Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2016 – 03:14 PM EDT

PDB ID	:	5IC8
Title	:	Structure of UTP6
Authors	:	Zhang, C.; Ye, K.
Deposited on	:	2016-02-23
Resolution	:	3.30 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:

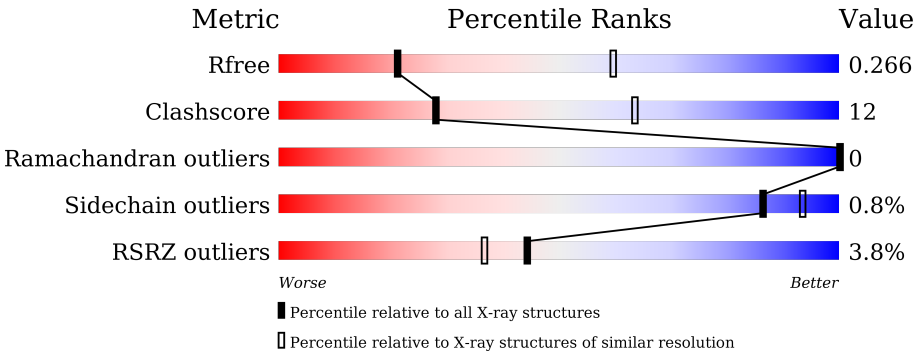
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	334	65% 19% • 15%
1	B	334	% 59% 25% 16%
1	C	334	5% 55% 21% 25%
1	D	334	7% 53% 25% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8581 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 Putative uncharacterized protein.

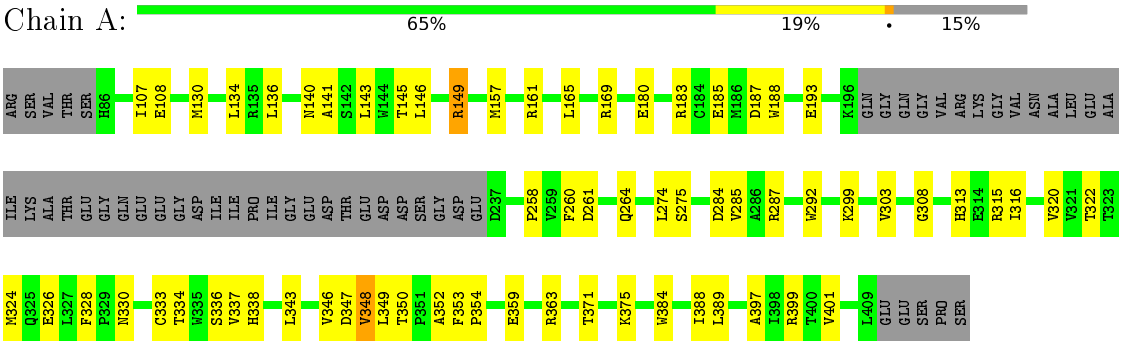
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2256	1441	416	386	13			
1	B	282	Total	C	N	O	S	0	0	0
			2239	1429	413	384	13			
1	C	252	Total	C	N	O	S	0	0	0
			2015	1296	372	334	13			
1	D	259	Total	C	N	O	S	0	0	0
			2071	1326	384	348	13			

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.

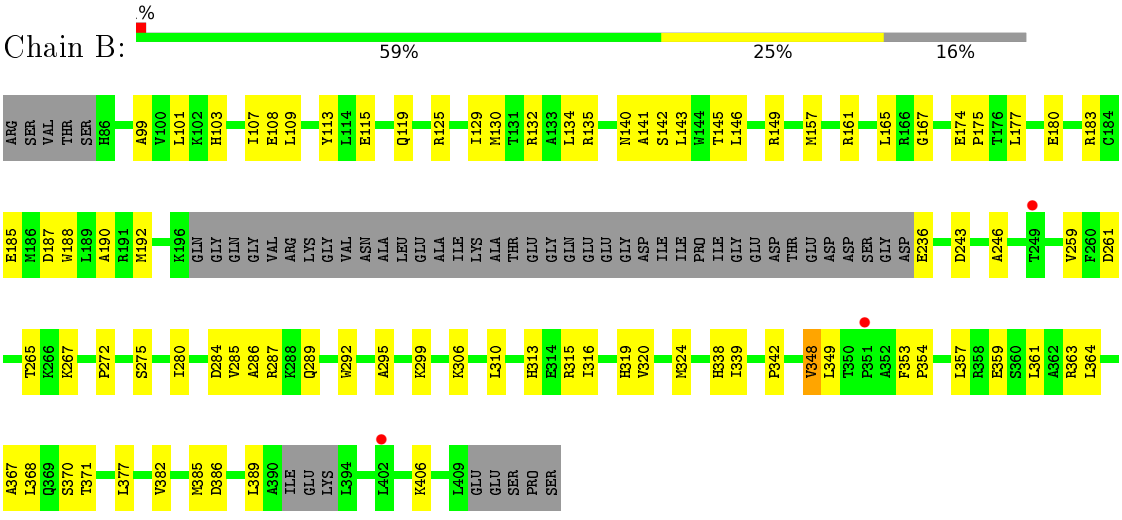
- Molecule 1: Putative uncharacterized protein

