Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2016 – 11:18 AM GMT

PDB ID	:	5BTN
Title	:	Crystal structure of a topoisomerase II complex
Authors	:	Blower, T.R.; Williamson, B.H.; Kerns, R.J.; Berger, J.M.
Deposited on	:	2015-06-03
Resolution	:	2.50 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 (i) symbol.

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

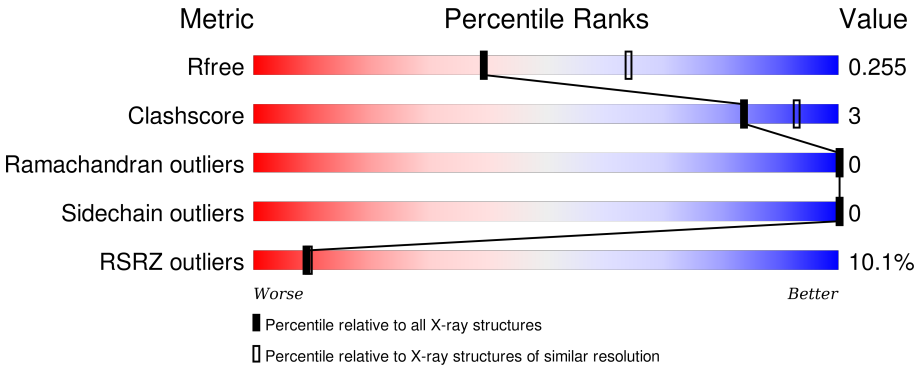
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	A	503	7% 94%
1	C	503	12% 92% 5%
2	B	253	9% 92% 5%
2	D	253	6% 90% 8%
3	E	24	25% 58% 29% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	24	21% 75% 13% 13%
4	F	24	29% 63% 25% 13%
4	G	24	25% 67% 21% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PTR	A	129	-	-	X	-
1	PTR	C	129	-	-	X	-
6	8MX	G	101	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26010 atoms, of which 12525 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	487	Total	C	H	N	O	P	S	0	1	0
			7693	2388	3854	704	733	1	13			
1	C	487	Total	C	H	N	O	P	S	0	1	0
			7690	2388	3851	704	733	1	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	SER	ALA	engineered mutation	UNP P9WG47
A	501	ILE	-	expression tag	UNP P9WG47
A	502	GLY	-	expression tag	UNP P9WG47
A	503	SER	-	expression tag	UNP P9WG47
A	504	GLY	-	expression tag	UNP P9WG47
C	90	SER	ALA	engineered mutation	UNP P9WG47
C	501	ILE	-	expression tag	UNP P9WG47
C	502	GLY	-	expression tag	UNP P9WG47
C	503	SER	-	expression tag	UNP P9WG47
C	504	GLY	-	expression tag	UNP P9WG47

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	245	Total	C	H	N	O	S	0	0	0
			3906	1217	1974	348	360	7			
2	D	247	Total	C	H	N	O	S	0	0	0
			3930	1224	1984	351	364	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	423	SER	-	expression tag	UNP P9WG45
B	424	ASN	-	expression tag	UNP P9WG45

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	425	ALA	-	expression tag	UNP P9WG45
D	423	SER	-	expression tag	UNP P9WG45
D	424	ASN	-	expression tag	UNP P9WG45
D	425	ALA	-	expression tag	UNP P9WG45

- Molecule 3 is a DNA chain called DNA substrate 24-mer GGTCATGAATGACTATGCAC GTAA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	21	Total 620	C 196	H 210	N 74	O 120	P 20	0	21	0
3	H	21	Total 616	C 196	H 206	N 74	O 120	P 20	0	21	0

