:1293:ARG:HH11	1:A:1293:ARG:HG2	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:HG3	1:B:1051:ARG:HH11	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:HG22	1:B:1272:VAL:O	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:1006:UF0:O1W	1:A:1138:SER:HB3	2.20	0.41
1:A:1016:LEU:O	1:A:1020:VAL:HG22	2.21	0.41
1:A:1054:PHE:O	1:A:1100:PRO:HB3	2.20	0.41
1:B:1138:SER:O	1:B:1139:LEU:C	2.63	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
1:A:1192:ARG:C	1:A:1195:GLU:HB3	2.46	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%)	30	22
All	All	590/658 (90%)	571 (97%)	18 (3%)	1 (0%)	43	36

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%)	225 (97%)	6 (3%)	40	35
1	B	218/259 (84%)	217 (100%)	1 (0%)	81	84
All	All	449/518 (87%)	442 (98%)	7 (2%)	55	54

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

Mol	Chain	Res	Type
1	A	973	LYS
1	A	1034	THR
1	A	1190	ILE
1	A	1198	LEU
1	A	1233	ASP

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Mol	Chain	Res	Type
1	A	1293	ARG
1	B	1145	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1005	HIS
1	A	1019	GLN
1	A	1028	GLN
1	A	1129	HIS
1	A	1201	GLN
1	A	1267	GLN
1	B	1019	GLN
1	B	1127	GLN
1	B	1145	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	1006	1	27,30,31	0.45	0	33,40,42	1.45	8 (24%)
1	UF0	B	1006	1	27,30,31	0.47	0	33,40,42	1.58	8 (24%)

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	A	1006	1	-	2/38/40/42	-
1	UF0	B	1006	1	-	2/38/40/42	-

There are no bond length outliers.

All (16) 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	-3.30	104.98	112.00
1	A	1006	UF0	C1I-C1H-N1F	-3.28	105.01	112.00
1	B	1006	UF0	C1H-N1F-C1E	2.49	127.02	122.55
1	A	1006	UF0	C1H-N1F-C1E	2.47	126.98	122.55
1	B	1006	UF0	C1N-N1O-C1U	2.25	127.01	122.82
1	B	1006	UF0	C1M-N1K-C1J	2.24	127.00	122.82
1	A	1006	UF0	C1N-N1O-C1U	2.24	126.99	122.82
1	A	1006	UF0	C1M-N1K-C1J	2.23	126.98	122.82
1	B	1006	UF0	O1-C1V-C1U	-2.20	109.49	113.95
1	A	1006	UF0	O1-C1V-C1U	-2.19	109.50	113.95
1	B	1006	UF0	C1N-C1M-N1K	-2.11	104.97	111.54
1	A	1006	UF0	C1N-C1M-N1K	-2.11	104.98	111.54
1	A	1006	UF0	C1M-C1N-N1O	-2.10	105.01	111.54
1	B	1006	UF0	C1M-C1N-N1O	-2.09	105.05	111.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1006	UF0	N1O-C1U-C1V-O1
1	A	1006	UF0	O1W-C1U-C1V-O1
1	B	1006	UF0	O1W-C1U-C1V-O1
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	A	1006	UF0	4	0
1	B	1006	UF0	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	319/329 (96%)	0.85	75 (23%) 2 1	14, 28, 73, 84	0
1	B	285/329 (86%)	0.61	31 (10%) 10 11	16, 30, 52, 70	0
All	All	604/658 (91%)	0.74	106 (17%) 4 4	14, 29, 66, 84	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1174	TRP	7.0
1	A	1186	VAL	5.8
1	A	990	CYS	5.0
1	A	1198	LEU	5.0
1	A	1183	ASP	4.7
1	A	1203	GLY	4.5
1	A	995	ALA	4.5
1	A	992	VAL	4.4
1	A	1199	ALA	4.4
1	A	972	PRO	4.4
1	B	1217	TYR	4.4
1	A	1205	THR	4.4
1	A	981	ALA	4.3
1	A	1002	LEU	4.3
1	B	1129	HIS	4.2
1	A	1187	LEU	4.2
1	A	1188	ALA	4.1
1	A	1181	GLY	4.1
1	A	988	LEU	4.1
1	A	1024	VAL	4.0
1	B	1109	ALA	4.0
1	A	1173	ASN	4.0
1	B	1207	THR	4.0
1	A	1201	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	1171	THR	3.6
1	A	975	GLY	3.6
1	A	1202	GLN	3.5
1	A	971	ALA	3.4
1	A	982	ALA	3.4
1	A	979	ILE	3.4
1	A	993	GLN	3.4
1	A	1197	PHE	3.4
1	B	1050	ARG	3.3
1	A	983	ALA	3.2
1	A	987	LEU	3.2
1	A	1014	ALA	3.2
1	A	994	ASP	3.1
1	A	997	ALA	3.1
1	A	1293	ARG	3.1
1	A	1182	LEU	3.1
1	A	1042	ILE	3.0
1	A	1184	PRO	3.0
1	B	1049	THR	3.0
1	A	970	ARG	3.0
1	B	1108	THR	3.0
1	A	1020	VAL	2.9
1	B	1228	HIS	2.9
1	A	996	ASP	2.9
1	A	980	ILE	2.9
1	A	1217	TYR	2.9
1	A	989	GLY	2.9
1	A	968	PRO	2.8
1	B	1272	VAL	2.8
1	B	1110	ALA	2.8
1	A	1195	GLU	2.8
1	A	1190	ILE	2.8
1	A	1200	ALA	2.7
1	B	1115	VAL	2.6
1	B	1249	MET	2.6
1	B	1293	ARG	2.6
1	B	1112	LEU	2.6
1	A	986	SER	2.6
1	A	1196	ALA	2.6
1	B	1218	ALA	2.6
1	A	1043	ASP	2.5
1	A	1041	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1001	ALA	2.5
1	B	1230	VAL	2.5
1	B	1102	PRO	2.5
1	A	1204	SER	2.5
1	B	1021	ALA	2.5
1	A	1049	THR	2.5
1	B	1211	THR	2.4
1	A	1191	ASN	2.4
1	A	984	PHE	2.4
1	B	1153	ALA	2.4
1	A	969	GLY	2.4
1	A	1016	LEU	2.3
1	A	1013	ALA	2.3
1	B	1104	GLY	2.3
1	B	1221	VAL	2.3
1	A	1207	THR	2.3
1	B	1125	GLU	2.3
1	B	1225	THR	2.3
1	A	1051	ARG	2.3
1	A	1248	GLY	2.3
1	A	1035	VAL	2.3
1	A	1172	GLN	2.2
1	A	1206	SER	2.2
1	A	1044	ALA	2.2
1	A	1228	HIS	2.2
1	B	1064	ASN	2.2
1	A	1247	GLU	2.2
1	A	1034	THR	2.2
1	B	1018	ARG	2.2
1	A	1175	GLN	2.2
1	A	974	ALA	2.2
1	A	1211	THR	2.1
1	A	1046	GLU	2.1
1	A	1015	GLN	2.1
1	B	1172	GLN	2.1
1	B	1020	VAL	2.1
1	A	1012	LEU	2.1
1	B	1103	ASN	2.1
1	A	1045	GLU	2.0
1	B	1215	GLY	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, 95th 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($\text{\AA}^2$)	Q<0.9
1	UF0	B	1006	31/32	0.91	0.12	26,35,42,43	0
1	UF0	A	1006	31/32	0.92	0.10	19,26,36,41	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.