Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID	:	2RBA
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

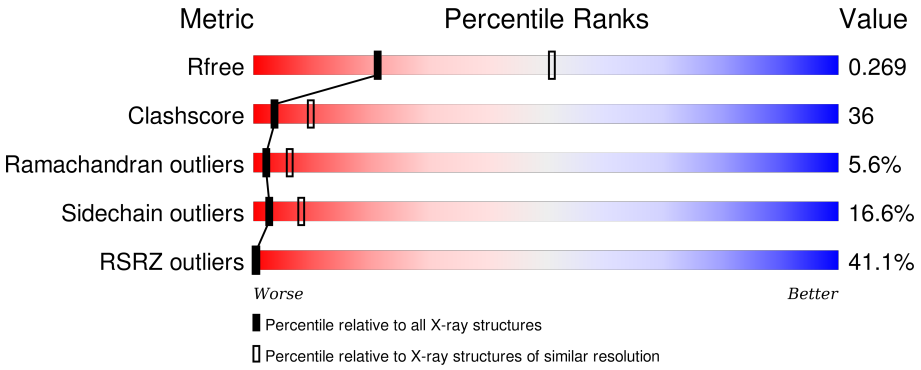
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.79 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	C	23	39% 13% 39% 48%
2	D	23	39% • 17% 78%
3	A	204	33% 33% 41% 14% • 11%
3	B	204	41% 43% 38% 7% • 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*DGP*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*DGP*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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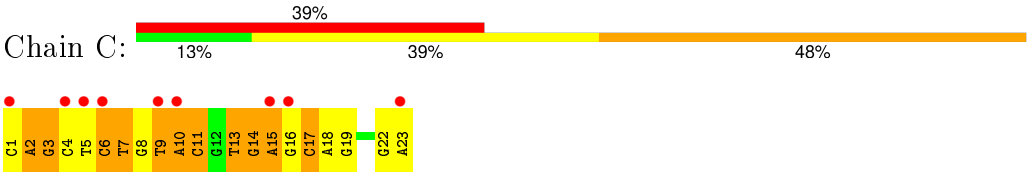
Chain	Residue	Modelled	Actual	Comment	Reference
B	107	HIS	-	EXPRESSION TAG	UNP Q13569
B	108	MET	-	EXPRESSION TAG	UNP Q13569
B	109	ALA	-	EXPRESSION TAG	UNP Q13569
B	110	SER	-	EXPRESSION TAG	UNP Q13569

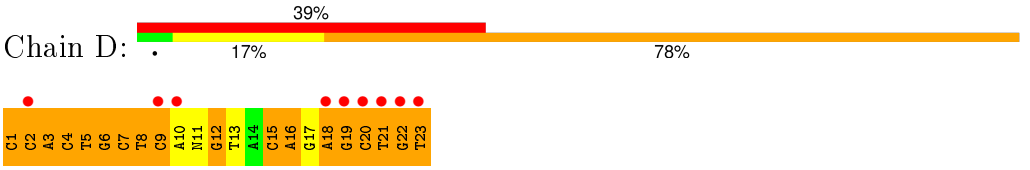
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

