Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 01:24 PM EDT

PDB ID	:	3FR7
Title	:	ketol-acid reductoisomerase (KARI) in complex with Mg2+
Authors	:	Guddat, L.W.; Leung, E.W.W.
Deposited on	:	2009-01-08
Resolution	:	1.55 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 ⓘ 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 ⓘ) were used in the production of this report:

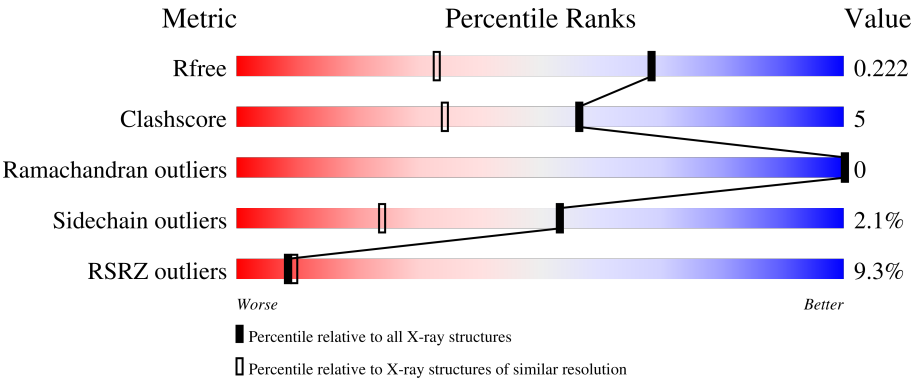
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	525	10% 84% 10% 6%
1	B	525	7% 85% 7% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8749 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 ketol-acid reductoisomerase (Os05g0573700 protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	31	0
			3969	2532	661	756	20			
1	B	490	Total	C	N	O	S	6	28	0
			3935	2510	657	748	20			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

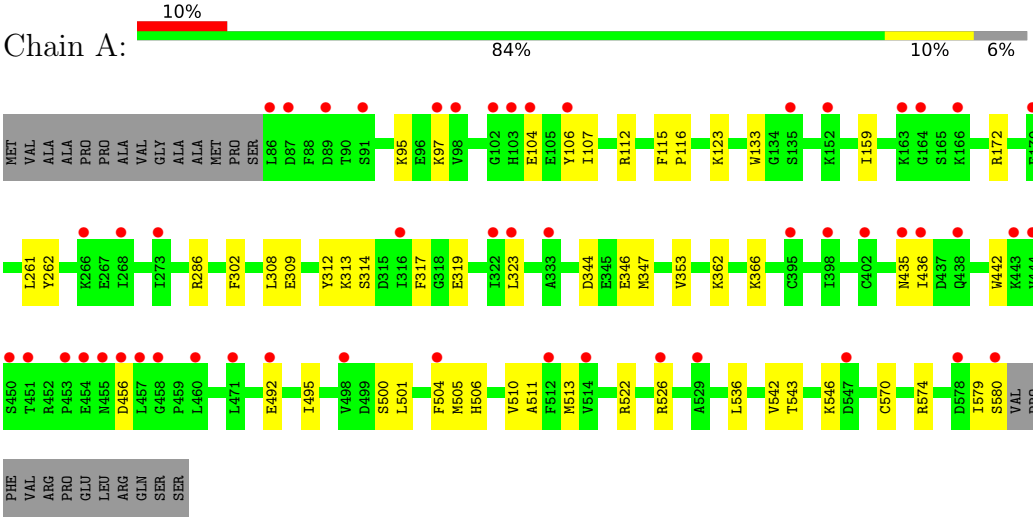
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	391	Total	O	0	0
			391	391		
3	B	449	Total	O	0	0
			449	449		

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.

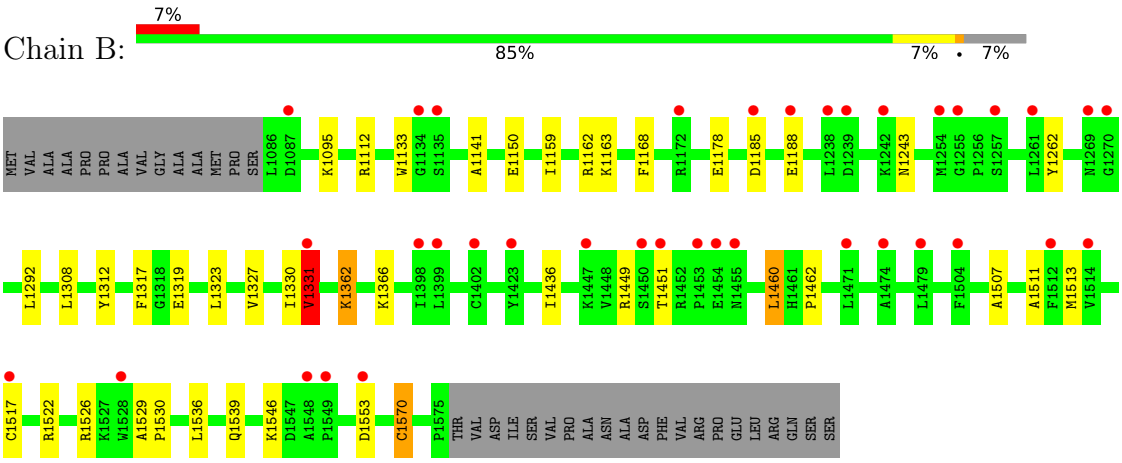
• Molecule 1: Putative ketol-acid reductoisomerase (Os05g0573700 protein)

