Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 03:22 AM EDT

PDB ID	:	3OBP
Title	:	Anaerobic complex of urate oxidase with uric acid
Authors	:	Gabison, L.; Chopard, C.; Colloc'h, N.; El Hajji, M.; Castro, B.; Chiadmi, M.; Prange, T.
Deposited on	:	2010-08-08
Resolution	:	1.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

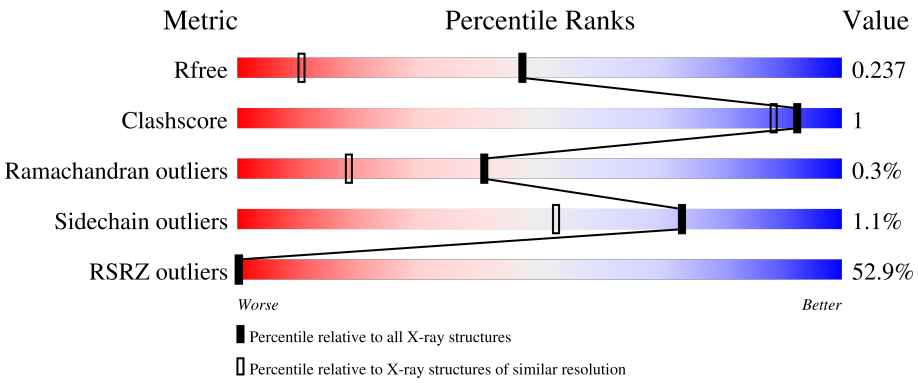
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

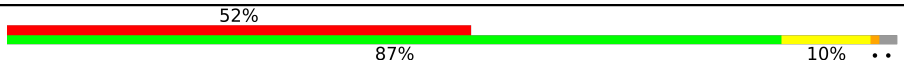
The reported resolution of this entry is 1.50 Å.

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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 of 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	302	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2653 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.

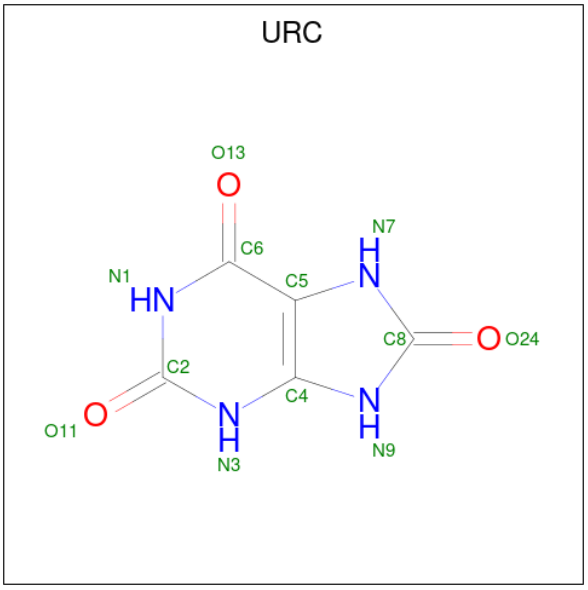
- Molecule 1 is a protein called Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2390	1510	412	459	9	0	9	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP Q00511

- Molecule 2 is URIC ACID (three-letter code: URC) (formula: $C_5H_4N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	5	4	3	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0

- Molecule 4 is water.

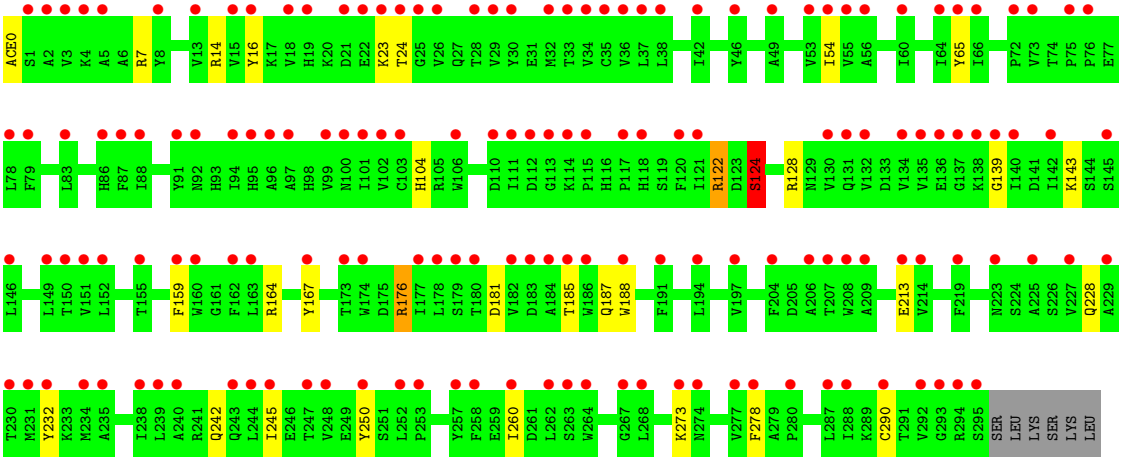
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	250	250	250	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Uricase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	79.85Å 96.29Å 105.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.50 23.17 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (10.00-1.50) 99.2 (23.17-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	11.03 (at 1.50Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.220 , 0.249 0.244 , 0.237	Depositor DCC
R_{free} test set	3897 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å^2)	4.4	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.28$, $< L^2 > = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	2653	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NA, URC