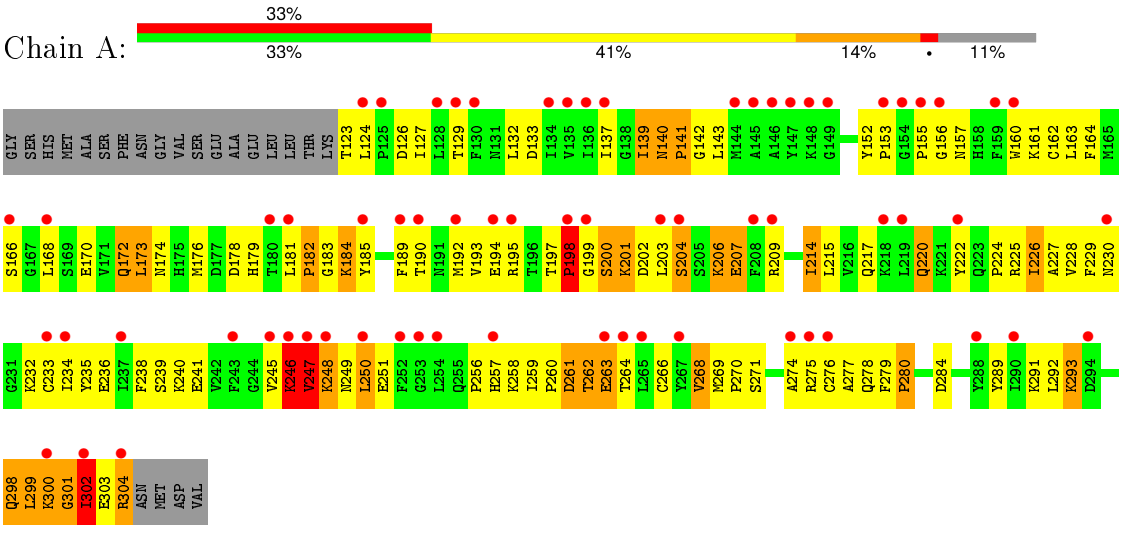
• Molecule 1: DNA (5'-D(*DCP*DAP*DGP*DCP*DTP*DCP*DTP*DGP*DTP*DAP*DCP*DGP*DTP*DGP*DAP*DGP*DCP*DAP*DGP*DTP*DGP*DGP*DA)-3')



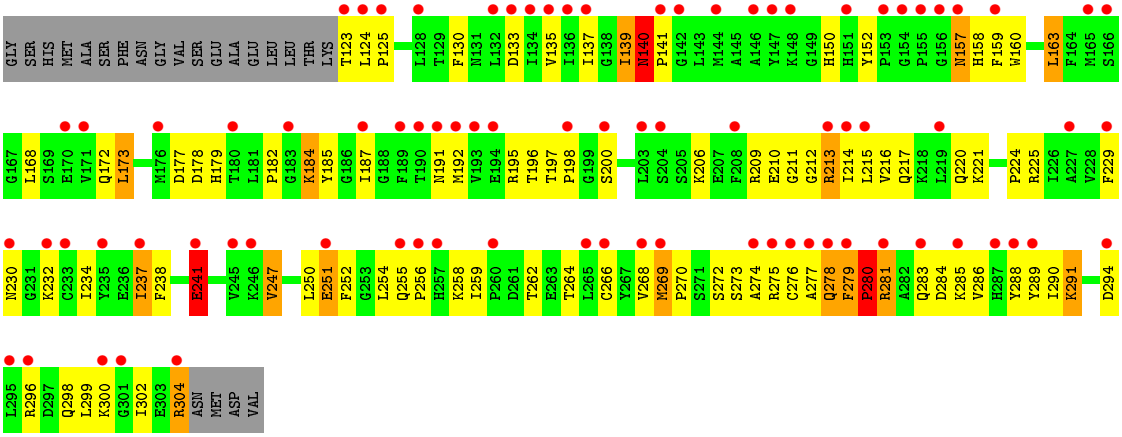
• Molecule 2: DNA (5'-D(*DCP*DCP*DAP*DCP*DTP*DGP*DCP*DTP*DCP*DAP*(3DR)P*DGP*DTP*DAP*DCP*DAP*DGP*DAP*DGP*DCP*DTP*DGP*DT)-3')



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



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


GLY SER HIS MET ALA SER PHE ASN GLY VAL SER GLU ALA GLU LEU LEU THR LYS T123 L124 P125 L128 T129 F130 N131 L132 D133 I134 V135 I136 I137 G138 I139 N140 P141 G142 L143 M144 A145 A146 Y147 K148 G149 H150 H151 Y152 P153 G154 P155 G156 N157 H158 F159 W160 L163 F164 M165 S166
G167 L168 S169 E170 V171 Q172 L173 M176 D177 D178 H179 T180 L181 P182 G183 K184 Y185 G186 I187 G188 F189 T190 N191 M192 V193 E194 R195 T196 T197 P198 G199 S200 L203 S204 S205 K206 E207 F208 R209 E210 G211 G212 R213 I214 L215 V216 Q217 K218 L219 Q220 K221 P224 R225 I226 A227 V228 F229
N230 G231 K232 C233 I234 Y235 E236 I237 F238 E241 V245 K246 V247 L250 E251 F252 G253 L254 Q255 P256 H257 K258 I259 P260 D261 T262 E263 T264 L265 C266 Y267 V268 M269 P270 S271 S272 S273 A274 R275 C276 A277 Q278 F279 P280 R281 A282 Q283 D284 K285 V286 H287 Y288 Y289 I290 K291 D294
L295 R296 D297 Q298 L299 K300 G301 I302 E303 R304 ASN MET ASP VAL

