



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:27 AM UTC

PDB ID : 2RBA / pdb_00002rba
Title : Structure of Human Thymine DNA Glycosylase Bound to Abasic and Undamaged DNA
Authors : Maiti, A.; Pozharski, E.; Drohat, A.C.
Deposited on : 2007-09-18
Resolution : 2.79 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

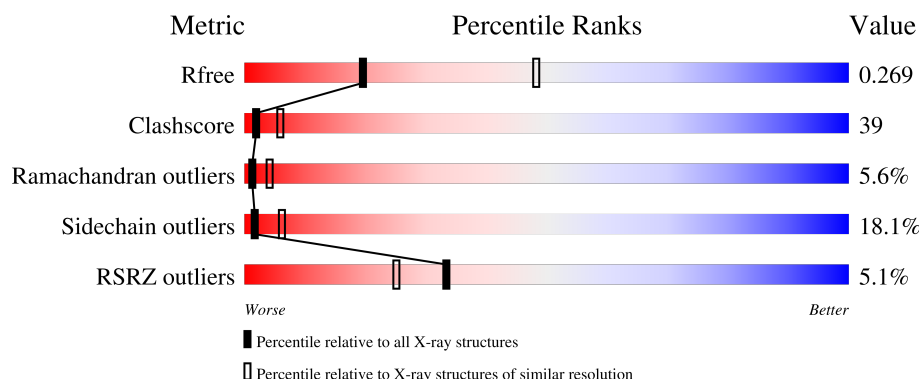
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	C	23	9% 17% 61% 22%
2	D	23	17% 13% 70% 17%
3	A	204	3% 27% 42% 16% 5% 11%
3	B	204	4% 35% 44% 9% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3845 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 DNA chain called DNA (5'-D(*DCP*DAP*DGP*DCP*DTP*DCP*DTP*DCP*DTP*DAP*DCP*DGP*DTP*DGP*DAP*DGP*DCP*DAP*DGP*DTP*DGP*DGP*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			473	225	90	136	22			

- Molecule 2 is a DNA chain called DNA (5'-D(*DCP*DCP*DAP*DCP*DTP*DGP*DCP*DTP*DCP*DAP*(3DR)P*DGP*DTP*DAP*DCP*DAP*DGP*DAP*DGP*DCP*DTP*DG P*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	23	Total	C	N	O	P	0	0	0
			456	218	81	135	22			

- Molecule 3 is a protein called G/T mismatch-specific thymine DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	182	Total	C	N	O	S	0	0	0
			1458	939	252	258	9			
3	B	182	Total	C	N	O	S	0	0	0
			1458	939	252	258	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP Q13569
A	106	SER	-	expression tag	UNP Q13569
A	107	HIS	-	expression tag	UNP Q13569
A	108	MET	-	expression tag	UNP Q13569
A	109	ALA	-	expression tag	UNP Q13569
A	110	SER	-	expression tag	UNP Q13569
B	105	GLY	-	expression tag	UNP Q13569
B	106	SER	-	expression tag	UNP Q13569

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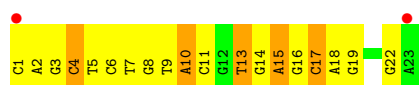
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Chain	Residue	Modelled	Actual	Comment	Reference
B	107	HIS	-	expression tag	UNP Q13569
B	108	MET	-	expression tag	UNP Q13569
B	109	ALA	-	expression tag	UNP Q13569
B	110	SER	-	expression tag	UNP Q13569

3 Residue-property plots

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.

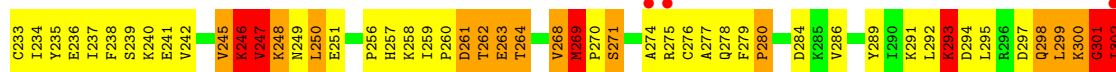
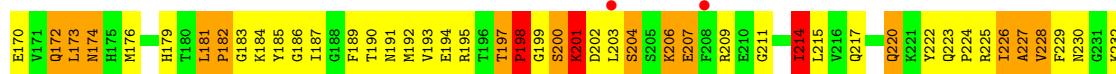
- Molecule 1: DNA (5'-D(*DCP*DAP*DGP*DCP*DTP*DCP*DTP*DGP*DTP*DAP*DCP*DCP*DTP*DGP*DAP*DGP*DCP*DAP*DGP*DTP*DGP*DGP*DA)-3')



- Molecule 2: DNA (5'-D(*DCP*DCP*DAP*DCP*DTP*DGP*DCP*DTP*DCP*DAP*(3DR)P*DGP*DTP*DAP*DCP*DAP*DGP*DAP*DGP*DCP*DTP*DGP*DT)-3')

