Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:43 PM GMT

PDB ID	:	1UYJ
Title	:	CLOSTRIDIUM PERFRINGENS EPSILON TOXIN SHOWS STRUCTURAL SIMILARITY WITH THE PORE FORMING TOXIN AEROLYSIN
Authors	:	Cole, A.R.; Gibert, M.; Poppoff, M.; Moss, D.S.; Titball, R.W.; Basak, A.K.
Deposited on	:	2004-03-02
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

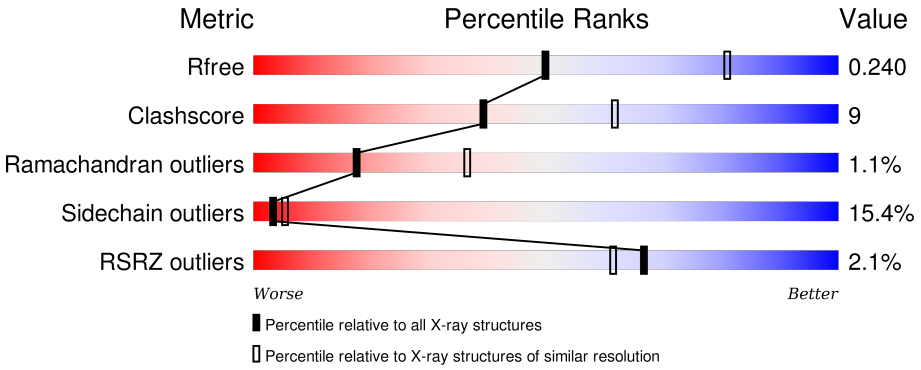
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	296	2% 66% 21% • 8%
1	B	296	2% 66% 21% • 8%
1	C	296	2% 66% 20% 6% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6320 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 EPSILON-TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2072	1303	338	426	5			
1	B	273	Total	C	N	O	S	0	0	0
			2088	1309	344	430	5			
1	C	273	Total	C	N	O	S	0	0	0
			2096	1319	345	427	5			

- Molecule 2 is URANIUM ATOM (three-letter code: U1) (formula: U).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	U	0	0
			5	5		
2	A	3	Total	U	0	0
			3	3		
2	C	4	Total	U	0	0
			4	4		

- Molecule 3 is water.

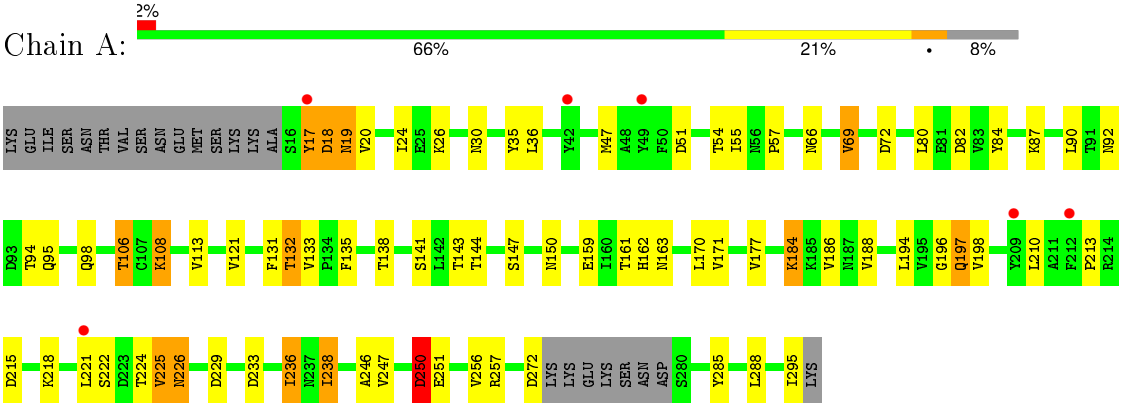
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	13	Total	O	0	0
			13	13		
3	C	28	Total	O	0	0
			28	28		

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 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.

