



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:21 PM UTC

PDB ID : 5GN2 / pdb_00005gn2
Title : Crystal structure of Uracil DNA glycosylase (BdiUNG) from Bradyrhizobium diazoefficiens
Authors : Patil, V.V.; Chembazhi, U.V.; Varshney, U.; Woo, E.
Deposited on : 2016-07-19
Resolution : 1.95 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

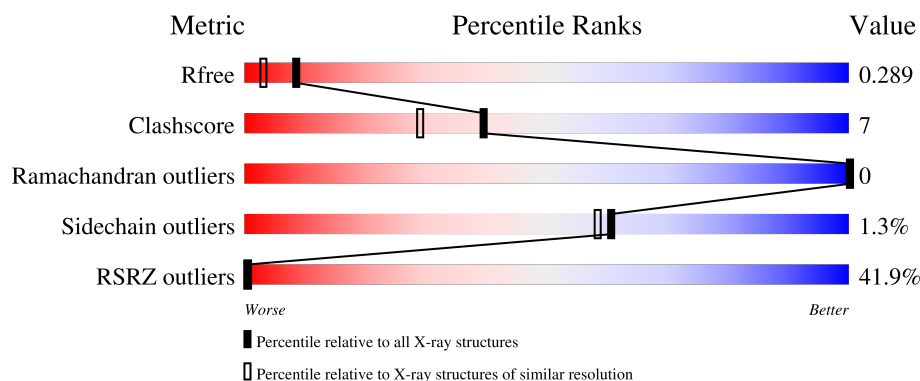
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	47% 86% 14%
1	B	272	31% 87% 12%
1	C	272	60% 78% 19%
1	D	272	29% 88% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8963 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	0	0	0
			2099	1344	368	381	6			
1	B	272	Total	C	N	O	S	0	0	0
			2099	1344	368	381	6			
1	C	272	Total	C	N	O	S	0	0	0
			2099	1344	368	381	6			
1	D	272	Total	C	N	O	S	0	0	0
			2099	1344	368	381	6			

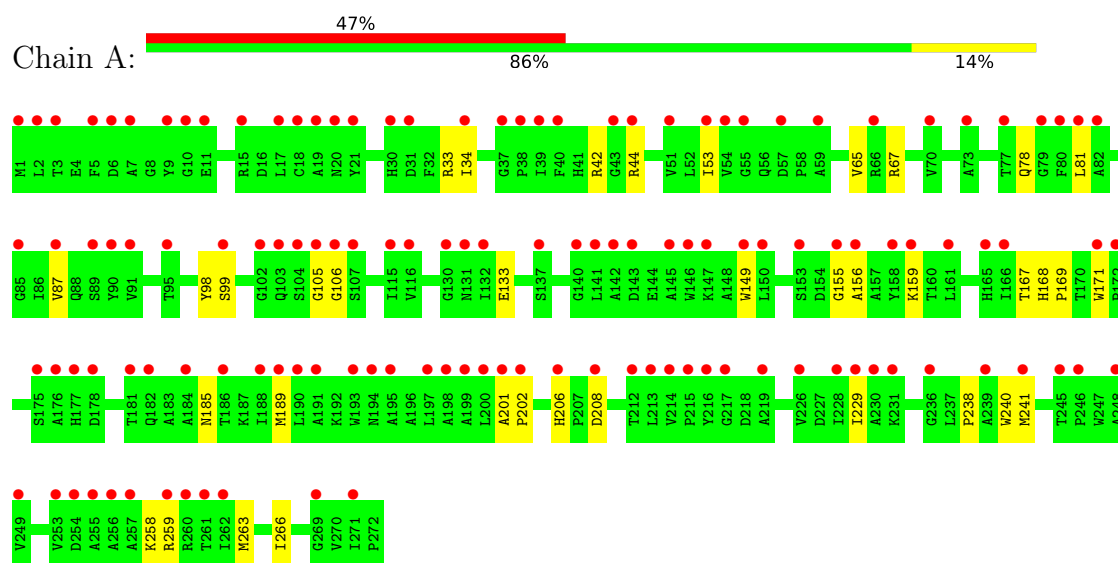
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	198	Total	O	0	0
			198	198		
2	B	176	Total	O	0	0
			176	176		
2	C	48	Total	O	0	0
			48	48		
2	D	145	Total	O	0	0
			145	145		