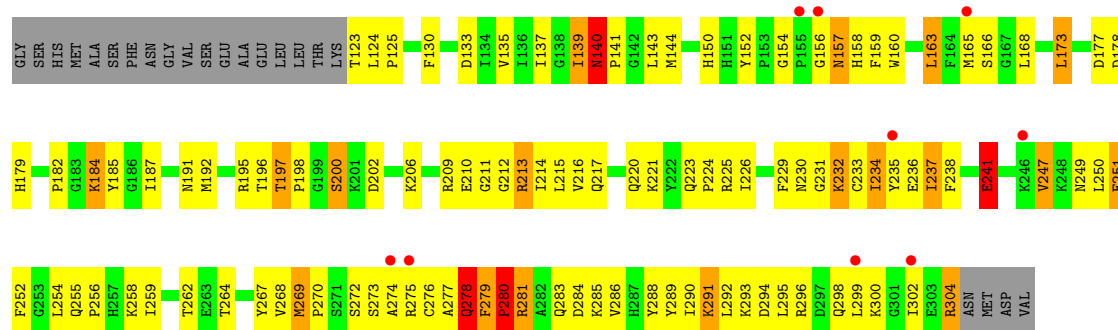


- Molecule 3: G/T mismatch-specific thymine DNA glycosylase



- Molecule 3: G/T mismatch-specific thymine DNA glycosylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	162.13Å 162.13Å 56.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.79 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.79) 97.5 (50.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.230 , 0.276 0.225 , 0.269	Depositor DCC
R_{free} test set	1048 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 181.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3845	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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	C	0.51	0/531	1.33	5/819 (0.6%)
2	D	0.50	0/497	1.42	3/762 (0.4%)
3	A	1.49	15/1495 (1.0%)	1.61	25/2015 (1.2%)
3	B	1.11	0/1495	1.31	10/2015 (0.5%)
All	All	1.17	15/4018 (0.4%)	1.44	43/5611 (0.8%)

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
3	A	1	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	268	VAL	CA-CB	-13.54	1.39	1.54
3	A	247	VAL	C-O	10.52	1.36	1.24
3	A	246	LYS	CD-CE	9.81	1.81	1.52
3	A	223	GLN	C-O	7.22	1.27	1.23
3	A	191	ASN	CA-C	-6.92	1.44	1.52
3	A	227	ALA	N-CA	-6.87	1.37	1.46
3	A	293	LYS	N-CA	6.71	1.54	1.46
3	A	135	VAL	C-O	6.70	1.31	1.24
3	A	248	LYS	N-CA	6.57	1.54	1.45
3	A	247	VAL	C-N	6.50	1.42	1.33
3	A	228	VAL	CA-CB	-6.01	1.46	1.53
3	A	145	ALA	CA-CB	-5.55	1.44	1.53
3	A	248	LYS	C-O	5.33	1.30	1.23
3	A	133	ASP	C-O	5.28	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	214	ILE	CA-CB	5.10	1.60	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	197	THR	CA-C-N	10.92	131.17	119.05
3	B	197	THR	C-N-CA	10.92	131.17	119.05
3	A	245	VAL	N-CA-C	10.33	122.83	107.75
3	A	302	ILE	CA-C-N	7.84	135.81	121.70
3	A	302	ILE	C-N-CA	7.84	135.81	121.70
3	A	197	THR	CA-C-N	7.67	129.43	119.84
3	A	197	THR	C-N-CA	7.67	129.43	119.84
3	A	302	ILE	N-CA-C	7.41	131.75	111.00
3	B	140	ASN	CA-C-N	-7.25	112.45	120.14
3	B	140	ASN	C-N-CA	-7.25	112.45	120.14
3	A	211	GLY	N-CA-C	-7.07	104.30	112.50
3	A	228	VAL	CB-CA-C	-6.81	102.20	111.33
3	A	269	MET	CA-C-N	-6.54	113.21	120.14
3	A	269	MET	C-N-CA	-6.54	113.21	120.14
3	A	226	ILE	CB-CA-C	-6.48	99.12	110.71
3	A	268	VAL	CB-CA-C	-6.31	104.38	111.45
3	A	148	LYS	N-CA-C	6.07	120.00	112.59
3	A	198	PRO	N-CA-C	5.96	124.76	112.47
3	A	301	GLY	CA-C-N	5.82	132.18	121.70
3	A	301	GLY	C-N-CA	5.82	132.18	121.70
3	B	232	LYS	N-CA-C	-5.75	104.21	111.11
3	A	130	PHE	N-CA-C	-5.71	101.57	110.42
1	C	17	DC	O4'-C1'-N1	5.71	116.97	108.40
3	B	223	GLN	CA-C-N	-5.70	114.38	120.03
3	B	223	GLN	C-N-CA	-5.70	114.38	120.03
1	C	4	DC	P-O5'-C5'	5.66	128.50	120.00
3	A	139	ILE	CB-CA-C	-5.66	104.41	112.22
3	A	181	LEU	CA-C-N	-5.65	112.78	119.84
3	A	181	LEU	C-N-CA	-5.65	112.78	119.84
3	A	242	VAL	N-CA-C	5.60	115.80	110.42
2	D	2	DC	P-O3'-C3'	5.51	128.46	120.20
1	C	10	DA	P-O3'-C3'	5.46	128.39	120.20
2	D	8	DT	P-O3'-C3'	5.40	128.30	120.20
3	B	295	LEU	N-CA-C	-5.28	105.44	111.14
1	C	13	DT	C4'-C3'-O3'	-5.28	102.08	110.00
3	A	174	ASN	N-CA-C	5.27	115.50	108.38
1	C	15	DA	P-O3'-C3'	5.22	128.04	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	DG	O5'-C5'-C4'	5.19	118.59	110.80
3	A	297	ASP	N-CA-C	5.09	118.27	111.75
3	A	271	SER	CA-C-N	-5.07	112.62	122.06
3	A	271	SER	C-N-CA	-5.07	112.62	122.06
3	B	278	GLN	CA-C-N	5.03	130.75	121.70
3	B	278	GLN	C-N-CA	5.03	130.75	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	302	ILE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	156	GLY	Peptide
3	A	198	PRO	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	C	473	0	260	29	0
2	D	456	0	257	28	0
3	A	1458	0	1469	122	0
3	B	1458	0	1469	124	0
All	All	3845	0	3455	285	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 39.

