Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 05:37 PM EDT

PDB ID	:	2FP0
Title	:	human ADP-ribosylhydrolase 3
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Deposited on	:	2006-01-15
Resolution	:	2.05 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 (1)) were used in the production of this report:

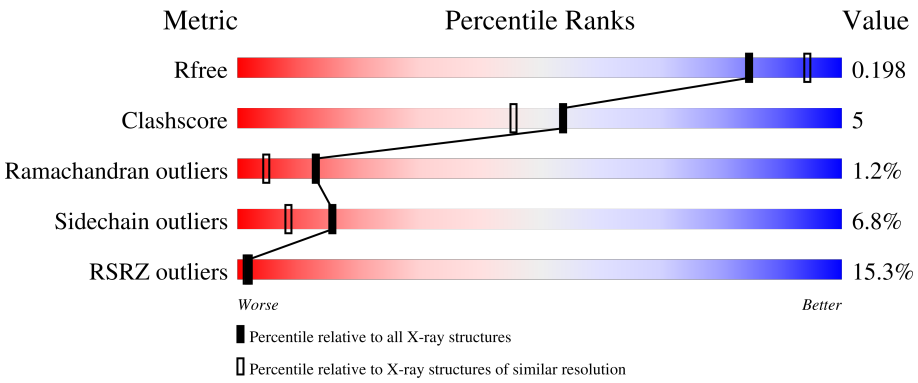
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	347	14% 78% 16% • • •
1	B	347	16% 84% 10% • • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5337 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 ADP-ribosylhydrolase like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2593	1622	443	513	15	0	0	0
1	B	339	2593	1622	443	513	15	0	0	0

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

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

- Molecule 3 is water.

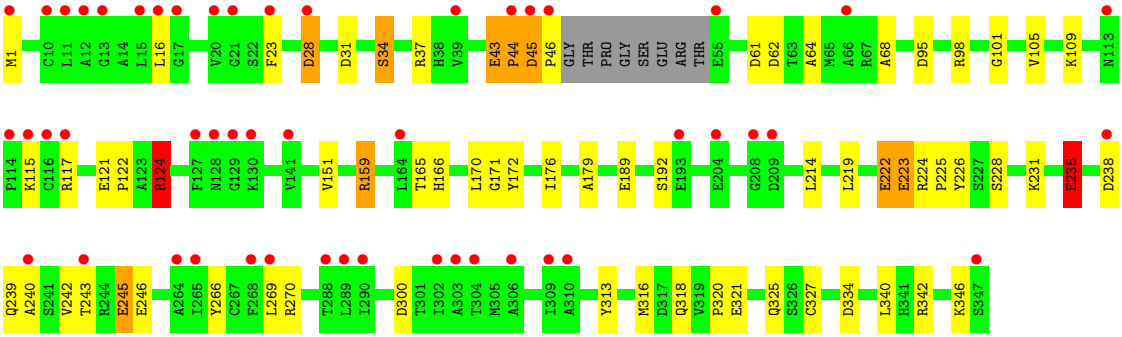
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	96	96	96	0	0
3	B	51	51	51	0	0

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.

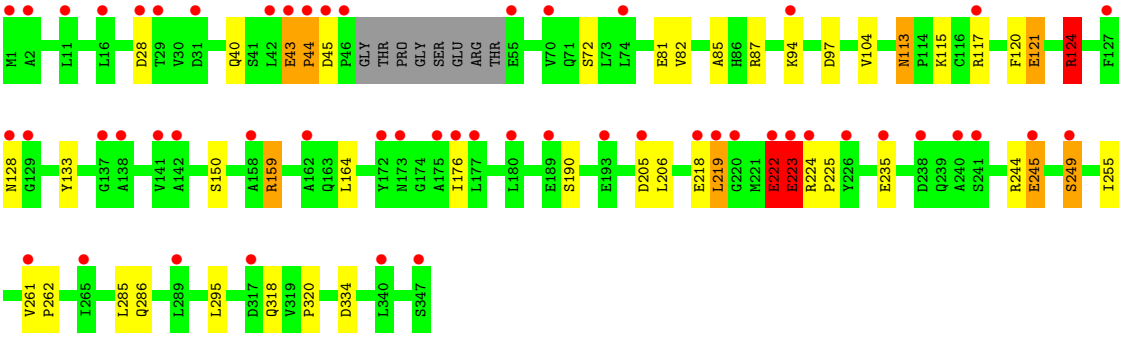
- Molecule 1: ADP-ribosylhydrolase like 2