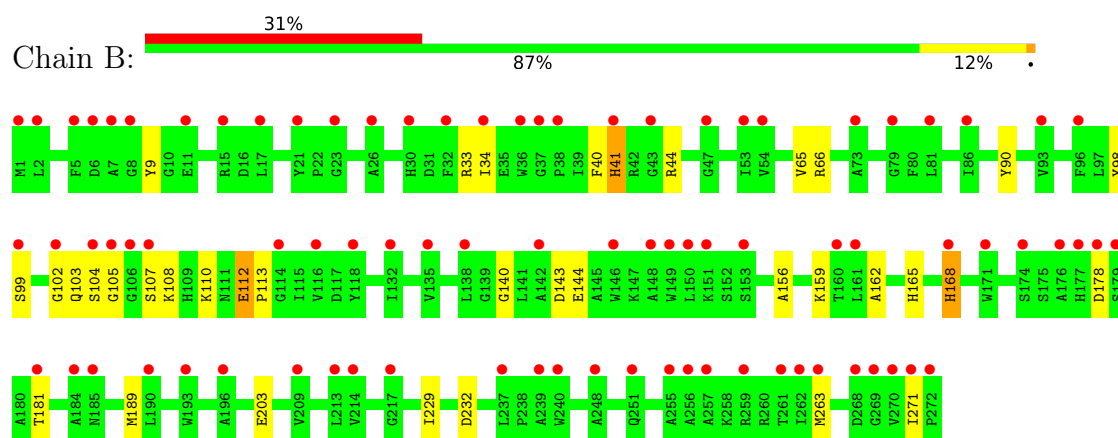
3 Residue-property plots [i](#)

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.

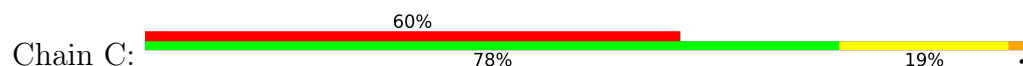
• Molecule 1: Blr0248 protein

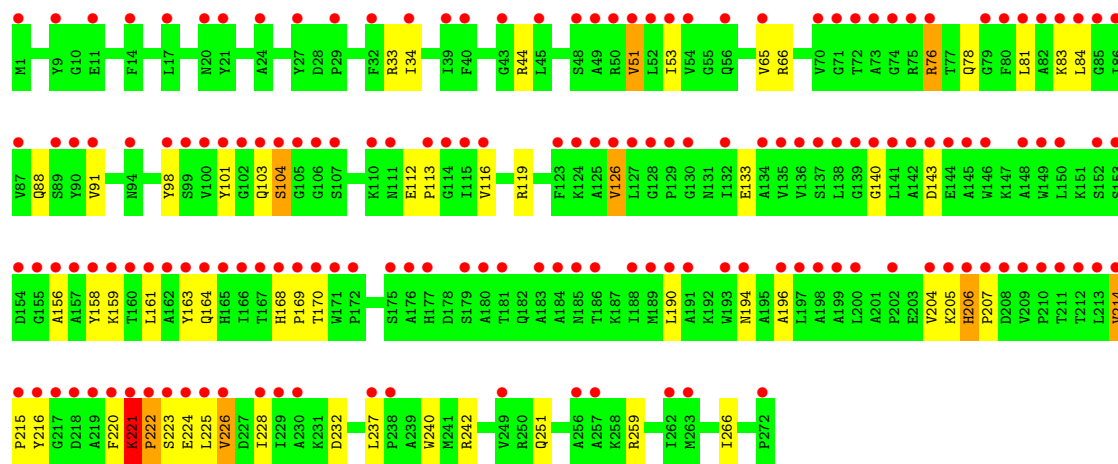


• Molecule 1: Blr0248 protein

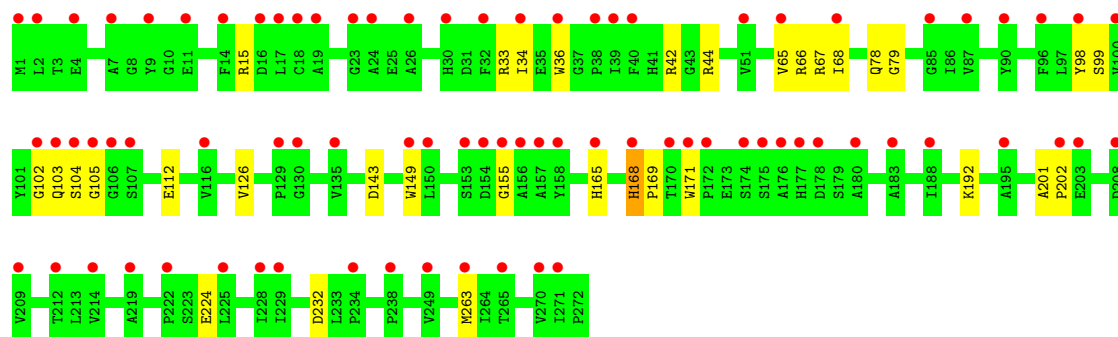
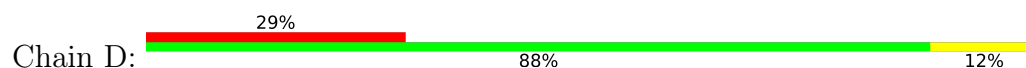


