Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 03:35 AM EDT

PDB ID	:	3IUK
Title	:	Crystal structure of putative bacterial protein of unknown function (DUF885, PF05960.1,) from Arthrobacter aurescens TC1, reveals fold similar to that of M32 carboxypeptidases
Authors	:	Nocek, B.; Chhor, G.; Cobb, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-08-31
Resolution	:	1.85 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:

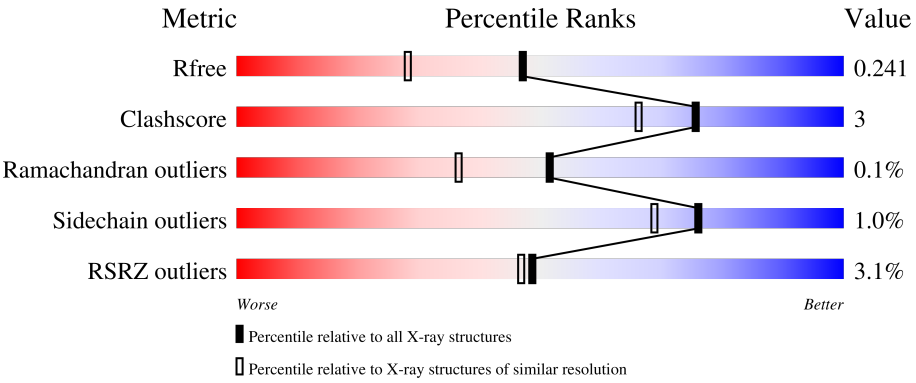
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	562	3% 93% 5%
1	B	562	3% 90% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10127 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.

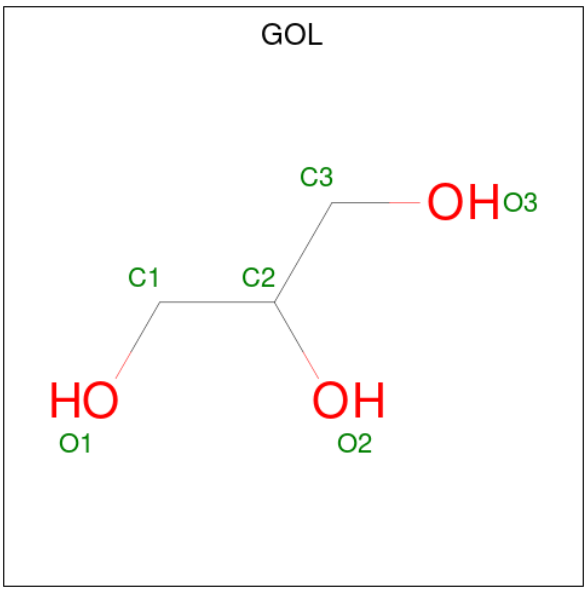
- Molecule 1 is a protein called uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	Se	0	8	0
			4331	2726	753	839	2	11			
1	B	550	Total	C	N	O	S	Se	0	0	0
			4262	2684	743	822	2	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A1R4M8
A	-1	ASN	-	expression tag	UNP A1R4M8
A	0	ALA	-	expression tag	UNP A1R4M8
B	-2	SER	-	expression tag	UNP A1R4M8
B	-1	ASN	-	expression tag	UNP A1R4M8
B	0	ALA	-	expression tag	UNP A1R4M8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is water.

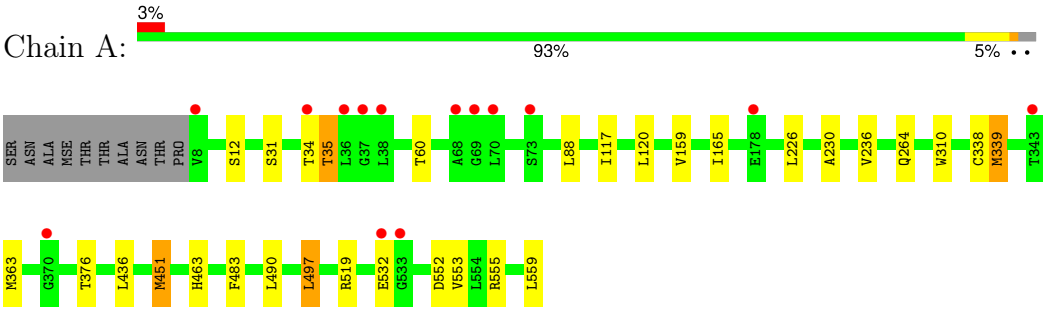
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	757	Total O 757 757	0	0
4	B	768	Total O 768 768	0	0

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.

