Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:12 PM GMT

PDB ID	:	4HK7
Title	:	Crystal structure of Cordyceps militaris IDCase in complex with uracil
Authors	:	Xu, S.; Zhu, J.; Ding, J.
Deposited on	:	2012-10-15
Resolution	:	2.19 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:

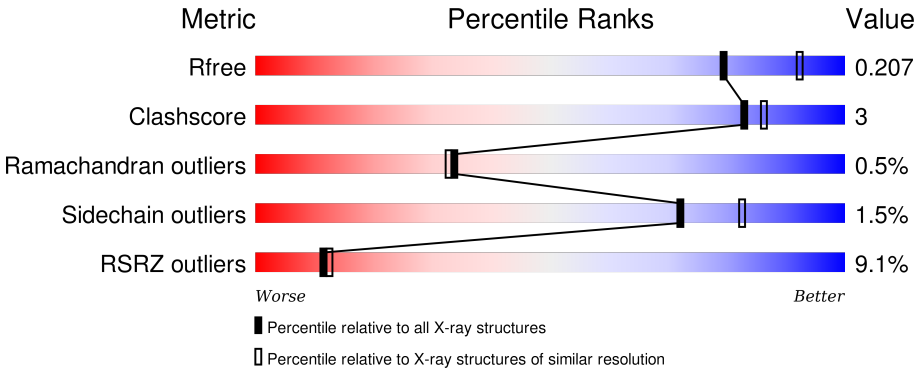
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.19 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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. 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	387	14% 88% 10%
1	B	387	10% 89% 8%
1	C	387	8% 87% 9%
1	D	387	3% 90% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12050 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 Uracil-5-carboxylate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2910	1870	504	522	14			
1	B	377	Total	C	N	O	S	0	0	0
			2890	1858	498	520	14			
1	C	375	Total	C	N	O	S	0	0	0
			2873	1848	495	516	14			
1	D	379	Total	C	N	O	S	0	0	0
			2910	1870	504	522	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP G3J531
A	-1	GLY	-	EXPRESSION TAG	UNP G3J531
A	0	SER	-	EXPRESSION TAG	UNP G3J531
A	377	LEU	-	EXPRESSION TAG	UNP G3J531
A	378	GLU	-	EXPRESSION TAG	UNP G3J531
A	379	HIS	-	EXPRESSION TAG	UNP G3J531
A	380	HIS	-	EXPRESSION TAG	UNP G3J531
A	381	HIS	-	EXPRESSION TAG	UNP G3J531
A	382	HIS	-	EXPRESSION TAG	UNP G3J531
A	383	HIS	-	EXPRESSION TAG	UNP G3J531
A	384	HIS	-	EXPRESSION TAG	UNP G3J531
B	-2	MET	-	EXPRESSION TAG	UNP G3J531
B	-1	GLY	-	EXPRESSION TAG	UNP G3J531
B	0	SER	-	EXPRESSION TAG	UNP G3J531
B	377	LEU	-	EXPRESSION TAG	UNP G3J531
B	378	GLU	-	EXPRESSION TAG	UNP G3J531
B	379	HIS	-	EXPRESSION TAG	UNP G3J531
B	380	HIS	-	EXPRESSION TAG	UNP G3J531
B	381	HIS	-	EXPRESSION TAG	UNP G3J531
B	382	HIS	-	EXPRESSION TAG	UNP G3J531
B	383	HIS	-	EXPRESSION TAG	UNP G3J531

