Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:15 am BST

PDB ID	:	5N1A
Title	:	Crystal structure of Utp4 from Chaetomium thermophilum
Authors	:	Calvino, F.R.; Ahmed, Y.L.; Wild, K.; Sinning, I.
Deposited on	:	2017-02-05
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

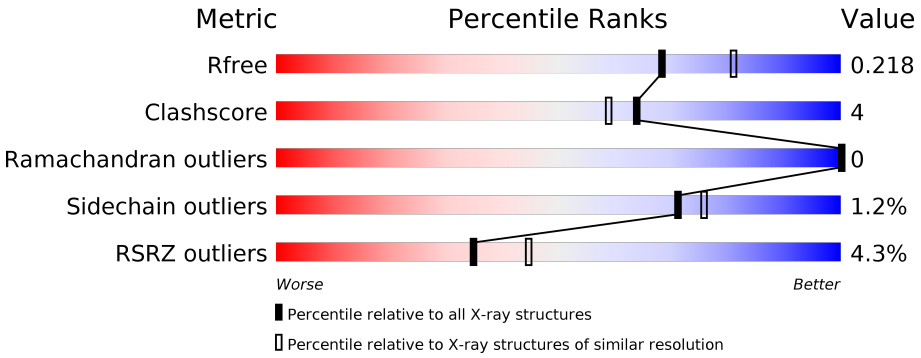
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	908	3% 68% 9% 23%
1	B	908	4% 69% 8% 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11717 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 utp4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	Se	0	1	0
			5527	3517	994	993	8	15			
1	B	706	Total	C	N	O	S	Se	0	1	0
			5542	3525	996	998	8	15			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	initiating methionine	UNP G0SCT7
A	-22	GLY	-	expression tag	UNP G0SCT7
A	-21	HIS	-	expression tag	UNP G0SCT7
A	-20	HIS	-	expression tag	UNP G0SCT7
A	-19	HIS	-	expression tag	UNP G0SCT7
A	-18	HIS	-	expression tag	UNP G0SCT7
A	-17	HIS	-	expression tag	UNP G0SCT7
A	-16	HIS	-	expression tag	UNP G0SCT7
A	-15	ASP	-	expression tag	UNP G0SCT7
A	-14	TYR	-	expression tag	UNP G0SCT7
A	-13	ASP	-	expression tag	UNP G0SCT7
A	-12	ILE	-	expression tag	UNP G0SCT7
A	-11	PRO	-	expression tag	UNP G0SCT7
A	-10	THR	-	expression tag	UNP G0SCT7
A	-9	THR	-	expression tag	UNP G0SCT7
A	-8	GLU	-	expression tag	UNP G0SCT7
A	-7	ASN	-	expression tag	UNP G0SCT7
A	-6	LEU	-	expression tag	UNP G0SCT7
A	-5	TYR	-	expression tag	UNP G0SCT7
A	-4	PHE	-	expression tag	UNP G0SCT7
A	-3	GLN	-	expression tag	UNP G0SCT7
A	-2	GLY	-	expression tag	UNP G0SCT7
A	-1	ALA	-	expression tag	UNP G0SCT7
A	0	HIS	-	expression tag	UNP G0SCT7
A	1	MSE	-	expression tag	UNP G0SCT7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MSE	-	initiating methionine	UNP G0SCT7
B	-22	GLY	-	expression tag	UNP G0SCT7
B	-21	HIS	-	expression tag	UNP G0SCT7
B	-20	HIS	-	expression tag	UNP G0SCT7
B	-19	HIS	-	expression tag	UNP G0SCT7
B	-18	HIS	-	expression tag	UNP G0SCT7
B	-17	HIS	-	expression tag	UNP G0SCT7
B	-16	HIS	-	expression tag	UNP G0SCT7
B	-15	ASP	-	expression tag	UNP G0SCT7
B	-14	TYR	-	expression tag	UNP G0SCT7
B	-13	ASP	-	expression tag	UNP G0SCT7
B	-12	ILE	-	expression tag	UNP G0SCT7
B	-11	PRO	-	expression tag	UNP G0SCT7
B	-10	THR	-	expression tag	UNP G0SCT7
B	-9	THR	-	expression tag	UNP G0SCT7
B	-8	GLU	-	expression tag	UNP G0SCT7
B	-7	ASN	-	expression tag	UNP G0SCT7
B	-6	LEU	-	expression tag	UNP G0SCT7
B	-5	TYR	-	expression tag	UNP G0SCT7
B	-4	PHE	-	expression tag	UNP G0SCT7
B	-3	GLN	-	expression tag	UNP G0SCT7
B	-2	GLY	-	expression tag	UNP G0SCT7
B	-1	ALA	-	expression tag	UNP G0SCT7
B	0	HIS	-	expression tag	UNP G0SCT7
B	1	MSE	-	expression tag	UNP G0SCT7

- Molecule 2 is water.