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	0.63	0/2491	1.48	35/3376 (1.0%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	ARG	NE-CZ-NH2	-12.81	113.90	120.30
1	A	14	ARG	NE-CZ-NH1	-9.71	115.44	120.30
1	A	128	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	0	ACE	O-C-N	8.86	136.87	122.70
1	A	104	HIS	CG-ND1-CE1	8.66	120.33	108.20
1	A	188	TRP	CD1-NE1-CE2	8.40	116.56	109.00
1	A	122	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	14	ARG	NH1-CZ-NH2	7.66	127.82	119.40
1	A	167	TYR	CB-CG-CD1	7.14	125.28	121.00
1	A	14	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	164	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	159	PHE	CB-CG-CD2	6.97	125.68	120.80
1	A	250	TYR	CB-CG-CD1	6.63	124.98	121.00
1	A	290[A]	CYS	CA-CB-SG	6.55	125.80	114.00
1	A	290[B]	CYS	CA-CB-SG	6.55	125.80	114.00
1	A	176	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	228	GLN	O-C-N	-6.49	112.32	122.70
1	A	16	TYR	O-C-N	6.27	132.74	122.70
1	A	124	SER	O-C-N	6.21	132.63	122.70
1	A	232	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	A	65[A]	TYR	CA-CB-CG	6.08	124.95	113.40
1	A	65[B]	TYR	CA-CB-CG	6.08	124.95	113.40
1	A	278	PHE	CB-CG-CD2	-5.98	116.61	120.80
1	A	104	HIS	ND1-CG-CD2	-5.88	97.77	106.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	TYR	CG-CD1-CE1	5.72	125.88	121.30
1	A	128	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	188	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	A	181	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	139	GLY	O-C-N	5.45	131.42	122.70
1	A	260	ILE	O-C-N	5.44	131.41	122.70
1	A	188	TRP	NE1-CE2-CD2	-5.39	101.91	107.30
1	A	16	TYR	CA-CB-CG	5.17	123.23	113.40
1	A	278	PHE	CB-CG-CD1	5.10	124.37	120.80
1	A	7	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	159	PHE	CG-CD2-CE2	5.08	126.38	120.80

There are no chirality outliers.

There are no planarity outliers.

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	2390	0	2351	7	0
2	A	12	0	4	1	0
3	A	1	0	0	0	0
4	A	250	0	0	3	0
All	All	2653	0	2355	7	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 1.

All (7) 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:54:ILE:HG12	4:A:1246:HOH:O	1.83	0.77
1:A:176:ARG:HH12	2:A:302:URC:HN3	1.36	0.71
1:A:242:GLN:O	1:A:245:ILE:HG12	2.07	0.54
1:A:273:LYS:HG3	4:A:1238:HOH:O	2.13	0.48
1:A:213[A]:GLU:HG3	4:A:1101:HOH:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23[B]:LYS:HG2	1:A:24:THR:HG23	1.99	0.43
1:A:143[B]:LYS:HE2	1:A:185:THR:HG21	2.00	0.43

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	303/302 (100%)	297 (98%)	5 (2%)	1 (0%)	41 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER

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	270/267 (101%)	267 (99%)	3 (1%)	73 53

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	SER
1	A	187	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	100	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
2	URC	A	302	-	8,13,13	1.43	1 (12%)	5,19,19	10.88	5 (100%)