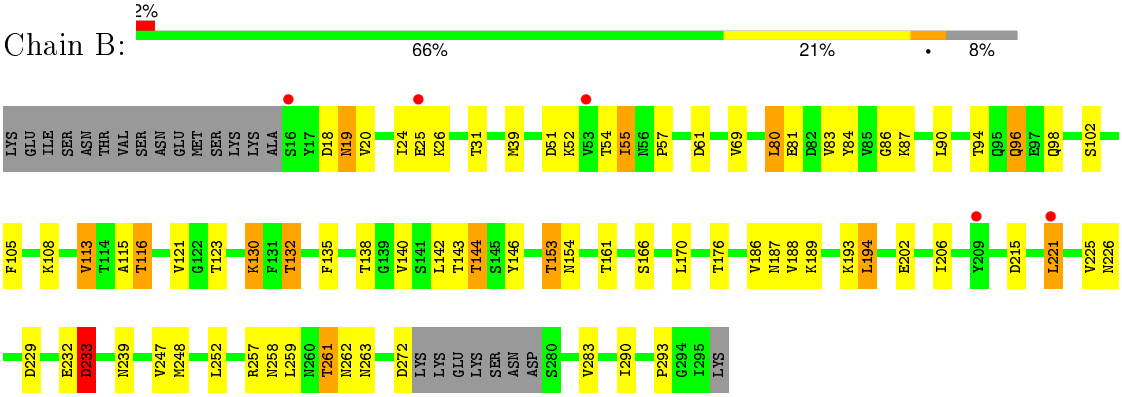
- Molecule 1: EPSILON-TOXIN

Chain A:



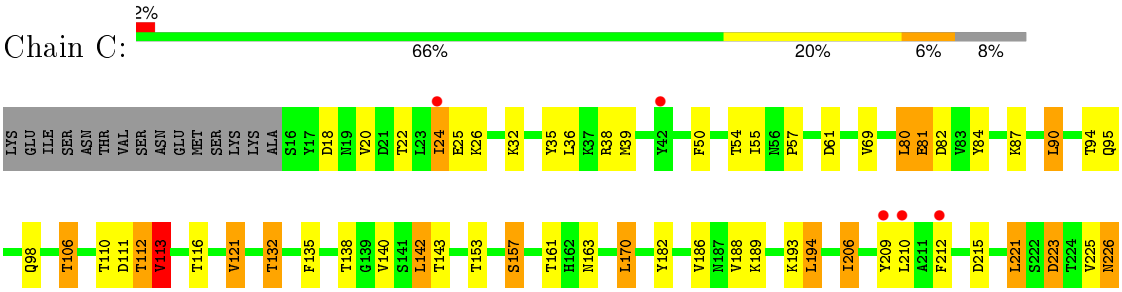
- Molecule 1: EPSILON-TOXIN

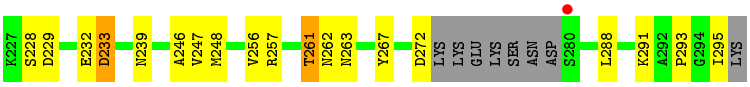
Chain B:



- Molecule 1: EPSILON-TOXIN

Chain C:




K227
S228
D229
E232
D233
N239
A246
V247
M248
V256
R257
T261
N262
N263
Y267
D272
LYS
LYS
GLU
LYS
SER
ASN
ASP
S280
L288
K291
A292
P293
G294
T295
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	125.96Å 125.96Å 121.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.60) 99.5 (49.78-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.43 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.290 0.241 , 0.240	Depositor DCC
R_{free} test set	1704 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.3	EDS
Estimated twinning fraction	0.180 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 33650 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6320	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.67 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0392e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: U1

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	0.60	0/2108	0.87	10/2879 (0.3%)
1	B	0.61	0/2125	0.84	6/2901 (0.2%)
1	C	0.65	0/2133	0.86	8/2910 (0.3%)
All	All	0.62	0/6366	0.86	24/8690 (0.3%)