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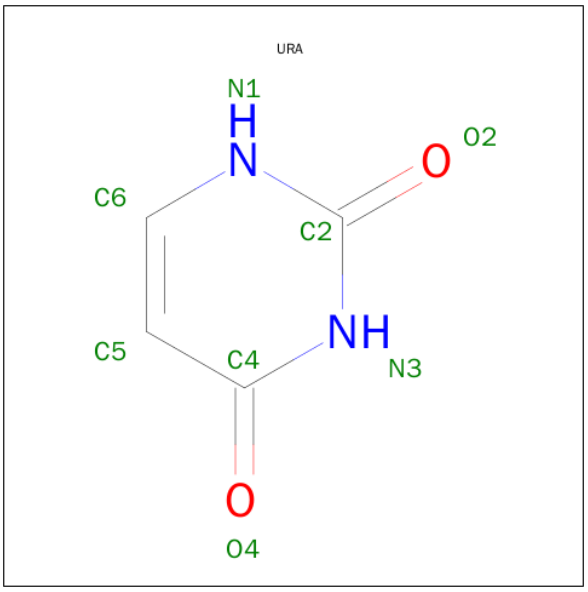
Chain	Residue	Modelled	Actual	Comment	Reference
B	384	HIS	-	EXPRESSION TAG	UNP G3J531
C	-2	MET	-	EXPRESSION TAG	UNP G3J531
C	-1	GLY	-	EXPRESSION TAG	UNP G3J531
C	0	SER	-	EXPRESSION TAG	UNP G3J531
C	377	LEU	-	EXPRESSION TAG	UNP G3J531
C	378	GLU	-	EXPRESSION TAG	UNP G3J531
C	379	HIS	-	EXPRESSION TAG	UNP G3J531
C	380	HIS	-	EXPRESSION TAG	UNP G3J531
C	381	HIS	-	EXPRESSION TAG	UNP G3J531
C	382	HIS	-	EXPRESSION TAG	UNP G3J531
C	383	HIS	-	EXPRESSION TAG	UNP G3J531
C	384	HIS	-	EXPRESSION TAG	UNP G3J531
D	-2	MET	-	EXPRESSION TAG	UNP G3J531
D	-1	GLY	-	EXPRESSION TAG	UNP G3J531
D	0	SER	-	EXPRESSION TAG	UNP G3J531
D	377	LEU	-	EXPRESSION TAG	UNP G3J531
D	378	GLU	-	EXPRESSION TAG	UNP G3J531
D	379	HIS	-	EXPRESSION TAG	UNP G3J531
D	380	HIS	-	EXPRESSION TAG	UNP G3J531
D	381	HIS	-	EXPRESSION TAG	UNP G3J531
D	382	HIS	-	EXPRESSION TAG	UNP G3J531
D	383	HIS	-	EXPRESSION TAG	UNP G3J531
D	384	HIS	-	EXPRESSION TAG	UNP G3J531

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 8 4 2 2	0	0
3	B	1	Total C N O 8 4 2 2	0	0
3	C	1	Total C N O 8 4 2 2	0	0
3	D	1	Total C N O 8 4 2 2	0	0

- Molecule 4 is water.

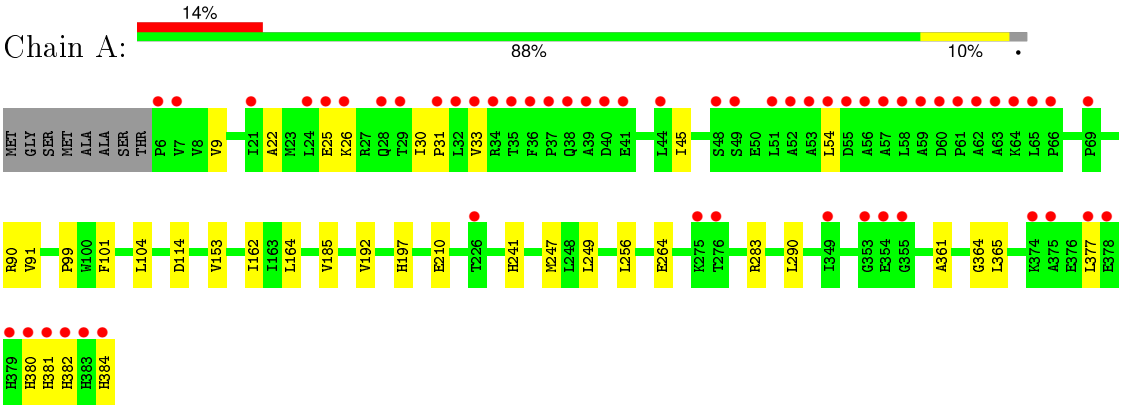
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	89	Total O 89 89	0	0
4	B	92	Total O 92 92	0	0
4	C	112	Total O 112 112	0	0
4	D	136	Total O 136 136	0	0

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 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.