Chain A:



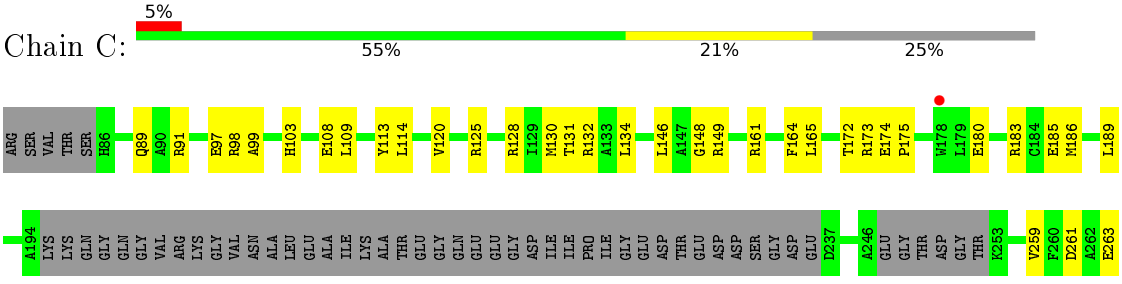
- Molecule 1: Putative uncharacterized protein

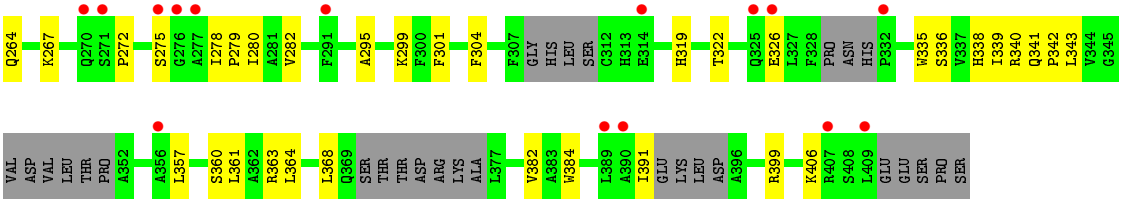
Chain B:



- Molecule 1: Putative uncharacterized protein

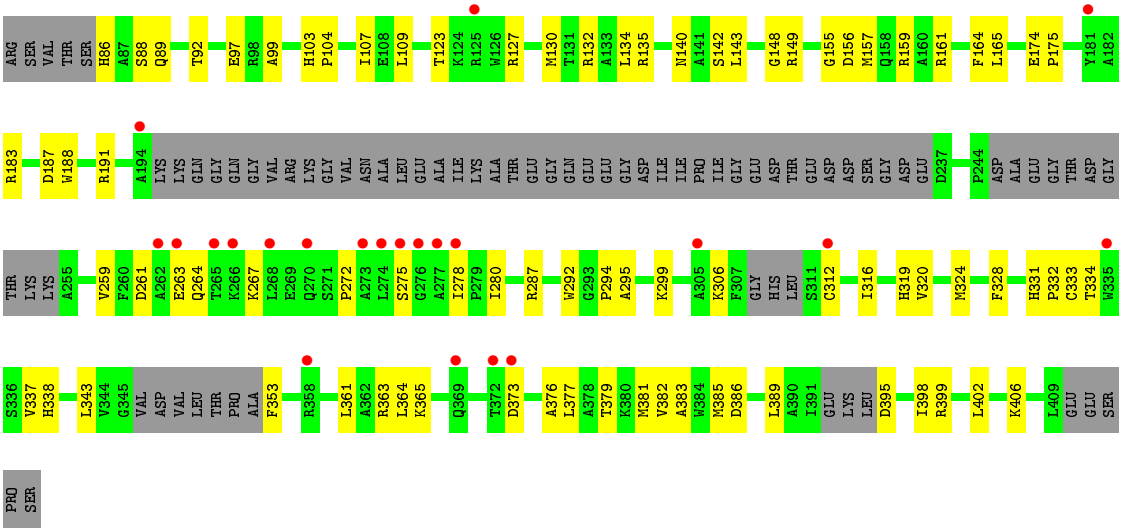
Chain C:





• Molecule 1: Putative uncharacterized protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.81Å 126.34Å 140.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.30 44.00 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.95-3.30) 93.8 (44.00-3.27)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.209 , 0.255 0.220 , 0.266	Depositor DCC
R_{free} test set	1922 reflections (7.83%)	DCC
Wilson B-factor (Å^2)	81.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8581	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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	0.62	0/2311	0.76	1/3125 (0.0%)
1	B	0.60	0/2293	0.72	0/3100
1	C	0.46	0/2060	0.61	0/2774
1	D	0.40	0/2120	0.57	0/2862
All	All	0.53	0/8784	0.67	1/11861 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	LEU	CA-CB-CG	6.02	129.15	115.30

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	2256	0	2296	45	0
1	B	2239	0	2271	58	0
1	C	2015	0	2054	47	0
1	D	2071	0	2098	56	0
All	All	8581	0	8719	202	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 12.

All (202) 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:D:386:ASP:OD1	1:D:406:LYS:NZ	2.08	0.87
1:B:130:MET:HE1	1:B:143:LEU:HB3	1.57	0.86
1:A:261:ASP:HB3	1:A:264:GLN:HG3	1.65	0.79
1:B:115:GLU:OE2	1:C:98:ARG:NH2	2.15	0.78
1:A:324:MET:HB3	1:A:334:THR:HG22	1.65	0.78
1:C:165:LEU:HD22	1:C:259:VAL:HG21	1.67	0.75
1:A:161:ARG:NH1	1:A:185:GLU:OE2	2.20	0.73
1:B:180:GLU:OE1	1:B:183:ARG:NH1	2.22	0.72
1:C:180:GLU:OE1	1:C:183:ARG:NH1	2.22	0.71
1:D:161:ARG:HH12	1:D:278:ILE:HG21	1.54	0.71
1:D:324:MET:HB3	1:D:334:THR:HG22	1.74	0.70
1:C:161:ARG:NH1	1:C:185:GLU:OE2	2.25	0.70
1:B:161:ARG:NH1	1:B:185:GLU:OE2	2.29	0.66
1:D:395:ASP:HB3	1:D:398:ILE:HD13	1.78	0.66
1:A:338:HIS:NE2	1:A:363:ARG:HD2	2.11	0.66
1:C:161:ARG:O	1:C:165:LEU:HG	1.96	0.66
1:C:97:GLU:OE2	1:C:132:ARG:NH2	2.30	0.64
1:C:343:LEU:HD13	1:C:384:TRP:HZ2	1.63	0.64
1:A:353:PHE:HB3	1:A:354:PRO:HD3	1.81	0.63
1:A:107:ILE:HD13	1:A:140:ASN:ND2	2.14	0.63
1:C:339:ILE:O	1:C:342:PRO:HD2	1.99	0.62
1:A:359:GLU:O	1:A:363:ARG:HG2	2.00	0.62
1:D:338:HIS:CG	1:D:363:ARG:HD3	2.35	0.61
1:D:149:ARG:NH1	1:D:183:ARG:HH12	1.99	0.61
1:C:280:ILE:HG23	1:C:319:HIS:CE1	2.36	0.61
1:A:145:THR:HG21	1:A:180:GLU:HG3	1.81	0.60
1:D:97:GLU:OE2	1:D:132:ARG:NH1	2.31	0.60
1:B:359:GLU:O	1:B:363:ARG:HG2	2.01	0.59
1:B:103:HIS:ND1	1:C:108:GLU:HG2	2.17	0.59
1:B:130:MET:CE	1:B:143:LEU:HB3	2.32	0.58
1:B:99:ALA:HB1	1:B:109:LEU:HD21	1.84	0.58
1:A:130:MET:HE1	1:A:143:LEU:HB3	1.85	0.57
1:A:328:PHE:O	1:A:334:THR:HG21	2.04	0.57
1:B:259:VAL:HG13	1:B:285:VAL:HG11	1.85	0.57