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	ASP	CB-CG-OD2	9.33	126.70	118.30
1	C	229	ASP	CB-CG-OD2	7.75	125.27	118.30
1	C	113	VAL	CB-CA-C	-7.24	97.64	111.40
1	C	215	ASP	CB-CG-OD2	7.07	124.66	118.30
1	B	215	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	257	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	82	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	215	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	223	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	229	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	272	ASP	CB-CG-OD2	5.85	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	229	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	257	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	111	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	51	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	17	TYR	N-CA-C	5.64	126.24	111.00
1	A	72	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	61	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	272	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	272	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	61	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	51	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	18	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	113	VAL	CB-CA-C	-5.10	101.71	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	26	LYS	Peptide
1	C	26	LYS	Peptide

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	2072	0	1939	34	0
1	B	2088	0	1979	32	0
1	C	2096	0	2004	42	0
2	A	3	0	0	0	0
2	B	5	0	0	0	0
2	C	4	0	0	0	0
3	A	11	0	0	0	0
3	B	13	0	0	1	0
3	C	28	0	0	3	0
All	All	6320	0	5922	108	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 9.

All (108) 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:66:ASN:HB2	1:A:197:GLN:HE22	1.47	0.78
1:A:184:LYS:HB2	1:A:250:ASP:OD1	1.84	0.77
1:B:144:THR:HG22	1:B:154:ASN:OD1	1.84	0.77
1:B:116:THR:HB	1:B:153:THR:HG22	1.69	0.75
1:A:198:VAL:HG23	1:A:238:ILE:HD12	1.68	0.74
1:B:24:ILE:HG21	1:B:221:LEU:HD13	1.70	0.74
1:A:94:THR:HG21	1:A:98:GLN:HE21	1.53	0.72
1:B:258:ASN:HB3	1:B:261:THR:HG22	1.70	0.71
1:C:295:ILE:C	3:C:2028:HOH:O	2.28	0.71
1:C:135:PHE:HB3	1:C:248:MET:HE1	1.73	0.71
1:B:108:LYS:HG2	1:B:161:THR:HG22	1.76	0.68
1:C:94:THR:HG21	1:C:98:GLN:NE2	2.10	0.67
1:B:132:THR:HB	1:B:143:THR:HG22	1.77	0.66
1:A:84:TYR:OH	1:A:87:LYS:HB2	1.96	0.65
1:C:263:ASN:HD22	1:C:293:PRO:HB3	1.61	0.65
1:C:257:ARG:HE	1:C:262:ASN:HD22	1.46	0.63
1:A:250:ASP:CG	1:A:251:GLU:H	2.02	0.62
1:C:94:THR:HG21	1:C:98:GLN:HE21	1.64	0.62
1:B:263:ASN:HD22	1:B:293:PRO:HB3	1.65	0.61
1:C:232:GLU:O	1:C:233:ASP:HB3	1.98	0.61
1:B:55:ILE:O	1:B:57:PRO:HD3	2.00	0.61
1:A:132:THR:HB	1:A:143:THR:HG22	1.82	0.61
1:B:194:LEU:O	1:B:239:ASN:HA	2.00	0.61
1:A:108:LYS:HG2	1:A:161:THR:HG22	1.84	0.59
1:C:135:PHE:CZ	1:C:186:VAL:HG11	2.38	0.59
1:C:32:LYS:NZ	1:C:50:PHE:O	2.35	0.59
1:C:132:THR:HB	1:C:143:THR:HG22	1.85	0.58
1:B:121:VAL:HG13	1:B:121:VAL:O	2.03	0.57
1:A:94:THR:HG21	1:A:98:GLN:NE2	2.19	0.57
1:C:267:TYR:OH	1:C:291:LYS:O	2.18	0.57
1:B:257:ARG:HE	1:B:262:ASN:HD22	1.53	0.56
1:A:108:LYS:CG	1:A:161:THR:HG22	2.36	0.56
1:A:18:ASP:HB2	1:A:236:ILE:HD11	1.88	0.55
1:A:198:VAL:CG2	1:A:238:ILE:HD12	2.35	0.55
1:C:138:THR:HG23	1:C:140:VAL:HG23	1.90	0.54
1:C:189:LYS:HE2	3:C:2022:HOH:O	2.08	0.54
1:C:24:ILE:HG21	1:C:221:LEU:HG	1.89	0.53