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	URC	A	302	-	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	URC	C6-N1	2.45	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	URC	C2-N1-C6	18.34	130.63	115.14
2	A	302	URC	C4-N9-C8	12.16	108.50	101.12
2	A	302	URC	C5-C6-N1	-8.89	111.27	123.43
2	A	302	URC	C4-C5-N7	4.39	113.92	109.47
2	A	302	URC	C4-C5-C6	-3.02	117.92	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	URC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	295/302 (97%)	2.27	156 (52%) 0 0	10, 18, 34, 78	1 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23[A]	LYS	10.1
1	A	295	SER	9.0
1	A	22	GLU	8.5
1	A	113	GLY	6.9
1	A	24	THR	6.9
1	A	111	ILE	6.5
1	A	1	SER	5.7
1	A	112	ASP	5.2
1	A	21	ASP	5.1
1	A	26	VAL	5.1
1	A	2	ALA	4.6
1	A	245	ILE	4.5
1	A	115	PRO	4.1
1	A	239	LEU	3.8
1	A	132	VAL	3.8
1	A	288	ILE	3.7
1	A	174	TRP	3.7
1	A	92	ASN	3.7
1	A	140	ILE	3.6
1	A	204	PHE	3.5
1	A	177	ILE	3.5
1	A	65[A]	TYR	3.5
1	A	264	TRP	3.4
1	A	101	ILE	3.4
1	A	146	LEU	3.4
1	A	91	TYR	3.4
1	A	3	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	18	VAL	3.4
1	A	110	ASP	3.4
1	A	268	LEU	3.4
1	A	135	VAL	3.3
1	A	227	VAL	3.3
1	A	188	TRP	3.3
1	A	178	LEU	3.3
1	A	34	VAL	3.3
1	A	99	VAL	3.3
1	A	248	VAL	3.3
1	A	186	TRP	3.2
1	A	278	PHE	3.2
1	A	38	LEU	3.2
1	A	142	ILE	3.2
1	A	159	PHE	3.2
1	A	290[A]	CYS	3.2
1	A	8	TYR	3.2
1	A	191	PHE	3.2
1	A	163	LEU	3.1
1	A	106	TRP	3.1
1	A	36	VAL	3.1
1	A	292	VAL	3.1
1	A	160	TRP	3.0
1	A	240	ALA	3.0
1	A	88	ILE	3.0
1	A	79	PHE	3.0
1	A	120	PHE	3.0
1	A	54	ILE	3.0
1	A	29	VAL	3.0
1	A	73	VAL	3.0
1	A	182	VAL	3.0
1	A	267	GLY	3.0
1	A	35	CYS	3.0
1	A	121	ILE	3.0
1	A	152	LEU	3.0
1	A	32	MET	3.0
1	A	114	LYS	2.9
1	A	102	VAL	2.9
1	A	16	TYR	2.9
1	A	250	TYR	2.9
1	A	25	GLY	2.9
1	A	277	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	2.9
1	A	184	ALA	2.9
1	A	134	VAL	2.9
1	A	30	TYR	2.9
1	A	287	LEU	2.9
1	A	55	VAL	2.9
1	A	262	LEU	2.8
1	A	258	PHE	2.8
1	A	64	ILE	2.8
1	A	197	VAL	2.8
1	A	138	LYS	2.8
1	A	219	PHE	2.8
1	A	149	LEU	2.7
1	A	260	ILE	2.7
1	A	53	VAL	2.7
1	A	37	LEU	2.7
1	A	225	ALA	2.7
1	A	274	ASN	2.7
1	A	180	THR	2.7
1	A	293	GLY	2.7
1	A	263	SER	2.7
1	A	232	TYR	2.7
1	A	56	ALA	2.7
1	A	137	GLY	2.7
1	A	185	THR	2.6
1	A	208	TRP	2.6
1	A	13	VAL	2.6
1	A	257	TYR	2.6
1	A	252	LEU	2.6
1	A	97	ALA	2.6
1	A	243	GLN	2.6
1	A	162	PHE	2.6
1	A	15	VAL	2.6
1	A	78	LEU	2.5
1	A	19	HIS	2.5
1	A	234	MET	2.5
1	A	136	GLU	2.5
1	A	5	ALA	2.5
1	A	49	ALA	2.5
1	A	87	PHE	2.5
1	A	118	HIS	2.5
1	A	130	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	183	ASP	2.4
1	A	28	THR	2.4
1	A	273	LYS	2.4
1	A	117	PRO	2.4
1	A	96	ALA	2.4
1	A	229	ALA	2.4
1	A	83	LEU	2.4
1	A	194	LEU	2.4
1	A	42	ILE	2.4
1	A	238	ILE	2.4
1	A	167	TYR	2.4
1	A	139	GLY	2.4
1	A	103	CYS	2.4
1	A	155	THR	2.4
1	A	206	ALA	2.3
1	A	46	TYR	2.3
1	A	150	THR	2.3
1	A	75	PRO	2.3
1	A	231[A]	MET	2.3
1	A	213[A]	GLU	2.3
1	A	214	VAL	2.3
1	A	72	PRO	2.3
1	A	207	THR	2.3
1	A	230	THR	2.2
1	A	247	THR	2.2
1	A	179	SER	2.2
1	A	60	ILE	2.2
1	A	4[A]	LYS	2.2
1	A	253	PRO	2.2
1	A	280	PRO	2.2
1	A	94	ILE	2.1
1	A	223	ASN	2.1
1	A	95	HIS	2.1
1	A	33	THR	2.1
1	A	76	PRO	2.1
1	A	294	ARG	2.1
1	A	151	VAL	2.1
1	A	145	SER	2.1
1	A	131	GLN	2.1
1	A	100	ASN	2.1
1	A	173	THR	2.1
1	A	209	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	235	ALA	2.1
1	A	66	ILE	2.0
1	A	86	HIS	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 monosaccharides 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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	URC	A	302	12/12	0.93	0.16	12,17,24,26	0
3	NA	A	850	1/1	0.97	0.13	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.