Chain A:



• Molecule 1: Putative ketol-acid reductoisomerase (Os05g0573700 protein)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.03Å 92.90Å 91.19Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	37.16 – 1.55 37.16 – 1.55	Depositor EDS
% Data completeness (in resolution range)	96.0 (37.16-1.55) 96.9 (37.16-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.230 0.194 , 0.222	Depositor DCC
R_{free} test set	7283 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8749	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 4.63% 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

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	0.58	0/4139	0.64	0/5586
1	B	0.59	1/4097 (0.0%)	0.66	2/5522 (0.0%)
All	All	0.59	1/8236 (0.0%)	0.65	2/11108 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1570	CYS	CB-SG	-6.04	1.72	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1331	VAL	CG1-CB-CG2	5.82	120.22	110.90
1	B	1460	LEU	CA-CB-CG	5.53	128.02	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	3969	0	4012	43	0
1	B	3935	0	3971	38	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	391	0	0	8	0
3	B	449	0	0	3	0
All	All	8749	0	7983	80	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 5.

All (80) 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:1362[B]:LYS:HG3	1:B:1366[B]:LYS:NZ	1.12	1.39
1:B:1362[B]:LYS:CG	1:B:1366[B]:LYS:NZ	2.08	1.14
1:B:1522:ARG:HG3	1:B:1526[A]:ARG:NH1	1.74	1.03
1:B:1362[B]:LYS:CG	1:B:1366[B]:LYS:HZ1	1.68	0.99
1:A:505:MET:HG2	1:A:513:MET:HG3	1.45	0.98
1:A:344[B]:ASP:OD1	1:A:347[B]:MET:HB2	1.72	0.89
1:B:1112[B]:ARG:NH1	1:B:1150[B]:GLU:OE2	2.07	0.88
1:B:1362[B]:LYS:HG3	1:B:1366[B]:LYS:HZ2	1.10	0.86
1:A:133:TRP:HZ3	1:A:159:ILE:HD13	1.40	0.86
1:A:123[B]:LYS:HD2	3:A:680:HOH:O	1.76	0.85
1:B:1522:ARG:HG3	1:B:1526[A]:ARG:HH12	1.41	0.85
1:A:133:TRP:HZ3	1:A:159:ILE:CD1	1.90	0.83
1:B:1362[B]:LYS:HG3	1:B:1366[B]:LYS:HZ1	1.00	0.82
1:B:1362[B]:LYS:HG3	1:B:1366[B]:LYS:HZ3	1.45	0.82
1:A:133:TRP:CZ3	1:A:159:ILE:HD13	2.15	0.81
1:A:505:MET:CG	1:A:513:MET:HG3	2.12	0.80
1:B:1522:ARG:CG	1:B:1526[A]:ARG:NH1	2.45	0.79
1:B:1362[A]:LYS:HE2	1:B:1366[A]:LYS:HE3	1.64	0.78
1:A:123[B]:LYS:HE2	1:A:286:ARG:HG2	1.67	0.76
1:A:323:LEU:HD22	1:A:501:LEU:HD12	1.67	0.76
1:A:353:VAL:HG11	3:A:851:HOH:O	1.86	0.74
1:A:123[B]:LYS:HD3	3:A:666:HOH:O	1.88	0.74
1:A:542:VAL:HG12	1:A:546:LYS:HE2	1.71	0.72
1:B:1112[B]:ARG:HH11	1:B:1150[B]:GLU:CD	1.93	0.72
1:B:1362[B]:LYS:HE2	1:B:1366[B]:LYS:HZ2	1.59	0.67
1:A:344[B]:ASP:OD1	1:A:347[B]:MET:CB	2.43	0.66
1:A:492[B]:GLU:HG3	3:A:735:HOH:O	1.95	0.65
1:B:1362[B]:LYS:CG	1:B:1366[B]:LYS:HZ2	1.92	0.65
