Full wwPDB X-ray Structure Validation Report (i)

Nov 9, 2021 – 01:09 pm GMT

PDB ID	:	6Z01
Title	:	DNA Topoisomerase
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Deposited on	:	2020-05-07
Resolution	:	1.90 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 (i) symbol.

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

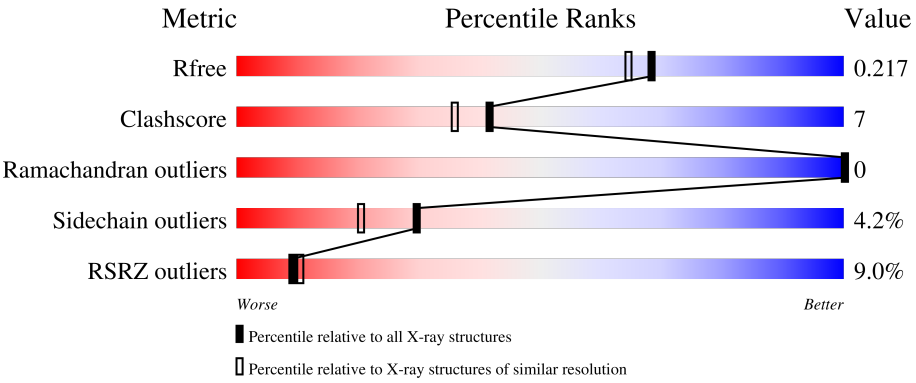
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	539	7% 83% 12%
1	B	539	10% 81% 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
2	CL	B	601	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9818 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	Se	0	0	0
			4346	2778	778	780	1	9			
1	B	517	Total	C	N	O	S	Se	0	3	0
			4339	2772	776	781	1	9			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Cl	0	0
			6	6		
2	B	6	Total	Cl	0	0
			6	6		

- Molecule 3 is water.

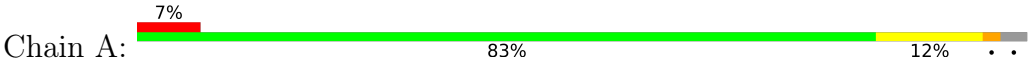
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	569	Total	O	0	0
			569	569		
3	B	552	Total	O	0	0
			552	552		

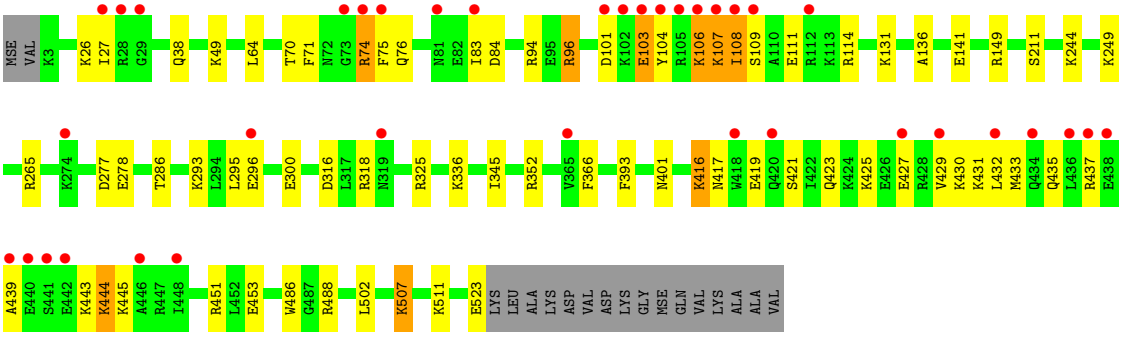
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA topoisomerase I

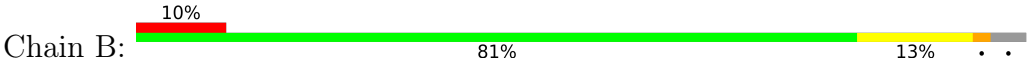
Chain A:

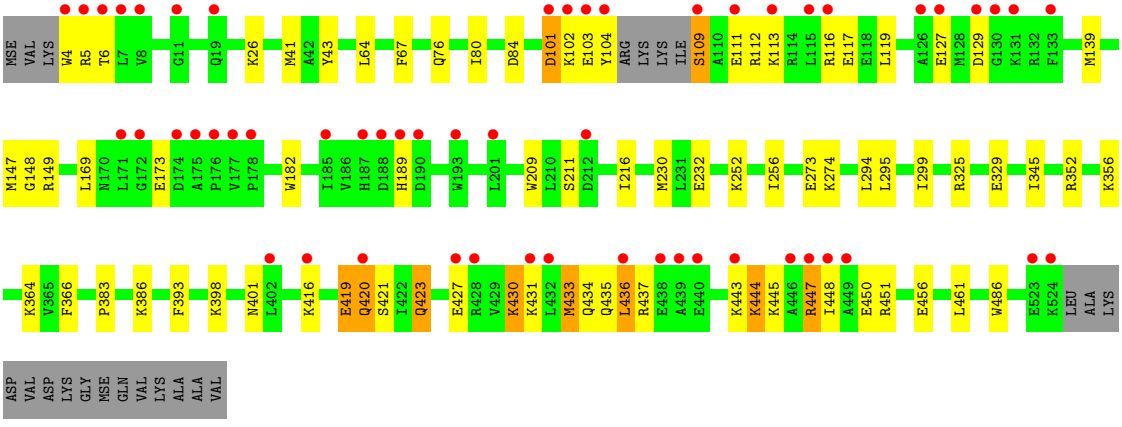




• Molecule 1: DNA topoisomerase I

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.20Å 96.59Å 94.56Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	35.44 – 1.90 35.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.44-1.90) 99.8 (35.44-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.180 , 0.217 0.180 , 0.217	Depositor DCC
R_{free} test set	4941 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9818	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.41	0/4435	0.53	1/5954 (0.0%)
1	B	0.42	0/4430	0.55	0/5946
All	All	0.42	0/8865	0.54	1/11900 (0.0%)

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	488	ARG	NE-CZ-NH2	-5.87	117.36	120.30