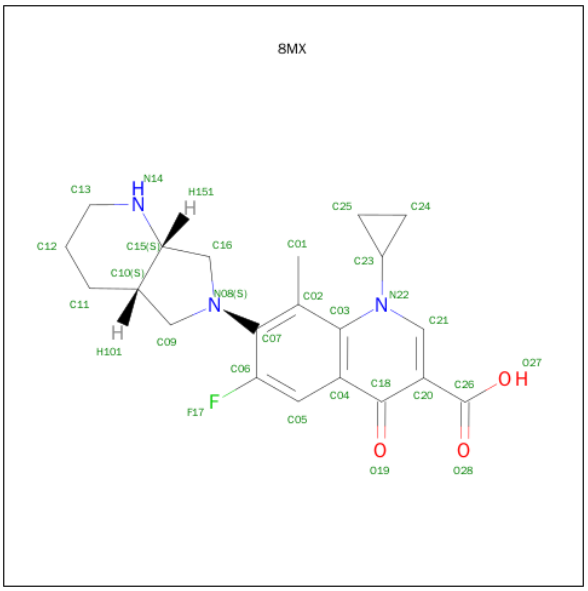
- Molecule 4 is a DNA chain called DNA substrate 24-mer TTACGTGCATAGTCATTCAT GACC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	21	Total 612	C 196	H 202	N 74	O 120	P 20	0	21	0
4	G	21	Total 608	C 196	H 198	N 74	O 120	P 20	0	21	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0
5	D	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	E	1	Total 1	Mg 1	0	0

- Molecule 6 is 1-cyclopropyl-6-fluoro-8-methyl-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyri din-6-yl]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (three-letter code: 8MX) (formula: $C_{21}H_{24}FN_3O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	G	1	Total	C	F	H	N	O	0	0
			51	21	1	23	3	3		
6	H	1	Total	C	F	H	N	O	0	0
			51	21	1	23	3	3		

- Molecule 7 is water.

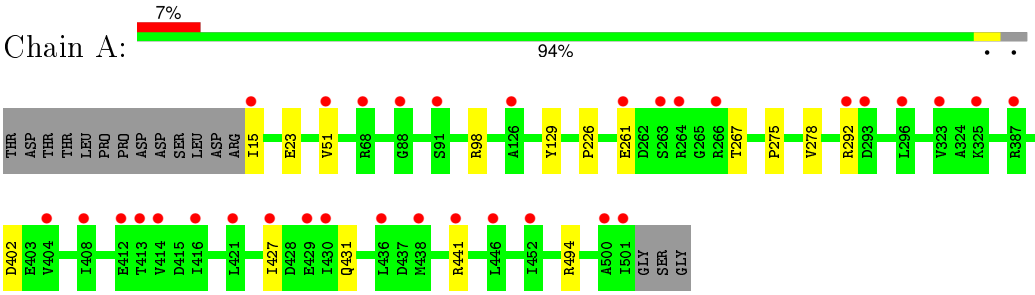
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	100	Total	O	0	0
			100	100		
7	B	31	Total	O	0	0
			31	31		
7	C	41	Total	O	0	0
			41	41		
7	D	29	Total	O	0	0
			29	29		
7	E	6	Total	O	0	0
			6	6		
7	F	5	Total	O	0	0
			5	5		
7	G	7	Total	O	0	0
			7	7		
7	H	10	Total	O	0	0
			10	10		

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.