1:A:504:PHE:HD2	1:A:513:MET:SD	2.19	0.65
1:A:314:SER:OG	1:A:492[B]:GLU:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ARG:HH21	1:A:526[A]:ARG:NH2	1.96	0.63
1:A:346[B]:GLU:H	1:A:346[B]:GLU:CD	2.02	0.63
1:A:505:MET:HG2	1:A:513:MET:CG	2.22	0.63
1:A:314:SER:HG	1:A:492[B]:GLU:HG2	1.63	0.63
1:A:172:ARG:HD2	3:A:612:HOH:O	2.00	0.62
1:A:526[A]:ARG:NE	3:A:922:HOH:O	2.33	0.62
1:A:504:PHE:CD2	1:A:513:MET:SD	2.93	0.61
1:B:1112[A]:ARG:NH1	1:B:1262:TYR:O	2.34	0.61
1:A:436:ILE:HD11	1:A:511:ALA:HA	1.82	0.60
1:B:1462:PRO:HG2	3:B:563:HOH:O	2.01	0.60
1:A:526[A]:ARG:HG2	3:A:922:HOH:O	2.03	0.59
1:B:1539:GLN:HG3	3:B:449:HOH:O	2.03	0.59
1:A:97:LYS:HD3	1:A:104:GLU:OE1	2.05	0.57
1:B:1436:ILE:HD11	1:B:1511:ALA:HA	1.86	0.57
1:A:95:LYS:HG2	1:A:106:TYR:CD2	2.41	0.56
1:A:500:SER:HA	1:A:580:SER:HB3	1.88	0.56
1:B:1513:MET:O	1:B:1517:CYS:HB2	2.06	0.55
1:A:543:THR:HA	1:A:546:LYS:HE3	1.90	0.54
1:B:1362[A]:LYS:CE	1:B:1366[A]:LYS:HE3	2.34	0.54
1:A:495[A]:ILE:HD12	1:A:574:ARG:HD3	1.89	0.54
1:A:261:LEU:HD11	1:A:579:ILE:HG22	1.91	0.53
1:A:435:ASN:O	1:B:1539:GLN:NE2	2.41	0.53
1:B:1522:ARG:HE	1:B:1526[A]:ARG:NH2	2.06	0.53
1:B:1522:ARG:HE	1:B:1526[A]:ARG:CZ	2.23	0.52
1:B:1141:ALA:HB1	1:B:1159:ILE:HD11	1.92	0.52
3:A:755:HOH:O	1:B:1546:LYS:HE2	2.13	0.49
1:B:1330:ILE:HG22	1:B:1536:LEU:HD11	1.95	0.49
1:B:1150[B]:GLU:HG3	3:B:544:HOH:O	2.12	0.49
1:A:319:GLU:HA	1:A:323:LEU:HB2	1.94	0.48
1:A:313:LYS:O	1:A:317:PHE:HB3	2.15	0.47
1:A:456:ASP:O	1:A:506:HIS:HE1	1.97	0.47
1:B:1449:ARG:NH2	1:B:1507:ALA:O	2.48	0.47
1:A:107:ILE:HD12	1:A:302:PHE:CD2	2.51	0.46
1:B:1529:ALA:HB3	1:B:1530:PRO:HD3	1.96	0.46
1:A:112:ARG:NH2	1:A:262:TYR:O	2.48	0.46
1:B:1362[B]:LYS:HE2	1:B:1366[B]:LYS:NZ	2.30	0.45
1:A:309[B]:GLU:HG2	1:A:313:LYS:HE3	1.98	0.45
1:B:1162:ARG:HD3	1:B:1163:LYS:O	2.17	0.45
1:B:1163:LYS:HA	1:B:1168:PHE:CD2	2.54	0.42
1:B:1319:GLU:HA	1:B:1323:LEU:HB2	2.01	0.42
1:B:1185:ASP:OD2	1:B:1188:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123[A]:LYS:HD3	1:A:123[A]:LYS:HA	1.90	0.41
1:B:1327:VAL:O	1:B:1331:VAL:HB	2.20	0.41
1:A:115:PHE:N	1:A:116:PRO:CD	2.83	0.41
1:B:1362[A]:LYS:CD	1:B:1366[A]:LYS:HE3	2.50	0.40
1:A:442:TRP:CH2	1:A:510:VAL:HB	2.55	0.40
1:A:362:LYS:HE2	1:A:366:LYS:HE2	2.03	0.40
1:B:1133:TRP:CD1	1:B:1133:TRP:O	2.74	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	524/525 (100%)	517 (99%)	7 (1%)	0	100	100
1	B	516/525 (98%)	509 (99%)	7 (1%)	0	100	100
All	All	1040/1050 (99%)	1026 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	439/432 (102%)	434 (99%)	5 (1%)	73	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	432/432 (100%)	417 (96%)	15 (4%)	36 9
All	All	871/864 (101%)	851 (98%)	20 (2%)	53 21