All (285) 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)
3:A:246:LYS:CD	3:A:246:LYS:CE	1.81	1.55
3:A:301:GLY:CA	3:A:303:GLU:HB2	1.68	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:301:GLY:HA2	3:A:303:GLU:CB	1.76	1.13
3:A:302:ILE:HG13	3:A:303:GLU:HG2	1.13	1.08
3:B:269:MET:HE1	3:B:288:TYR:HB3	1.37	1.05
3:B:279:PHE:HB3	3:B:284:ASP:HB2	1.34	1.05
3:B:213:ARG:HH11	3:B:213:ARG:HB2	1.23	1.00
3:A:268:VAL:CG1	3:A:269:MET:N	2.23	0.99
3:A:268:VAL:HG12	3:A:269:MET:N	1.78	0.99
3:B:269:MET:CE	3:B:288:TYR:HB3	1.93	0.97
3:A:301:GLY:HA2	3:A:303:GLU:HB2	0.97	0.96
3:B:158:HIS:HD2	3:B:285:LYS:HZ3	1.10	0.96
3:A:198:PRO:HB2	3:A:199:GLY:O	1.67	0.93
3:B:158:HIS:HD2	3:B:285:LYS:NZ	1.67	0.91
3:B:276:CYS:HB3	3:B:280:PRO:HG2	1.55	0.89
3:B:139:ILE:HD12	3:B:139:ILE:H	1.38	0.89
3:A:302:ILE:HG13	3:A:303:GLU:CG	2.02	0.89
3:A:268:VAL:HG13	3:A:269:MET:H	1.42	0.85
3:B:269:MET:HA	3:B:269:MET:HE3	1.58	0.83
3:B:133:ASP:HA	3:B:225:ARG:HD2	1.62	0.82
1:C:18:DA:C2	3:B:277:ALA:HB2	2.16	0.81
2:D:15:DC:H2''	2:D:16:DA:OP2	1.80	0.80
3:B:276:CYS:HB3	3:B:280:PRO:CG	2.12	0.80
3:B:158:HIS:CD2	3:B:285:LYS:NZ	2.49	0.79
3:B:197:THR:HB	3:B:198:PRO:HD2	1.64	0.79
3:B:269:MET:CE	3:B:269:MET:HA	2.14	0.78
3:B:259:ILE:HB	3:B:262:THR:OG1	1.85	0.77
3:B:278:GLN:HB2	3:B:279:PHE:CG	2.22	0.74
3:A:155:PRO:HA	3:A:157:ASN:H	1.52	0.74
3:A:246:LYS:CD	3:A:246:LYS:NZ	2.49	0.74
1:C:17:DC:H4'	3:B:275:ARG:HE	1.53	0.73
2:D:12:DG:C8	2:D:12:DG:H5''	2.25	0.72
3:A:199:GLY:HA3	3:A:200:SER:HB2	1.71	0.72
3:A:124:LEU:HD23	3:A:141:PRO:HB3	1.71	0.71
2:D:18:DA:H2''	2:D:19:DG:OP2	1.90	0.71
2:D:12:DG:O3'	3:A:271:SER:HB2	1.91	0.71
2:D:16:DA:H2''	2:D:17:DG:OP2	1.89	0.70
3:B:291:LYS:HE2	3:B:291:LYS:HA	1.74	0.70
3:B:124:LEU:HD12	3:B:125:PRO:HD2	1.73	0.69
3:A:193:VAL:HG12	3:A:194:GLU:N	2.08	0.69
3:A:301:GLY:HA2	3:A:303:GLU:CA	2.23	0.69
2:D:19:DG:H2''	2:D:20:DC:OP2	1.93	0.68
3:B:139:ILE:HD12	3:B:139:ILE:N	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:209:ARG:HG2	3:A:241:GLU:OE2	1.94	0.67
3:B:157:ASN:ND2	3:B:272:SER:OG	2.26	0.67
1:C:1:DC:H2''	1:C:2:DA:N7	2.10	0.67
3:A:301:GLY:N	3:A:303:GLU:HB2	2.09	0.67
3:B:274:ALA:HA	3:B:280:PRO:HG3	1.77	0.66
1:C:7:DT:H2''	1:C:8:DG:OP2	1.96	0.66
3:A:269:MET:HG3	3:A:270:PRO:CD	2.26	0.66
3:B:213:ARG:HB2	3:B:213:ARG:NH1	2.04	0.65
3:B:213:ARG:HH11	3:B:213:ARG:CB	2.05	0.65
2:D:8:DT:H2''	2:D:9:DC:O5'	1.96	0.65
3:B:278:GLN:CG	3:B:279:PHE:O	2.45	0.65
1:C:3:DG:H1'	1:C:4:DC:O5'	1.96	0.64
3:B:139:ILE:O	3:B:140:ASN:HB3	1.96	0.64
3:B:209:ARG:HH11	3:B:209:ARG:HG3	1.61	0.64
1:C:19:DG:H4'	3:B:278:GLN:NE2	2.13	0.64
3:B:278:GLN:HG2	3:B:279:PHE:O	1.97	0.63
3:B:279:PHE:HB3	3:B:284:ASP:CB	2.21	0.62
3:B:299:LEU:O	3:B:302:ILE:HG22	1.98	0.62
3:B:252:PHE:HB2	3:B:288:TYR:CE2	2.34	0.62
3:B:269:MET:HE2	3:B:288:TYR:HB3	1.81	0.62
3:B:139:ILE:H	3:B:139:ILE:CD1	2.10	0.62
3:B:158:HIS:CD2	3:B:285:LYS:HZ3	2.02	0.61
3:B:150:HIS:HD2	3:B:178:ASP:OD1	1.83	0.61
3:B:286:VAL:O	3:B:290:ILE:HG12	2.01	0.61
3:B:291:LYS:HE3	3:B:294:ASP:OD2	2.01	0.61
3:A:299:LEU:O	3:A:302:ILE:HG12	2.00	0.61
3:B:224:PRO:O	3:B:264:THR:HG23	2.00	0.61
3:B:283:GLN:HA	3:B:286:VAL:HG23	1.83	0.61
3:A:197:THR:HB	3:A:198:PRO:HD2	1.82	0.61