1:A:330:ASN:ND2	1:A:371:THR:O	2.37	0.57
1:A:322:THR:O	1:A:326:GLU:HG3	2.05	0.57
1:D:130:MET:HE2	1:D:134:LEU:HD22	1.87	0.57
1:D:272:PRO:HG2	1:D:275:SER:HB3	1.87	0.56
1:A:130:MET:CE	1:A:134:LEU:HG	2.35	0.56
1:B:107:ILE:HD12	1:B:107:ILE:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLY:HA2	1:D:191:ARG:HH22	1.71	0.56
1:D:187:ASP:O	1:D:191:ARG:HG3	2.06	0.56
1:D:328:PHE:O	1:D:334:THR:HG21	2.06	0.56
1:B:275:SER:O	1:B:315:ARG:NH2	2.34	0.55
1:D:123:THR:O	1:D:127:ARG:HG3	2.05	0.55
1:A:108:GLU:CD	1:A:108:GLU:H	2.10	0.55
1:C:391:ILE:HD11	1:C:399:ARG:HH22	1.71	0.55
1:D:324:MET:HE1	1:D:337:VAL:HG11	1.89	0.55
1:B:286:ALA:HA	1:B:289:GLN:HG2	1.88	0.55
1:B:386:ASP:OD1	1:B:406:LYS:NZ	2.26	0.55
1:D:338:HIS:O	1:D:363:ARG:NH1	2.31	0.55
1:B:243:ASP:HB3	1:B:246:ALA:HB2	1.88	0.54
1:B:382:VAL:HG13	1:B:406:LYS:HE3	1.89	0.54
1:C:343:LEU:HD13	1:C:384:TRP:CZ2	2.41	0.54
1:A:130:MET:CE	1:A:143:LEU:HB3	2.38	0.54
1:A:338:HIS:O	1:A:363:ARG:NH1	2.40	0.54
1:B:338:HIS:NE2	1:B:363:ARG:HD2	2.22	0.54
1:B:367:ALA:HB1	1:B:377:LEU:HD21	1.89	0.54
1:D:280:ILE:HG23	1:D:319:HIS:CE1	2.43	0.54
1:B:353:PHE:HB3	1:B:354:PRO:HD3	1.90	0.54
1:A:157:MET:HE3	1:A:188:TRP:CD1	2.42	0.54
1:C:335:TRP:O	1:C:339:ILE:HG13	2.07	0.54
1:C:341:GLN:HB3	1:C:342:PRO:HD3	1.88	0.54
1:C:357:LEU:O	1:C:361:LEU:HD13	2.08	0.54
1:D:140:ASN:HB3	1:D:143:LEU:HD12	1.89	0.54
1:C:99:ALA:HB1	1:C:109:LEU:HD21	1.90	0.54
1:B:338:HIS:O	1:B:363:ARG:NH1	2.41	0.53
1:B:339:ILE:O	1:B:342:PRO:HD2	2.09	0.53
1:D:280:ILE:HG23	1:D:319:HIS:HE1	1.74	0.53
1:A:260:PHE:HE1	1:A:285:VAL:HG21	1.74	0.53
1:B:364:LEU:O	1:B:368:LEU:HG	2.08	0.53
1:B:130:MET:CE	1:B:134:LEU:HG	2.39	0.53
1:D:99:ALA:HB1	1:D:109:LEU:HD21	1.90	0.53
1:C:382:VAL:HG13	1:C:406:LYS:HG3	1.90	0.52
1:C:165:LEU:HD22	1:C:259:VAL:CG2	2.39	0.52
1:D:132:ARG:O	1:D:135:ARG:HB3	2.10	0.52
1:A:141:ALA:O	1:A:145:THR:HG23	2.10	0.52
1:A:384:TRP:CE2	1:A:388:ILE:HD11	2.45	0.52
1:B:157:MET:HG3	1:B:188:TRP:CD1	2.45	0.52
1:B:320:VAL:HG12	1:B:324:MET:CE	2.39	0.51
1:C:295:ALA:O	1:C:299:LYS:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:ASP:O	1:D:399:ARG:HG2	2.10	0.51
1:B:280:ILE:HG23	1:B:319:HIS:CD2	2.45	0.51
1:C:272:PRO:HG2	1:C:275:SER:HB3	1.92	0.51
1:B:310:LEU:O	1:B:313:HIS:ND1	2.32	0.51
1:C:301:PHE:HE1	1:C:340:ARG:HE	1.59	0.51
1:A:130:MET:HE2	1:A:134:LEU:HG	1.93	0.51
1:B:130:MET:HE2	1:B:134:LEU:HG	1.93	0.51
1:A:316:ILE:O	1:A:320:VAL:HG23	2.11	0.50
1:A:287:ARG:HA	1:A:292:TRP:CD2	2.47	0.50
1:D:130:MET:HE3	1:D:143:LEU:HB3	1.93	0.50
1:D:156:ASP:OD2	1:D:159:ARG:HG3	2.11	0.50
1:A:260:PHE:CE1	1:A:285:VAL:HG21	2.45	0.50