• Molecule 1: Blr0248 protein





• Molecule 1: Blr0248 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.65Å 90.03Å 255.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.52 – 1.95 30.52 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.52-1.95) 98.6 (30.52-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.245 , 0.290 0.251 , 0.289	Depositor DCC
R_{free} test set	2000 reflections (1.68%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8963	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	0.59	1/2159 (0.0%)	0.90	2/2944 (0.1%)
1	B	0.62	1/2159 (0.0%)	0.88	5/2944 (0.2%)
1	C	0.61	4/2159 (0.2%)	1.01	12/2944 (0.4%)
1	D	0.56	0/2159	0.88	4/2944 (0.1%)
All	All	0.60	6/8636 (0.1%)	0.92	23/11776 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	237	LEU	C-N	6.73	1.41	1.33
1	C	214	VAL	CA-CB	6.21	1.60	1.53
1	B	40	PHE	C-O	-5.39	1.17	1.23
1	C	222	PRO	N-CD	5.32	1.55	1.47
1	A	169	PRO	N-CD	5.19	1.55	1.47
1	C	207	PRO	N-CD	5.04	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	GLY	N-CA-C	-8.88	101.41	112.77
1	C	84	LEU	N-CA-C	-7.38	103.85	112.92
1	A	105	GLY	N-CA-C	7.18	121.87	112.25
1	C	104	SER	N-CA-C	-6.91	97.81	108.31
1	C	237	LEU	CA-C-N	-6.84	113.61	120.31
1	C	237	LEU	C-N-CA	-6.84	113.61	120.31
1	C	168	HIS	CA-C-N	6.45	126.95	119.47
1	C	168	HIS	C-N-CA	6.45	126.95	119.47
1	D	103	GLN	N-CA-C	-6.12	102.17	110.68
1	D	168	HIS	CA-C-N	6.00	126.43	119.47
1	D	168	HIS	C-N-CA	6.00	126.43	119.47
1	B	112	GLU	CA-C-N	5.95	125.66	119.05
1	B	112	GLU	C-N-CA	5.95	125.66	119.05
1	A	106	GLY	N-CA-C	-5.80	107.14	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ARG	CB-CG-CD	5.79	124.62	111.30
1	B	168	HIS	CA-C-N	5.78	126.18	119.47
1	B	168	HIS	C-N-CA	5.78	126.18	119.47
1	D	102	GLY	N-CA-C	-5.62	99.87	113.18
1	C	221	LYS	CA-C-N	-5.59	113.16	118.97
1	C	221	LYS	C-N-CA	-5.59	113.16	118.97
1	B	140	GLY	N-CA-C	5.30	119.55	112.77
1	C	206	HIS	CA-C-N	-5.21	113.32	119.84
1	C	206	HIS	C-N-CA	-5.21	113.32	119.84

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	2099	0	2072	21	0
1	B	2099	0	2072	22	0
1	C	2099	0	2069	51	0
1	D	2099	0	2072	21	0
2	A	198	0	0	1	0
2	B	176	0	0	1	0
2	C	48	0	0	2	0
2	D	145	0	0	3	0
All	All	8963	0	8285	112	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 7.