4 Data and refinement statistics (i)

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 35.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.79) 97.6 (35.10-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [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 (5.39%)	DCC
Wilson B-factor (Å^2)	95.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 178.9	EDS
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 20503 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.10	0/531	1.98	23/819 (2.8%)
2	D	1.15	0/497	2.29	42/762 (5.5%)
3	A	1.18	6/1495 (0.4%)	1.21	8/2015 (0.4%)
3	B	0.91	1/1495 (0.1%)	0.93	0/2015
All	All	1.07	7/4018 (0.2%)	1.46	73/5611 (1.3%)

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
3	A	1	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	LYS	CD-CE	12.25	1.81	1.51
3	A	268	VAL	CA-CB	-7.35	1.39	1.54
3	B	266	CYS	CB-SG	-6.82	1.70	1.82
3	A	247	VAL	C-O	6.78	1.36	1.23
3	A	266	CYS	CB-SG	-6.59	1.71	1.82
3	A	184	LYS	CE-NZ	5.48	1.62	1.49
3	A	184	LYS	CD-CE	5.42	1.64	1.51

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	12	DG	O4'-C4'-C3'	-12.97	98.22	106.00
1	C	17	DC	O4'-C1'-N1	12.81	116.97	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	7	DC	O4'-C1'-N1	10.12	115.08	108.00
1	C	15	DA	O4'-C1'-N9	-8.76	101.87	108.00
2	D	4	DC	O4'-C1'-N1	8.59	114.01	108.00
2	D	15	DC	O4'-C1'-N1	8.19	113.73	108.00
2	D	10	DA	O4'-C1'-N9	7.78	113.45	108.00
3	A	302	ILE	N-CA-C	7.69	131.75	111.00
2	D	19	DG	O4'-C1'-N9	7.45	113.21	108.00
2	D	2	DC	P-O3'-C3'	7.30	128.46	119.70
1	C	10	DA	P-O3'-C3'	7.24	128.39	119.70
2	D	8	DT	P-O3'-C3'	7.17	128.30	119.70
1	C	11	DC	O4'-C1'-N1	7.10	112.97	108.00
2	D	8	DT	C2-N3-C4	-7.08	122.95	127.20
2	D	4	DC	C2-N3-C4	7.05	123.42	119.90
1	C	15	DA	P-O3'-C3'	6.95	128.04	119.70
2	D	1	DC	C1'-O4'-C4'	-6.90	103.20	110.10
3	A	178	ASP	CB-CG-OD2	-6.86	112.13	118.30
2	D	15	DC	C1'-O4'-C4'	-6.79	103.31	110.10
2	D	18	DA	P-O3'-C3'	6.63	127.65	119.70
2	D	8	DT	C5-C4-O4	-6.50	120.35	124.90
2	D	13	DT	C5-C4-O4	-6.35	120.45	124.90
2	D	5	DT	N3-C4-O4	6.30	123.68	119.90
2	D	9	DC	C1'-O4'-C4'	-6.29	103.81	110.10
2	D	16	DA	C5-C6-N1	6.24	120.82	117.70
3	A	226	ILE	CB-CA-C	-6.24	99.12	111.60