Chain A:



- Molecule 1: ADP-ribosylhydrolase like 2

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	57.33Å 60.63Å 102.88Å 90.00° 96.43° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 24.42 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.05) 98.8 (24.42-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.231 0.195 , 0.198	Depositor DCC
R_{free} test set	896 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5337	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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 (i)

5.1 Standard geometry (i)

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	1.20	9/2639 (0.3%)	1.11	16/3564 (0.4%)
1	B	0.99	1/2639 (0.0%)	0.89	6/3564 (0.2%)
All	All	1.10	10/5278 (0.2%)	1.00	22/7128 (0.3%)

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	0	2
1	B	0	2
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	TYR	CD1-CE1	8.12	1.51	1.39
1	B	121	GLU	CG-CD	6.92	1.62	1.51
1	A	64	ALA	CA-CB	-6.36	1.39	1.52
1	A	68	ALA	CA-CB	-6.21	1.39	1.52
1	A	240	ALA	CA-CB	5.54	1.64	1.52
1	A	171	GLY	N-CA	-5.38	1.38	1.46
1	A	235	GLU	CB-CG	5.34	1.62	1.52
1	A	172	TYR	CD1-CE1	-5.31	1.31	1.39
1	A	266	TYR	CE2-CZ	-5.07	1.31	1.38
1	A	179	ALA	CA-CB	5.06	1.63	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	ARG	NE-CZ-NH2	-13.50	113.55	120.30
1	A	61	ASP	CB-CG-OD2	-11.07	108.34	118.30
1	A	61	ASP	CB-CG-OD1	9.36	126.72	118.30
1	A	316	MET	CG-SD-CE	8.72	114.16	100.20
1	A	270	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	342	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	98	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	124	ARG	CG-CD-NE	6.44	125.32	111.80
1	A	300	ASP	CB-CG-OD1	6.32	123.98	118.30
1	B	44	PRO	N-CA-C	6.28	128.43	112.10
1	A	340	LEU	CB-CG-CD2	6.24	121.61	111.00
1	B	97	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	214	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	159	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	124	ARG	CG-CD-NE	5.63	123.62	111.80
1	A	95	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	270	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	159	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	43	GLU	C-N-CD	-5.44	108.63	120.60
1	B	43	GLU	C-N-CA	5.25	144.03	122.00
1	A	95	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	37	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	GLU	Peptide
1	A	43	GLU	Peptide
1	B	222	GLU	Peptide
1	B	43	GLU	Peptide