3:B:269:MET:CE	3:B:288:TYR:CB	2.74	0.60
3:A:198:PRO:CB	3:A:199:GLY:O	2.46	0.60
3:B:276:CYS:CB	3:B:280:PRO:HG2	2.31	0.60
3:B:158:HIS:CD2	3:B:285:LYS:HZ1	2.20	0.60
1:C:19:DG:H5'	3:B:276:CYS:SG	2.42	0.60
2:D:17:DG:OP2	2:D:17:DG:H2'	2.02	0.59
1:C:8:DG:H2''	1:C:9:DT:O5'	2.02	0.59
3:A:200:SER:C	3:A:202:ASP:H	2.11	0.59
3:B:185:TYR:O	3:B:187:ILE:HG13	2.02	0.59
3:B:197:THR:HB	3:B:198:PRO:CD	2.33	0.59
3:B:135:VAL:HG12	3:B:135:VAL:O	2.02	0.59
3:B:283:GLN:HA	3:B:286:VAL:CG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:193:VAL:CG1	3:A:194:GLU:N	2.65	0.58
3:A:199:GLY:HA3	3:A:200:SER:CB	2.34	0.58
3:B:232:LYS:HE2	3:B:252:PHE:CZ	2.39	0.58
3:A:142:GLY:HA2	3:A:197:THR:O	2.05	0.57
3:B:277:ALA:HB3	3:B:278:GLN:OE1	2.04	0.57
3:A:141:PRO:HD2	3:A:195:ARG:O	2.05	0.57
3:A:263:GLU:OE1	3:A:263:GLU:HA	2.04	0.57
3:A:166:SER:CB	3:A:289:TYR:HB3	2.34	0.56
3:B:252:PHE:HB2	3:B:288:TYR:HE2	1.70	0.56
3:A:279:PHE:HD2	3:A:284:ASP:O	1.88	0.56
3:A:182:PRO:O	3:A:184:LYS:N	2.38	0.56
3:A:193:VAL:HG11	3:A:203:LEU:HD22	1.87	0.56
3:B:269:MET:HE2	3:B:270:PRO:CD	2.36	0.56
3:B:250:LEU:HD12	3:B:251:GLU:N	2.20	0.56
2:D:5:DT:C4	2:D:6:DG:O6	2.59	0.56
3:B:269:MET:HE3	3:B:269:MET:CA	2.32	0.56
3:A:164:PHE:CD2	3:A:172:GLN:HB2	2.40	0.56
3:A:247:VAL:HG21	3:A:250:LEU:HD13	1.89	0.55
2:D:11:3DR:OP1	3:A:157:ASN:ND2	2.39	0.55
3:A:197:THR:HB	3:A:198:PRO:CD	2.36	0.55
3:B:269:MET:HE2	3:B:270:PRO:HD2	1.89	0.55
3:B:184:LYS:HG2	3:B:185:TYR:CE2	2.41	0.55
3:A:299:LEU:O	3:A:302:ILE:CG1	2.55	0.55
3:A:274:ALA:C	3:A:276:CYS:H	2.15	0.54
3:A:168:LEU:CD2	3:A:293:LYS:HG2	2.37	0.54
3:A:170:GLU:OE1	3:A:170:GLU:N	2.38	0.54
3:B:285:LYS:O	3:B:289:TYR:HD1	1.89	0.54
1:C:5:DT:H2''	1:C:6:DC:OP2	2.07	0.54
1:C:18:DA:H1'	3:B:276:CYS:SG	2.48	0.54
1:C:18:DA:H2	3:B:277:ALA:HB2	1.68	0.54
3:B:209:ARG:HG3	3:B:209:ARG:NH1	2.19	0.54
3:B:276:CYS:HB3	3:B:280:PRO:CD	2.37	0.54
2:D:1:DC:O2	2:D:2:DC:N3	2.41	0.53
3:A:132:LEU:O	3:A:224:PRO:HA	2.09	0.53
3:A:139:ILE:HA	3:A:234:ILE:HG21	1.90	0.53
3:A:291:LYS:O	3:A:292:LEU:C	2.50	0.53
3:B:209:ARG:O	3:B:213:ARG:NH1	2.41	0.53
3:A:140:ASN:CG	3:A:203:LEU:HD11	2.32	0.53
3:B:135:VAL:HG12	3:B:137:ILE:CG1	2.38	0.53
2:D:19:DG:OP2	2:D:19:DG:H2'	2.08	0.53
3:B:269:MET:HE1	3:B:288:TYR:CB	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:193:VAL:CG1	3:A:194:GLU:H	2.20	0.53
3:A:170:GLU:OE1	3:A:185:TYR:OH	2.17	0.52
3:B:135:VAL:O	3:B:137:ILE:HG13	2.08	0.52
3:B:278:GLN:HB2	3:B:279:PHE:CD1	2.44	0.52
3:A:256:PRO:HB2	3:A:257:HIS:CE1	2.44	0.52
3:A:174:ASN:C	3:A:174:ASN:OD1	2.52	0.52
3:A:235:TYR:O	3:A:236:GLU:C	2.51	0.52
3:A:166:SER:CB	3:A:289:TYR:CB	2.88	0.52
2:D:6:DG:H4'	2:D:7:DC:OP1	2.10	0.52
3:B:184:LYS:O	3:B:184:LYS:HG3	2.09	0.51
3:A:155:PRO:HA	3:A:157:ASN:N	2.22	0.51
3:B:216:VAL:O	3:B:220:GLN:HG3	2.10	0.51
1:C:16:DG:N2	2:D:8:DT:O2	2.44	0.51
3:A:262:THR:OG1	3:A:264:THR:HB	2.10	0.51
3:A:140:ASN:ND2	3:A:203:LEU:HD11	2.26	0.51
3:A:137:ILE:HD13	3:A:215:LEU:HD11	1.93	0.51
3:A:204:SER:HB3	3:A:207:GLU:HG3	1.92	0.51
3:B:273:SER:OG	3:B:275:ARG:HB2	2.11	0.51
3:A:166:SER:HB2	3:A:289:TYR:CB	2.40	0.51
3:B:230:ASN:O	3:B:234:ILE:HG22	2.11	0.51
1:C:15:DA:H5'	3:A:155:PRO:HB2	1.93	0.51