1	C	6	DC	C2-N3-C4	6.20	123.00	119.90
1	C	9	DT	P-O3'-C3'	6.18	127.12	119.70
2	D	12	DG	P-O3'-C3'	6.16	127.10	119.70
1	C	14	DG	O4'-C1'-N9	-6.14	103.70	108.00
2	D	13	DT	O4'-C1'-C2'	-6.12	101.01	105.90
1	C	7	DT	C4-C5-C7	6.04	122.63	119.00
1	C	23	DA	C5-C6-N1	6.01	120.70	117.70
2	D	16	DA	C5-C6-N6	-5.99	118.91	123.70
3	A	246	LYS	CD-CE-NZ	-5.96	97.99	111.70
2	D	4	DC	C3'-C2'-C1'	-5.95	95.36	102.50
2	D	21	DT	O4'-C4'-C3'	-5.93	102.13	104.50
2	D	4	DC	C5-C4-N4	5.88	124.32	120.20
2	D	15	DC	N1-C2-O2	5.88	122.43	118.90
2	D	9	DC	P-O3'-C3'	5.86	126.73	119.70
2	D	16	DA	C6-N1-C2	-5.84	115.09	118.60
1	C	11	DC	C5-C4-N4	5.84	124.29	120.20
2	D	3	DA	C3'-C2'-C1'	-5.80	95.54	102.50
2	D	8	DT	C6-C5-C7	-5.76	119.44	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	7	DC	N1-C2-O2	5.73	122.34	118.90
3	A	126	ASP	CB-CG-OD2	5.67	123.41	118.30
2	D	4	DC	C1'-O4'-C4'	-5.66	104.44	110.10
3	A	302	ILE	C-N-CA	5.64	135.81	121.70
2	D	12	DG	C6-N1-C2	-5.63	121.72	125.10
1	C	2	DA	P-O3'-C3'	5.62	126.44	119.70
2	D	6	DG	P-O3'-C3'	5.55	126.37	119.70
1	C	23	DA	C6-N1-C2	-5.46	115.32	118.60
3	A	302	ILE	CA-C-N	5.39	129.06	117.20
2	D	23	DT	C5-C4-O4	-5.39	121.13	124.90
2	D	12	DG	C4-C5-N7	-5.38	108.65	110.80
1	C	3	DG	O4'-C1'-N9	5.30	111.71	108.00
3	A	178	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	14	DG	P-O3'-C3'	5.26	126.01	119.70
1	C	13	DT	C1'-O4'-C4'	-5.21	104.89	110.10
2	D	20	DC	O4'-C4'-C3'	-5.21	102.42	104.50
1	C	9	DT	C1'-O4'-C4'	-5.18	104.92	110.10
1	C	6	DC	N1-C2-O2	5.17	122.00	118.90
2	D	22	DG	O4'-C1'-N9	5.17	111.62	108.00
2	D	8	DT	C4-C5-C7	5.13	122.08	119.00
1	C	11	DC	N3-C4-N4	-5.13	114.41	118.00
1	C	7	DT	C5-C4-O4	-5.13	121.31	124.90
1	C	3	DG	P-O3'-C3'	5.12	125.84	119.70
2	D	8	DT	O4'-C1'-N1	5.07	111.55	108.00
2	D	13	DT	C1'-O4'-C4'	-5.06	105.04	110.10
2	D	21	DT	O4'-C1'-N1	5.06	111.54	108.00
2	D	5	DT	C5-C4-O4	-5.03	121.38	124.90
1	C	7	DT	P-O3'-C3'	5.02	125.72	119.70
1	C	6	DC	O4'-C1'-N1	5.01	111.51	108.00

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	27	0
2	D	456	0	257	28	0
3	A	1458	0	1469	114	0
3	B	1458	0	1469	110	0
All	All	3845	0	3455	263	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 36.