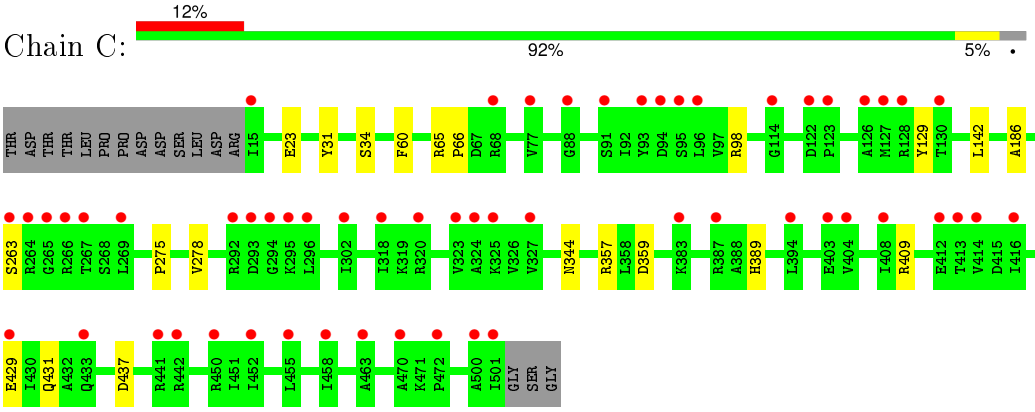
- Molecule 1: DNA gyrase subunit A

Chain A:



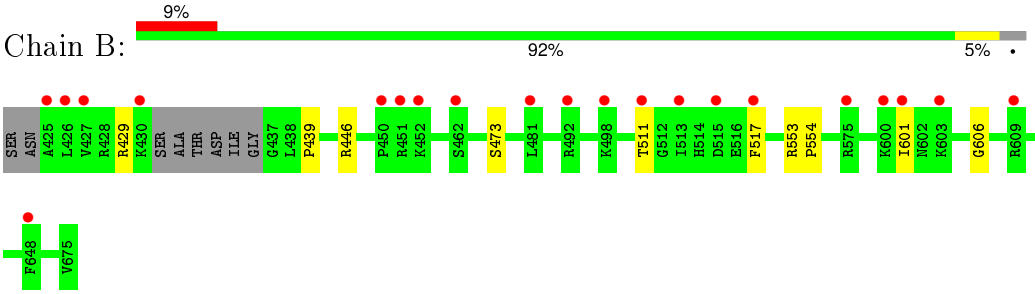
- Molecule 1: DNA gyrase subunit A

Chain C:



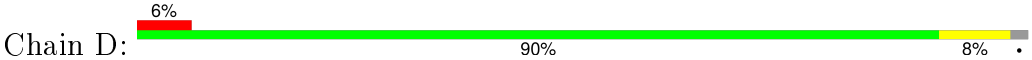
- Molecule 2: DNA gyrase subunit B

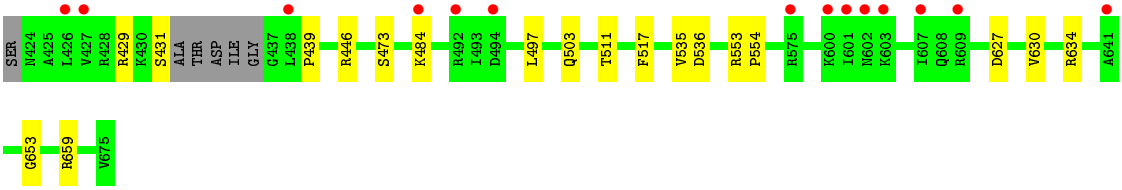
Chain B:



- Molecule 2: DNA gyrase subunit B

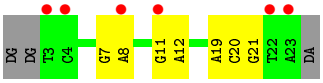
Chain D:





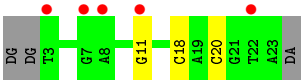
• Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA

Chain E:



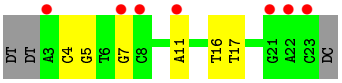
• Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA

Chain H:



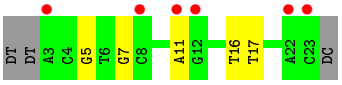
• Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC

Chain F:



• Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.34Å 82.91Å 129.08Å 90.00° 108.78° 90.00°	Depositor
Resolution (Å)	49.65 – 2.50 49.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.65-2.50) 94.3 (49.19-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.251 0.235 , 0.255	Depositor DCC
R_{free} test set	3566 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 70976 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26010	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: MG, 8MX, PTR