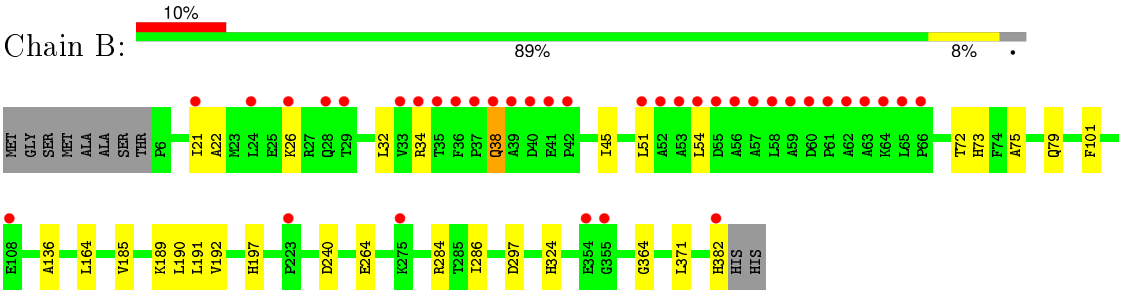
- Molecule 1: Uracil-5-carboxylate decarboxylase

Chain A:



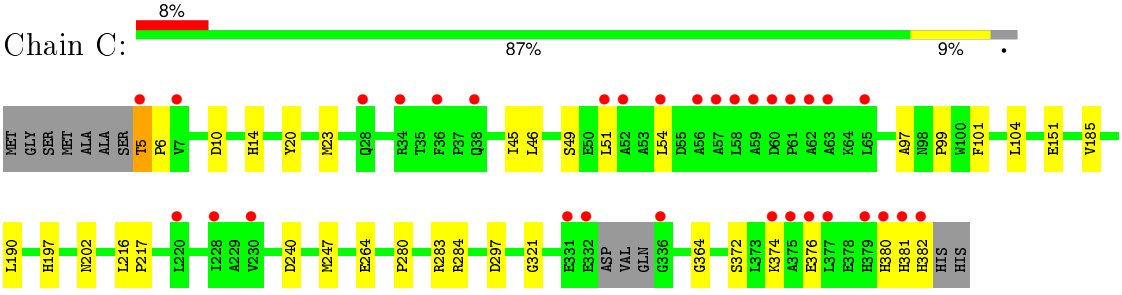
- Molecule 1: Uracil-5-carboxylate decarboxylase

Chain B:



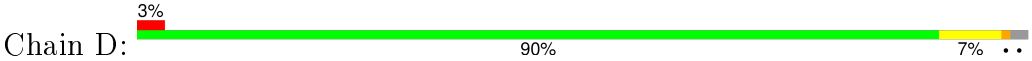
- Molecule 1: Uracil-5-carboxylate decarboxylase

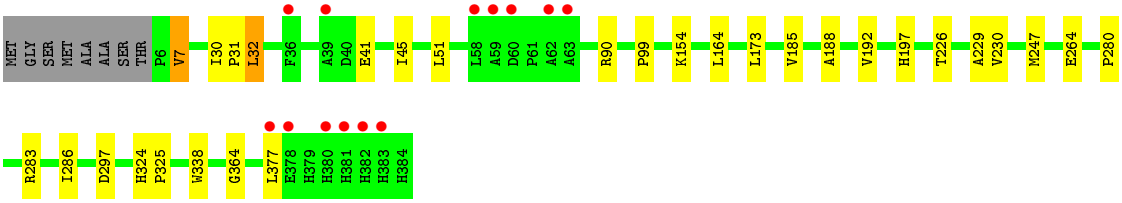
Chain C:



- Molecule 1: Uracil-5-carboxylate decarboxylase

Chain D:




MET
GLY
SER
MET
ALA
ALA
SER
THR
P6
V7
I30
P31
L32
F36
A39
D40
E41
T45
L51
L58
A59
D60
P61
A62
A63
R90
P99
K154
L164
L173
V185
A188
V192
H197
T226
A229
V230
M247
E264
P280

R283
I286
D297
H324
P325
W338
G364
L377
E378
H379
H380
H381
H382
H383
H384

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.33Å 144.92Å 77.31Å 90.00° 97.14° 90.00°	Depositor
Resolution (Å)	76.73 – 2.19 41.80 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (76.73-2.19) 99.2 (41.80-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.153 , 0.210 0.150 , 0.207	Depositor DCC
R_{free} test set	4324 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.1	EDS
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 86074 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12050	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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, 0.375 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: ZN, URA

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	0.47	0/2988	0.55	0/4069
1	B	0.47	0/2966	0.53	0/4039
1	C	0.47	0/2948	0.53	0/4014
1	D	0.49	1/2988 (0.0%)	0.55	0/4069
All	All	0.48	1/11890 (0.0%)	0.54	0/16191

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338	TRP	CD2-CE2	5.22	1.47	1.41

There are no bond angle outliers.