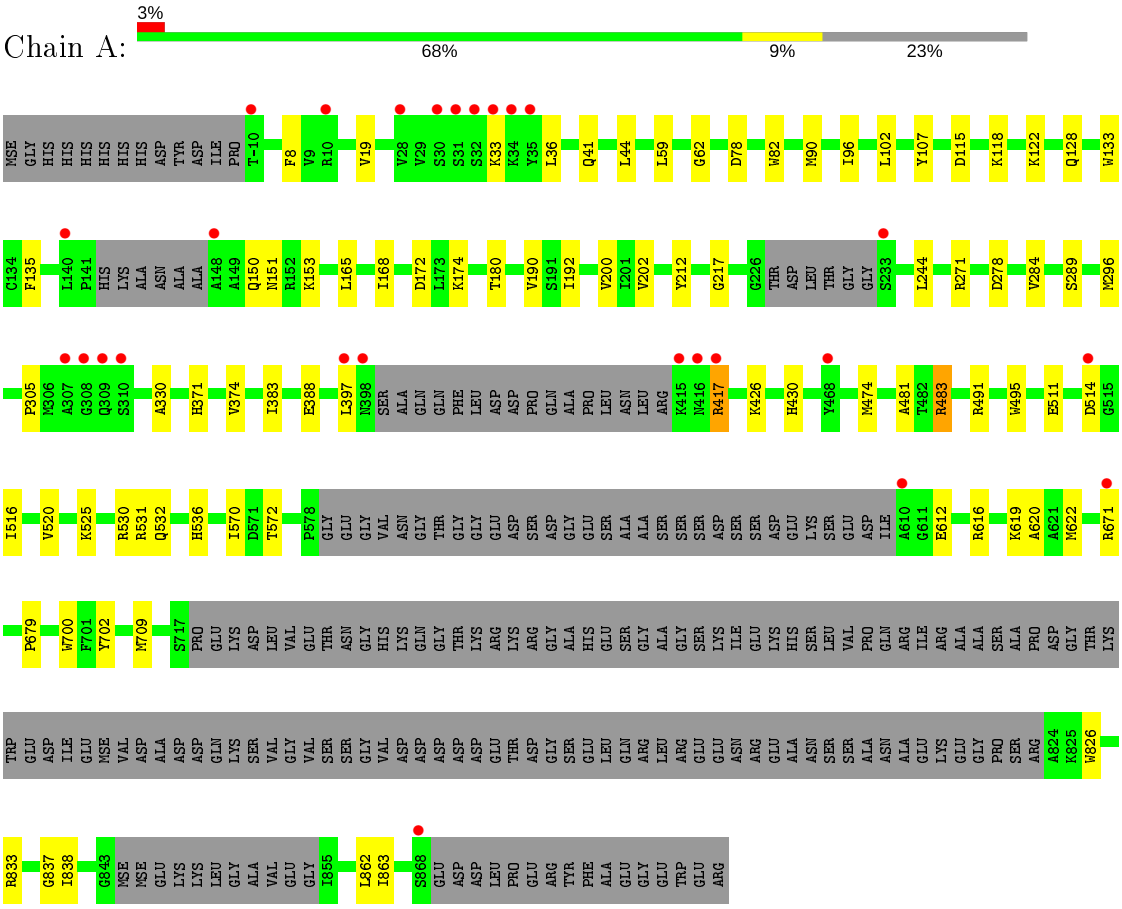
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	347	Total O 347 347	0	0
2	B	301	Total O 301 301	0	0

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.