All (263) 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:CE	3:A:246:LYS:CD	1.81	1.55
3:A:301:GLY:CA	3:A:303:GLU:HB2	1.68	1.22
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	1.36	1.06
3:B:279:PHE:HB3	3:B:284:ASP:HB2	1.34	1.05
3:B:213:ARG:HB2	3:B:213:ARG:HH11	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:B:158:HIS:HD2	3:B:285:LYS:HZ3	1.09	0.97
3:A:301:GLY:HA2	3:A:303:GLU:HB2	0.97	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:H	3:B:139:ILE:HD12	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:133:ASP:HA	3:B:225:ARG:HD2	1.62	0.82
3:B:269:MET:HE3	3:B:269:MET:HA	1.60	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:199:GLY:HA3	3:A:200:SER:HB2	1.71	0.72
2:D:12:DG:C8	2:D:12:DG:H5"	2.25	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:HA	3:B:291:LYS:HE2	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
3:B:139:ILE:HD12	3:B:139:ILE:N	2.07	0.68
2:D:19:DG:H2"	2:D:20:DC:OP2	1.93	0.68
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
3:A:301:GLY:N	3:A:303:GLU:HB2	2.09	0.67
1:C:1:DC:H2"	1:C:2:DA:N7	2.10	0.67
3:B:274:ALA:HA	3:B:280:PRO:HG3	1.77	0.66
3:B:158:HIS:CD2	3:B:285:LYS:HZ3	2.01	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:NH1	3:B:213:ARG:HB2	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:209:ARG:HH11	3:B:209:ARG:HG3	1.61	0.64
3:B:139:ILE:O	3:B:140:ASN:HB3	1.96	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:139:ILE:CD1	3:B:139:ILE:H	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	3:B:288:TYR:HB3	1.82	0.60
3:B:269:MET:CE	3:B:288:TYR:CB	2.74	0.60
3:B:276:CYS:CB	3:B:280:PRO:HG2	2.31	0.60
3:A:198:PRO:CB	3:A:199:GLY:O	2.46	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
3:B:197:THR:HB	3:B:198:PRO:CD	2.33	0.59
1:C:8:DG:H2"	1:C:9:DT:O5'	2.02	0.59
3:B:185:TYR:O	3:B:187:ILE:HG13	2.02	0.59
3:B:135:VAL:HG12	3:B:135:VAL:O	2.02	0.59
3:B:158:HIS:CD2	3:B:285:LYS:HZ1	2.21	0.59
3:B:283:GLN:HA	3:B:286:VAL:CG2	2.34	0.58
3:A:193:VAL:CG1	3:A:194:GLU:N	2.65	0.58
3:B:232:LYS:HE2	3:B:252:PHE:CZ	2.39	0.58
3:A:199:GLY:HA3	3:A:200:SER:CB	2.34	0.58
3:A:142:GLY:HA2	3:A:197:THR:O	2.05	0.57
3:B:269:MET:HE2	3:B:270:PRO:CD	2.35	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:B:252:PHE:HB2	3:B:288:TYR:HE2	1.70	0.56
3:A:166:SER:CB	3:A:289:TYR:HB3	2.34	0.56
3:A:279:PHE:HD2	3:A:284:ASP:O	1.88	0.56
3:A:193:VAL:HG11	3:A:203:LEU:HD22	1.87	0.56
3:A:182:PRO:O	3:A:184:LYS:N	2.38	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: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
3:B:269:MET:HE2	3:B:270:PRO:HD2	1.88	0.55
3:A:197:THR:HB	3:A:198:PRO:CD	2.36	0.55
2:D:11:3DR:OP1	3:A:157:ASN:ND2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:200:SER:C	3:A:202:ASP:H	2.11	0.54
3:B:269:MET:HE3	3:B:269:MET:CA	2.33	0.54
3:A:170:GLU:N	3:A:170:GLU:OE1	2.38	0.54
3:A:168:LEU:CD2	3:A:293:LYS:HG2	2.37	0.54
3:B:269:MET:HE1	3:B:288:TYR:CB	2.24	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:276:CYS:HB3	3:B:280:PRO:CD	2.37	0.54
3:B:209:ARG:HG3	3:B:209:ARG:NH1	2.19	0.54
3:B:209:ARG:O	3:B:213:ARG:NH1	2.41	0.53
3:A:139:ILE:HA	3:A:234:ILE:HG21	1.90	0.53
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:B:135:VAL:HG12	3:B:137:ILE:CG1	2.38	0.53
2:D:19:DG:H2'	2:D:19:DG:OP2	2.08	0.53
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: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:B:273:SER:OG	3:B:275:ARG:HB2	2.11	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: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
2:D:3:DA:OP2	2:D:3:DA:H2'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:274:ALA:C	3:A:276:CYS:H	2.15	0.50
3:A:200:SER:N	3:A:202:ASP:OD2	2.45	0.49
