Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:42 am BST

PDB ID	:	5GN3
Title	:	Structure of selenomethionine-labelled Uracil DNA glycosylase (BdiUNG) from Bradyrhizobium diazoefficiens
Authors	:	Patil, V.V.; Chembazhi, U.V.; Varshney, U.; Woo, E.
Deposited on	:	2016-07-19
Resolution	:	2.28 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 following versions of software and data (see references ⓘ) were used in the production of this report:

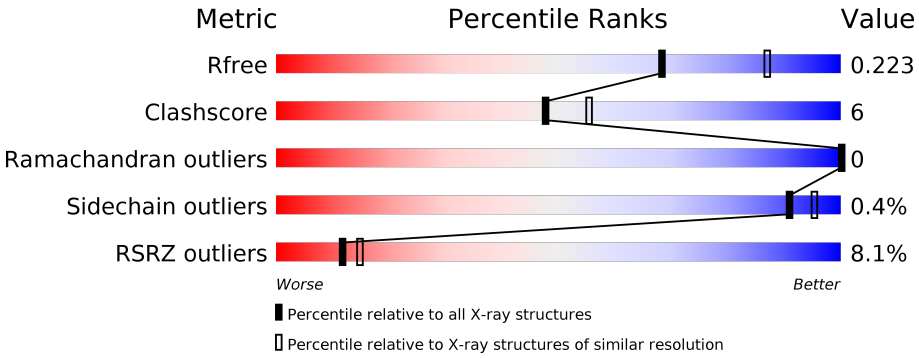
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 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	272	5% 89% 10%
1	B	272	4% 87% 13%
1	C	272	18% 88% 12%
1	D	272	6% 90% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9017 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 Blr0248 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	Se	0	0	0
			2099	1344	368	381	1	5			
1	B	272	Total	C	N	O	S	Se	0	0	0
			2099	1344	368	381	1	5			
1	C	272	Total	C	N	O	S	Se	0	0	0
			2099	1344	368	381	1	5			
1	D	272	Total	C	N	O	S	Se	0	0	0
			2099	1344	368	381	1	5			

- Molecule 2 is water.

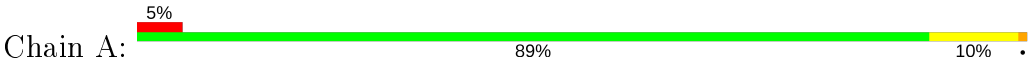
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	203	Total	O	0	0
			203	203		
2	B	190	Total	O	0	0
			190	190		
2	C	67	Total	O	0	0
			67	67		
2	D	161	Total	O	0	0
			161	161		

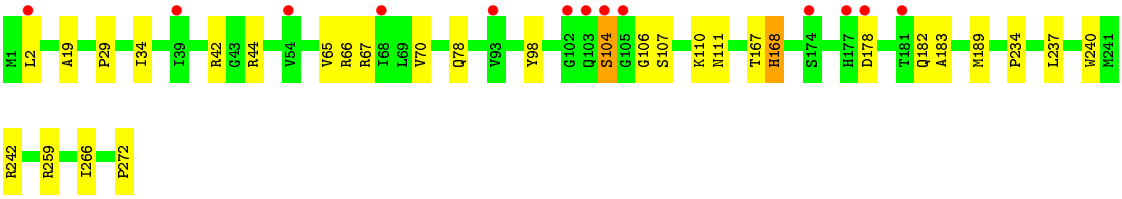
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Blr0248 protein

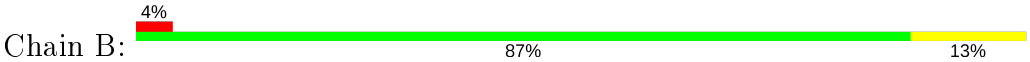
Chain A:

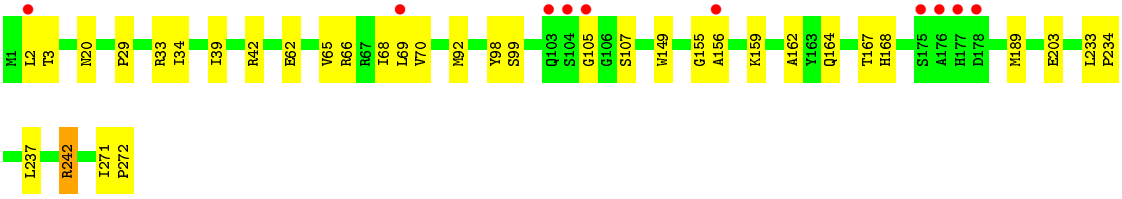




- Molecule 1: Blr0248 protein

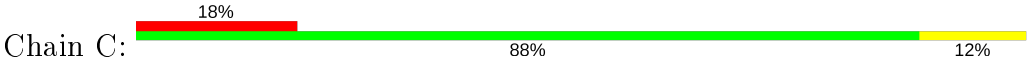
Chain B:

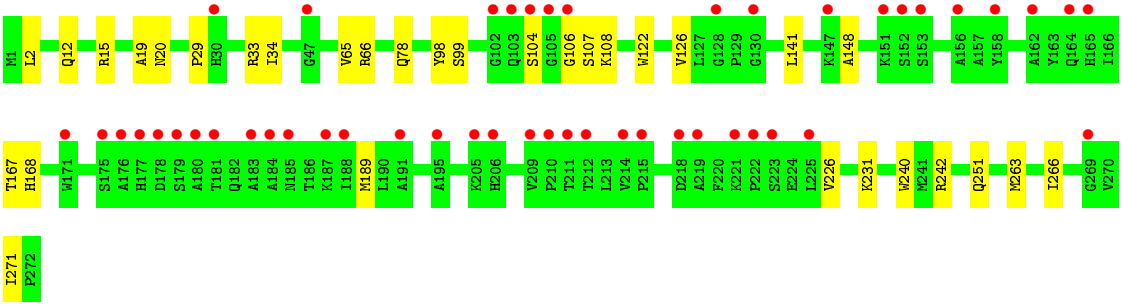




- Molecule 1: Blr0248 protein

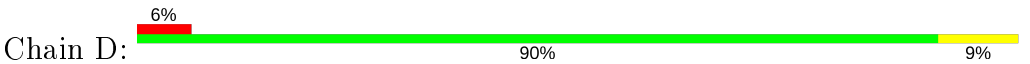
Chain C:

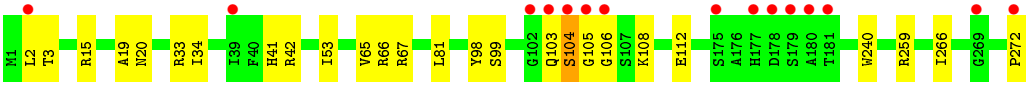




- Molecule 1: Blr0248 protein

Chain D:




M1
L2
T3
R15
A19
N20
R33
I34
I39
F40
H41
R42
I53
V65
R66
R67
L81
Y98
S99
G102
Q103
S104
G105
G106
S107
K108
E112
S175
A176
H177
D178
S179
A180
T181
W240
R259
I266
G269
P272

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.96Å 90.07Å 256.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.99 – 2.28 30.99 – 2.28	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.99-2.28) 90.0 (30.99-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.00 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.180 , 0.212 0.203 , 0.223	Depositor DCC
R_{free} test set	1980 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	1.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9017	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 3.92% 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

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	0.53	0/2155	0.64	2/2932 (0.1%)
1	B	0.48	0/2155	0.64	2/2932 (0.1%)
1	C	0.48	0/2155	0.58	0/2932
1	D	0.54	0/2155	0.61	1/2932 (0.0%)
All	All	0.51	0/8620	0.61	5/11728 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	242	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	B	242	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	44	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	D	104	SER	N-CA-C	7.10	130.16	111.00
1	A	168	HIS	C-N-CD	5.23	139.38	128.40

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	2099	0	2072	29	0
1	B	2099	0	2072	33	0
1	C	2099	0	2072	30	0
1	D	2099	0	2072	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	203	0	0	5	0
2	B	190	0	0	5	0
2	C	67	0	0	4	0
2	D	161	0	0	3	0
All	All	9017	0	8288	101	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 6.