All (112) 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:C:216:TYR:CE1	1:C:224:GLU:OE2	1.67	1.44
1:C:216:TYR:HE1	1:C:224:GLU:CD	1.46	1.23
1:C:216:TYR:HE1	1:C:224:GLU:OE2	0.92	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:TYR:CE1	1:C:224:GLU:CD	2.28	0.97
1:C:220:PHE:HD2	1:C:224:GLU:HG2	1.30	0.95
1:C:216:TYR:CZ	1:C:224:GLU:OE2	2.25	0.89
1:D:42:ARG:NH2	1:D:78:GLN:OE1	2.08	0.87
1:C:220:PHE:CD2	1:C:224:GLU:HG2	2.16	0.79
1:D:44:ARG:NH2	1:D:232:ASP:OD1	2.15	0.79
1:D:104:SER:H	1:D:105:GLY:HA2	1.46	0.77
1:B:110:LYS:NZ	1:B:144:GLU:OE1	2.18	0.75
1:C:51:VAL:HG21	1:C:81:LEU:HD22	1.68	0.73
1:A:65:VAL:HG22	1:A:241:MET:HE2	1.72	0.70
1:D:104:SER:N	1:D:105:GLY:HA2	2.07	0.69
1:D:143:ASP:HB2	1:D:165:HIS:HD2	1.60	0.66
1:D:42:ARG:HG3	1:D:67:ARG:HB3	1.80	0.64
1:C:220:PHE:HD2	1:C:224:GLU:CG	2.09	0.63
1:C:44:ARG:NH2	1:C:232:ASP:OD1	2.33	0.62
1:B:143:ASP:HB2	1:B:165:HIS:HD2	1.64	0.61
1:C:53:ILE:HD11	1:C:81:LEU:HD21	1.84	0.60
1:C:76:ARG:NH2	1:C:169:PRO:O	2.37	0.58
1:B:178:ASP:OD2	1:B:181:THR:OG1	2.12	0.58
1:A:42:ARG:NH1	1:A:78:GLN:OE1	2.25	0.57
1:C:216:TYR:OH	1:C:224:GLU:OE2	2.22	0.57
1:A:168:HIS:O	1:A:189:MET:HE1	2.04	0.57
1:A:53:ILE:HD11	1:A:81:LEU:HD21	1.87	0.56
1:D:104:SER:N	1:D:105:GLY:CA	2.68	0.56
1:C:251:GLN:NE2	2:C:305:HOH:O	2.38	0.56
1:C:158:TYR:HD1	1:C:161:LEU:HB2	1.71	0.56
1:C:204:VAL:HG12	1:C:204:VAL:O	2.05	0.55
1:D:149:TRP:O	1:D:155:GLY:HA3	2.07	0.55
1:D:33:ARG:HD2	1:D:99:SER:HB3	1.89	0.54
1:A:34:ILE:HA	1:A:98:TYR:CD1	2.42	0.54
1:B:143:ASP:HB2	1:B:165:HIS:CD2	2.43	0.54
1:D:34:ILE:HA	1:D:98:TYR:CD1	2.43	0.54
1:C:156:ALA:O	1:C:159:LYS:HG3	2.08	0.54
1:B:102:GLY:C	1:B:104:SER:H	2.15	0.53
1:C:143:ASP:OD1	1:C:163:TYR:OH	2.21	0.53
1:C:78:GLN:HB3	1:C:226:VAL:HG13	1.91	0.52
1:A:238:PRO:HD2	1:A:241:MET:SD	2.49	0.52
1:C:158:TYR:CD1	1:C:161:LEU:HD22	2.44	0.51
1:C:116:VAL:HG12	1:C:119:ARG:NH2	2.26	0.51
1:D:42:ARG:HD3	1:D:68:ILE:O	2.11	0.50
1:C:78:GLN:CB	1:C:226:VAL:HG13	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HD2	1:B:99:SER:HB3	1.94	0.50
1:C:116:VAL:HG12	1:C:119:ARG:HH22	1.77	0.49
1:A:259:ARG:HG2	1:B:271:ILE:HD13	1.95	0.49
1:A:44:ARG:NH2	1:A:229:ILE:HD11	2.28	0.49
1:A:167:THR:HG22	1:A:189:MET:HE2	1.95	0.49
1:C:83:LYS:HE3	1:C:214:VAL:O	2.12	0.49
1:C:34:ILE:HA	1:C:98:TYR:CD1	2.49	0.48
1:D:168:HIS:ND1	2:D:301:HOH:O	2.11	0.48
1:A:263:MET:SD	1:B:263:MET:HG3	2.54	0.47
1:B:162:ALA:CB	1:B:203:GLU:HG2	2.44	0.47
1:A:149:TRP:O	1:A:155:GLY:HA3	2.15	0.47
1:C:216:TYR:CE1	1:C:224:GLU:OE1	2.65	0.47
1:B:34:ILE:HA	1:B:98:TYR:CD1	2.49	0.47
1:C:101:TYR:CD2	1:C:259:ARG:NH1	2.83	0.46
1:B:44:ARG:NH2	1:B:229:ILE:HD11	2.30	0.46
1:B:65:VAL:O	1:B:66:ARG:HB2	2.16	0.46