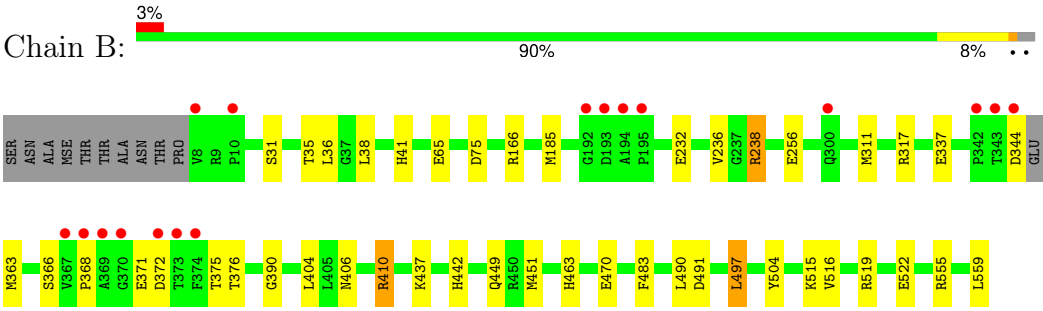
• Molecule 1: uncharacterized protein

Chain A:



• Molecule 1: uncharacterized protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.61Å 85.39Å 115.49Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 37.10 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-1.85) 99.3 (37.10-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.163 , 0.220 0.190 , 0.241	Depositor DCC
R_{free} test set	4915 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10127	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL

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	0.89	0/4442	0.84	3/6014 (0.0%)
1	B	0.96	3/4348 (0.1%)	0.85	7/5890 (0.1%)
All	All	0.92	3/8790 (0.0%)	0.84	10/11904 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	ASP	CB-CG	-5.89	1.39	1.51
1	B	232	GLU	CG-CD	5.50	1.60	1.51
1	B	516	VAL	CB-CG2	5.01	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	MSE	CG-SE-CE	-12.40	71.61	98.90
1	B	410	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	B	519	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	519	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	166	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	363	MSE	CG-SE-CE	-5.36	87.12	98.90
1	B	75	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	185	MSE	CG-SE-CE	-5.25	87.36	98.90
1	B	238	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	238	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	4331	0	4198	18	0
1	B	4262	0	4111	35	0
2	A	6	0	8	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	757	0	0	5	0
4	B	768	0	0	10	0
All	All	10127	0	8317	53	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 (53) 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:B:451:MSE:HG2	1:B:490:LEU:HD22	1.53	0.89
1:A:31:SER:O	1:A:35:THR:HG23	1.91	0.71
1:B:368:PRO:HB2	1:B:371:GLU:OE1	1.92	0.69
1:B:375:THR:HG22	4:B:568:HOH:O	1.97	0.65
1:A:555[A]:ARG:HG3	1:A:559:LEU:HD22	1.79	0.64
1:A:555[B]:ARG:HG2	1:A:559:LEU:HD22	1.79	0.63
1:A:555[A]:ARG:CG	1:A:559:LEU:HD22	2.29	0.62
1:B:238:ARG:NH2	1:B:256:GLU:OE1	2.31	0.61
1:B:31:SER:O	1:B:35:THR:HG23	2.00	0.60
1:B:41:HIS:HE1	4:B:878:HOH:O	1.82	0.60
1:B:555:ARG:CG	1:B:559:LEU:HD23	2.33	0.58
1:B:317:ARG:HD2	4:B:678:HOH:O	2.05	0.57
1:B:406:ASN:O	1:B:410:ARG:HG3	2.04	0.57
1:A:236:VAL:H	1:A:463:HIS:HD2	1.52	0.56
1:B:337:GLU:OE1	1:B:362:ARG:NH1	2.39	0.56
1:B:236:VAL:H	1:B:463:HIS:HD2	1.55	0.54
1:B:555:ARG:O	1:B:559:LEU:HD22	2.09	0.53
1:B:36:LEU:HB3	1:B:38:LEU:HD13	1.90	0.53
1:B:368:PRO:CG	1:B:371:GLU:OE1	2.57	0.53
1:A:553:VAL:HG23	4:A:570:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ARG:HG3	1:B:559:LEU:HD23	1.91	0.52
1:B:368:PRO:CB	1:B:371:GLU:OE1	2.57	0.52
1:B:442:HIS:HD2	4:B:730:HOH:O	1.94	0.51
1:A:12:SER:HB2	4:A:1631:HOH:O	2.10	0.50
1:B:470:GLU:HG2	4:B:1368:HOH:O	2.10	0.50
1:B:449:GLN:HE22	1:B:515:LYS:NZ	2.11	0.49
1:B:65:GLU:HG3	4:B:1081:HOH:O	2.12	0.49
1:B:483:PHE:CZ	1:B:497:LEU:HD13	2.48	0.49
1:A:451:MSE:HG3	1:A:490:LEU:HG	1.95	0.48
1:B:463:HIS:HE1	1:B:504:TYR:O	1.95	0.48
1:B:368:PRO:HG2	1:B:371:GLU:OE1	2.14	0.48
1:B:449:GLN:HE22	1:B:515:LYS:HZ2	1.62	0.48
1:B:555:ARG:HG3	1:B:559:LEU:CD2	2.43	0.48
1:B:522:GLU:CD	4:B:590:HOH:O	2.53	0.47
1:B:555:ARG:HG2	1:B:559:LEU:HD23	1.95	0.47
1:A:264:GLN:NE2	4:A:1619:HOH:O	2.47	0.47
1:B:344:ASP:HA	1:B:366:SER:OG	2.14	0.47
1:B:555:ARG:O	1:B:559:LEU:CD2	2.63	0.47
1:A:165:ILE:HD12	1:A:230:ALA:HB2	1.98	0.46
1:A:310:TRP:CZ2	1:A:376:THR:HB	2.51	0.46
1:A:436:LEU:HD11	4:A:1706:HOH:O	2.16	0.45
1:B:311:MSE:SE	1:B:363:MSE:HE3	2.66	0.45
1:A:552:ASP:OD1	4:A:1543:HOH:O	2.21	0.45
1:A:338:CYS:O	1:A:339:MSE:HE3	2.17	0.45
1:B:36:LEU:CB	1:B:38:LEU:HD13	2.47	0.44
1:B:238:ARG:NH2	1:B:256:GLU:CD	2.71	0.44
1:A:483:PHE:CZ	1:A:497:LEU:HD13	2.53	0.44
1:A:117:ILE:HD12	1:A:120:LEU:HD12	2.00	0.44
1:B:437:LYS:HE2	4:B:882:HOH:O	2.19	0.42
1:B:470:GLU:CG	4:B:1368:HOH:O	2.67	0.41
1:A:159:VAL:HG13	1:A:226:LEU:HG	2.03	0.41
1:A:60:THR:HG23	1:A:88:LEU:HG	2.03	0.40
1:B:41:HIS:CE1	4:B:878:HOH:O	2.66	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	558/562 (99%)	550 (99%)	8 (1%)	0	100	100
1	B	546/562 (97%)	535 (98%)	10 (2%)	1 (0%)	47	33
All	All	1104/1124 (98%)	1085 (98%)	18 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	390	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	443/432 (102%)	438 (99%)	5 (1%)	73	65
1	B	431/432 (100%)	427 (99%)	4 (1%)	78	72
All	All	874/864 (101%)	865 (99%)	9 (1%)	76	69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	35	THR
1	A	339	MSE
1	A	497	LEU
1	A	532	GLU