1:B:108:GLU:HG2	1:C:103:HIS:ND1	2.27	0.50
1:B:284:ASP:O	1:B:287:ARG:HB3	2.12	0.50
1:B:367:ALA:O	1:B:370:SER:OG	2.21	0.50
1:C:342:PRO:HB2	1:C:360:SER:HB3	1.94	0.50
1:D:338:HIS:ND1	1:D:363:ARG:HD3	2.27	0.50
1:A:333:CYS:O	1:A:336:SER:HB3	2.12	0.50
1:C:338:HIS:ND1	1:C:363:ARG:HD3	2.28	0.49
1:C:130:MET:CE	1:C:134:LEU:HG	2.42	0.49
1:D:107:ILE:HD13	1:D:140:ASN:ND2	2.28	0.49
1:D:165:LEU:HD22	1:D:259:VAL:HG11	1.95	0.49
1:B:295:ALA:O	1:B:299:LYS:HG3	2.13	0.49
1:B:385:MET:O	1:B:389:LEU:HG	2.13	0.49
1:D:140:ASN:OD1	1:D:142:SER:HB2	2.13	0.49
1:A:299:LYS:O	1:A:303:VAL:HG23	2.13	0.49
1:C:174:GLU:HA	1:C:175:PRO:HD3	1.70	0.49
1:A:169:ARG:HD2	1:A:258:PRO:HA	1.95	0.48
1:A:338:HIS:CD2	1:A:363:ARG:HD2	2.47	0.48
1:C:278:ILE:O	1:C:282:VAL:HG23	2.12	0.48
1:C:361:LEU:O	1:C:364:LEU:HG	2.13	0.48
1:C:263:GLU:O	1:C:267:LYS:HG2	2.13	0.48
1:D:383:ALA:O	1:D:386:ASP:HB2	2.14	0.48
1:D:149:ARG:NH1	1:D:183:ARG:NH1	2.62	0.47
1:D:263:GLU:O	1:D:267:LYS:HG2	2.15	0.47
1:B:236:GLU:OE1	1:B:236:GLU:N	2.48	0.46
1:D:156:ASP:OD2	1:D:159:ARG:NH1	2.48	0.46
1:D:306:LYS:HE3	1:D:306:LYS:HB2	1.77	0.46
1:B:161:ARG:O	1:B:165:LEU:HG	2.14	0.46
1:B:357:LEU:O	1:B:361:LEU:HD13	2.15	0.46
1:C:261:ASP:HB3	1:C:264:GLN:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:MET:HE2	1:C:304:PHE:CE1	2.51	0.46
1:D:389:LEU:HB3	1:D:402:LEU:HD11	1.97	0.46
1:A:324:MET:HE1	1:A:337:VAL:HG11	1.98	0.46
1:B:287:ARG:HA	1:B:292:TRP:CD2	2.50	0.46
1:B:145:THR:HG21	1:B:180:GLU:HG3	1.98	0.46
1:B:141:ALA:O	1:B:145:THR:HG23	2.16	0.45
1:C:336:SER:OG	1:C:340:ARG:NH1	2.49	0.45
1:D:287:ARG:HA	1:D:292:TRP:CE3	2.51	0.45
1:A:149:ARG:NH2	1:A:187:ASP:OD2	2.44	0.45
1:D:361:LEU:O	1:D:364:LEU:HG	2.15	0.45
1:B:306:LYS:H	1:B:306:LYS:HG2	1.54	0.45
1:B:125:ARG:O	1:B:129:ILE:HG12	2.17	0.45
1:C:114:LEU:HD13	1:C:146:LEU:HD23	1.98	0.45
1:D:86:HIS:O	1:D:89:GLN:HB2	2.16	0.45
1:B:132:ARG:O	1:B:135:ARG:HB3	2.17	0.45
1:B:174:GLU:HA	1:B:175:PRO:HD3	1.86	0.45
1:C:148:GLY:HA3	1:C:164:PHE:CE2	2.52	0.44
1:C:280:ILE:HG23	1:C:319:HIS:HE1	1.78	0.44
1:C:278:ILE:HB	1:C:279:PRO:HD3	2.00	0.44
1:B:157:MET:HG3	1:B:188:TRP:CG	2.52	0.44
1:C:97:GLU:OE1	1:C:113:TYR:OH	2.22	0.44
1:B:316:ILE:O	1:B:320:VAL:HG23	2.16	0.44
1:A:350:THR:HG22	1:A:352:ALA:H	1.82	0.44
1:B:272:PRO:HG2	1:B:275:SER:HB3	1.98	0.44
1:D:165:LEU:HD22	1:D:259:VAL:CG1	2.48	0.44
1:B:267:LYS:HA	1:B:267:LYS:HD3	1.79	0.43
1:C:134:LEU:HA	1:C:134:LEU:HD23	1.91	0.43
1:D:312:CYS:O	1:D:316:ILE:HG12	2.17	0.43
1:B:119:GLN:OE1	1:C:91:ARG:HB3	2.18	0.43
1:A:375:LYS:HE2	1:A:375:LYS:HB3	1.86	0.43
1:A:193:GLU:HG2	1:A:274:LEU:HD23	2.01	0.43