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	2910	0	2908	21	0
1	B	2890	0	2894	18	0
1	C	2873	0	2878	18	0
1	D	2910	0	2908	14	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	8	0	3	0	0
3	B	8	0	3	0	0
3	C	8	0	3	0	0
3	D	8	0	3	0	0
4	A	89	0	0	3	0
4	B	92	0	0	0	0
4	C	112	0	0	0	0
4	D	136	0	0	0	0
All	All	12050	0	11600	71	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 3.

All (71) 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:382:HIS:CB	4:A:574:HOH:O	2.24	0.84
1:A:382:HIS:HB3	4:A:574:HOH:O	1.76	0.84
1:A:25:GLU:HG3	1:A:33:VAL:O	1.80	0.82
1:A:31:PRO:HG3	1:A:99:PRO:HG3	1.77	0.65
1:B:72:THR:OG1	1:B:79:GLN:NE2	2.31	0.64
1:B:38:GLN:HE21	1:B:38:GLN:H	1.45	0.63
1:D:280:PRO:O	1:D:283:ARG:HB2	2.02	0.60
1:A:153:VAL:HG21	1:A:162:ILE:HD11	1.85	0.59
1:D:7:VAL:HG12	1:D:90:ARG:HB3	1.85	0.59
1:A:382:HIS:CG	4:A:574:HOH:O	2.56	0.58
1:C:374:LYS:HB3	1:C:376:GLU:OE2	2.04	0.57
1:D:30:ILE:HD13	1:D:51:LEU:CD2	2.36	0.56
1:B:38:GLN:NE2	1:B:38:GLN:H	2.03	0.55
1:C:185:VAL:HG13	1:C:190:LEU:HB2	1.89	0.54
1:A:247:MET:HE3	1:A:249:LEU:HD21	1.90	0.53
1:B:32:LEU:HD13	1:B:34:ARG:HG2	1.91	0.53
1:C:372:SER:HB2	1:C:381:HIS:O	2.10	0.52
1:D:154:LYS:HD3	1:D:188:ALA:HB1	1.90	0.51
1:A:380:HIS:ND1	1:A:381:HIS:HD2	2.08	0.51
1:C:5:THR:N	1:C:6:PRO:HD3	2.26	0.51
1:B:191:LEU:HD22	1:B:371:LEU:HD21	1.91	0.51
1:C:264:GLU:CD	1:C:283:ARG:HH22	2.14	0.51
1:D:297:ASP:C	1:D:297:ASP:OD1	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:THR:N	1:C:6:PRO:CD	2.74	0.50
1:A:264:GLU:OE1	1:A:283:ARG:NH2	2.44	0.49
1:C:264:GLU:OE1	1:C:283:ARG:NH2	2.45	0.49
1:B:240:ASP:OD1	1:B:284:ARG:HD3	2.13	0.49
1:C:45:ILE:HD13	1:C:54:LEU:HD13	1.95	0.49
1:C:101:PHE:HB3	1:C:104:LEU:HD12	1.94	0.49
1:B:21:ILE:HD12	1:B:75:ALA:HB2	1.95	0.47
1:B:264:GLU:HG2	1:B:286:ILE:HG22	1.98	0.46
1:D:7:VAL:HG21	1:D:377:LEU:HD13	1.96	0.46
1:A:185:VAL:HG11	1:A:192:VAL:HG22	1.98	0.46
1:A:9:VAL:HG22	1:A:91:VAL:HB	1.97	0.45
1:B:45:ILE:HG21	1:B:54:LEU:HD22	1.99	0.45
1:A:380:HIS:O	1:A:384:HIS:HB2	2.16	0.45
1:B:101:PHE:CE2	1:B:136:ALA:HB3	2.51	0.45
1:C:297:ASP:OD1	1:C:297:ASP:C	2.56	0.45
1:D:31:PRO:HG3	1:D:99:PRO:CG	2.47	0.45
1:C:20:TYR:HA	1:C:23:MET:HE2	1.98	0.45
1:C:14:HIS:HB3	1:C:97:ALA:HB2	1.99	0.45
1:C:49:SER:HB3	1:C:202:ASN:ND2	2.32	0.45