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	0.21	0/3882	0.40	0/5254
1	C	0.21	0/3882	0.39	0/5254
2	B	0.21	0/1960	0.38	0/2634
2	D	0.22	0/1974	0.38	0/2653
3	E	0.56	0/458	0.95	0/704
3	H	0.53	0/458	0.97	0/704
4	F	0.53	0/458	0.94	0/704
4	G	0.51	0/458	0.93	0/704
All	All	0.28	0/13530	0.51	0/18611

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3839	3854	3853	24	0
1	C	3839	3851	3853	21	0
2	B	1932	1974	1973	7	0
2	D	1946	1984	1984	14	0
3	E	410	210	210	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	410	206	206	5	0
4	F	410	202	202	7	0
4	G	410	198	198	7	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	G	28	23	0	1	0
6	H	28	23	0	2	0
7	A	100	0	0	2	0
7	B	31	0	0	0	0
7	C	41	0	0	0	0
7	D	29	0	0	0	0
7	E	6	0	0	1	0
7	F	5	0	0	0	0
7	G	7	0	0	0	0
7	H	10	0	0	0	0
All	All	13485	12525	12479	67	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 3.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:OE1	1:A:267:THR:HG22	1.59	1.02
1:C:129:PTR:O3P	4:G:11[B]:DA:C5'	2.12	0.97
1:A:261:GLU:OE1	1:A:267:THR:CG2	2.17	0.92
1:C:129:PTR:O3P	3:E:11[A]:DG:H4'	1.73	0.88
1:A:292:ARG:NH2	2:D:431:SER:O	2.08	0.85
1:C:98:ARG:NH1	4:F:7[A]:DG:OP1	2.12	0.81
3:E:21[A]:DG:N2	4:F:4[A]:DC:O2	2.12	0.80
2:D:653:GLY:O	2:D:659:ARG:NH2	2.14	0.80
1:A:129:PTR:O2P	3:H:11[B]:DG:H4'	1.85	0.77
1:A:129:PTR:O2P	4:F:11[A]:DA:C5'	2.32	0.77
1:C:129:PTR:O3P	4:G:11[B]:DA:C4'	2.34	0.75
4:G:7[B]:DG:N2	3:H:18[B]:DC:O2	2.20	0.75
1:C:129:PTR:O3P	3:E:11[A]:DG:C4'	2.34	0.74
1:A:129:PTR:O2P	3:H:11[B]:DG:C5'	2.37	0.73
1:C:129:PTR:O3P	3:E:11[A]:DG:C5'	2.37	0.72
1:C:129:PTR:O3P	4:G:11[B]:DA:H4'	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ARG:NH1	1:C:359:ASP:OD1	2.26	0.68
2:D:429:ARG:NH1	2:D:439:PRO:O	2.28	0.67
2:D:659:ARG:NH1	3:E:19[A]:DA:OP1	2.28	0.66
1:A:129:PTR:O2P	3:H:11[B]:DG:C4'	2.44	0.66
1:A:129:PTR:O2P	4:F:11[A]:DA:H4'	1.96	0.65
2:B:429:ARG:NH1	2:B:439:PRO:O	2.30	0.65
1:C:262:ASP:OD1	1:C:263:SER:N	2.37	0.58
1:A:441:ARG:NE	1:C:437:ASP:OD1	2.38	0.56
1:A:98:ARG:NH2	3:E:7[A]:DG:OP1	2.38	0.56
1:A:261:GLU:OE1	1:A:267:THR:HG21	2.05	0.56
1:A:261:GLU:HG2	7:A:696:HOH:O	2.07	0.55
1:C:389:HIS:O	1:C:431:GLN:NE2	2.40	0.54
1:A:98:ARG:CZ	3:E:7[A]:DG:OP1	2.58	0.51
1:C:31:TYR:HA	2:D:535:VAL:CG1	2.40	0.51
4:G:5[B]:DG:N2	3:H:20[B]:DC:O2	2.43	0.51
1:A:98:ARG:NH1	3:E:7[A]:DG:OP1	2.44	0.50
6:H:101:8MX:C01	6:H:101:8MX:C09	2.90	0.50
2:B:446:ARG:NH1	2:B:473:SER:OG	2.45	0.50
2:D:484:LYS:NZ	2:D:536:ASP:O	2.45	0.49
1:A:226:PRO:O	1:A:494:ARG:NH2	2.46	0.49
