



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 05:46 PM GMT

PDB ID : 1WS3
Title : Urate oxidase from aspergillus flavus complexed with uracil
Authors : Retailleau, P.; Colloc'h, N.; Vivares, D.; Bonnete, F.; Castro, B.; El Hajji, M.; Prange, T.
Deposited on : 2004-10-29
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

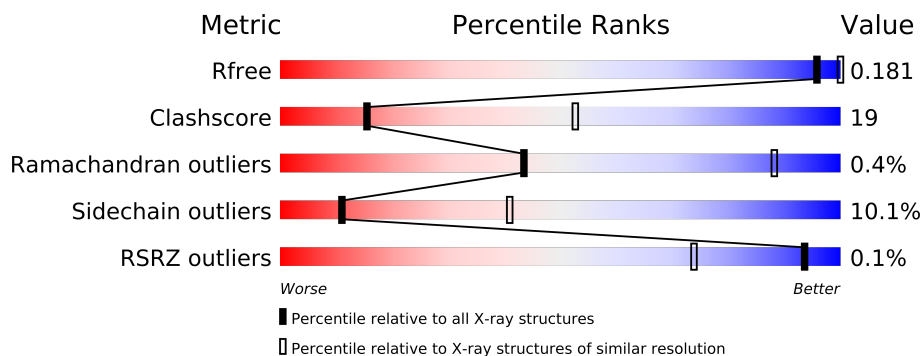
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	
1	C	301	
1	D	301	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	URA	A	900	-	X
2	URA	B	1900	-	X
2	URA	C	2900	-	X
2	URA	D	3900	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9507 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

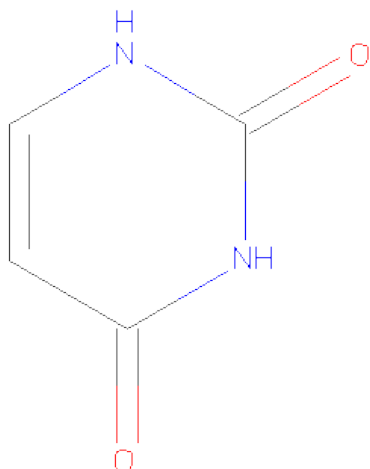
- Molecule 1 is a protein called Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	1
			2363	1493	410	453	7			
1	B	296	Total	C	N	O	S	0	0	1
			2363	1493	410	453	7			
1	C	299	Total	C	N	O	S	0	0	1
			2386	1508	414	457	7			
1	D	296	Total	C	N	O	S	0	0	1
			2363	1493	410	453	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
B	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
C	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
D	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511

- Molecule 2 is URACIL (three-letter code: URA) (formula: C₄H₄N₂O₂).



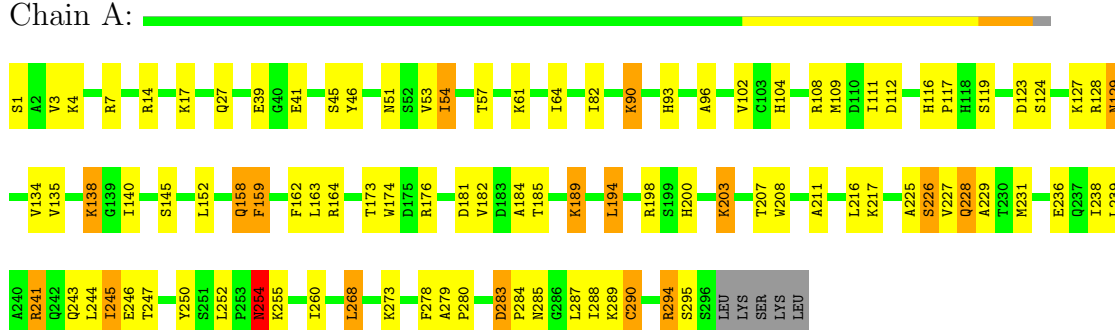
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	2	2		
2	B	1	Total	C	N	O	0	0
			8	4	2	2		
2	C	1	Total	C	N	O	0	0
			8	4	2	2		
2	D	1	Total	C	N	O	0	0
			8	4	2	2		

3 Residue-property plots

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.

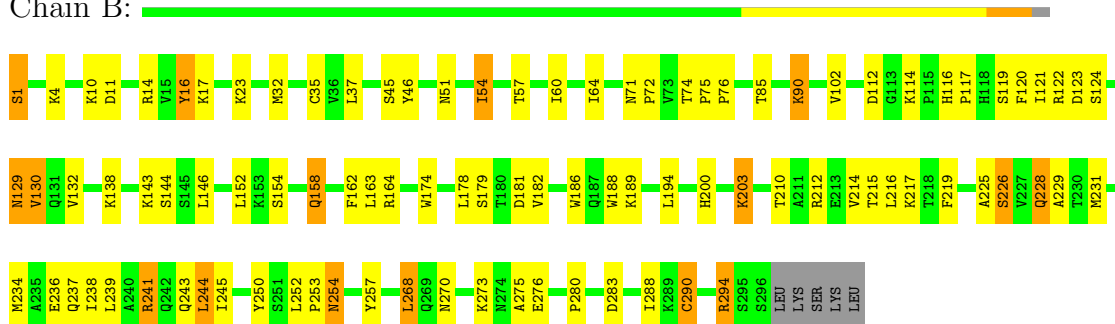
• Molecule 1: Uricase

Chain A:



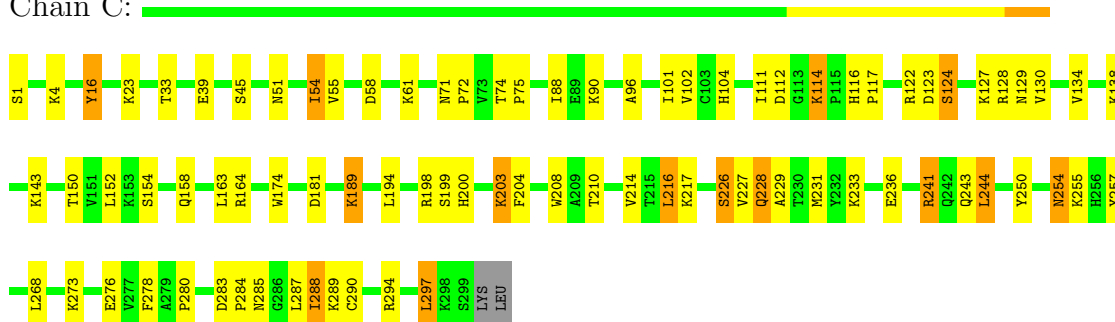
• Molecule 1: Uricase

Chain B:



• Molecule 1: Uricase

Chain C:



• Molecule 1: Uricase

Chain D:

LEU	A211	I111	S1
	L216	G13	K4
	K217	K114	
	F219	S119	R7
			T8
	N223	D123	G9
	S224	S124	K10
	A225		D11
	S226	K127	V13
	V227	R128	R14
	Q228	N129	
	A229	V130	K17
	T230		
	M231	V134	T33
	E236	K138	V36
	Q237		
	L238	I142	E41
		K143	I42
	R241		E43
	Q242	L146	T44
	Q243		S45
	L244	L149	
	Y250	K153	D50
		S154	N51
	P253	T155	S52
	N254	M156	V53
	K255	S157	I54
		Q158	V55
	L260		D58
		F162	
	L268	L163	K61
	Q269	R164	
		L170	A68
	A275	K171	K69
	E276		Q70
	F278	V174	P75
	A279	L178	P76
	P280		E77
		D181	I88
	D283		E89
	P284	V188	K90
	N285	K189	
		L194	H93
	L288		I94
	K289		H95
	C290		
		S199	V99
		H200	I100
	R294		I101
	S295	K203	V102
	L296	F204	C103
	LEU		H104
	LVS		
	SER	W208	T110
	LVS		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.60Å 140.60Å 151.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.20 36.07 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-3.20) 99.9 (36.07-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 3.18Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.146 , 0.200 0.148 , 0.181	Depositor DCC
R_{free} test set	2885 reflections (11.22%)	DCC
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 10.6	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 28896 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9507	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 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, 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	0.64	1/2407 (0.0%)	0.81	1/3267 (0.0%)
1	B	0.63	0/2407	0.78	1/3267 (0.0%)
1	C	0.63	0/2430	0.79	1/3297 (0.0%)
1	D	0.62	0/2407	0.78	0/3267
All	All	0.63	1/9651 (0.0%)	0.79	3/13098 (0.0%)

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	1	0
1	B	0	1
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	PHE	CG-CD2	-5.16	1.31	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ASN	CB-CA-C	5.89	122.19	110.40
1	B	254	ASN	CB-CA-C	5.26	120.93	110.40
1	C	254	ASN	CB-CA-C	5.01	120.42	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	254	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	SAC	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2363	0	2324	91	0
1	B	2363	0	2324	87	0
1	C	2386	0	2353	88	0
1	D	2363	0	2324	113	0
2	A	8	0	3	0	0
2	B	8	0	3	1	0
2	C	8	0	3	1	0
2	D	8	0	3	1	0
All	All	9507	0	9337	352	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 352 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:294:ARG:HG2	1:B:294:ARG:HH11	1.03	1.12
1:B:116:HIS:ND1	1:B:117:PRO:HD2	1.73	1.04
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.25	1.01
1:D:200:HIS:HD2	1:D:203:LYS:NZ	1.59	0.98
1:A:294:ARG:HG2	1:A:294:ARG:HH11	1.32	0.95