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	LEU
1	A	312	TYR
1	A	536	LEU
1	A	570[A]	CYS
1	A	570[B]	CYS
1	B	1095	LYS
1	B	1178	GLU
1	B	1243	ASN
1	B	1292	LEU
1	B	1308	LEU
1	B	1312	TYR
1	B	1317	PHE
1	B	1331	VAL
1	B	1362[A]	LYS
1	B	1362[B]	LYS
1	B	1451	THR
1	B	1460	LEU
1	B	1553[A]	ASP
1	B	1553[B]	ASP
1	B	1570	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	269	ASN
1	A	341	GLN
1	A	506	HIS
1	B	1243	ASN
1	B	1269	ASN
1	B	1538	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	495/525 (94%)	0.74	55 (11%) 5 5	15, 20, 29, 47	1 (0%)
1	B	490/525 (93%)	0.61	37 (7%) 13 16	15, 20, 30, 41	1 (0%)
All	All	985/1050 (93%)	0.68	92 (9%) 8 9	15, 20, 29, 47	2 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1454	GLU	6.5
1	A	457	LEU	6.4
1	B	1455	ASN	6.1
1	A	450	SER	5.9
1	A	451	THR	5.7
1	A	455	ASN	5.5
1	A	454	GLU	5.3
1	A	447	LYS	5.3
1	A	106	TYR	4.9
1	A	453	PRO	4.9
1	A	456	ASP	4.8
1	B	1548	ALA	4.5
1	A	504	PHE	4.4
1	B	1450	SER	4.3
1	A	446	GLU	3.9
1	B	1504	PHE	3.8
1	A	163[A]	LYS	3.8
1	A	164	GLY	3.7
1	A	443	LYS	3.6
1	B	1135[A]	SER	3.5
1	A	91[A]	SER	3.4
1	A	135	SER	3.4
1	B	1254[A]	MET	3.3
1	B	1423[A]	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	3.3
1	A	458	GLY	3.2
1	A	436	ILE	3.2
1	B	1134	GLY	3.2
1	B	1447	LYS	3.1
1	A	97	LYS	3.0
1	B	1255	GLY	3.0
1	A	89[A]	ASP	3.0
1	A	87	ASP	2.9
1	B	1517	CYS	2.8
1	A	435	ASN	2.8
1	A	102	GLY	2.8
1	A	166[A]	LYS	2.8
1	B	1451	THR	2.8
1	A	512	PHE	2.8
1	A	86	LEU	2.8
1	A	98[A]	VAL	2.8
1	B	1549	PRO	2.7
1	A	438	GLN	2.7
1	B	1479	LEU	2.7
1	A	580	SER	2.6
1	B	1331	VAL	2.6
1	B	1270	GLY	2.6
1	B	1553[A]	ASP	2.6
1	A	333	ALA	2.6
1	A	460[A]	LEU	2.5
1	A	179	GLU	2.5
1	A	258	VAL	2.5
1	B	1185	ASP	2.5
1	B	1398	ILE	2.5
1	B	1087	ASP	2.4
1	A	514	VAL	2.4
1	B	1238	LEU	2.4
1	B	1399	LEU	2.4
1	B	1188	GLU	2.4
1	A	322	ILE	2.4
1	B	1172	ARG	2.4
1	A	471	LEU	2.4
1	A	266	LYS	2.3
1	B	1402	CYS	2.3
1	B	1261	LEU	2.3
1	A	526[A]	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	273	ILE	2.3
1	A	402	CYS	2.3
1	B	1269	ASN	2.3
1	A	395	CYS	2.2
1	A	316	ILE	2.2
1	A	578	ASP	2.2
1	A	152	LYS	2.2
1	B	1453	PRO	2.2
1	A	323	LEU	2.2
1	A	492[A]	GLU	2.2
1	B	1474	ALA	2.2
1	B	1512	PHE	2.2
1	A	498	VAL	2.1
1	A	103	HIS	2.1
1	B	1242[A]	LYS	2.1
1	A	268	ILE	2.1
1	A	398	ILE	2.1
1	A	529	ALA	2.1
1	B	1514	VAL	2.1
1	A	104	GLU	2.1
1	B	1471	LEU	2.1
1	B	1257	SER	2.0
1	A	547	ASP	2.0
1	B	1239	ASP	2.0
1	B	1528	TRP	2.0
1	A	444	VAL	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	MG	A	1580	1/1	0.92	0.12	37,37,37,37	0
2	MG	B	1598	1/1	0.97	0.19	24,24,24,24	0
2	MG	A	1576	1/1	0.98	0.22	22,22,22,22	0
2	MG	B	1597	1/1	0.99	0.02	17,17,17,17	0
2	MG	A	1577	1/1	0.99	0.15	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.