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	2593	0	2521	35	0
1	B	2593	0	2521	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	96	0	0	1	0
3	B	51	0	0	1	0
All	All	5337	0	5042	54	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 (54) 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:45:ASP:HB3	1:A:46:PRO:HA	1.41	1.02
1:A:45:ASP:HB3	1:A:46:PRO:CA	2.03	0.88
1:A:45:ASP:CB	1:A:46:PRO:HA	2.10	0.80
1:A:44:PRO:HB2	1:A:45:ASP:HA	1.64	0.80
1:A:235:GLU:OE2	1:A:235:GLU:O	2.02	0.77
1:A:16:LEU:HD23	1:A:327:CYS:SG	2.33	0.68
1:A:165:THR:OG1	1:A:166:HIS:HD2	1.76	0.68
1:A:124:ARG:HH11	1:A:124:ARG:HG3	1.60	0.67
1:A:245:GLU:H	1:A:245:GLU:CD	2.03	0.61
1:A:23:PHE:HB2	3:A:456:HOH:O	2.00	0.61
1:B:113:ASN:HD22	1:B:115:LYS:N	2.00	0.59
1:B:113:ASN:HD22	1:B:115:LYS:H	1.48	0.59
1:B:113:ASN:ND2	1:B:115:LYS:H	2.01	0.58
1:B:124:ARG:HH11	1:B:124:ARG:HG3	1.70	0.56
1:A:45:ASP:CB	1:A:46:PRO:CA	2.77	0.56
1:A:44:PRO:HB2	1:A:45:ASP:OD1	2.06	0.54
1:B:285:LEU:H	1:B:318:GLN:NE2	2.06	0.54
1:A:243:THR:OG1	1:A:246:GLU:HG3	2.07	0.54
1:A:43:GLU:N	1:A:44:PRO:HD3	2.24	0.53
1:A:44:PRO:HB2	1:A:45:ASP:CA	2.39	0.52
1:B:72:SER:HB2	1:B:87:ARG:HD2	1.92	0.52
1:B:133:TYR:CE2	1:B:219:LEU:HD11	2.46	0.51
1:A:159:ARG:HB2	1:A:176:ILE:HD11	1.93	0.50
1:B:244:ARG:HG2	1:B:295:LEU:HD23	1.93	0.50
1:A:165:THR:OG1	1:A:166:HIS:CD2	2.62	0.49
1:A:170:LEU:O	1:A:226:TYR:OH	2.21	0.48
1:A:44:PRO:CB	1:A:45:ASP:HA	2.39	0.48
1:B:206:LEU:HD22	3:B:552:HOH:O	2.14	0.48
1:B:286:GLN:NE2	1:B:320:PRO:HG3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:CG1	1:A:109:LYS:HE3	2.46	0.46
1:B:159:ARG:HB2	1:B:176:ILE:HD11	1.98	0.46
1:A:318:GLN:O	1:A:320:PRO:HD3	2.18	0.44
1:A:224:ARG:N	1:A:225:PRO:CD	2.81	0.44
1:A:223:GLU:HA	1:A:225:PRO:HD3	2.00	0.44
1:B:223:GLU:HA	1:B:225:PRO:HD3	2.00	0.44
1:A:31:ASP:HB3	1:A:34:SER:HB3	2.00	0.43
1:A:124:ARG:O	1:A:124:ARG:NH1	2.52	0.43
1:A:46:PRO:HB2	1:B:120:PHE:HB2	2.01	0.43
1:A:321:GLU:O	1:A:325:GLN:HG3	2.19	0.43
1:A:245:GLU:CD	1:A:245:GLU:N	2.69	0.43
1:A:165:THR:HG1	1:A:166:HIS:HD2	1.65	0.43
1:A:192:SER:CB	1:A:269:LEU:HD22	2.50	0.42
1:A:101:GLY:O	1:A:105:VAL:HG23	2.19	0.42
1:B:81:GLU:HG2	1:B:82:VAL:N	2.34	0.42
1:B:222:GLU:O	1:B:223:GLU:O	2.37	0.42
1:B:245:GLU:O	1:B:249:SER:HB2	2.20	0.42
1:A:228:SER:HA	1:A:231:LYS:HE3	2.03	0.41
1:A:16:LEU:CD2	1:A:327:CYS:SG	3.08	0.41
1:B:85:ALA:HB2	1:B:164:LEU:HD22	2.02	0.41
1:A:124:ARG:HH11	1:A:124:ARG:CG	2.31	0.41
1:B:255:ILE:HD12	1:B:255:ILE:N	2.35	0.41
1:B:224:ARG:N	1:B:225:PRO:CD	2.84	0.41
1:B:261:VAL:HB	1:B:262:PRO:HD3	2.02	0.41
1:A:121:GLU:HB3	1:A:122:PRO:HD3	2.02	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	335/347 (96%)	323 (96%)	8 (2%)	4 (1%)	13 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	335/347 (96%)	320 (96%)	11 (3%)	4 (1%)	13 5
All	All	670/694 (96%)	643 (96%)	19 (3%)	8 (1%)	13 5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	45	ASP
1	A	223	GLU
1	B	28	ASP
1	B	44	PRO
1	B	223	GLU
1	B	45	ASP
1	A	44	PRO

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	273/279 (98%)	255 (93%)	18 (7%)	16 9
1	B	273/279 (98%)	254 (93%)	19 (7%)	15 7
All	All	546/558 (98%)	509 (93%)	37 (7%)	16 8

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	28	ASP
1	A	34	SER
1	A	62	ASP
1	A	115	LYS
1	A	117	ARG
1	A	124	ARG
1	A	151	VAL

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Mol	Chain	Res	Type
1	A	189	GLU
1	A	219	LEU
1	A	222	GLU
1	A	235	GLU
1	A	238	ASP
1	A	239	GLN
1	A	242	VAL
1	A	245	GLU
1	A	334	ASP
1	A	346	LYS
1	B	40	GLN
1	B	94	LYS
1	B	104	VAL
1	B	113	ASN
1	B	117	ARG
1	B	121	GLU
1	B	124	ARG
1	B	128	ASN
1	B	150	SER
1	B	190	SER
1	B	205	ASP
1	B	218	GLU
1	B	219	LEU
1	B	222	GLU
1	B	223	GLU
1	B	235	GLU
1	B	245	GLU
1	B	249	SER
1	B	334	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	90	GLN
1	A	126	GLN
1	A	152	GLN
1	A	166	HIS
1	A	198	GLN
1	B	27	HIS
1	B	38	HIS
1	B	40	GLN