1:C:44:ARG:HA	1:C:44:ARG:HD3	1.83	0.46
1:D:168:HIS:CE1	1:D:171:TRP:HB2	2.52	0.45
1:A:156:ALA:O	1:A:159:LYS:HG3	2.17	0.45
1:C:91:VAL:HG11	1:C:126:VAL:HG11	1.99	0.45
1:C:76:ARG:NH2	1:C:170:THR:HA	2.32	0.45
1:C:91:VAL:HG11	1:C:126:VAL:CG1	2.46	0.45
1:B:44:ARG:HA	1:B:44:ARG:HD3	1.81	0.44
1:C:76:ARG:HD3	2:C:334:HOH:O	2.17	0.44
1:C:205:LYS:O	1:C:206:HIS:CG	2.70	0.44
1:C:240:TRP:CZ2	1:C:266:ILE:HG12	2.53	0.44
1:C:33:ARG:HG3	1:C:101:TYR:HB2	2.00	0.44
1:C:103:GLN:C	1:C:104:SER:HG	2.21	0.44
1:C:190:LEU:HD21	1:C:220:PHE:CE2	2.52	0.44
1:C:221:LYS:O	1:C:222:PRO:C	2.57	0.44
1:B:156:ALA:HA	1:B:159:LYS:HE3	1.99	0.44
1:C:103:GLN:O	1:C:104:SER:OG	2.23	0.44
1:C:103:GLN:O	1:C:104:SER:C	2.61	0.43
1:C:112:GLU:HA	1:C:113:PRO:HD3	1.90	0.43
1:A:201:ALA:HB3	1:A:202:PRO:HD3	2.00	0.43
1:C:133:GLU:OE1	1:C:206:HIS:ND1	2.37	0.43
1:D:65:VAL:O	1:D:66:ARG:HB2	2.18	0.43
1:D:112:GLU:OE1	2:D:302:HOH:O	2.22	0.43
1:C:65:VAL:O	1:C:66:ARG:HB2	2.18	0.42
1:D:15:ARG:NH2	2:D:305:HOH:O	2.30	0.42
1:A:171:TRP:CZ3	1:A:185:ASN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLU:HA	1:B:113:PRO:HD3	1.81	0.42
1:C:83:LYS:HB2	1:C:83:LYS:HE2	1.79	0.42
1:B:9:TYR:CE1	1:B:41:HIS:CE1	3.07	0.42
1:A:33:ARG:HD2	1:A:99:SER:HB3	2.01	0.42
1:D:79:GLY:HA3	1:D:224:GLU:O	2.19	0.42
1:B:103:GLN:C	1:B:105:GLY:H	2.27	0.42
1:B:168:HIS:O	1:B:189:MET:HE1	2.20	0.42
1:D:192:LYS:HB2	1:D:192:LYS:HE3	1.64	0.42
1:C:164:GLN:HG2	1:C:196:ALA:HA	2.02	0.42
1:B:98:TYR:HA	2:B:333:HOH:O	2.19	0.41
1:C:194:ASN:OD1	1:C:216:TYR:HB2	2.20	0.41
1:D:201:ALA:HB3	1:D:202:PRO:HD3	2.02	0.41
1:C:101:TYR:CZ	1:C:259:ARG:HD2	2.56	0.41
1:A:42:ARG:HG3	1:A:67:ARG:HB3	2.02	0.41
1:C:228:ILE:O	1:C:242:ARG:HD2	2.20	0.41
1:D:168:HIS:HA	1:D:169:PRO:HD3	1.89	0.41
1:A:87:VAL:HG22	1:A:208:ASP:CB	2.51	0.41
1:B:90:TYR:OH	1:B:232:ASP:OD2	2.34	0.41
1:B:107:SER:HB2	1:B:110:LYS:HD3	2.03	0.41
1:A:258:LYS:NZ	2:A:317:HOH:O	2.53	0.40
1:C:266:ILE:HD11	1:D:36:TRP:CE2	2.56	0.40
1:A:133:GLU:OE2	1:A:206:HIS:ND1	2.42	0.40
1:A:167:THR:HG22	1:A:189:MET:CE	2.51	0.40
1:A:240:TRP:CZ2	1:A:266:ILE:HG12	2.56	0.40
1:C:214:VAL:HA	1:C:215:PRO:HD2	1.91	0.40
1:B:102:GLY:C	1:B:104:SER:N	2.79	0.40
1:C:221:LYS:O	1:C:224:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	263 (97%)	7 (3%)	0	100	100
1	B	270/272 (99%)	260 (96%)	10 (4%)	0	100	100
1	C	270/272 (99%)	255 (94%)	15 (6%)	0	100	100
1	D	270/272 (99%)	263 (97%)	7 (3%)	0	100	100
All	All	1080/1088 (99%)	1041 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	213/213 (100%)	213 (100%)	0	100	100
1	B	213/213 (100%)	211 (99%)	2 (1%)	70	70
1	C	213/213 (100%)	206 (97%)	7 (3%)	33	24
1	D	213/213 (100%)	211 (99%)	2 (1%)	70	70
All	All	852/852 (100%)	841 (99%)	11 (1%)	61	58