1:C:46:LEU:HD22	1:C:99:PRO:HD3	2.00	0.44
1:B:22:ALA:O	1:B:26:LYS:HE2	2.18	0.44
1:A:264:GLU:CD	1:A:283:ARG:HH22	2.20	0.44
1:B:297:ASP:C	1:B:297:ASP:OD1	2.57	0.44
1:C:10:ASP:OD1	1:C:321:GLY:HA2	2.18	0.44
1:A:30:ILE:HG12	1:A:45:ILE:HG22	2.00	0.44
1:C:280:PRO:O	1:C:283:ARG:HB2	2.18	0.43
1:D:226:THR:O	1:D:230:VAL:HG23	2.18	0.43
1:A:361:ALA:HA	1:A:365:LEU:HB2	2.00	0.43
1:D:32:LEU:HD12	1:D:45:ILE:HB	2.01	0.43
1:A:256:LEU:HD23	1:A:290:LEU:HD21	2.01	0.43
1:B:189:LYS:HE2	1:B:382:HIS:CD2	2.54	0.43
1:A:45:ILE:HD13	1:A:54:LEU:HD13	2.00	0.42
1:A:22:ALA:O	1:A:26:LYS:HG2	2.20	0.42
1:B:185:VAL:HG11	1:B:192:VAL:HG22	2.01	0.42
1:A:185:VAL:HG11	1:A:192:VAL:CG2	2.50	0.42
1:D:173:LEU:HD12	1:D:229:ALA:HB1	2.02	0.42
1:D:31:PRO:HG3	1:D:99:PRO:HG3	2.01	0.42
1:C:240:ASP:OD1	1:C:284:ARG:HD3	2.20	0.42
1:B:185:VAL:HG13	1:B:190:LEU:HB2	2.02	0.41
1:D:264:GLU:HG2	1:D:286:ILE:HG22	2.01	0.41
1:B:21:ILE:CD1	1:B:75:ALA:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:HG11	1:D:192:VAL:HG22	2.02	0.41
1:A:91:VAL:HG21	1:A:377:LEU:HD21	2.02	0.40
1:A:101:PHE:HB3	1:A:104:LEU:HD12	2.03	0.40
1:B:73:HIS:CD2	1:B:324:HIS:HE2	2.39	0.40
1:D:324:HIS:HA	1:D:325:PRO:HA	1.86	0.40
1:B:191:LEU:CD2	1:B:371:LEU:HD21	2.52	0.40
1:C:216:LEU:HB2	1:C:217:PRO:HD3	2.03	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	377/387 (97%)	364 (97%)	11 (3%)	2 (0%)	34	33
1	B	375/387 (97%)	364 (97%)	9 (2%)	2 (0%)	34	33
1	C	371/387 (96%)	359 (97%)	10 (3%)	2 (0%)	34	33
1	D	377/387 (97%)	367 (97%)	8 (2%)	2 (0%)	34	33
All	All	1500/1548 (97%)	1454 (97%)	38 (2%)	8 (0%)	34	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	197	HIS
1	D	197	HIS
1	A	197	HIS
1	B	197	HIS
1	B	364	GLY
1	A	364	GLY
1	C	364	GLY
1	D	364	GLY

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	308/313 (98%)	303 (98%)	5 (2%)	70	81
1	B	306/313 (98%)	303 (99%)	3 (1%)	82	90
1	C	304/313 (97%)	298 (98%)	6 (2%)	63	74
1	D	308/313 (98%)	303 (98%)	5 (2%)	70	81
All	All	1226/1252 (98%)	1207 (98%)	19 (2%)	72	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	114	ASP
1	A	164	LEU
1	A	210	GLU
1	A	241	HIS
1	B	38	GLN
1	B	51	LEU
1	B	164	LEU
1	C	5	THR
1	C	51	LEU
1	C	151	GLU
1	C	247	MET
1	C	380	HIS
1	C	382	HIS
1	D	7	VAL
1	D	32	LEU
1	D	41	GLU
1	D	164	LEU
1	D	247	MET