1:C:428:ASP:OD1	1:C:429:GLU:N	2.43	0.49
3:E:12[A]:DA:OP1	7:E:201:HOH:O	2.16	0.48
1:A:129:PTR:O2P	4:F:11[A]:DA:C4'	2.51	0.46
1:A:427:ILE:CG2	1:A:431:GLN:HB2	2.45	0.46
1:A:23:GLU:OE1	2:B:634:ARG:NH1	2.49	0.45
1:C:60:PHE:HB2	1:C:142:LEU:HD13	1.99	0.45
1:A:51:VAL:HG11	3:E:8[A]:DA:H5'	1.99	0.45
1:A:275:PRO:HG2	1:A:278:VAL:HG21	1.99	0.45
1:A:15:ILE:HD12	2:B:633:LEU:HB2	1.99	0.44
1:C:275:PRO:HG2	1:C:278:VAL:HG21	1.99	0.44
4:F:16[A]:DT:C6	4:F:17[A]:DT:H72	2.53	0.44
1:C:31:TYR:HA	2:D:535:VAL:HG13	2.00	0.43
1:C:186:ALA:O	1:C:344:ASN:ND2	2.52	0.43
2:D:446:ARG:NH2	2:D:473:SER:OG	2.51	0.43
2:D:627:ASP:HB3	2:D:630:VAL:HG22	1.99	0.43
1:A:98:ARG:NH1	4:G:7[B]:DG:OP1	2.51	0.43
1:C:34:SER:OG	2:D:535:VAL:HG11	2.19	0.43
1:C:23:GLU:OE1	2:D:634:ARG:NH1	2.51	0.43
6:H:101:8MX:C23	6:H:101:8MX:C01	2.97	0.43
2:B:511:THR:HG21	2:B:517:PHE:CE2	2.53	0.43
6:G:101:8MX:C23	6:G:101:8MX:C01	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:553:ARG:N	2:B:554:PRO:CD	2.83	0.42
3:E:20[A]:DC:O2	4:F:5[A]:DG:N2	2.51	0.42
2:D:497:LEU:O	2:D:503:GLN:NE2	2.51	0.42
1:C:65:ARG:HB3	1:C:66:PRO:HD2	2.01	0.41
4:G:16[B]:DT:C6	4:G:17[B]:DT:H72	2.55	0.41
2:D:553:ARG:N	2:D:554:PRO:CD	2.83	0.41
1:A:402:ASP:OD1	1:C:409:ARG:NH1	2.52	0.41
2:B:601:ILE:HG22	2:B:606:GLY:HA2	2.03	0.41
1:A:261:GLU:CG	7:A:696:HOH:O	2.65	0.41
2:D:511:THR:HG21	2:D:517:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/503 (96%)	467 (96%)	18 (4%)	0	100	100
1	C	485/503 (96%)	468 (96%)	17 (4%)	0	100	100
2	B	241/253 (95%)	232 (96%)	9 (4%)	0	100	100
2	D	243/253 (96%)	235 (97%)	8 (3%)	0	100	100
All	All	1454/1512 (96%)	1402 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/421 (97%)	408 (100%)	0	100	100
1	C	408/421 (97%)	408 (100%)	0	100	100
2	B	205/211 (97%)	205 (100%)	0	100	100
2	D	207/211 (98%)	207 (100%)	0	100	100
All	All	1228/1264 (97%)	1228 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	PTR	A	129	1	13,16,17	0.75	0	19,22,24	0.89	1 (5%)
1	PTR	C	129	1	13,16,17	0.75	0	19,22,24	0.91	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
1	PTR	A	129	1	-	0/9/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	C	129	1	-	0/9/11/13	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(^{o})	Ideal(^{o})
1	A	129	PTR	O-C-CA	-2.07	120.17	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	129	PTR	6	0
1	C	129	PTR	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
6	8MX	G	101	5	23,32,32	5.92	10 (43%)	30,49,49	2.68	16 (53%)
6	8MX	H	101	5	23,32,32	5.85	9 (39%)	30,49,49	3.12	18 (60%)