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Mol	Chain	Res	Type
1	B	113	ASN
1	B	128	ASN
1	B	211	GLN
1	B	318	GLN
1	B	324	GLN
1	B	325	GLN

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, 4 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 (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	339/347 (97%)	0.82	50 (14%)	2	2	39, 47, 60, 69	0
1	B	339/347 (97%)	1.02	54 (15%)	1	1	41, 47, 59, 71	0
All	All	678/694 (97%)	0.92	104 (15%)	2	1	39, 47, 60, 71	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	PRO	11.6
1	B	46	PRO	11.6
1	B	45	ASP	11.0
1	B	219	LEU	7.4
1	A	115	LYS	7.4
1	B	222	GLU	6.4
1	A	114	PRO	5.9
1	B	128	ASN	5.5
1	B	347	SER	5.0
1	A	347	SER	4.6
1	B	28	ASP	4.4
1	A	44	PRO	4.4
1	A	116	CYS	4.3
1	A	208	GLY	4.3
1	A	128	ASN	4.2
1	B	249	SER	4.1
1	B	245	GLU	3.9
1	B	31	ASP	3.9
1	A	289	LEU	3.9
1	B	238	ASP	3.8
1	A	55	GLU	3.8
1	B	16	LEU	3.8
1	B	172	TYR	3.7
1	A	46	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	177	LEU	3.7
1	B	117	ARG	3.7
1	B	226	TYR	3.7
1	A	193	GLU	3.7
1	B	240	ALA	3.6
1	A	117	ARG	3.6
1	B	241	SER	3.6
1	B	235	GLU	3.6
1	B	193	GLU	3.5
1	B	289	LEU	3.5
1	A	45	ASP	3.4
1	B	127	PHE	3.4
1	A	1	MET	3.3
1	B	141	VAL	3.3
1	B	29	THR	3.2
1	A	11	LEU	3.2
1	B	11	LEU	3.2
1	A	130	LYS	3.2
1	B	1	MET	3.1
1	A	127	PHE	3.1
1	A	20	VAL	3.1
1	B	189	GLU	3.0
1	B	317	ASP	3.0
1	B	205	ASP	3.0
1	B	142	ALA	2.9
1	A	265	ILE	2.9
1	A	164	LEU	2.9
1	B	129	GLY	2.9
1	B	55	GLU	2.9
1	A	303	ALA	2.9
1	B	223	GLU	2.8
1	A	209	ASP	2.8
1	A	309	ILE	2.8
1	B	176	ILE	2.7
1	B	224	ARG	2.7
1	B	175	ALA	2.6
1	B	180	LEU	2.6
1	B	43	GLU	2.6
1	B	261	VAL	2.6
1	A	17	GLY	2.6
1	A	269	LEU	2.6
1	A	39	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	264	ALA	2.5
1	B	220	GLY	2.5
1	A	240	ALA	2.5
1	A	113	ASN	2.4
1	A	238	ASP	2.4
1	A	306	ALA	2.4
1	B	138	ALA	2.4
1	A	304	THR	2.4
1	A	28	ASP	2.4
1	A	288	THR	2.4
1	A	243	THR	2.3
1	B	173	ASN	2.3
1	B	340	LEU	2.3
1	A	10	CYS	2.3
1	A	129	GLY	2.3
1	B	137	GLY	2.3
1	A	21	GLY	2.3
1	B	2	ALA	2.3
1	A	268	PHE	2.2
1	A	15	LEU	2.2
1	A	141	VAL	2.2
1	A	302	ILE	2.2
1	A	16	LEU	2.2
1	B	265	ILE	2.2
1	B	218	GLU	2.2
1	B	70	VAL	2.2
1	A	204	GLU	2.2
1	A	66	ALA	2.2
1	A	12	ALA	2.1
1	B	158	ALA	2.1
1	A	23	PHE	2.1
1	A	13	GLY	2.1
1	B	162	ALA	2.1
1	A	310	ALA	2.0
1	A	290	ILE	2.0
1	B	94	LYS	2.0
1	B	42	LEU	2.0
1	B	74	LEU	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	MG	A	402	1/1	0.95	0.06	29,29,29,29	0
2	MG	B	502	1/1	0.97	0.07	37,37,37,37	0
2	MG	A	401	1/1	0.98	0.05	19,19,19,19	0
2	MG	B	501	1/1	0.99	0.05	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.