3:A:235:TYR:CE2	3:A:239:SER:HB2	2.47	0.49
3:A:226:ILE:HG22	3:A:227:ALA:N	2.26	0.49
3:A:172:GLN:HE21	3:A:172:GLN:HA	1.77	0.49
3:A:127:ILE:HG21	3:A:179:HIS:HA	1.93	0.49
3:B:269:MET:HE2	3:B:288:TYR:CB	2.42	0.49
3:A:291:LYS:O	3:A:292:LEU:C	2.50	0.48
3:A:140:ASN:CG	3:A:203:LEU:HD11	2.32	0.48
3:B:130:PHE:HE2	3:B:221:LYS:O	1.95	0.48
3:A:217:GLN:HA	3:A:220:GLN:HG3	1.96	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:B:274:ALA:HA	3:B:280:PRO:CG	2.42	0.48
3:A:214:ILE:HD13	3:A:215:LEU:N	2.28	0.48
3:A:259:ILE:HG23	3:A:260:PRO:HD2	1.96	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
3:B:140:ASN:HA	3:B:191:ASN:CB	2.44	0.47
2:D:20:DC:H6	2:D:20:DC:OP2	1.97	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:235:TYR:O	3:A:236:GLU:C	2.51	0.47
3:A:174:ASN:C	3:A:174:ASN:OD1	2.52	0.47
3:B:247:VAL:HG22	3:B:250:LEU:HB2	1.97	0.47
3:B:124:LEU:HD23	3:B:141:PRO:HB3	1.96	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: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:CA	3:A:172:GLN:HE21	2.28	0.46
3:B:296:ARG:HD2	3:B:300:LYS:HD3	1.97	0.46
3:A:201:LYS:NZ	3:A:201:LYS:HB2	2.29	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: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
3:B:291:LYS:CE	3:B:291:LYS:HA	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:DT:H6	2:D:21:DT:OP2	1.98	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:NE	3:B:304:ARG:H	2.14	0.46
3:B:278:GLN:HG3	3:B:279:PHE:O	2.16	0.46
3:B:213:ARG:NH1	3:B:213:ARG:CB	2.73	0.46
2:D:8:DT:C2'	2:D:9:DC:O5'	2.62	0.46
3:B:304:ARG:HE	3:B:304:ARG:H	1.63	0.46
3:B:197:THR:CB	3:B:198:PRO:CD	2.94	0.45
3:B:259:ILE:CG1	3:B:264:THR:HB	2.46	0.45
3:B:279:PHE:CD2	3:B:279:PHE:N	2.84	0.45
3:B:140:ASN:ND2	3:B:195:ARG:O	2.40	0.45
3:B:229:PHE:CD1	3:B:229:PHE:N	2.84	0.45
1:C:14:DG:H2"	1:C:15:DA:C8	2.51	0.45
3:A:166:SER:HB2	3:A:289:TYR:HB3	1.96	0.45
3:A:160:TRP:O	3:A:172:GLN:NE2	2.32	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
1:C:10:DA:H2"	1:C:11:DC:O5'	2.17	0.44
3:A:233:CYS:HA	3:A:236:GLU:HB3	1.99	0.44
3:A:174:ASN:O	3:A:176:MET:N	2.50	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:224:PRO:O	3:A:225:ARG:C	2.53	0.44
3:A:259:ILE:HG13	3:A:264:THR:CG2	2.48	0.44
3:B:274:ALA:C	3:B:276:CYS:H	2.21	0.44
3:A:172:GLN:HE21	3:A:173:LEU:N	2.16	0.44
3:B:272:SER:HA	3:B:285:LYS:HE3	2.00	0.43
3:A:304:ARG:HG3	3:A:304:ARG:NH1	2.33	0.43
1:C:19:DG:O6	2:D:3:DA:N6	2.51	0.43
3:A:230:ASN:OD1	3:A:271:SER:HA	2.18	0.43
3:B:252:PHE:CB	3:B:288:TYR:CE2	3.01	0.43
3:B:209:ARG:C	3:B:211:GLY:N	2.72	0.43
3:A:263:GLU:OE1	3:A:263:GLU:CA	2.67	0.43
3:A:232:LYS:O	3:A:234:ILE:N	2.51	0.43
1:C:22:DG:N2	2:D:1:DC:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:280:PRO:O	3:B:281:ARG:HB2	2.19	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:A:304:ARG:CG	3:A:304:ARG:HH11	2.32	0.42
3:A:229:PHE:CD1	3:A:229:PHE:N	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:A:200:SER:C	3:A:202:ASP:N	2.73	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: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:276:CYS:SG	3:B:277:ALA:N	2.92	0.41
1:C:22:DG:O5'	1:C:22:DG:H8	2.03	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
3:B:252:PHE:CE2	3:B:270:PRO:HA	2.56	0.41
3:B:168:LEU:HD12	3:B:289:TYR:HD2	1.85	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:137:ILE:CD1	3:A:215:LEU:HD11	2.51	0.41
3:B:178:ASP:OD1	3:B:179:HIS:N	2.54	0.40
3:A:152:TYR:N	3:A:153:PRO:HD3	2.36	0.40
1:C:9:DT:H2"	1:C:10:DA:OP2	2.20	0.40
3:A:292:LEU:HD12	3:A:292:LEU:HA	1.74	0.40
2:D:22:DG:H2"	2:D:23:DT:OP2	2.21	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 3
3	B	180/204 (88%)	147 (82%)	26 (14%)	7 (4%)	4 12
All	All	360/408 (88%)	275 (76%)	65 (18%)	20 (6%)	2 6