3:A:133:ASP:OD2	3:A:300:LYS:NZ	2.44	0.51
3:A:162:CYS:O	3:A:166:SER:N	2.37	0.51
3:A:168:LEU:HD21	3:A:293:LYS:HG2	1.93	0.51
3:B:159:PHE:CZ	3:B:163:LEU:HD13	2.46	0.50
3:B:269:MET:HE2	3:B:288:TYR:CB	2.40	0.50
2:D:3:DA:OP2	2:D:3:DA:H2'	2.11	0.50
1:C:19:DG:H5'	3:B:276:CYS:HG	1.75	0.50
1:C:5:DT:P	3:A:246:LYS:HZ1	2.35	0.49
3:A:200:SER:N	3:A:202:ASP:OD2	2.45	0.49
3:A:226:ILE:HG22	3:A:227:ALA:N	2.26	0.49
3:A:235:TYR:CE2	3:A:239:SER:HB2	2.47	0.49
3:A:127:ILE:HG21	3:A:179:HIS:HA	1.93	0.49
3:A:172:GLN:HA	3:A:172:GLN:HE21	1.77	0.49
3:A:224:PRO:O	3:A:225:ARG:C	2.53	0.49
3:B:274:ALA:C	3:B:276:CYS:H	2.21	0.48
3:A:217:GLN:HA	3:A:220:GLN:HG3	1.96	0.48
3:B:130:PHE:HE2	3:B:221:LYS:O	1.95	0.48
3:A:277:ALA:O	3:A:280:PRO:HD3	2.13	0.48
3:B:209:ARG:HA	3:B:241:GLU:OE2	2.13	0.48
3:A:214:ILE:HD13	3:A:215:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:274:ALA:HA	3:B:280:PRO:CG	2.42	0.48
3:A:259:ILE:HG23	3:A:260:PRO:HD2	1.96	0.48
3:B:209:ARG:C	3:B:211:GLY:N	2.72	0.48
3:B:279:PHE:N	3:B:280:PRO:O	2.46	0.48
3:A:299:LEU:O	3:A:303:GLU:HG3	2.14	0.47
2:D:20:DC:OP2	2:D:20:DC:H6	1.97	0.47
3:B:140:ASN:HA	3:B:191:ASN:CB	2.44	0.47
3:A:152:TYR:HB2	3:A:160:TRP:HE1	1.79	0.47
3:A:235:TYR:HA	3:A:238:PHE:HB3	1.96	0.47
3:B:232:LYS:HE2	3:B:252:PHE:CE1	2.48	0.47
3:A:189:PHE:O	3:A:190:THR:HB	2.14	0.47
3:A:233:CYS:HA	3:A:236:GLU:CB	2.44	0.47
3:B:124:LEU:HD23	3:B:141:PRO:HB3	1.96	0.47
3:B:247:VAL:HG22	3:B:250:LEU:HB2	1.97	0.47
3:B:252:PHE:HD2	3:B:268:VAL:HG12	1.80	0.47
3:A:181:LEU:CD2	3:A:189:PHE:CZ	2.97	0.47
3:A:193:VAL:HG12	3:A:194:GLU:H	1.75	0.47
3:A:172:GLN:HE21	3:A:172:GLN:CA	2.28	0.46
3:A:201:LYS:HB2	3:A:201:LYS:NZ	2.29	0.46
3:B:296:ARG:HD2	3:B:300:LYS:HD3	1.97	0.46
3:A:152:TYR:HB2	3:A:160:TRP:NE1	2.30	0.46
3:A:259:ILE:HG13	3:A:264:THR:HG22	1.96	0.46
3:A:228:VAL:HG11	3:A:269:MET:HE2	1.98	0.46
3:B:254:LEU:HD12	3:B:255:GLN:N	2.29	0.46
1:C:18:DA:N6	2:D:4:DC:H42	2.13	0.46
3:A:181:LEU:HD22	3:A:189:PHE:CZ	2.51	0.46
2:D:21:DT:OP2	2:D:21:DT:H6	1.98	0.46
3:B:291:LYS:HA	3:B:291:LYS:CE	2.38	0.46
3:A:206:LYS:O	3:A:209:ARG:N	2.47	0.46
3:A:261:ASP:O	3:A:262:THR:HG22	2.14	0.46
3:B:304:ARG:H	3:B:304:ARG:NE	2.14	0.46
3:B:213:ARG:NH1	3:B:213:ARG:CB	2.73	0.46
3:B:278:GLN:HG3	3:B:279:PHE:O	2.16	0.46
2:D:8:DT:C2'	2:D:9:DC:O5'	2.62	0.46
3:B:304:ARG:H	3:B:304:ARG:HE	1.63	0.46
3:B:197:THR:CB	3:B:198:PRO:CD	2.94	0.45
3:B:165:MET:HE2	3:B:165:MET:HA	1.96	0.45
3:B:259:ILE:CG1	3:B:264:THR:HB	2.46	0.45
3:B:279:PHE:N	3:B:279:PHE:CD2	2.84	0.45
3:B:140:ASN:ND2	3:B:195:ARG:O	2.40	0.45
3:B:229:PHE:N	3:B:229:PHE:CD1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:DG:H2''	1:C:15:DA:C8	2.51	0.45
3:A:160:TRP:O	3:A:172:GLN:NE2	2.32	0.45
3:A:166:SER:HB2	3:A:289:TYR:HB3	1.96	0.45
2:D:17:DG:H4'	2:D:18:DA:OP1	2.17	0.45
3:B:255:GLN:HB3	3:B:256:PRO:HD2	1.99	0.45
1:C:18:DA:N6	2:D:4:DC:N4	2.65	0.45
3:A:248:LYS:HG3	3:A:249:ASN:N	2.31	0.45
3:A:143:LEU:HG	3:A:198:PRO:HA	1.99	0.45
1:C:22:DG:H22	2:D:1:DC:C1'	2.31	0.44
3:A:185:TYR:O	3:A:186:GLY:C	2.58	0.44
1:C:10:DA:H2''	1:C:11:DC:O5'	2.17	0.44
3:A:174:ASN:O	3:A:176:MET:N	2.50	0.44
3:A:206:LYS:O	3:A:207:GLU:C	2.60	0.44
3:A:233:CYS:HA	3:A:236:GLU:HB3	1.99	0.44