1:C:94:THR:HG22	1:C:95:GLN:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:CZ	1:A:186:VAL:HG11	2.44	0.52
1:C:110:THR:HG22	1:C:112:THR:HG22	1.93	0.51
1:A:196:GLY:O	1:A:238:ILE:HD13	2.10	0.51
1:B:130:LYS:NZ	1:B:130:LYS:HB3	2.26	0.50
1:A:132:THR:CB	1:A:143:THR:HG22	2.41	0.50
1:B:187:ASN:HD21	1:B:189:LYS:CE	2.25	0.50
1:B:19:ASN:ND2	1:B:20:VAL:HG12	2.27	0.49
1:B:135:PHE:CZ	1:B:186:VAL:HG11	2.47	0.49
1:A:184:LYS:CB	1:A:250:ASP:OD1	2.58	0.49
1:C:94:THR:HG22	1:C:95:GLN:H	1.77	0.49
1:A:19:ASN:C	1:A:19:ASN:ND2	2.65	0.49
1:B:135:PHE:HB3	1:B:248:MET:CE	2.42	0.49
1:B:187:ASN:HD21	1:B:189:LYS:NZ	2.11	0.49
1:C:225:VAL:O	1:C:226:ASN:HB3	2.11	0.48
1:C:261:THR:HG22	1:C:263:ASN:H	1.77	0.48
1:A:250:ASP:CG	1:A:251:GLU:N	2.66	0.48
1:A:92:ASN:ND2	1:A:171:VAL:O	2.45	0.47
1:C:106:THR:HG22	1:C:163:ASN:OD1	2.14	0.47
1:C:194:LEU:O	1:C:239:ASN:HA	2.15	0.47
1:A:106:THR:HG22	1:A:163:ASN:OD1	2.14	0.47
1:B:258:ASN:HB2	1:B:293:PRO:HG2	1.96	0.47
1:B:115:ALA:HB1	1:B:146:TYR:CZ	2.50	0.46
1:A:113:VAL:HG23	1:A:246:ALA:HB2	1.96	0.46
1:C:225:VAL:O	1:C:226:ASN:CB	2.64	0.46
1:B:84:TYR:OH	1:B:87:LYS:HB2	2.15	0.46
1:B:138:THR:HG23	1:B:283:VAL:HG21	1.96	0.46
1:C:55:ILE:O	1:C:57:PRO:HD3	2.16	0.46
1:B:232:GLU:O	1:B:233:ASP:HB3	2.16	0.46
1:C:84:TYR:OH	1:C:87:LYS:HB2	2.16	0.46
1:C:113:VAL:HG13	1:C:246:ALA:HB2	1.97	0.46
1:A:69:VAL:HG22	1:A:131:PHE:CD1	2.52	0.45
1:C:170:LEU:HB3	1:C:295:ILE:HD13	1.98	0.45
1:B:258:ASN:O	1:B:262:ASN:N	2.49	0.45
1:C:248:MET:HB2	1:C:248:MET:HE3	1.93	0.45
1:C:226:ASN:ND2	1:C:228:SER:OG	2.49	0.45
1:A:247:VAL:HG13	1:A:247:VAL:O	2.17	0.45
1:A:225:VAL:O	1:A:226:ASN:CG	2.55	0.44
1:B:176:THR:HG22	1:B:259:LEU:HD12	1.99	0.44
1:A:162:HIS:HB3	1:A:285:TYR:CE2	2.52	0.44
1:B:138:THR:HG22	1:B:140:VAL:HG23	1.98	0.44
1:C:189:LYS:CE	3:C:2022:HOH:O	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASP:O	1:A:238:ILE:HA	2.17	0.43
1:C:232:GLU:O	1:C:233:ASP:CB	2.64	0.43
1:C:121:VAL:HG13	1:C:121:VAL:O	2.18	0.43
1:B:86:GLY:HA3	1:B:105:PHE:CE1	2.52	0.43
1:A:19:ASN:ND2	1:A:20:VAL:HG22	2.34	0.43
1:C:35:TYR:OH	1:C:212:PHE:HB3	2.19	0.43
1:A:35:TYR:OH	1:A:213:PRO:O	2.23	0.42
1:C:209:TYR:CD1	1:C:210:LEU:HG	2.54	0.42
1:A:55:ILE:O	1:A:57:PRO:HD3	2.19	0.42
1:C:112:THR:HB	1:C:157:SER:HB3	2.00	0.42
1:C:82:ASP:HB3	1:C:182:TYR:CD1	2.54	0.42
1:B:19:ASN:HD22	1:B:20:VAL:N	2.18	0.42
1:A:133:VAL:CG1	1:A:133:VAL:O	2.67	0.42
1:B:232:GLU:O	1:B:233:ASP:CB	2.68	0.42
1:C:20:VAL:HG12	1:C:22:THR:HB	2.01	0.42
1:A:133:VAL:HG13	1:A:133:VAL:O	2.20	0.41
1:B:261:THR:HG23	1:B:263:ASN:H	1.85	0.41
1:C:106:THR:CG2	1:C:163:ASN:OD1	2.69	0.41
1:B:96:GLN:O	1:B:98:GLN:HG2	2.20	0.41
1:C:80:LEU:HD13	1:C:81:GLU:HG3	2.02	0.41
1:A:121:VAL:O	1:A:121:VAL:HG13	2.21	0.41
1:B:135:PHE:HB3	1:B:248:MET:HE3	2.03	0.40
1:B:52:LYS:CB	3:B:2002:HOH:O	2.69	0.40
1:A:94:THR:HG22	1:A:95:GLN:N	2.37	0.40
1:C:24:ILE:CG2	1:C:221:LEU:HD12	2.51	0.40
1:A:162:HIS:HB3	1:A:285:TYR:HE2	1.87	0.40
1:C:206:ILE:HD13	1:C:206:ILE:O	2.22	0.40
1:C:90:LEU:HA	1:C:90:LEU:HD12	1.97	0.40
1:C:142:LEU:HD12	1:C:142:LEU:HA	1.94	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	269/296 (91%)	244 (91%)	21 (8%)	4 (2%)	13 26
1	B	269/296 (91%)	247 (92%)	19 (7%)	3 (1%)	17 36
1	C	269/296 (91%)	252 (94%)	15 (6%)	2 (1%)	26 51
All	All	807/888 (91%)	743 (92%)	55 (7%)	9 (1%)	17 36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	TYR
1	A	210	LEU
1	C	226	ASN
1	C	233	ASP
1	B	80	LEU
1	B	233	ASP
1	A	226	ASN
1	A	26	LYS
1	B	225	VAL