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

Mol	Chain	Res	Type
1	A	73	HIS
1	A	202	ASN
1	A	381	HIS
1	B	38	GLN
1	B	73	HIS
1	B	79	GLN
1	B	335	GLN
1	B	346	GLN
1	C	202	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	URA	A	403	2	4,8,8	2.07	1 (25%)	6,10,10	8.56	4 (66%)
3	URA	B	402	2	4,8,8	2.23	1 (25%)	6,10,10	8.60	4 (66%)
3	URA	C	402	2	4,8,8	2.04	1 (25%)	6,10,10	8.23	4 (66%)
3	URA	D	403	2	4,8,8	1.88	1 (25%)	6,10,10	8.72	4 (66%)

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
3	URA	A	403	2	-	0/0/0/0	0/1/1/1
3	URA	B	402	2	-	0/0/0/0	0/1/1/1
3	URA	C	402	2	-	0/0/0/0	0/1/1/1
3	URA	D	403	2	-	0/0/0/0	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	URA	C4-N3	3.61	1.39	1.33
3	C	402	URA	C4-N3	3.95	1.40	1.33
3	A	403	URA	C4-N3	3.97	1.40	1.33
3	B	402	URA	C4-N3	4.31	1.41	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	URA	N1-C2-N3	-14.23	119.25	128.33
3	A	403	URA	N1-C2-N3	-14.00	119.40	128.33
3	D	403	URA	N1-C2-N3	-13.95	119.43	128.33
3	C	402	URA	N1-C2-N3	-13.86	119.49	128.33
3	D	403	URA	C5-C6-N1	-3.21	120.23	123.90
3	A	403	URA	C5-C6-N1	-3.13	120.33	123.90
3	B	402	URA	C5-C6-N1	-2.53	121.01	123.90
3	C	402	URA	C5-C6-N1	-2.53	121.01	123.90
3	B	402	URA	C4-N3-C2	4.98	119.08	114.14
3	A	403	URA	C4-N3-C2	5.03	119.12	114.14
3	C	402	URA	C4-N3-C2	5.38	119.47	114.14
3	D	403	URA	C4-N3-C2	5.45	119.54	114.14
3	C	402	URA	C6-N1-C2	13.24	120.92	114.40
3	A	403	URA	C6-N1-C2	14.30	121.44	114.40
3	B	402	URA	C6-N1-C2	14.43	121.50	114.40
3	D	403	URA	C6-N1-C2	14.75	121.66	114.40