All (101) 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:106:GLY:CA	1:A:107:SER:OG	1.97	1.11
1:C:19:ALA:O	1:D:2:LEU:HD12	1.51	1.09
1:B:168:HIS:O	1:B:189:MSE:HE1	1.59	1.02
1:A:106:GLY:HA3	1:A:107:SER:OG	1.60	0.98
1:A:106:GLY:HA2	1:A:107:SER:OG	1.64	0.94
1:A:242:ARG:NH1	2:A:301:HOH:O	2.00	0.94
1:A:78:GLN:NE2	2:A:302:HOH:O	2.02	0.90
1:B:68:ILE:HD11	1:B:92:MSE:HB2	1.57	0.87
1:B:62:GLU:HG3	1:B:70:VAL:HG22	1.58	0.85
1:C:242:ARG:NH1	2:C:301:HOH:O	2.10	0.85
1:B:164:GLN:OE1	2:B:301:HOH:O	1.98	0.79
1:D:15:ARG:NH2	2:D:302:HOH:O	2.13	0.79
1:C:19:ALA:O	1:D:2:LEU:CD1	2.31	0.76
1:A:168:HIS:O	1:A:189:MSE:HE1	1.85	0.76
1:C:33:ARG:NE	2:C:304:HOH:O	2.20	0.74
1:D:112:GLU:OE1	2:D:301:HOH:O	2.05	0.73
1:C:108:LYS:O	1:C:108:LYS:HG2	1.88	0.73
1:C:20:ASN:ND2	1:D:2:LEU:HD13	2.02	0.73
1:C:20:ASN:CG	1:D:2:LEU:HD13	2.09	0.72
1:A:183:ALA:O	2:A:303:HOH:O	2.07	0.71
1:B:168:HIS:O	1:B:189:MSE:CE	2.37	0.70
1:C:12:GLN:HE21	1:C:15:ARG:HH21	1.38	0.70
1:B:68:ILE:HD11	1:B:92:MSE:CB	2.22	0.70
1:C:2:LEU:HD12	1:D:19:ALA:O	1.90	0.70
1:D:104:SER:C	1:D:106:GLY:HA3	2.13	0.69
1:D:104:SER:O	1:D:106:GLY:HA3	1.92	0.69
1:B:3:THR:HG23	2:B:341:HOH:O	1.94	0.68
1:C:19:ALA:HB1	1:D:2:LEU:HD11	1.74	0.68
1:A:106:GLY:CA	1:A:107:SER:CB	2.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:HG22	1:A:189:MSE:CE	2.27	0.64
1:D:15:ARG:NH1	2:D:306:HOH:O	2.30	0.64
1:C:148:ALA:O	2:C:302:HOH:O	2.16	0.62
1:B:62:GLU:CG	1:B:70:VAL:HG22	2.28	0.62
1:C:20:ASN:OD1	1:D:2:LEU:HD13	1.99	0.61
1:D:42:ARG:HG3	1:D:67:ARG:HB3	1.82	0.61
1:A:19:ALA:HB1	1:B:2:LEU:HD11	1.82	0.61
1:C:34:ILE:HA	1:C:98:TYR:CD1	2.37	0.60
1:C:19:ALA:CB	1:D:2:LEU:HD11	2.32	0.59
1:A:167:THR:CG2	1:A:189:MSE:CE	2.83	0.56
1:D:103:GLN:O	1:D:104:SER:OG	2.22	0.55
1:B:242:ARG:NE	2:B:302:HOH:O	2.18	0.54
1:B:39:ILE:HD12	2:B:305:HOH:O	2.07	0.54
1:B:42:ARG:HH21	1:B:69:LEU:HB3	1.72	0.54
1:A:19:ALA:O	1:B:2:LEU:HD12	2.07	0.54
1:B:34:ILE:HA	1:B:98:TYR:CD1	2.43	0.53
1:C:251:GLN:OE1	1:C:263:MSE:HE3	2.09	0.53
1:A:34:ILE:HA	1:A:98:TYR:CD1	2.44	0.52
1:B:234:PRO:HD2	1:B:237:LEU:HD22	1.92	0.52
1:A:111:ASN:HB2	2:A:401:HOH:O	2.09	0.52
1:D:106:GLY:C	1:D:108:LYS:H	2.13	0.51
1:A:240:TRP:CZ2	1:A:266:ILE:HG12	2.45	0.51
1:B:33:ARG:HD2	1:B:99:SER:HB3	1.93	0.51
1:C:168:HIS:O	1:C:189:MSE:HE1	2.10	0.51
1:D:34:ILE:HA	1:D:98:TYR:CD1	2.45	0.51
1:A:234:PRO:HD2	1:A:237:LEU:HD22	1.94	0.50
1:C:2:LEU:HD13	1:D:20:ASN:OD1	2.11	0.50
1:C:104:SER:C	1:C:106:GLY:H	2.14	0.50