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	294/301 (98%)	279 (95%)	15 (5%)	0	100	100
1	B	294/301 (98%)	276 (94%)	17 (6%)	1 (0%)	50	91
1	C	297/301 (99%)	283 (95%)	11 (4%)	3 (1%)	22	74
1	D	294/301 (98%)	277 (94%)	16 (5%)	1 (0%)	50	91
All	All	1179/1204 (98%)	1115 (95%)	59 (5%)	5 (0%)	43	88

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	SER
1	B	23	LYS
1	C	124	SER
1	C	23	LYS
1	C	204	PHE

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	260/266 (98%)	232 (89%)	28 (11%)	9	37
1	B	260/266 (98%)	230 (88%)	30 (12%)	8	35
1	C	263/266 (99%)	243 (92%)	20 (8%)	19	60
1	D	260/266 (98%)	233 (90%)	27 (10%)	10	39
All	All	1043/1064 (98%)	938 (90%)	105 (10%)	11	41

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	226	SER
1	C	4	LYS
1	D	241	ARG
1	B	228	GLN
1	B	268	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	86	HIS
1	C	129	ASN
1	D	200	HIS
1	B	243	GLN
1	D	228	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 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	SAC	A	1	1	8,8,9	8.62	4 (50%)	6,9,11	2.39	3 (50%)
1	SAC	B	1	1	8,8,9	6.70	2 (25%)	6,9,11	0.82	0
1	SAC	C	1	1	8,8,9	8.76	3 (37%)	6,9,11	1.50	1 (16%)
1	SAC	D	1	1	8,8,9	7.64	2 (25%)	6,9,11	2.05	2 (33%)

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	SAC	A	1	1	-	0/6/8/10	0/0/0/0
1	SAC	B	1	1	-	0/6/8/10	0/0/0/0
1	SAC	C	1	1	-	0/6/8/10	0/0/0/0
1	SAC	D	1	1	-	0/6/8/10	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	SAC	O-C	24.50	1.28	1.11
1	A	1	SAC	O-C	23.52	1.27	1.11
1	D	1	SAC	O-C	21.29	1.26	1.11
1	B	1	SAC	O-C	18.57	1.24	1.11
1	A	1	SAC	OAC-C1A	3.88	1.31	1.23

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	SAC	CA-N-C1A	-4.27	116.08	122.01
1	A	1	SAC	OAC-C1A-N	-3.86	113.84	121.90
1	C	1	SAC	CA-N-C1A	-3.42	117.27	122.01
1	A	1	SAC	CB-CA-N	3.12	113.38	109.48
1	A	1	SAC	C2A-C1A-N	2.24	120.49	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands 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	$\# Z > 2$
2	URA	A	900	-	8,8,8	2.27	4 (50%)	6,10,10	1.14	0
2	URA	B	1900	-	8,8,8	2.31	4 (50%)	6,10,10	1.37	1 (16%)
2	URA	C	2900	-	8,8,8	2.09	2 (25%)	6,10,10	1.23	1 (16%)
2	URA	D	3900	-	8,8,8	2.29	4 (50%)	6,10,10	1.25	1 (16%)

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
2	URA	A	900	-	-	0/0/0/0	0/1/1/1
2	URA	B	1900	-	-	0/0/0/0	0/1/1/1
2	URA	C	2900	-	-	0/0/0/0	0/1/1/1
2	URA	D	3900	-	-	0/0/0/0	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1900	URA	C2-N1	4.79	1.46	1.37
2	D	3900	URA	C2-N1	4.78	1.46	1.37
2	A	900	URA	C2-N1	4.64	1.46	1.37
2	C	2900	URA	C2-N1	4.26	1.45	1.37
2	B	1900	URA	C6-N1	2.48	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1900	URA	C5-C6-N1	2.22	123.14	120.67
2	D	3900	URA	C5-C6-N1	2.12	123.03	120.67
2	C	2900	URA	C5-C6-N1	2.08	122.98	120.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	296/301 (98%)	-0.56	0 100 100	12, 31, 57, 76	0
1	B	296/301 (98%)	-0.54	0 100 100	16, 30, 56, 77	0
1	C	299/301 (99%)	-0.55	0 100 100	12, 31, 57, 75	0
1	D	296/301 (98%)	-0.56	0 100 100	13, 31, 54, 80	0
All	All	1187/1204 (98%)	-0.55	0 93 100	12, 31, 56, 80	0

There are no RSRZ outliers to report.

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

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SAC	D	1	9/10	0.18	2.57	43,49,60,71	0
1	SAC	B	1	9/10	0.30	1.67	42,57,69,71	0
1	SAC	A	1	9/10	0.23	1.59	46,59,63,79	0
1	SAC	C	1	9/10	0.19	-0.16	47,58,65,78	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	URA	B	1900	8/8	0.48	7.93	45,46,47,47	8
2	URA	C	2900	8/8	0.34	5.77	44,45,47,47	8
2	URA	D	3900	8/8	0.39	4.81	41,42,43,43	8
2	URA	A	900	8/8	0.35	4.64	42,43,44,44	8

6.5 Other polymers ⓘ

There are no such residues in this entry.