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	HIS
1	B	108	LYS
1	C	51	VAL
1	C	88	GLN
1	C	126	VAL
1	C	221	LYS
1	C	223	SER
1	C	225	LEU
1	C	226	VAL
1	D	126	VAL
1	D	263	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	B	111	ASN
1	B	165	HIS
1	D	88	GLN
1	D	165	HIS
1	D	185	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	272/272 (100%)	2.05	129 (47%) 0 0	28, 40, 60, 87	0
1	B	272/272 (100%)	1.72	84 (30%) 1 1	30, 40, 57, 94	0
1	C	272/272 (100%)	2.61	163 (59%) 0 0	36, 62, 86, 94	0
1	D	272/272 (100%)	1.70	80 (29%) 1 1	33, 43, 59, 95	0
All	All	1088/1088 (100%)	2.02	456 (41%) 0 0	28, 43, 78, 95	0

All (456) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	GLY	8.0
1	C	104	SER	7.6
1	C	199	ALA	6.4
1	C	155	GLY	6.2
1	A	11	GLU	6.0
1	D	102	GLY	6.0
1	C	210	PRO	5.7
1	C	162	ALA	5.7
1	C	167	THR	5.5
1	A	104	SER	5.5
1	C	156	ALA	5.4
1	A	103	GLN	5.3
1	C	51	VAL	5.2
1	C	224	GLU	5.1
1	C	86	ILE	5.1
1	A	176	ALA	5.1
1	C	193	TRP	5.0
1	C	106	GLY	4.9
1	C	132	ILE	4.8
1	C	186	THR	4.8
1	C	49	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	135	VAL	4.6
1	A	87	VAL	4.6
1	C	209	VAL	4.6
1	C	222	PRO	4.6
1	C	212	THR	4.5
1	A	30	HIS	4.4
1	C	229	ILE	4.4
1	D	1	MET	4.4
1	A	142	ALA	4.4
1	C	180	ALA	4.4
1	C	71	GLY	4.3
1	C	166	ILE	4.3
1	C	102	GLY	4.3
1	C	145	ALA	4.3
1	D	2	LEU	4.3
1	C	116	VAL	4.3
1	C	176	ALA	4.3
1	C	149	TRP	4.3
1	C	158	TYR	4.2
1	C	163	TYR	4.2
1	C	191	ALA	4.2
1	C	213	LEU	4.2
1	A	53	ILE	4.2
1	C	134	ALA	4.2
1	C	214	VAL	4.2
1	C	148	ALA	4.1
1	C	226	VAL	4.1
1	C	219	ALA	4.1
1	C	141	LEU	4.1
1	A	166	ILE	4.0
1	C	161	LEU	4.0
1	C	150	LEU	4.0
1	D	176	ALA	4.0
1	C	171	TRP	3.9
1	C	82	ALA	3.9
1	C	126	VAL	3.9
1	C	216	TYR	3.9
1	C	146	TRP	3.9
1	A	20	ASN	3.8
1	C	139	GLY	3.8
1	C	183	ALA	3.8
1	B	270	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	20	ASN	3.8
1	B	1	MET	3.8
1	A	150	LEU	3.8
1	A	269	GLY	3.8
1	C	79	GLY	3.8
1	B	142	ALA	3.7
1	A	102	GLY	3.7
1	C	157	ALA	3.7
1	C	123	PHE	3.7
1	A	81	LEU	3.6
1	C	206	HIS	3.6
1	D	105	GLY	3.6
1	C	207	PRO	3.6
1	C	52	LEU	3.6
1	C	81	LEU	3.6
1	A	141	LEU	3.6
1	A	193	TRP	3.6
1	C	85	GLY	3.6
1	C	100	VAL	3.5
1	C	220	PHE	3.5
1	D	172	PRO	3.5
1	B	150	LEU	3.5
1	C	190	LEU	3.5
1	B	114	GLY	3.5
1	C	189	MET	3.5
1	C	107	SER	3.5
1	C	211	THR	3.5
1	C	130	GLY	3.4
1	A	19	ALA	3.4
1	A	197	LEU	3.4
1	A	38	PRO	3.4
1	B	34	ILE	3.4
1	D	155	GLY	3.4
1	C	24	ALA	3.4
1	C	256	ALA	3.4
1	D	104	SER	3.4
1	C	194	ASN	3.4
1	B	38	PRO	3.4
1	B	168	HIS	3.4
1	A	155	GLY	3.4
1	B	269	GLY	3.4
1	A	171	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	96	PHE	3.4
1	C	84	LEU	3.4
1	A	181	THR	3.4
1	C	160	THR	3.4
1	A	91	VAL	3.3
1	B	2	LEU	3.3
1	B	106	GLY	3.3
1	C	114	GLY	3.3
1	C	223	SER	3.3
1	C	53	ILE	3.3
1	C	115	ILE	3.3
1	C	142	ALA	3.3
1	B	30	HIS	3.3
1	A	21	TYR	3.3
1	C	1	MET	3.3
1	C	83	LYS	3.3
1	A	31	ASP	3.3
1	C	137	SER	3.3
1	C	39	ILE	3.2
1	A	219	ALA	3.2
1	C	74	GLY	3.2
1	D	11	GLU	3.2
1	B	271	ILE	3.2