3:A:161:LYS:HA	3:A:172:GLN:OE1	2.17	0.44
2:D:12:DG:H4'	3:A:271:SER:OG	2.18	0.44
3:B:212:GLY:HA2	3:B:215:LEU:HB3	2.00	0.44
3:A:259:ILE:HG13	3:A:264:THR:CG2	2.48	0.44
3:B:267:TYR:C	3:B:267:TYR:CD2	2.96	0.44
3:A:172:GLN:HE21	3:A:173:LEU:N	2.16	0.44
3:B:166:SER:C	3:B:168:LEU:H	2.26	0.44
3:B:272:SER:HA	3:B:285:LYS:HE3	2.00	0.43
3:A:304:ARG:NH1	3:A:304:ARG:HG3	2.33	0.43
1:C:19:DG:O6	2:D:3:DA:N6	2.51	0.43
3:A:200:SER:C	3:A:202:ASP:N	2.73	0.43
3:A:230:ASN:OD1	3:A:271:SER:HA	2.18	0.43
3:A:263:GLU:OE1	3:A:263:GLU:CA	2.67	0.43
3:B:200:SER:C	3:B:202:ASP:H	2.25	0.43
3:B:232:LYS:O	3:B:233:CYS:C	2.60	0.43
3:B:252:PHE:CB	3:B:288:TYR:CE2	3.01	0.43
1:C:22:DG:N2	2:D:1:DC:C2	2.87	0.43
3:A:232:LYS:O	3:A:234:ILE:N	2.51	0.43
1:C:13:DT:H2'	1:C:14:DG:C8	2.54	0.43
3:A:228:VAL:HG21	3:A:292:LEU:CD2	2.49	0.43
2:D:6:DG:C2	2:D:7:DC:C2	3.07	0.43
3:B:152:TYR:HB2	3:B:160:TRP:HE1	1.84	0.43
3:B:280:PRO:O	3:B:281:ARG:HB2	2.19	0.43
3:B:225:ARG:C	3:B:226:ILE:HG13	2.44	0.42
3:A:294:ASP:O	3:A:295:LEU:C	2.59	0.42
3:A:304:ARG:HH11	3:A:304:ARG:CG	2.32	0.42
3:B:154:GLY:C	3:B:156:GLY:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:162:CYS:O	3:A:163:LEU:C	2.62	0.42
3:A:229:PHE:N	3:A:229:PHE:CD1	2.88	0.42
1:C:22:DG:H8	1:C:22:DG:P	2.42	0.42
3:A:129:THR:O	3:A:222:TYR:CD2	2.73	0.42
2:D:8:DT:H2'	2:D:9:DC:O4'	2.19	0.42
3:A:298:GLN:O	3:A:300:LYS:N	2.53	0.42
3:A:268:VAL:CG1	3:A:269:MET:H	1.97	0.42
3:B:143:LEU:O	3:B:144:MET:C	2.63	0.42
3:B:231:GLY:O	3:B:232:LYS:C	2.62	0.41
3:B:133:ASP:O	3:B:225:ARG:HB2	2.20	0.41
1:C:6:DC:H2''	1:C:7:DT:O5'	2.20	0.41
3:B:235:TYR:O	3:B:236:GLU:C	2.63	0.41
3:A:181:LEU:O	3:A:182:PRO:O	2.38	0.41
3:A:260:PRO:O	3:A:261:ASP:CB	2.68	0.41
3:B:173:LEU:HB3	3:B:177:ASP:OD1	2.20	0.41
3:B:291:LYS:O	3:B:292:LEU:C	2.62	0.41
1:C:22:DG:H8	1:C:22:DG:O5'	2.03	0.41
3:B:215:LEU:O	3:B:216:VAL:C	2.62	0.41
3:B:276:CYS:SG	3:B:277:ALA:N	2.92	0.41
3:A:172:GLN:HE21	3:A:173:LEU:H	1.69	0.41
3:B:232:LYS:NZ	3:B:250:LEU:O	2.53	0.41
1:C:14:DG:H2''	1:C:15:DA:H8	1.86	0.41
3:A:256:PRO:HB2	3:A:257:HIS:ND1	2.36	0.41
3:A:303:GLU:O	3:A:304:ARG:C	2.63	0.41
3:B:168:LEU:HD12	3:B:289:TYR:HD2	1.85	0.41
3:B:252:PHE:CE2	3:B:270:PRO:HA	2.56	0.41
3:A:137:ILE:CD1	3:A:215:LEU:HD11	2.51	0.41
3:A:152:TYR:N	3:A:153:PRO:HD3	2.36	0.40
3:A:279:PHE:O	3:A:280:PRO:C	2.63	0.40
3:B:178:ASP:OD1	3:B:179:HIS:N	2.54	0.40
3:B:292:LEU:O	3:B:293:LYS:C	2.64	0.40
1:C:9:DT:H2''	1:C:10:DA:OP2	2.20	0.40
2:D:22:DG:H2''	2:D:23:DT:OP2	2.21	0.40
3:A:292:LEU:HD12	3:A:292:LEU:HA	1.74	0.40
1:C:3:DG:H2''	1:C:4:DC:OP2	2.20	0.40
3:A:184:LYS:HG2	3:A:185:TYR:CE2	2.56	0.40
3:B:237:ILE:HG22	3:B:238:PHE:N	2.36	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	
3	A	180/204 (88%)	128 (71%)	39 (22%)	13 (7%)	1	2
3	B	180/204 (88%)	147 (82%)	26 (14%)	7 (4%)	2	8
All	All	360/408 (88%)	275 (76%)	65 (18%)	20 (6%)	1	4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	182	PRO
3	A	183	GLY
3	A	200	SER
3	A	206	LYS
3	A	207	GLU
3	B	140	ASN
3	B	280	PRO
3	A	299	LEU
3	B	200	SER
3	B	281	ARG
3	B	241	GLU
3	A	201	LYS
3	A	261	ASP
3	B	210	GLU
3	A	141	PRO
3	A	301	GLY
3	A	140	ASN
3	A	302	ILE
3	A	280	PRO
3	B	182	PRO