1:A:19:ALA:HB1	1:B:2:LEU:CD1	2.42	0.49
1:B:242:ARG:NH2	2:B:302:HOH:O	2.30	0.48
1:C:29:PRO:HB2	1:D:272:PRO:HG3	1.95	0.48
1:C:12:GLN:HE21	1:C:15:ARG:NH2	2.08	0.48
1:C:231:LYS:HE2	1:C:231:LYS:HB2	1.73	0.47
1:C:271:ILE:HD13	1:D:259:ARG:HG2	1.97	0.46
1:D:65:VAL:O	1:D:66:ARG:HB2	2.15	0.46
1:C:122:TRP:O	1:C:126:VAL:HG13	2.16	0.45
2:C:318:HOH:O	1:D:3:THR:HG23	2.16	0.45
1:C:65:VAL:O	1:C:66:ARG:HB2	2.16	0.45
1:A:42:ARG:HG3	1:A:67:ARG:HB3	1.97	0.45
1:D:105:GLY:N	1:D:106:GLY:HA3	2.32	0.44
1:A:29:PRO:HB2	1:B:272:PRO:HG3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:HG2	1:B:29:PRO:HB2	2.00	0.43
1:B:42:ARG:NE	1:B:69:LEU:O	2.51	0.43
1:A:167:THR:HB	1:A:189:MSE:HE2	2.00	0.43
1:D:33:ARG:HD2	1:D:99:SER:HB3	2.01	0.43
1:C:33:ARG:HD2	1:C:99:SER:HB3	2.01	0.43
1:C:167:THR:HB	1:C:189:MSE:HE2	2.01	0.43
1:D:108:LYS:O	1:D:108:LYS:HG2	2.19	0.43
1:A:65:VAL:O	1:A:66:ARG:HB2	2.19	0.43
1:B:68:ILE:HD11	1:B:92:MSE:C	2.38	0.42
1:C:107:SER:HB3	1:C:141:LEU:HD21	2.01	0.42
1:A:2:LEU:HD12	1:B:20:ASN:OD1	2.19	0.42
1:B:162:ALA:CB	1:B:203:GLU:HG2	2.49	0.42
1:A:178:ASP:O	1:A:182:GLN:HG3	2.20	0.42
1:A:104:SER:C	1:A:106:GLY:N	2.73	0.42
1:B:105:GLY:C	1:B:107:SER:H	2.22	0.42
1:A:167:THR:CG2	1:A:189:MSE:HE2	2.49	0.42
1:D:53:ILE:HD11	1:D:81:LEU:HD21	2.02	0.41
1:C:20:ASN:HD21	1:D:2:LEU:HD13	1.79	0.41
1:A:110:LYS:HE2	2:A:392:HOH:O	2.21	0.41
1:B:167:THR:HB	1:B:189:MSE:HE2	2.02	0.41
1:B:65:VAL:O	1:B:66:ARG:HB2	2.21	0.41
1:B:156:ALA:HA	1:B:159:LYS:HE3	2.02	0.41
1:B:62:GLU:HA	1:B:70:VAL:HG21	2.03	0.41
1:C:78:GLN:HB3	1:C:226:VAL:HB	2.02	0.41
1:A:167:THR:HG22	1:A:189:MSE:HE2	2.03	0.41
1:B:233:LEU:HD22	1:B:242:ARG:HD3	2.02	0.41
1:B:62:GLU:CD	1:B:70:VAL:HG22	2.42	0.41
1:D:240:TRP:CZ2	1:D:266:ILE:HG12	2.56	0.41
1:A:259:ARG:HG2	1:B:271:ILE:HD13	2.03	0.40
1:B:149:TRP:O	1:B:155:GLY:HA3	2.22	0.40
1:C:240:TRP:CZ2	1:C:266:ILE:HG12	2.57	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	270/272 (99%)	262 (97%)	8 (3%)	0	100	100
1	B	270/272 (99%)	261 (97%)	9 (3%)	0	100	100
1	C	270/272 (99%)	259 (96%)	11 (4%)	0	100	100
1	D	270/272 (99%)	260 (96%)	10 (4%)	0	100	100
All	All	1080/1088 (99%)	1042 (96%)	38 (4%)	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	213/208 (102%)	211 (99%)	2 (1%)	78	88
1	B	213/208 (102%)	213 (100%)	0	100	100
1	C	213/208 (102%)	213 (100%)	0	100	100
1	D	213/208 (102%)	212 (100%)	1 (0%)	88	94
All	All	852/832 (102%)	849 (100%)	3 (0%)	91	95