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
6	8MX	G	101	5	-	0/4/33/33	1/4/5/5
6	8MX	H	101	5	-	0/4/33/33	0/4/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	101	8MX	C16-C15	-18.25	1.20	1.52
6	G	101	8MX	C16-C15	-16.48	1.23	1.52
6	H	101	8MX	C09-C10	-15.77	1.28	1.53
6	G	101	8MX	C09-C10	-14.91	1.30	1.53
6	H	101	8MX	C04-C03	-3.56	1.38	1.41
6	G	101	8MX	C04-C03	-3.12	1.39	1.41
6	H	101	8MX	C12-C11	-2.43	1.46	1.53
6	G	101	8MX	C12-C11	-2.06	1.47	1.53
6	G	101	8MX	C07-N08	2.08	1.47	1.40
6	H	101	8MX	C15-N14	2.12	1.49	1.47
6	H	101	8MX	C05-C06	2.30	1.39	1.35
6	G	101	8MX	C09-N08	2.88	1.50	1.46
6	H	101	8MX	C12-C13	3.17	1.65	1.49
6	G	101	8MX	C15-N14	3.30	1.51	1.47
6	G	101	8MX	C12-C13	3.75	1.68	1.49
6	H	101	8MX	C10-C15	8.27	1.64	1.53
6	H	101	8MX	C16-N08	9.13	1.58	1.46
6	G	101	8MX	C10-C15	10.48	1.67	1.53
6	G	101	8MX	C16-N08	11.57	1.62	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	101	8MX	C16-N08-C09	-7.51	102.06	112.21
6	G	101	8MX	C21-N22-C23	-6.94	111.36	119.25
6	H	101	8MX	C21-N22-C23	-6.36	112.02	119.25
6	H	101	8MX	C09-N08-C07	-5.98	113.67	122.82
6	H	101	8MX	C13-N14-C15	-5.32	108.02	111.58
6	G	101	8MX	C09-N08-C07	-4.97	115.21	122.82
6	G	101	8MX	C16-N08-C07	-4.41	116.08	122.82
6	G	101	8MX	C05-C04-C18	-3.77	115.25	121.47
6	H	101	8MX	C05-C04-C18	-3.39	115.88	121.47
6	G	101	8MX	C13-N14-C15	-3.25	109.40	111.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	101	8MX	C16-C15-C10	-3.22	101.18	104.81
6	H	101	8MX	C01-C02-C07	-3.19	115.12	121.67
6	G	101	8MX	C16-N08-C09	-2.98	108.18	112.21
6	H	101	8MX	C16-N08-C07	-2.71	118.67	122.82
6	G	101	8MX	C06-C07-N08	-2.58	114.38	121.74
6	H	101	8MX	C11-C10-C15	-2.53	110.28	113.56
6	H	101	8MX	C02-C03-C04	-2.41	117.91	120.19
6	H	101	8MX	F17-C06-C05	-2.36	116.73	120.18
6	G	101	8MX	C02-C03-C04	-2.22	118.09	120.19
6	G	101	8MX	C01-C02-C07	-2.13	117.29	121.67
6	H	101	8MX	C20-C18-C04	-2.10	118.28	121.92
6	G	101	8MX	C20-C18-C04	-2.10	118.28	121.92
6	H	101	8MX	C05-C06-C07	-2.10	120.22	123.29
6	H	101	8MX	C05-C04-C03	2.13	120.83	118.12
6	G	101	8MX	C01-C02-C03	2.21	123.38	120.20
6	G	101	8MX	C02-C07-N08	2.37	125.28	119.91
6	H	101	8MX	C01-C02-C03	2.61	123.95	120.20
6	G	101	8MX	C05-C04-C03	2.62	121.45	118.12
6	G	101	8MX	C16-C15-C10	2.80	107.97	104.81
6	H	101	8MX	C23-N22-C03	3.32	125.19	120.95
6	H	101	8MX	F17-C06-C07	3.34	123.05	118.34
6	G	101	8MX	C23-N22-C03	4.05	126.13	120.95
6	H	101	8MX	C18-C04-C03	4.30	123.29	119.73
6	G	101	8MX	C18-C04-C03	4.31	123.29	119.73