1:B:348:VAL:HA	1:B:349:LEU:HA	1.64	0.43
1:D:157:MET:HG3	1:D:188:TRP:CG	2.53	0.43
1:D:261:ASP:HB3	1:D:264:GLN:HG3	2.00	0.42
1:D:316:ILE:O	1:D:320:VAL:HG23	2.19	0.42
1:A:308:GLY:O	1:A:313:HIS:CD2	2.72	0.42
1:B:146:LEU:HA	1:B:146:LEU:HD12	1.71	0.42
1:B:157:MET:CE	1:B:188:TRP:HB2	2.49	0.42
1:D:161:ARG:O	1:D:165:LEU:HG	2.18	0.42
1:D:361:LEU:O	1:D:365:LYS:HG3	2.18	0.42
1:B:134:LEU:HA	1:B:134:LEU:HD23	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:HIS:HA	1:D:104:PRO:HD2	1.91	0.42
1:D:148:GLY:HA3	1:D:164:PHE:CE2	2.54	0.42
1:D:174:GLU:HA	1:D:175:PRO:HD3	1.82	0.42
1:D:295:ALA:O	1:D:299:LYS:HG3	2.20	0.42
1:A:146:LEU:HA	1:A:146:LEU:HD12	1.84	0.42
1:A:161:ARG:O	1:A:165:LEU:HG	2.19	0.42
1:B:261:ASP:O	1:B:265:THR:HG23	2.20	0.42
1:D:287:ARG:HA	1:D:292:TRP:CD2	2.55	0.42
1:D:294:PRO:HB2	1:D:333:CYS:SG	2.60	0.42
1:D:373:ASP:OD2	1:D:376:ALA:N	2.29	0.42
1:C:172:THR:HG23	1:C:173:ARG:HD2	2.02	0.41
1:C:149:ARG:HH12	1:C:183:ARG:HH22	1.67	0.41
1:D:381:MET:O	1:D:385:MET:HG3	2.20	0.41
1:A:348:VAL:HA	1:A:349:LEU:HA	1.77	0.41
1:C:128:ARG:O	1:C:131:THR:HB	2.20	0.41
1:C:322:THR:O	1:C:326:GLU:HG3	2.20	0.41
1:A:180:GLU:OE1	1:A:183:ARG:NH1	2.53	0.41
1:B:140:ASN:OD1	1:B:142:SER:HB2	2.21	0.41
1:C:89:GLN:NE2	1:C:120:VAL:HB	2.36	0.41
1:B:190:ALA:HA	1:B:310:LEU:HD21	2.02	0.41
1:D:379:THR:O	1:D:382:VAL:HG22	2.20	0.41
1:A:284:ASP:O	1:A:287:ARG:HB3	2.20	0.41
1:C:364:LEU:O	1:C:368:LEU:HG	2.21	0.41
1:D:331:HIS:HA	1:D:332:PRO:HD3	1.95	0.41
1:D:332:PRO:HB3	1:D:377:LEU:HB2	2.02	0.41
1:A:343:LEU:HD23	1:A:346:VAL:HG21	2.01	0.41
1:A:275:SER:O	1:A:315:ARG:NH2	2.53	0.41
1:B:167:GLY:HA3	1:B:177:LEU:HD21	2.02	0.41
1:C:125:ARG:HD2	1:C:125:ARG:HH11	1.71	0.41
1:A:347:ASP:N	1:A:347:ASP:OD1	2.53	0.40
1:A:397:ALA:O	1:A:401:VAL:HG12	2.21	0.40
1:A:384:TRP:O	1:A:388:ILE:HG13	2.21	0.40
1:B:142:SER:O	1:B:146:LEU:HB2	2.22	0.40
1:D:88:SER:O	1:D:92:THR:HG23	2.20	0.40
1:A:389:LEU:O	1:A:399:ARG:NH1	2.54	0.40
1:D:343:LEU:HD21	1:D:353:PHE:HD1	1.87	0.40
1:B:149:ARG:NH1	1:B:187:ASP:OD2	2.49	0.40
1:B:320:VAL:HG12	1:B:324:MET:HE2	2.04	0.40
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	280/334 (84%)	277 (99%)	3 (1%)	0	100	100
1	B	276/334 (83%)	272 (99%)	4 (1%)	0	100	100
1	C	236/334 (71%)	235 (100%)	1 (0%)	0	100	100
1	D	247/334 (74%)	244 (99%)	3 (1%)	0	100	100
All	All	1039/1336 (78%)	1028 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	231/271 (85%)	229 (99%)	2 (1%)	84	92
1	B	229/271 (84%)	224 (98%)	5 (2%)	60	84
1	C	203/271 (75%)	203 (100%)	0	100	100
1	D	211/271 (78%)	211 (100%)	0	100	100
All	All	874/1084 (81%)	867 (99%)	7 (1%)	86	93