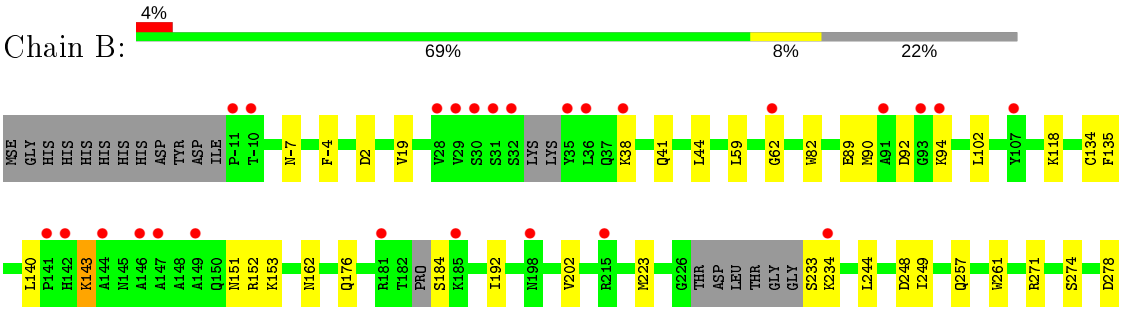
- Molecule 1: utp4

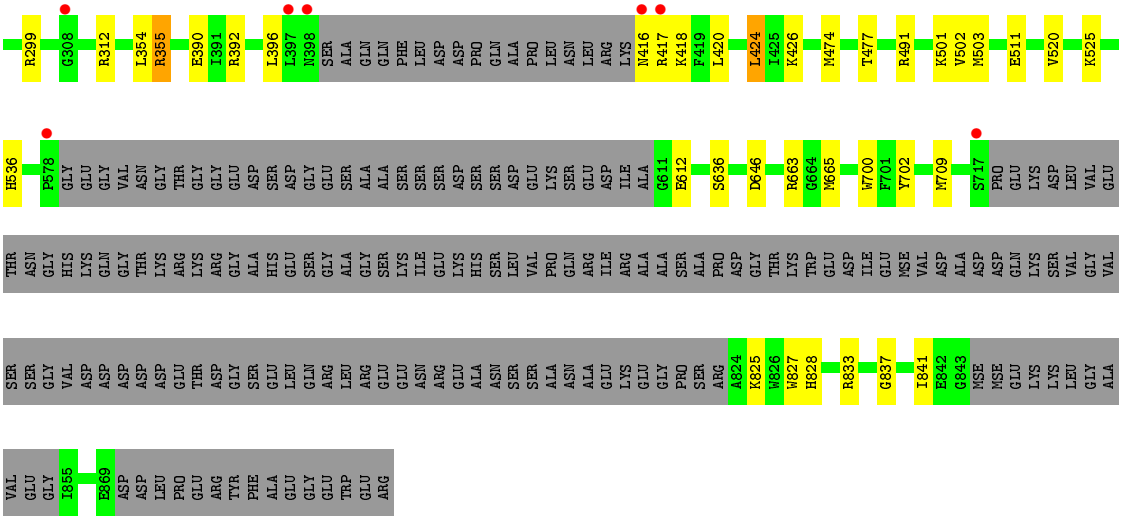
Chain A:



- Molecule 1: utp4

Chain B:




R299 G308 R312 L354 R355 E390 I391 R392 L396 L397 N398 SER ALA GLN GLN PHE LEU ASP ASP PRO GLN ALA PRO LEU ASN LEU ARG LYS N416 R417 K418 F419 L420 L424 I425 K426 M474 T477 R491 K501 V502 M503 E511 V520 K525
H536 P578 GLY GLU GLY VAL ASN GLY THR GLY GLY GLU ASP SER ASP GLY GLU SER ALA ALA SER SER SER ASP SER SER ASP GLU LYS SER GLU ASP ILE ALA G611 E612 S636 D646 R663 G664 M665 W700 F701 Y702 M709 S717 PRO GLU LYS ASP LEU VAL GLU
THR ASN GLY HIS LYS GLN GLY THR LYS ARG LYS ARG GLY ALA HIS GLU SER GLY ALA GLY SER LYS ILE GLU LYS HIS SER LEU VAL PRO GLN ARG ILE ARG ALA ALA SER ALA PRO ASP GLY THR LYS TRP GLU ASP ILE GLU MSE VAL ASP ALA ASP ASP GLN LYS SER VAL GLY VAL
SER SER GLY VAL ASP ASP ASP ASP GLU THR ASP GLY SER GLU LEU GLN ARG LEU ARG GLU GLU GLU ASN ARG GLU ALA ASN SER SER ALA ASN ALA GLU LYS GLU GLY PRO SER ARG A824 K825 W826 W827 H828 R833 G837 I841 E842 G843 MSE MSE GLU LYS LYS LEU GLY ALA
VAL GLU GLY I855 E869 ASP ASP LEU PRO GLU ARG TYR PHE ALA GLU GLY GLU TRP GLU ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.03Å 81.59Å 112.30Å 90.00° 110.55° 90.00°	Depositor
Resolution (Å)	47.53 – 2.15 47.53 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.53-2.15) 99.9 (47.53-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.183 , 0.220 0.180 , 0.218	Depositor DCC
R_{free} test set	4684 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11717	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/5644	0.58	6/7626 (0.1%)
1	B	0.29	0/5663	0.66	12/7653 (0.2%)
All	All	0.28	0/11307	0.62	18/15279 (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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	LYS	CA-CB-CG	17.05	150.91	113.40
1	B	234	LYS	CA-CB-CG	11.19	138.02	113.40
1	B	312	ARG	CB-CG-CD	-9.77	86.20	111.60
1	B	38	LYS	CB-CA-C	-9.39	91.61	110.40
1	B	424	LEU	CB-CG-CD1	-9.33	95.13	111.00
1	A	525	LYS	CD-CE-NZ	-8.66	91.78	111.70
1	B	38	LYS	CB-CG-CD	8.26	133.06	111.60
1	B	312	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	A	417	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	B	312	ARG	CG-CD-NE	7.83	128.23	111.80
1	B	424	LEU	CB-CG-CD2	7.56	123.84	111.00
1	A	671	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	B	312	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	B	38	LYS	CG-CD-CE	-6.29	93.04	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	525	LYS	CB-CG-CD	-5.61	97.01	111.60
1	B	234	LYS	CD-CE-NZ	5.51	124.38	111.70
1	A	671	ARG	NE-CZ-NH2	5.06	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	ARG	Sidechain
1	B	511	GLU	Sidechain

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	5527	0	5553	51	1
1	B	5542	0	5550	42	2
2	A	347	0	0	7	1
2	B	301	0	0	8	0
All	All	11717	0	11103	92	2

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 4.