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	101	8MX	C10-C11-C12-C13-C15-N14

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	101	8MX	1	0
6	H	101	8MX	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	486/503 (96%)	0.82	36 (7%) 17 19	35, 56, 107, 166	0
1	C	486/503 (96%)	0.94	61 (12%) 5 5	35, 58, 107, 167	0
2	B	245/253 (96%)	0.86	22 (8%) 12 12	43, 64, 98, 128	0
2	D	247/253 (97%)	0.70	14 (5%) 27 31	39, 60, 97, 151	0
3	E	21/24 (87%)	1.85	6 (28%) 1 0	55, 95, 182, 204	21 (100%)
3	H	21/24 (87%)	1.41	5 (23%) 1 1	27, 57, 124, 182	21 (100%)
4	F	21/24 (87%)	1.66	7 (33%) 0 0	63, 86, 175, 196	21 (100%)
4	G	21/24 (87%)	1.68	6 (28%) 1 0	27, 51, 143, 181	21 (100%)
All	All	1548/1608 (96%)	0.89	157 (10%) 9 9	27, 60, 110, 204	84 (5%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	23[A]	DA	10.8
1	C	501	ILE	10.1
1	A	293	ASP	9.9
4	G	23[B]	DC	8.9
1	A	501	ILE	8.2
1	C	264	ARG	7.0
1	A	408	ILE	6.1
1	A	412	GLU	6.0
2	B	426	LEU	5.9
2	D	426	LEU	5.7
1	A	264	ARG	5.4
1	C	422	ILE	5.3
1	A	292	ARG	5.2
1	C	404	VAL	5.0
2	B	427	VAL	4.7
1	C	292	ARG	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	387	ARG	4.6
1	A	401	LEU	4.3
2	D	601	ILE	4.1
1	A	500	ALA	4.1
1	C	327	VAL	4.1
2	B	601	ILE	4.1
1	C	387	ARG	3.7
1	A	266	ARG	3.7
3	E	22[A]	DT	3.6
1	C	500	ALA	3.6
1	C	470	ALA	3.6
1	C	463	ALA	3.5
2	B	603	LYS	3.5
1	A	323	VAL	3.5
4	F	3[A]	DA	3.4
3	H	3[B]	DT	3.4
1	A	15	ILE	3.3
1	C	427	ILE	3.3
1	C	412	GLU	3.3
2	D	603	LYS	3.2
4	F	23[A]	DC	3.2
1	C	452	ILE	3.2
1	C	414	VAL	3.1
1	C	127	MET	3.1
1	A	414	VAL	3.0
1	A	446	LEU	3.0
1	A	441	ARG	3.0
3	H	11[B]	DG	3.0
2	B	492	ARG	3.0
3	E	11[A]	DG	2.9
1	C	293	ASP	2.9
1	C	450	ARG	2.9
1	A	427	ILE	2.9
1	C	266	ARG	2.8
1	C	318	ILE	2.8
1	C	128[A]	ARG	2.8
1	C	126	ALA	2.8
1	C	261	GLU	2.8
1	C	294	GLY	2.8
1	C	408	ILE	2.8
1	C	325	LYS	2.8
4	F	22[A]	DA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	575	ARG	2.8
2	B	513	ILE	2.8
1	C	15	ILE	2.8
1	C	442	ARG	2.7
2	B	600	LYS	2.7
1	C	265	GLY	2.7
1	C	429	GLU	2.7
2	D	609	ARG	2.6
1	A	430	ILE	2.6
1	A	91	SER	2.6
2	B	430	LYS	2.6