1	C	228	ILE	3.2
1	C	197	LEU	3.2
1	B	32	PHE	3.2
1	A	177	HIS	3.2
1	C	168	HIS	3.2
1	C	263	MET	3.2
1	C	188	ILE	3.1
1	C	101	TYR	3.1
1	C	103	GLN	3.1
1	B	214	VAL	3.1
1	C	14	PHE	3.1
1	C	221	LYS	3.1
1	A	261	THR	3.1
1	A	239	ALA	3.1
1	D	26	ALA	3.1
1	B	105	GLY	3.1
1	D	90	TYR	3.1
1	C	87	VAL	3.1
1	C	181	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	26	ALA	3.1
1	A	271	ILE	3.1
1	D	130	GLY	3.1
1	C	90	TYR	3.1
1	C	208	ASP	3.1
1	D	209	VAL	3.1
1	D	103	GLN	3.1
1	A	140	GLY	3.1
1	D	19	ALA	3.1
1	A	54	VAL	3.0
1	D	116	VAL	3.0
1	C	89	SER	3.0
1	A	106	GLY	3.0
1	C	198	ALA	3.0
1	C	127	LEU	3.0
1	A	158	TYR	3.0
1	D	228	ILE	3.0
1	C	249	VAL	3.0
1	A	107	SER	3.0
1	A	201	ALA	3.0
1	C	11	GLU	3.0
1	D	168	HIS	2.9
1	A	214	VAL	2.9
1	A	178	ASP	2.9
1	B	43	GLY	2.9
1	C	177	HIS	2.9
1	A	213	LEU	2.9
1	B	190	LEU	2.9
1	C	56	GLN	2.9
1	C	200	LEU	2.9
1	C	225	LEU	2.9
1	C	237	LEU	2.9
1	C	204	VAL	2.9
1	A	1	MET	2.9
1	A	7	ALA	2.9
1	A	156	ALA	2.9
1	A	257	ALA	2.9
1	C	184	ALA	2.9
1	B	138	LEU	2.9
1	C	136	VAL	2.9
1	A	59	ALA	2.9
1	A	15	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	150	LEU	2.9
1	A	55	GLY	2.9
1	C	185	ASN	2.8
1	D	51	VAL	2.8
1	C	172	PRO	2.8
1	A	82	ALA	2.8
1	C	154	ASP	2.8
1	A	99	SER	2.8
1	B	104	SER	2.8
1	C	128	GLY	2.8
1	B	21	TYR	2.8
1	A	44	ARG	2.8
1	A	161	LEU	2.8
1	A	262	ILE	2.8
1	D	188	ILE	2.8
1	A	216	TYR	2.8
1	A	255	ALA	2.8
1	A	105	GLY	2.8
1	C	110	LYS	2.8
1	A	34	ILE	2.8
1	C	215	PRO	2.8
1	D	202	PRO	2.8
1	A	116	VAL	2.8
1	A	226	VAL	2.8
1	A	175	SER	2.7
1	A	194	ASN	2.7
1	B	79	GLY	2.7
1	B	161	LEU	2.7
1	A	5	PHE	2.7
1	A	40	PHE	2.7
1	B	179	SER	2.7
1	B	93	VAL	2.7
1	A	248	ALA	2.7
1	B	7	ALA	2.7
1	C	125	ALA	2.7
1	D	195	ALA	2.7
1	A	79	GLY	2.7
1	C	140	GLY	2.7
1	B	178	ASP	2.7
1	A	66	ARG	2.7
1	C	153	SER	2.7
1	C	179	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	34	ILE	2.7
1	C	70	VAL	2.7
1	A	37	GLY	2.6
1	A	43	GLY	2.6
1	A	184	ALA	2.6
1	A	256	ALA	2.6
1	B	257	ALA	2.6
1	D	40	PHE	2.6
1	D	170	THR	2.6
1	C	124	LYS	2.6
1	C	43	GLY	2.6
1	D	65	VAL	2.6
1	C	196	ALA	2.6
1	C	98	TYR	2.6
1	A	165	HIS	2.6
1	D	208	ASP	2.6
1	D	180	ALA	2.6
1	B	181	THR	2.6
1	C	9	TYR	2.6
1	C	21	TYR	2.6
1	C	32	PHE	2.6
1	A	228	ILE	2.6
1	A	130	GLY	2.6
1	A	195	ALA	2.6
1	C	111	ASN	2.6
1	A	18	CYS	2.5
1	B	213	LEU	2.5
1	D	149	TRP	2.5
1	B	37	GLY	2.5
1	D	68	ILE	2.5
1	D	271	ILE	2.5
1	C	94	ASN	2.5
1	D	87	VAL	2.5
1	D	4	GLU	2.5
1	A	9	TYR	2.5
1	C	17	LEU	2.5
1	A	217	GLY	2.5
1	B	8	GLY	2.5
1	D	171	TRP	2.5
1	A	153	SER	2.5
1	D	175	SER	2.5
1	A	199	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	24	ALA	2.5
1	C	72	THR	2.5
1	D	135	VAL	2.5
1	D	212	THR	2.5
1	D	265	THR	2.5
1	A	172	PRO	2.5
1	A	215	PRO	2.5
1	B	5	PHE	2.5
1	B	185	ASN	2.5
1	C	48	SER	2.5
1	C	262	ILE	2.5
1	A	73	ALA	2.5
1	A	159	LYS	2.5
1	D	178	ASP	2.5
1	C	238	PRO	2.5
1	D	129	PRO	2.5
1	D	23	GLY	2.4
1	D	177	HIS	2.4
1	A	137	SER	2.4
1	C	99	SER	2.4
1	B	263	MET	2.4
1	D	263	MET	2.4
1	A	245	THR	2.4