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%)	133 (83%)	27 (17%)	2 7
3	B	160/178 (90%)	134 (84%)	26 (16%)	3 8
All	All	320/356 (90%)	267 (83%)	53 (17%)	3 8

All (53) 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	192	MET
3	A	198	PRO
3	A	204	SER
3	A	214	ILE
3	A	220	GLN
3	A	240	LYS
3	A	245	VAL
3	A	246	LYS
3	A	247	VAL
3	A	248	LYS
3	A	250	LEU
3	A	251	GLU
3	A	258	LYS
3	A	262	THR
3	A	263	GLU
3	A	275	ARG
3	A	278	GLN
3	A	293	LYS
3	A	298	GLN
3	A	300	LYS
3	A	302	ILE
3	A	304	ARG
3	B	123	THR
3	B	139	ILE
3	B	140	ASN
3	B	157	ASN

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Mol	Chain	Res	Type
3	B	163	LEU
3	B	172	GLN
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	237	ILE
3	B	241	GLU
3	B	247	VAL
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

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

Mol	Chain	Res	Type
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
3	B	179	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	7,11,12	0.51	0	8,14,17	0.82	0

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.

There are no bond angle outliers.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	C	23/23 (100%)	1.96	9 (39%) 0 0	77, 143, 198, 202	0
2	D	22/23 (95%)	1.80	9 (40%) 0 0	88, 151, 198, 203	0
3	A	182/204 (89%)	2.11	67 (36%) 0 0	72, 94, 108, 117	0
3	B	182/204 (89%)	2.21	83 (45%) 0 0	78, 99, 135, 154	0
All	All	409/454 (90%)	2.13	168 (41%) 0 0	72, 97, 162, 203	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	203	LEU	14.8
3	B	203	LEU	12.6
3	A	154	GLY	9.9
3	A	147	TYR	9.5
3	A	155	PRO	9.3
3	A	146	ALA	9.0
3	B	274	ALA	8.4
3	B	165	MET	8.2
3	A	274	ALA	7.9
3	B	275	ARG	7.7
3	B	246	LYS	7.7
3	B	278	GLN	7.3
3	A	125	PRO	7.2
3	A	204	SER	7.1
1	C	6	DC	6.8
3	A	149	GLY	6.6
3	A	208	PHE	6.1
3	B	204	SER	6.1
3	B	156	GLY	6.1
2	D	22	DG	5.9
3	B	235	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
3	A	246	LYS	5.8
1	C	16	DG	5.8
3	A	304	ARG	5.8
3	A	275	ARG	5.7
3	B	279	PHE	5.5
3	B	154	GLY	5.4
3	B	166	SER	5.3
3	A	290	ILE	5.3
2	D	23	DT	5.2
3	B	157	ASN	5.1
2	D	21	DT	5.1
3	A	185	TYR	5.0
3	B	192	MET	5.0
3	A	252	PHE	5.0
3	B	155	PRO	4.7
3	B	147	TYR	4.7
3	B	288	TYR	4.6
3	A	245	VAL	4.6
3	A	234	ILE	4.5
3	A	302	ILE	4.5
3	B	266	CYS	4.5
3	B	128	LEU	4.4
3	A	198	PRO	4.4
3	A	254	LEU	4.3