1	C	320	ARG	2.6
3	H	22[B]	DT	2.6
1	A	261	GLU	2.6
1	C	416	ILE	2.6
1	C	91	SER	2.6
1	A	404	VAL	2.5
2	D	494	ASP	2.5
1	C	269	LEU	2.5
1	A	325	LYS	2.5
4	G	22[B]	DA	2.5
2	B	451	ARG	2.5
2	B	648	PHE	2.5
4	G	12[B]	DG	2.5
4	F	8[A]	DC	2.4
1	A	436	LEU	2.4
1	C	263	SER	2.4
1	C	114	GLY	2.4
1	A	394	LEU	2.4
4	G	11[B]	DA	2.4
1	C	383	LYS	2.4
1	C	130	THR	2.4
1	A	421	LEU	2.4
4	F	11[A]	DA	2.4
1	A	296	LEU	2.4
2	D	438	LEU	2.4
2	D	602	ASN	2.4
2	D	484	LYS	2.4
1	C	267	THR	2.4
4	F	7[A]	DG	2.3
1	A	452	ILE	2.3
2	B	450	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	252	ARG	2.3
1	C	441	ARG	2.3
4	G	3[B]	DA	2.3
1	A	126	ALA	2.3
1	A	413	THR	2.3
1	C	413	THR	2.3
1	C	296	LEU	2.3
2	B	481	LEU	2.3
4	G	8[B]	DC	2.3
1	C	455	LEU	2.3
1	A	263	SER	2.3
1	C	458	ILE	2.3
3	H	8[B]	DA	2.2
1	A	51	VAL	2.2
1	C	88	GLY	2.2
2	B	517	PHE	2.2
4	F	21[A]	DG	2.2
1	C	302	ILE	2.2
2	D	600	LYS	2.2
1	A	429	GLU	2.2
1	C	95	SER	2.2
1	C	323	VAL	2.2
1	A	68	ARG	2.2
2	D	641	ALA	2.2
1	C	394	LEU	2.2
2	B	462	SER	2.2
2	D	492	ARG	2.2
2	B	498	LYS	2.2
1	C	94	ASP	2.2
1	C	122	ASP	2.2
3	E	3[A]	DT	2.2
1	C	96	LEU	2.2
1	C	295	LYS	2.1
1	C	433	GLN	2.1
1	C	123	PRO	2.1
3	H	7[B]	DG	2.1
1	C	93	TYR	2.1
2	B	515	ASP	2.1
2	D	575	ARG	2.1
2	B	511	THR	2.1
2	D	607	ILE	2.1
2	B	452	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	438	MET	2.1
1	C	324	ALA	2.1
2	D	427	VAL	2.1
2	B	616	MET	2.0
1	C	472	PRO	2.0
2	B	609	ARG	2.0
3	E	8[A]	DA	2.0
1	A	88	GLY	2.0
3	E	4[A]	DC	2.0
2	B	425	ALA	2.0
1	A	395	VAL	2.0
1	C	77	VAL	2.0
1	C	68	ARG	2.0
1	A	416	ILE	2.0
1	C	403	GLU	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
1	PTR	C	129	16/17	0.96	0.31	-	47,51,74,78	0
1	PTR	A	129	16/17	0.96	0.25	-	43,48,68,70	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
6	8MX	G	101	28/28	0.88	0.37	2.17	56,78,113,113	0
5	MG	E	101	1/1	0.99	0.31	0.85	74,74,74,74	0
6	8MX	H	101	28/28	0.90	0.32	0.76	47,65,141,141	0
5	MG	B	701	1/1	0.93	0.27	-0.46	37,37,37,37	0
5	MG	D	701	1/1	0.93	0.19	-1.04	32,32,32,32	0
5	MG	C	601	1/1	0.97	0.19	-1.36	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.