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

Mol	Chain	Res	Type
1	A	70	VAL
1	A	104	SER
1	D	41	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	GLN
1	B	251	GLN

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Mol	Chain	Res	Type
1	C	165	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	267/272 (98%)	0.14	13 (4%)	29	35	14, 25, 45, 82	0
1	B	267/272 (98%)	0.09	10 (3%)	41	47	16, 25, 43, 84	0
1	C	267/272 (98%)	0.93	48 (17%)	1	1	25, 48, 71, 83	0
1	D	267/272 (98%)	0.06	15 (5%)	24	29	19, 29, 46, 73	0
All	All	1068/1088 (98%)	0.31	86 (8%)	12	15	14, 29, 63, 84	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	GLN	8.6
1	C	103	GLN	7.0
1	B	103	GLN	6.6
1	C	176	ALA	6.3
1	B	177	HIS	5.6
1	C	102	GLY	5.5
1	C	177	HIS	5.1
1	C	152	SER	5.0
1	D	2	LEU	4.9
1	C	175	SER	4.8
1	B	104	SER	4.8
1	D	103	GLN	4.7
1	A	104	SER	4.7
1	D	105	GLY	4.6
1	C	222	PRO	4.6
1	C	105	GLY	4.6
1	C	209	VAL	4.4
1	A	177	HIS	4.2
1	D	102	GLY	4.1
1	B	178	ASP	4.0
1	B	105	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	106	GLY	4.0
1	C	211	THR	3.9
1	C	210	PRO	3.8
1	C	181	THR	3.8
1	C	178	ASP	3.8
1	C	104	SER	3.8
1	A	178	ASP	3.7
1	C	180	ALA	3.6
1	D	177	HIS	3.5
1	D	106	GLY	3.5
1	C	171	TRP	3.4
1	C	218	ASP	3.4
1	C	188	ILE	3.3
1	C	153	SER	3.3
1	C	221	LYS	3.2
1	D	175	SER	3.2
1	B	2	LEU	3.1
1	C	184	ALA	3.1
1	D	178	ASP	3.0
1	C	205	LYS	2.9
1	C	158	TYR	2.9
1	A	39	ILE	2.9
1	C	223	SER	2.9
1	D	272	PRO	2.9
1	B	69	LEU	2.8
1	C	183	ALA	2.8
1	C	162	ALA	2.8
1	C	219	ALA	2.8
1	D	179	SER	2.8
1	C	179	SER	2.7
1	C	156	ALA	2.6
1	A	2	LEU	2.6
1	A	105	GLY	2.6
1	C	191	ALA	2.6
1	A	54	VAL	2.6
1	D	269	GLY	2.6
1	D	104	SER	2.6
1	D	181	THR	2.6
1	C	206	HIS	2.5
1	C	147	LYS	2.5
1	C	151	LYS	2.4
1	C	225	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	156	ALA	2.3
1	B	176	ALA	2.3
1	C	212	THR	2.3
1	C	269	GLY	2.3
1	C	47	GLY	2.2
1	D	39	ILE	2.2
1	C	185	ASN	2.2
1	C	30	HIS	2.2
1	A	174	SER	2.2
1	C	130	GLY	2.2
1	C	164	GLN	2.2
1	C	187	LYS	2.1
1	A	93	VAL	2.1
1	A	68	ILE	2.1
1	C	214	VAL	2.1
1	C	128	GLY	2.1
1	A	102	GLY	2.1
1	D	180	ALA	2.1
1	C	165	HIS	2.0
1	C	195	ALA	2.0
1	B	175	SER	2.0
1	A	181	THR	2.0
1	C	215	PRO	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.