3	A	195	ARG	4.1
1	C	23	DA	4.0
3	A	144	MET	4.0
3	B	148	LYS	4.0
3	A	128	LEU	3.9
3	B	289	TYR	3.9
3	B	219	LEU	3.9
2	D	2	DC	3.9
3	A	222	TYR	3.8
3	B	237	ILE	3.8
3	B	245	VAL	3.8
3	A	219	LEU	3.8
3	A	243	PHE	3.7
1	C	4	DC	3.7
3	A	199	GLY	3.6
3	B	277	ALA	3.6
3	B	214	ILE	3.6
3	A	194	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	156	GLY	3.6
3	B	265	LEU	3.5
3	A	233	CYS	3.4
3	A	257	HIS	3.4
3	B	281	ARG	3.4
3	A	288	TYR	3.3
3	B	123	THR	3.3
3	A	153	PRO	3.3
3	A	145	ALA	3.3
3	B	294	ASP	3.3
3	B	135	VAL	3.3
3	B	124	LEU	3.3
1	C	1	DC	3.3
3	A	276	CYS	3.2
3	A	189	PHE	3.2
3	A	137	ILE	3.2
3	B	187	ILE	3.2
3	B	159	PHE	3.2
2	D	9	DC	3.2
1	C	5	DT	3.2
3	B	132	LEU	3.2
1	C	15	DA	3.1
3	B	136	ILE	3.1
3	B	189	PHE	3.1
3	A	248	LYS	3.0
3	A	247	VAL	3.0
1	C	9	DT	3.0
3	B	304	ARG	3.0
3	B	230	ASN	3.0
3	B	251	GLU	3.0
3	B	256	PRO	3.0
3	B	260	PRO	3.0
2	D	10	DA	2.9
3	B	171	VAL	2.9
3	B	300	LYS	2.8
3	A	159	PHE	2.8
2	D	18	DA	2.8
3	A	192	MET	2.8
3	B	257	HIS	2.7
3	A	168	LEU	2.7
3	B	193	VAL	2.7
3	B	296	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	10	DA	2.7
3	B	141	PRO	2.6
3	A	218	LYS	2.6
3	B	146	ALA	2.6
3	A	263	GLU	2.6
3	B	269	MET	2.6
3	B	151	HIS	2.6
3	B	190	THR	2.5
3	A	124	LEU	2.5
3	B	295	LEU	2.5
3	B	180	THR	2.5
3	B	301	GLY	2.5
3	A	129	THR	2.5
3	B	215	LEU	2.5
3	B	176	MET	2.5
3	B	134	ILE	2.5
2	D	19	DG	2.5
3	B	125	PRO	2.5
3	B	208	PHE	2.4
3	B	268	VAL	2.4
3	B	144	MET	2.4
3	B	213	ARG	2.4
3	A	250	LEU	2.4
3	A	300	LYS	2.4
3	B	198	PRO	2.4
2	D	20	DC	2.4
3	B	276	CYS	2.4
3	A	130	PHE	2.3
3	A	237	ILE	2.3
3	A	265	LEU	2.3
3	A	166	SER	2.3
3	B	227	ALA	2.3
3	B	241	GLU	2.3
3	B	137	ILE	2.3
3	A	136	ILE	2.3
3	A	181	LEU	2.3
3	B	285	LYS	2.3
3	A	267	TYR	2.2
3	B	232	LYS	2.2
3	A	264	THR	2.2
3	A	294	ASP	2.2
3	B	194	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	180	THR	2.2
3	A	134	ILE	2.1
3	B	287	HIS	2.1
3	B	233	CYS	2.1
3	A	148	LYS	2.1
3	A	135	VAL	2.1
3	A	190	THR	2.1
3	A	253	GLY	2.1
3	A	160	TRP	2.1
3	A	230	ASN	2.1
3	B	153	PRO	2.1
3	B	200	SER	2.1
3	B	283	GLN	2.1
3	B	142	GLY	2.1
3	B	255	GLN	2.0
3	B	170	GLU	2.0
3	B	183	GLY	2.0
3	B	191	ASN	2.0
3	A	209	ARG	2.0
3	B	133	ASP	2.0
3	B	229	PHE	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	3DR	D	11	11/12	0.45	0.60	-	124,131,137,140	0

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.