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	4346	0	4395	51	0
1	B	4339	0	4380	72	0
2	A	6	0	0	1	0
2	B	6	0	0	3	0
3	A	569	0	0	13	0
3	B	552	0	0	9	0
All	All	9818	0	8775	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (122) 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:B:113:LYS:HG2	1:B:116:ARG:HH21	1.30	0.95
1:B:451:ARG:HH21	1:B:451:ARG:HB2	1.33	0.92
1:B:447:ARG:NH1	1:B:451:ARG:HH11	1.71	0.89
1:A:507:LYS:NZ	3:A:702:HOH:O	2.09	0.83
1:A:149:ARG:NH2	3:A:705:HOH:O	2.15	0.80
1:A:443:LYS:NZ	3:A:703:HOH:O	2.14	0.80
1:A:107:LYS:HG3	1:A:108:ILE:HG22	1.65	0.79
1:A:421:SER:O	3:A:701:HOH:O	2.00	0.79
1:B:451:ARG:HB2	1:B:451:ARG:NH2	1.98	0.78
1:A:94:ARG:NH1	3:A:708:HOH:O	2.18	0.76
1:B:398:LYS:HD2	1:B:461:LEU:HD21	1.68	0.76
1:A:141:GLU:HG3	2:A:606:CL:CL	2.23	0.74
1:A:511:LYS:NZ	3:A:709:HOH:O	2.20	0.73
1:B:447:ARG:HH11	1:B:451:ARG:HH11	1.34	0.73
1:A:417:ASN:ND2	3:A:710:HOH:O	2.23	0.72
1:B:43:TYR:OH	3:B:801:HOH:O	2.06	0.72
1:B:448:ILE:HA	1:B:451:ARG:NH1	2.06	0.69
1:B:41:MSE:HE1	1:B:67:PHE:HA	1.75	0.69
1:B:232:GLU:OE1	3:B:802:HOH:O	2.11	0.68
1:B:295:LEU:O	1:B:325:ARG:NH2	2.25	0.68
1:A:131:LYS:NZ	1:B:419:GLU:OE2	2.23	0.67
1:B:76[B]:GLN:OE1	3:B:803:HOH:O	2.12	0.67
1:A:453:GLU:OE2	3:A:704:HOH:O	2.14	0.66
1:B:448:ILE:HG12	1:B:451:ARG:HH12	1.62	0.63
1:B:436:LEU:HD12	1:B:448:ILE:HB	1.82	0.61
1:B:456:GLU:OE1	3:B:804:HOH:O	2.16	0.61
1:A:295:LEU:O	1:A:325:ARG:NH2	2.24	0.61
1:B:364:LYS:HD3	3:B:805:HOH:O	2.01	0.59
1:B:273:GLU:HB2	2:B:601:CL:CL	2.39	0.59
1:A:316:ASP:OD1	1:A:318:ARG:HG2	2.03	0.59
1:B:26:LYS:HB2	1:B:84:ASP:HB3	1.84	0.58
1:A:103:GLU:O	1:A:108:ILE:HG23	2.02	0.58
1:B:41:MSE:HE1	1:B:67:PHE:CA	2.33	0.57
1:B:273:GLU:OE1	3:B:805:HOH:O	2.16	0.57
1:A:49:LYS:O	3:A:707:HOH:O	2.18	0.57
1:A:523:GLU:OE2	3:A:706:HOH:O	2.17	0.57
1:A:26:LYS:HB2	1:A:84:ASP:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ILE:HD13	1:B:345:ILE:HD13	1.85	0.57
1:B:433:MSE:HB3	1:B:434:GLN:NE2	2.21	0.56
1:A:430:LYS:NZ	1:A:433:MSE:HE1	2.19	0.56
1:B:109:SER:OG	1:B:109:SER:O	2.23	0.55
1:B:64:LEU:HD11	1:B:80:ILE:HG12	1.89	0.54
1:B:423:GLN:O	1:B:427:GLU:N	2.30	0.54
1:A:439:ALA:HB3	1:A:445:LYS:HD3	1.89	0.54
1:B:41:MSE:HE2	1:B:67:PHE:HD1	1.72	0.54
1:B:436:LEU:HG	1:B:445:LYS:HG2	1.91	0.53
1:B:109:SER:N	3:B:815:HOH:O	2.42	0.52
1:A:111:GLU:OE2	1:A:114:ARG:NH1	2.43	0.51
1:B:433:MSE:HB3	1:B:434:GLN:HE22	1.75	0.51
1:B:139:MSE:HG3	2:B:604:CL:CL	2.47	0.51
1:A:393:PHE:CE1	1:A:486:TRP:CD1	2.98	0.51
1:B:448:ILE:HA	1:B:451:ARG:HH12	1.76	0.50
1:A:419:GLU:O	1:A:423:GLN:HG3	2.11	0.50
1:B:113:LYS:HG2	1:B:116:ARG:NH2	2.13	0.50
1:B:430:LYS:O	1:B:433:MSE:HB2	2.12	0.50
1:B:448:ILE:HG23	1:B:451:ARG:HH22	1.77	0.49
1:A:423:GLN:O	1:A:427:GLU:HG3	2.13	0.49
1:B:41:MSE:CE	1:B:67:PHE:HA	2.42	0.49
1:B:112:ARG:HH22	1:B:113:LYS:HG3	1.78	0.48
1:B:112:ARG:NH2	1:B:113:LYS:HG3	2.28	0.48
1:B:448:ILE:HG12	1:B:451:ARG:NH1	2.27	0.48
1:B:256:ILE:HA	1:B:345:ILE:HD11	1.96	0.48
1:A:106:LYS:HA	1:A:109:SER:HB2	1.94	0.48
1:B:149:ARG:HA	1:B:230:MSE:HE2	1.94	0.48
1:A:27:ILE:HG12	1:A:83:ILE:HG12	1.96	0.48
1:A:74:ARG:HG3	1:A:75:PHE:CD2	2.49	0.48
1:B:444:LYS:O	1:B:448:ILE:HG13	2.13	0.47
1:A:293:LYS:HE2	1:A:300:GLU:HB2	1.97	0.47
1:A:244:LYS:NZ	3:A:723:HOH:O	2.46	0.47
1:B:393:PHE:CE1	1:B:486:TRP:CD1	3.02	0.47
1:B:434:GLN:HA	1:B:437:ARG:HB2	1.96	0.47
1:B:364:LYS:NZ	3:B:830:HOH:O	2.47	0.47
1:B:420:GLN:HA	1:B:423:GLN:HG3	1.97	0.47
1:B:252:LYS:O	1:B:256:ILE:HG12	2.16	0.46
1:B:431:LYS:O	1:B:435:GLN:HB2	2.16	0.46
1:A:96:ARG:NH2	3:A:724:HOH:O	2.46	0.46
1:A:444:LYS:HD3	1:A:444:LYS:HA	1.56	0.46
1:B:209:TRP:HB2	1:B:216:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ILE:HD13	1:B:345:ILE:CD1	2.45	0.46
1:B:448:ILE:HA	1:B:451:ARG:CZ	2.45	0.46
1:A:433:MSE:O	1:A:437:ARG:HG3	2.15	0.46
1:B:325:ARG:O	1:B:329:GLU:HG3	2.16	0.46
1:A:106:LYS:HA	1:A:106:LYS:HD3	1.39	0.45
1:B:383:PRO:HD2	1:B:386:LYS:HD2	1.97	0.45
1:B:436:LEU:HB2	1:B:448:ILE:HB	1.98	0.45
1:A:108:ILE:CG1	1:A:108:ILE:O	2.65	0.45
1:A:432:LEU:HD21	1:A:451:ARG:NH1	2.31	0.45
1:B:447:ARG:HH11	1:B:447:ARG:HG2	1.80	0.44
1:B:113:LYS:O	1:B:117:GLU:HB2	2.17	0.44
1:B:352:ARG:HG2	1:B:356:LYS:HE3	1.98	0.44
1:B:169:LEU:HD11	1:B:182:TRP:CE2	2.53	0.44
1:B:4:TRP:CE2	1:B:189:HIS:HA	2.51	0.44
1:B:6:THR:HG22	1:B:129:ASP:HA	1.99	0.44
1:B:430:LYS:HA	1:B:430:LYS:HD3	1.56	0.44
1:A:433:MSE:HE3	1:A:433:MSE:HB2	1.72	0.44
1:A:104:TYR:CZ	1:A:352:ARG:HD2	2.54	0.43
1:A:345:ILE:HD13	1:A:345:ILE:HA	1.84	0.43
1:A:431:LYS:O	1:A:435:GLN:HG3	2.19	0.43
1:A:416:LYS:HE2	1:A:417:ASN:ND2	2.34	0.42
1:A:38:GLN:HG2	1:A:70:THR:OG1	2.19	0.42
1:A:136:ALA:HB2	1:A:211:SER:HA	2.01	0.42
1:B:173:GLU:CD	1:B:189:HIS:HE2	2.23	0.42
1:A:107:LYS:HG3	1:A:108:ILE:N	2.35	0.42
1:A:430:LYS:HA	1:A:433:MSE:CE	2.50	0.42
1:B:273:GLU:HG3	2:B:601:CL:CL	2.57	0.42
1:A:430:LYS:HA	1:A:430:LYS:HD3	1.73	0.42
1:A:430:LYS:CE	1:A:433:MSE:HE1	2.50	0.41
1:B:436:LEU:HB2	1:B:448:ILE:CG2	2.50	0.41
1:B:102:LYS:HB3	1:B:104:TYR:CE1	2.55	0.41
1:B:148:GLY:O	1:B:230:MSE:HE2	2.20	0.41
1:B:456:GLU:HG3	3:B:975:HOH:O	2.20	0.41
1:A:425:LYS:O	1:A:429:VAL:HG12	2.20	0.41
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.86	0.41
1:B:41:MSE:HE1	1:B:67:PHE:N	2.34	0.41
1:B:416:LYS:HE3	1:B:416:LYS:HB3	1.72	0.41
1:A:277:ASP:OD1	1:A:278:GLU:N	2.54	0.41
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.88	0.41
1:B:294:LEU:HD23	1:B:299:ILE:HG23	2.03	0.41
1:A:249:LYS:NZ	3:A:736:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PHE:O	1:A:76:GLN:NE2	2.54	0.40
1:B:101:ASP:O	1:B:103:GLU:HG2	2.21	0.40
1:B:447:ARG:HG2	1:B:447:ARG:O	2.21	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	519/539 (96%)	508 (98%)	11 (2%)	0	100	100
1	B	516/539 (96%)	511 (99%)	5 (1%)	0	100	100
All	All	1035/1078 (96%)	1019 (98%)	16 (2%)	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	458/462 (99%)	442 (96%)	16 (4%)	36	27
1	B	458/462 (99%)	436 (95%)	22 (5%)	25	16
All	All	916/924 (99%)	878 (96%)	38 (4%)	30	21