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Mol	Chain	Res	Type
1	B	376	THR
1	B	404	LEU
1	B	491	ASP
1	B	497	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	264	GLN
1	A	279	GLN
1	A	411	ASN
1	A	449	GLN
1	A	463	HIS
1	A	496	GLN
1	B	138	ASN
1	B	300	GLN
1	B	442	HIS
1	B	449	GLN
1	B	463	HIS

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 4 ligands modelled in this entry, 3 are 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	GOL	A	1001	-	5,5,5	0.37	0	5,5,5	0.66	0

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	GOL	A	1001	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	GOL	C1-C2-C3-O3
2	A	1001	GOL	O2-C2-C3-O3
2	A	1001	GOL	O1-C1-C2-C3
2	A	1001	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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

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	541/562 (96%)	-0.06	16 (2%)	50	48	4, 10, 21, 30	0
1	B	539/562 (95%)	-0.11	18 (3%)	46	44	3, 9, 23, 32	0
All	All	1080/1124 (96%)	-0.09	34 (3%)	49	47	3, 10, 22, 32	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	THR	4.5
1	A	8	VAL	4.4
1	B	370	GLY	4.1
1	A	69	GLY	4.0
1	B	369	ALA	3.8
1	A	370	GLY	3.8
1	A	346	GLY	3.7
1	B	8	VAL	3.6
1	B	194	ALA	3.6
1	A	38	LEU	3.6
1	B	374	PHE	3.4
1	B	192	GLY	3.3
1	A	343	THR	3.2
1	A	532	GLU	3.0
1	A	34	THR	3.0
1	A	37	GLY	2.9
1	B	193	ASP	2.9
1	A	73	SER	2.9
1	A	345	GLU	2.9
1	B	368	PRO	2.9
1	B	342	PRO	2.7
1	B	367	VAL	2.6
1	B	347	GLY	2.4
1	B	344	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	372	ASP	2.3
1	A	70	LEU	2.2
1	B	10	PRO	2.1
1	B	195	PRO	2.1
1	B	300	GLN	2.1
1	A	36	LEU	2.1
1	B	373	THR	2.1
1	A	178	GLU	2.1
1	A	68	ALA	2.0
1	A	533	GLY	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, 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	B-factors(Å^2)	Q<0.9
2	GOL	A	1001	6/6	0.84	0.19	41,43,43,43	0
3	MG	A	561	1/1	0.92	0.11	35,35,35,35	0
3	MG	A	560	1/1	0.97	0.17	19,19,19,19	0
3	MG	B	560	1/1	0.99	0.23	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.