1	A	57	ASP	2.4
1	C	143	ASP	2.4
1	C	217	GLY	2.4
1	A	200	LEU	2.4
1	B	81	LEU	2.4
1	C	205	LYS	2.4
1	A	254	ASP	2.4
1	B	261	THR	2.4
1	C	257	ALA	2.4
1	C	29	PRO	2.4
1	D	222	PRO	2.4
1	A	70	VAL	2.4
1	B	171	TRP	2.4
1	D	249	VAL	2.4
1	C	152	SER	2.4
1	A	2	LEU	2.4
1	C	138	LEU	2.4
1	D	158	TYR	2.4
1	D	154	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	39	ILE	2.4
1	B	176	ALA	2.4
1	B	255	ALA	2.4
1	D	234	PRO	2.4
1	A	253	VAL	2.4
1	A	149	TRP	2.4
1	D	36	TRP	2.4
1	D	174	SER	2.4
1	A	80	PHE	2.3
1	D	14	PHE	2.3
1	A	3	THR	2.3
1	C	144	GLU	2.3
1	B	262	ILE	2.3
1	D	157	ALA	2.3
1	A	202	PRO	2.3
1	B	41	HIS	2.3
1	B	217	GLY	2.3
1	D	270	VAL	2.3
1	B	239	ALA	2.3
1	A	39	ILE	2.3
1	A	189	MET	2.3
1	A	229	ILE	2.3
1	B	132	ILE	2.3
1	B	174	SER	2.3
1	B	6	ASP	2.3
1	D	18	CYS	2.3
1	B	17	LEU	2.3
1	A	186	THR	2.3
1	C	170	THR	2.3
1	B	73	ALA	2.3
1	B	102	GLY	2.3
1	C	164	GLN	2.3
1	A	206	HIS	2.3
1	B	177	HIS	2.3
1	B	36	TRP	2.2
1	A	90	TYR	2.2
1	A	198	ALA	2.2
1	C	27	TYR	2.2
1	C	129	PRO	2.2
1	C	202	PRO	2.2
1	D	38	PRO	2.2
1	A	89	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	153	SER	2.2
1	B	53	ILE	2.2
1	B	86	ILE	2.2
1	C	218	ASP	2.2
1	B	135	VAL	2.2
1	D	100	VAL	2.2
1	C	159	LYS	2.2
1	A	17	LEU	2.2
1	B	11	GLU	2.2
1	B	237	LEU	2.2
1	A	10	GLY	2.2
1	A	85	GLY	2.2
1	B	272	PRO	2.2
1	C	272	PRO	2.2
1	A	191	ALA	2.2
1	D	156	ALA	2.2
1	D	183	ALA	2.2
1	B	146	TRP	2.2
1	B	240	TRP	2.2
1	A	115	ILE	2.2
1	D	34	ILE	2.2
1	D	229	ILE	2.2
1	C	75	ARG	2.2
1	C	65	VAL	2.2
1	A	190	LEU	2.2
1	A	6	ASP	2.2
1	B	23	GLY	2.2
1	B	107	SER	2.2
1	B	153	SER	2.2
1	C	113	PRO	2.2
1	B	248	ALA	2.2
1	D	96	PHE	2.2
1	A	260	ARG	2.2
1	B	259	ARG	2.2
1	A	249	VAL	2.2
1	B	116	VAL	2.2
1	B	251	GLN	2.2
1	C	54	VAL	2.2
1	C	91	VAL	2.2
1	A	212	THR	2.2
1	D	107	SER	2.2
1	D	225	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	256	ALA	2.2
1	C	230	ALA	2.2
1	A	241	MET	2.1
1	D	9	TYR	2.1
1	B	193	TRP	2.1
1	A	208	ASP	2.1
1	A	51	VAL	2.1
1	D	214	VAL	2.1
1	B	99	SER	2.1
1	C	45	LEU	2.1
1	A	131	ASN	2.1
1	D	32	PHE	2.1
1	A	143	ASP	2.1
1	B	268	ASP	2.1
1	C	76	ARG	2.1
1	D	85	GLY	2.1
1	D	106	GLY	2.1
1	D	17	LEU	2.1
1	A	132	ILE	2.1
1	D	16	ASP	2.1
1	D	98	TYR	2.1
1	A	259	ARG	2.1
1	C	50	ARG	2.1
1	C	175	SER	2.1
1	A	147	LYS	2.1
1	A	146	TRP	2.1
1	B	54	VAL	2.1
1	B	149	TRP	2.1
1	C	165	HIS	2.1
1	D	30	HIS	2.1
1	D	165	HIS	2.1
1	A	246	PRO	2.1
1	A	230	ALA	2.1
1	B	148	ALA	2.1
1	B	184	ALA	2.1
1	B	196	ALA	2.1
1	D	7	ALA	2.1
1	B	15	ARG	2.1
1	A	231	LYS	2.0
1	B	151	LYS	2.0
1	B	118	TYR	2.0
1	A	236	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	47	GLY	2.0
1	B	209	VAL	2.0
1	C	169	PRO	2.0
1	A	145	ALA	2.0
1	C	73	ALA	2.0
1	D	219	ALA	2.0
1	D	203	GLU	2.0
1	A	188	ILE	2.0
1	C	40	PHE	2.0
1	C	80	PHE	2.0
1	A	77	THR	2.0
1	A	95	THR	2.0
1	A	182	GLN	2.0
1	B	160	THR	2.0
1	D	238	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 oligosaccharides 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.