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	
3	A	160/178 (90%)	128 (80%)	32 (20%)	1	4
3	B	160/178 (90%)	134 (84%)	26 (16%)	2	8
All	All	320/356 (90%)	262 (82%)	58 (18%)	2	6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	123	THR
3	A	139	ILE
3	A	163	LEU
3	A	172	GLN
3	A	173	LEU
3	A	187	ILE
3	A	192	MET
3	A	198	PRO
3	A	201	LYS
3	A	204	SER
3	A	214	ILE
3	A	220	GLN
3	A	237	ILE
3	A	240	LYS
3	A	245	VAL
3	A	246	LYS
3	A	247	VAL
3	A	250	LEU
3	A	251	GLU
3	A	258	LYS
3	A	262	THR
3	A	263	GLU
3	A	264	THR
3	A	269	MET
3	A	275	ARG
3	A	278	GLN
3	A	286	VAL
3	A	293	LYS
3	A	298	GLN
3	A	300	LYS
3	A	302	ILE

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Mol	Chain	Res	Type
3	A	304	ARG
3	B	123	THR
3	B	139	ILE
3	B	157	ASN
3	B	163	LEU
3	B	173	LEU
3	B	184	LYS
3	B	192	MET
3	B	196	THR
3	B	206	LYS
3	B	213	ARG
3	B	214	ILE
3	B	217	GLN
3	B	234	ILE
3	B	237	ILE
3	B	241	GLU
3	B	247	VAL
3	B	249	ASN
3	B	251	GLU
3	B	258	LYS
3	B	269	MET
3	B	278	GLN
3	B	279	PHE
3	B	280	PRO
3	B	291	LYS
3	B	298	GLN
3	B	304	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	191	ASN
3	A	220	GLN
3	A	249	ASN
3	A	298	GLN
3	B	150	HIS
3	B	157	ASN
3	B	158	HIS
3	B	172	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	3DR	D	11	2	8,11,12	0.52	0	7,14,17	1.44	1 (14%)