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	379/387 (97%)	0.74	56 (14%) 3 3	23, 35, 70, 94	0
1	B	377/387 (97%)	0.46	37 (9%) 10 10	24, 35, 68, 94	0
1	C	375/387 (96%)	0.29	32 (8%) 13 14	22, 31, 59, 86	0
1	D	379/387 (97%)	0.04	13 (3%) 49 50	21, 29, 52, 74	0
All	All	1510/1548 (97%)	0.38	138 (9%) 11 12	21, 33, 63, 94	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	10.0
1	B	61	PRO	8.2
1	A	37	PRO	8.0
1	A	60	ASP	7.9
1	A	381	HIS	7.7
1	B	40	ASP	7.5
1	A	61	PRO	7.5
1	B	59	ALA	7.4
1	B	58	LEU	7.2
1	B	37	PRO	7.0
1	A	62	ALA	6.9
1	B	35	THR	6.8
1	B	56	ALA	6.7
1	B	60	ASP	6.6
1	A	57	ALA	6.5
1	A	382	HIS	6.5
1	A	35	THR	6.5
1	C	59	ALA	6.4
1	A	36	PHE	6.4
1	C	58	LEU	6.4
1	A	34	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	380	HIS	6.2
1	A	39	ALA	6.1
1	A	51	LEU	6.0
1	B	57	ALA	6.0
1	A	63	ALA	5.9
1	B	38	GLN	5.9
1	B	62	ALA	5.8
1	A	383	HIS	5.8
1	A	6	PRO	5.6
1	A	56	ALA	5.6
1	C	382	HIS	5.6
1	D	59	ALA	5.5
1	A	38	GLN	5.4
1	B	65	LEU	5.3
1	B	21	ILE	5.3
1	A	65	LEU	5.2
1	B	52	ALA	5.2
1	C	332	GLU	5.2
1	A	40	ASP	5.2
1	A	58	LEU	5.1
1	C	375	ALA	5.1
1	C	63	ALA	5.0
1	A	54	LEU	4.9
1	B	63	ALA	4.8
1	B	36	PHE	4.8
1	A	377	LEU	4.7
1	B	28	GLN	4.6
1	A	44	LEU	4.6
1	C	51	LEU	4.5
1	A	53	ALA	4.4
1	C	376	GLU	4.4
1	C	60	ASP	4.4
1	C	379	HIS	4.4
1	C	56	ALA	4.3
1	C	62	ALA	4.3
1	B	39	ALA	4.2
1	B	55	ASP	4.2
1	A	355	GLY	4.1
1	A	384	HIS	4.1
1	A	48	SER	4.1
1	C	381	HIS	4.1
1	B	53	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	51	LEU	4.1
1	A	28	GLN	4.0
1	A	33	VAL	4.0
1	B	54	LEU	4.0
1	A	55	ASP	3.9
1	A	375	ALA	3.9
1	B	34	ARG	3.9
1	D	58	LEU	3.9
1	C	5	THR	3.8
1	C	54	LEU	3.8
1	A	49	SER	3.7
1	A	52	ALA	3.7
1	D	62	ALA	3.7
1	C	57	ALA	3.6
1	A	379	HIS	3.5
1	A	26	LYS	3.5
1	C	61	PRO	3.4
1	D	382	HIS	3.4
1	B	64	LYS	3.4
1	B	26	LYS	3.3
1	D	60	ASP	3.2
1	C	34	ARG	3.2
1	C	380	HIS	3.2
1	A	374	LYS	3.2
1	B	33	VAL	3.2
1	A	378	GLU	3.1
1	B	66	PRO	3.1
1	D	378	GLU	3.0
1	C	36	PHE	2.9
1	D	381	HIS	2.9
1	A	66	PRO	2.9
1	C	377	LEU	2.9
1	C	52	ALA	2.8
1	C	38	GLN	2.7
1	D	380	HIS	2.7
1	A	29	THR	2.7
1	A	24	LEU	2.6
1	C	331	GLU	2.6
1	A	31	PRO	2.6
1	D	63	ALA	2.5
1	A	25	GLU	2.5
1	C	336	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	275	LYS	2.5
1	C	65	LEU	2.5
1	C	28	GLN	2.5
1	B	29	THR	2.4
1	B	42	PRO	2.4
1	A	276	THR	2.4
1	B	355	GLY	2.4
1	C	7	VAL	2.4
1	A	7	VAL	2.3
1	B	108	GLU	2.3
1	B	382	HIS	2.3
1	D	39	ALA	2.3
1	B	354	GLU	2.3
1	A	69	PRO	2.3
1	A	32	LEU	2.3
1	D	377	LEU	2.3
1	B	24	LEU	2.2
1	A	41	GLU	2.2
1	D	383	HIS	2.2
1	A	21	ILE	2.2
1	B	223	PRO	2.2
1	C	230	VAL	2.2
1	B	41	GLU	2.2
1	C	220	LEU	2.2
1	A	353	GLY	2.1
1	C	374	LYS	2.1
1	D	36	PHE	2.1
1	A	349	ILE	2.1
1	B	275	LYS	2.1
1	A	226	THR	2.0
1	C	228	ILE	2.0
1	A	64	LYS	2.0
1	A	354	GLU	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 (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
3	URA	D	403	8/8	0.99	0.12	0.30	24,25,26,28	0
3	URA	C	402	8/8	0.99	0.11	-0.05	23,24,25,26	0
3	URA	B	402	8/8	0.96	0.13	-0.37	27,31,32,36	0
2	ZN	D	401	1/1	0.99	0.11	-0.84	31,31,31,31	0
2	ZN	A	401	1/1	1.00	0.09	-0.90	33,33,33,33	0
2	ZN	C	401	1/1	1.00	0.10	-0.92	28,28,28,28	0
3	URA	A	403	8/8	0.98	0.10	-0.92	29,33,35,37	0
2	ZN	B	401	1/1	1.00	0.10	-1.62	34,34,34,34	0
2	ZN	A	402	1/1	0.97	0.13	-1.87	52,52,52,52	0
2	ZN	D	402	1/1	0.99	0.05	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.