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

Mol	Chain	Res	Type
1	A	149	ARG
1	A	348	VAL

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Mol	Chain	Res	Type
1	B	101	LEU
1	B	113	TYR
1	B	192	MET
1	B	348	VAL
1	B	371	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	319	HIS

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	284/334 (85%)	-0.24	0 100 100	37, 64, 101, 118	0
1	B	282/334 (84%)	-0.14	3 (1%) 82 78	39, 64, 118, 158	0
1	C	252/334 (75%)	0.23	16 (6%) 23 19	51, 125, 182, 196	0
1	D	259/334 (77%)	0.37	22 (8%) 13 10	61, 138, 177, 189	0
All	All	1077/1336 (80%)	0.04	41 (3%) 44 37	37, 87, 171, 196	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	276	GLY	6.4
1	D	273	ALA	6.3
1	D	274	LEU	5.5
1	D	277	ALA	4.3
1	D	275	SER	4.1
1	D	268	LEU	4.0
1	D	265	THR	3.7
1	B	351	PRO	3.3
1	D	372	THR	3.1
1	C	390	ALA	3.1
1	D	194	ALA	3.1
1	D	358	ARG	3.0
1	D	263	GLU	2.9
1	D	270	GLN	2.9
1	B	249	THR	2.9
1	B	402	LEU	2.9
1	C	325	GLN	2.9
1	D	312	CYS	2.8
1	D	369	GLN	2.7
1	C	326	GLU	2.7
1	C	275	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	314	GLU	2.7
1	C	271	SER	2.6
1	C	332	PRO	2.6
1	D	181	TYR	2.6
1	C	276	GLY	2.5
1	D	305	ALA	2.5
1	C	270	GLN	2.4
1	C	291	PHE	2.4
1	C	407	ARG	2.4
1	D	278	ILE	2.3
1	D	335	TRP	2.3
1	C	277	ALA	2.3
1	D	262	ALA	2.3
1	C	409	LEU	2.2
1	D	266	LYS	2.2
1	C	389	LEU	2.2
1	D	125	ARG	2.2
1	D	373	ASP	2.2
1	C	178	TRP	2.2
1	C	356	ALA	2.1

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 (i)

There are no carbohydrates 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.