All (92) 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:371:HIS:CD2	1:A:483:ARG:NH1	1.74	1.53
1:A:371:HIS:CD2	1:A:483:ARG:HH11	1.51	1.12
1:A:371:HIS:CD2	1:A:483:ARG:HH12	1.70	0.93
1:A:371:HIS:HD2	1:A:483:ARG:NH1	1.53	0.91
1:B:424:LEU:HD12	1:B:426:LYS:HE2	1.56	0.86
1:A:514:ASP:OD1	1:B:184:SER:OG	2.09	0.71
1:A:19:VAL:HG13	1:A:44:LEU:HD11	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:VAL:HG11	1:A:863:ILE:HD13	1.74	0.68
1:B:271:ARG:NH1	2:B:911:HOH:O	2.30	0.65
1:A:78:ASP:HB2	1:A:107:TYR:CZ	2.32	0.64
1:B:41:GLN:HA	1:B:41:GLN:OE1	1.99	0.62
1:B:19:VAL:HG13	1:B:44:LEU:HD11	1.80	0.62
1:A:474:MSE:HE3	1:A:520:VAL:HG11	1.80	0.61
1:A:491:ARG:NH2	1:A:612:GLU:OE1	2.31	0.61
1:B:491:ARG:NH2	1:B:612:GLU:OE1	2.28	0.60
1:B:663:ARG:HE	1:B:665:MSE:HE2	1.66	0.59
1:B:501:LYS:HB3	1:B:503:MSE:HE3	1.84	0.59
1:A:531:ARG:NH1	2:A:902:HOH:O	2.22	0.59
1:A:33:LYS:HB3	1:A:36:LEU:HD12	1.86	0.58
1:B:92:ASP:OD1	1:B:94:LYS:HB2	2.03	0.58
1:A:616[A]:ARG:HH21	1:A:620:ALA:HB1	1.68	0.58
1:B:118:LYS:NZ	2:B:913:HOH:O	2.36	0.57
1:A:78:ASP:OD1	2:A:901:HOH:O	2.17	0.57
1:A:371:HIS:CG	1:A:483:ARG:HH12	2.20	0.56
1:A:570:ILE:O	2:A:902:HOH:O	2.17	0.55
1:B:274:SER:O	1:B:299:ARG:NH1	2.39	0.55
1:B:-7:ASN:ND2	1:B:2:ASP:OD1	2.40	0.55
1:A:619:LYS:HD2	1:A:622:MSE:SE	2.56	0.54
1:A:174:LYS:NZ	2:A:911:HOH:O	2.41	0.53
1:A:8:PHE:CZ	1:A:383:ILE:HD11	2.43	0.52
1:A:511:GLU:HG2	1:A:516:ILE:HD13	1.91	0.52
1:B:700:TRP:CE2	1:B:709:MSE:HG3	2.45	0.52
1:A:168:ILE:HA	1:A:172:ASP:O	2.09	0.52
1:B:59:LEU:HB2	1:B:62:GLY:O	2.10	0.52
1:B:153:LYS:NZ	1:B:176:GLN:OE1	2.33	0.52
1:A:700:TRP:CE2	1:A:709:MSE:HG3	2.45	0.52
1:B:355:ARG:NH2	2:B:906:HOH:O	2.25	0.51
1:B:192:ILE:HG12	1:B:202:VAL:HG12	1.92	0.51
1:B:474:MSE:HE3	1:B:520:VAL:HG11	1.93	0.51
1:A:531:ARG:HD3	2:A:967:HOH:O	2.11	0.50
1:B:89:GLU:HG2	1:B:90:MSE:O	2.11	0.50
1:B:244:LEU:HD12	1:B:248:ASP:HB2	1.93	0.50
1:A:133:TRP:HE3	1:A:190:VAL:HG12	1.77	0.50
1:B:162:ASN:ND2	2:B:907:HOH:O	2.26	0.50
1:A:192:ILE:HG13	1:A:202:VAL:HG12	1.95	0.49
1:B:82:TRP:CE2	1:B:102:LEU:HD13	2.47	0.49
1:B:-4:PHE:HB3	1:B:827:TRP:CD1	2.48	0.49
1:A:150:GLN:N	1:A:150:GLN:OE1	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LYS:HE3	1:B:536:HIS:CE1	2.48	0.48
1:A:8:PHE:HZ	1:A:383:ILE:HD11	1.78	0.48
1:B:354:LEU:HB3	2:B:903:HOH:O	2.12	0.48
1:A:82:TRP:CE2	1:A:102:LEU:HD13	2.50	0.47
1:B:503:MSE:HE1	1:B:525:LYS:HG2	1.96	0.46
1:A:41:GLN:HG3	2:A:1222:HOH:O	2.15	0.46
1:B:418:LYS:HD2	1:B:420:LEU:HD12	1.95	0.46
1:A:90:MSE:SE	1:A:96:ILE:HD11	2.65	0.46
1:B:223:MSE:HB3	1:B:261:TRP:CZ3	2.50	0.45
1:A:200:VAL:CG1	1:A:212:TYR:HB2	2.46	0.45
1:A:244:LEU:HD23	1:A:284:VAL:HG11	1.99	0.45
1:A:838:ILE:HG12	1:A:862:LEU:HG	1.99	0.45
1:A:115:ASP:HB2	1:A:122:LYS:HB2	1.99	0.44
1:B:134:CYS:SG	1:B:192:ILE:HG13	2.57	0.44
1:A:59:LEU:HB2	1:A:62:GLY:O	2.17	0.44
1:A:481:ALA:HB2	1:A:495:TRP:CD1	2.53	0.44
1:B:396:LEU:HD12	1:B:841:ILE:HD13	1.99	0.43
1:B:90:MSE:SE	1:B:536:HIS:HB3	2.68	0.43
1:A:271:ARG:HH11	1:A:271:ARG:HG3	1.83	0.43
1:A:702:TYR:CE2	1:A:837:GLY:HA2	2.53	0.43
1:A:133:TRP:CE3	1:A:190:VAL:HG12	2.53	0.43
1:A:388:GLU:HA	1:A:430:HIS:CD2	2.54	0.43
1:B:477:THR:O	2:B:901:HOH:O	2.21	0.43
1:A:289:SER:O	1:A:305:PRO:HD3	2.19	0.43
1:B:249:ILE:HB	1:B:261:TRP:HB2	2.00	0.43
1:B:502:VAL:O	1:B:503:MSE:HE2	2.18	0.43
1:A:180:THR:HG22	1:A:217:GLY:O	2.19	0.43
1:B:702:TYR:CE1	1:B:837:GLY:HA2	2.54	0.42
1:A:90:MSE:HE2	1:A:536:HIS:HB3	2.02	0.42
1:B:257:GLN:OE1	2:B:902:HOH:O	2.21	0.42
1:A:118:LYS:HE2	2:A:947:HOH:O	2.19	0.42
1:B:416:ASN:OD1	1:B:417:ARG:N	2.50	0.42
1:A:426:LYS:HD3	1:A:426:LYS:HA	1.81	0.42
1:B:833:ARG:NH1	2:B:930:HOH:O	2.52	0.42
1:B:636:SER:HB3	1:B:646:ASP:HB2	2.02	0.42
1:B:140:LEU:HD23	1:B:152:ARG:HD3	2.02	0.41
1:B:390:GLU:OE2	1:B:392:ARG:NE	2.53	0.41
1:A:19:VAL:HG12	1:A:330:ALA:HB3	2.02	0.41
1:B:503:MSE:SE	1:B:525:LYS:HG2	2.71	0.41
1:A:153:LYS:HB3	1:A:165:LEU:HD11	2.03	0.41
1:A:397:LEU:HA	1:A:397:LEU:HD23	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:OD1	1:A:153:LYS:NZ	2.54	0.41
1:A:572:THR:H	1:A:616[A]:ARG:NH2	2.19	0.41
1:A:679:PRO:HB3	1:A:826:TRP:CZ2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:NE2	1:B:151:ASN:OD1[4_546]	2.11	0.09
1:B:143:LYS:NZ	2:A:911:HOH:O[4_556]	2.16	0.04