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	3DR	D	11	2	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	11	3DR	O4'-C4'-C3'	2.97	108.09	103.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	11	3DR	1	0

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	C	23/23 (100%)	0.67	2 (8%) 16 11	77, 143, 198, 202	0
2	D	22/23 (95%)	1.04	4 (18%) 3 2	88, 151, 198, 203	0
3	A	182/204 (89%)	0.37	6 (3%) 49 39	72, 94, 108, 117	0
3	B	182/204 (89%)	0.47	9 (4%) 35 27	78, 99, 135, 154	0
All	All	409/454 (90%)	0.47	21 (5%) 33 25	72, 97, 162, 203	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	275	ARG	5.2
3	B	275	ARG	5.1
2	D	12	DG	4.2
3	A	274	ALA	3.8
1	C	23	DA	3.4
2	D	23	DT	3.2
3	B	274	ALA	2.9
2	D	13	DT	2.9
3	B	302	ILE	2.8
3	A	302	ILE	2.7
3	B	299	LEU	2.7
3	A	155	PRO	2.7
1	C	1	DC	2.7
3	B	165	MET	2.6
3	A	208	PHE	2.6
3	B	155	PRO	2.6
3	B	156	GLY	2.4
2	D	10	DA	2.2
3	B	246	LYS	2.2
3	A	203	LEU	2.2
3	B	235	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
2	3DR	D	11	11/12	0.82	0.28	124,131,137,140	0

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.