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	220/267 (82%)	183 (83%)	37 (17%)	2 4
1	B	230/267 (86%)	193 (84%)	37 (16%)	3 5
1	C	230/267 (86%)	199 (86%)	31 (14%)	5 8
All	All	680/801 (85%)	575 (85%)	105 (15%)	3 5

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	19	ASN
1	A	24	ILE
1	A	30	ASN

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	47	MET
1	A	54	THR
1	A	69	VAL
1	A	80	LEU
1	A	90	LEU
1	A	106	THR
1	A	108	LYS
1	A	132	THR
1	A	138	THR
1	A	141	SER
1	A	144	THR
1	A	147	SER
1	A	150	ASN
1	A	159	GLU
1	A	170	LEU
1	A	177	VAL
1	A	184	LYS
1	A	188	VAL
1	A	194	LEU
1	A	197	GLN
1	A	218	LYS
1	A	221	LEU
1	A	222	SER
1	A	224	THR
1	A	225	VAL
1	A	233	ASP
1	A	236	ILE
1	A	238	ILE
1	A	250	ASP
1	A	256	VAL
1	A	288	LEU
1	A	295	ILE
1	B	18	ASP
1	B	19	ASN
1	B	25	GLU
1	B	31	THR
1	B	39	MET
1	B	54	THR
1	B	55	ILE
1	B	69	VAL
1	B	80	LEU