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	690/908 (76%)	680 (99%)	10 (1%)	0	100	100
1	B	691/908 (76%)	676 (98%)	15 (2%)	0	100	100
All	All	1381/1816 (76%)	1356 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	595/740 (80%)	588 (99%)	7 (1%)	71	76
1	B	596/740 (80%)	589 (99%)	7 (1%)	71	76
All	All	1191/1480 (80%)	1177 (99%)	14 (1%)	71	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	PHE
1	A	278	ASP
1	A	296	MSE
1	A	483	ARG
1	A	530	ARG
1	A	532	GLN
1	A	833	ARG
1	B	135	PHE
1	B	143	LYS
1	B	233	SER
1	B	278	ASP
1	B	355	ARG
1	B	825	LYS
1	B	828	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	688/908 (75%)	0.05	26 (3%)	40	49	22, 37, 68, 115	1 (0%)
1	B	691/908 (76%)	0.19	33 (4%)	30	39	26, 40, 75, 126	0
All	All	1379/1816 (75%)	0.12	59 (4%)	35	45	22, 38, 72, 126	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	SER	6.8
1	B	146	ALA	6.3
1	A	32	SER	5.6
1	B	36	LEU	5.6
1	B	147	ALA	5.2
1	B	181	ARG	5.1
1	B	142	HIS	5.1
1	A	148	ALA	5.0
1	A	417	ARG	5.0
1	B	416	ASN	4.9
1	B	30	SER	4.9
1	A	308	GLY	4.3
1	B	29	VAL	4.2
1	B	398	ASN	4.2
1	B	234	LYS	4.1
1	B	38	LYS	4.1
1	B	35	TYR	4.0
1	A	307	ALA	3.8
1	B	-11	PRO	3.7
1	A	30	SER	3.6
1	B	308	GLY	3.6
1	A	416	ASN	3.4
1	A	31	SER	3.3
1	A	397	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	35	TYR	3.2
1	B	144	ALA	3.2
1	B	28	VAL	3.2
1	A	415	LYS	3.2
1	B	417	ARG	3.1
1	A	-10	THR	3.1
1	A	28	VAL	3.1
1	B	91	ALA	3.0
1	B	397	LEU	3.0
1	A	309	GLN	2.9
1	B	93	GLY	2.9
1	B	107	TYR	2.8
1	B	62	GLY	2.8
1	A	34	LYS	2.7
1	A	868	SER	2.7
1	B	141	PRO	2.7
1	B	31	SER	2.6
1	B	94	LYS	2.5
1	A	233	SER	2.5
1	A	33	LYS	2.5
1	B	198	ASN	2.4
1	A	671	ARG	2.3
1	B	578	PRO	2.3
1	A	310	SER	2.3
1	B	-10	THR	2.3
1	A	140	LEU	2.2
1	B	185	LYS	2.2
1	A	610	ALA	2.1
1	B	717	SER	2.1
1	B	215	ARG	2.1
1	A	468	TYR	2.1
1	A	398	ASN	2.1
1	B	149	ALA	2.1
1	A	514	ASP	2.0
1	A	10	ARG	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.