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Mol	Chain	Res	Type
1	B	81	GLU
1	B	83	VAL
1	B	90	LEU
1	B	94	THR
1	B	96	GLN
1	B	102	SER
1	B	113	VAL
1	B	116	THR
1	B	123	THR
1	B	130	LYS
1	B	132	THR
1	B	142	LEU
1	B	144	THR
1	B	153	THR
1	B	166	SER
1	B	170	LEU
1	B	188	VAL
1	B	193	LYS
1	B	194	LEU
1	B	202	GLU
1	B	206	ILE
1	B	221	LEU
1	B	226	ASN
1	B	233	ASP
1	B	247	VAL
1	B	252	LEU
1	B	261	THR
1	B	290	ILE
1	C	24	ILE
1	C	25	GLU
1	C	36	LEU
1	C	38	ARG
1	C	39	MET
1	C	54	THR
1	C	69	VAL
1	C	80	LEU
1	C	81	GLU
1	C	90	LEU
1	C	106	THR
1	C	112	THR
1	C	113	VAL
1	C	116	THR

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Mol	Chain	Res	Type
1	C	121	VAL
1	C	132	THR
1	C	142	LEU
1	C	153	THR
1	C	157	SER
1	C	161	THR
1	C	170	LEU
1	C	188	VAL
1	C	193	LYS
1	C	194	LEU
1	C	206	ILE
1	C	221	LEU
1	C	223	ASP
1	C	247	VAL
1	C	256	VAL
1	C	261	THR
1	C	288	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	30	ASN
1	A	56	ASN
1	A	66	ASN
1	A	98	GLN
1	A	150	ASN
1	A	197	GLN
1	A	226	ASN
1	A	262	ASN
1	B	19	ASN
1	B	152	ASN
1	B	187	ASN
1	B	226	ASN
1	B	260	ASN
1	B	262	ASN
1	B	263	ASN
1	B	281	ASN
1	C	98	GLN
1	C	152	ASN
1	C	174	ASN
1	C	226	ASN

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Mol	Chain	Res	Type
1	C	260	ASN
1	C	262	ASN
1	C	263	ASN
1	C	265	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 12 ligands modelled in this entry, 12 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

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	273/296 (92%)	0.11	6 (2%)	65	59	33, 48, 73, 79	0
1	B	273/296 (92%)	0.19	5 (1%)	71	66	31, 47, 72, 78	0
1	C	273/296 (92%)	0.20	6 (2%)	65	59	30, 46, 72, 78	0
All	All	819/888 (92%)	0.17	17 (2%)	67	61	30, 47, 72, 79	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	TYR	4.3
1	A	49	TYR	4.2
1	A	221	LEU	3.5
1	C	209	TYR	3.4
1	A	17	TYR	2.9
1	B	221	LEU	2.8
1	B	25	GLU	2.6
1	A	212	PHE	2.5
1	C	280	SER	2.3
1	C	42	TYR	2.2
1	A	42	TYR	2.2
1	B	16	SER	2.2
1	C	212	PHE	2.1
1	C	24	ILE	2.1
1	B	209	TYR	2.1
1	C	210	LEU	2.0
1	B	53	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	U1	C	1296	1/1	0.99	0.17	-0.54	51,51,51,51	0
2	U1	B	1296	1/1	0.99	0.17	-0.85	57,57,57,57	0
2	U1	A	1296	1/1	0.99	0.16	-1.49	58,58,58,58	0
2	U1	A	1298	1/1	0.82	0.22	-	61,61,61,61	1
2	U1	C	1298	1/1	0.96	0.31	-	65,65,65,65	1
2	U1	B	1298	1/1	0.87	0.27	-	63,63,63,63	1
2	U1	A	1297	1/1	0.77	0.22	-	67,67,67,67	1
2	U1	B	1299	1/1	0.94	0.17	-	59,59,59,59	1
2	U1	B	1297	1/1	0.80	0.28	-	69,69,69,69	1
2	U1	C	1297	1/1	0.96	0.19	-	57,57,57,57	1
2	U1	C	1299	1/1	0.83	0.30	-	88,88,88,88	1
2	U1	B	1300	1/1	0.92	0.34	-	74,74,74,74	1

6.5 Other polymers (i)

There are no such residues in this entry.