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	96	ARG
1	A	101	ASP
1	A	103	GLU
1	A	106	LYS
1	A	107	LYS
1	A	108	ILE
1	A	265	ARG
1	A	286	THR
1	A	296	GLU
1	A	336	LYS
1	A	366	PHE
1	A	401	ASN
1	A	416	LYS
1	A	444	LYS
1	A	507	LYS
1	B	5	ARG
1	B	101	ASP
1	B	109	SER
1	B	111	GLU
1	B	119	LEU
1	B	127	GLU
1	B	147	MSE
1	B	211	SER
1	B	274	LYS
1	B	366	PHE
1	B	401	ASN
1	B	419	GLU
1	B	420	GLN
1	B	421	SER
1	B	423	GLN
1	B	430	LYS
1	B	433	MSE
1	B	436	LEU
1	B	443	LYS
1	B	444	LYS
1	B	447	ARG
1	B	450	GLU

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

Mol	Chain	Res	Type
1	A	420	GLN

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Mol	Chain	Res	Type
1	B	10	ASN
1	B	81	ASN
1	B	420	GLN
1	B	434	GLN
1	B	435	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	512/539 (94%)	0.35	37 (7%) 15 17	21, 37, 78, 114	0
1	B	508/539 (94%)	0.55	55 (10%) 5 6	18, 36, 87, 102	0
All	All	1020/1078 (94%)	0.45	92 (9%) 9 10	18, 37, 86, 114	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	TYR	10.3
1	B	436	LEU	10.0
1	B	446	ALA	8.6
1	A	439	ALA	6.5
1	B	133	PHE	6.4
1	B	104	TYR	6.1
1	B	4	TRP	5.7
1	B	172	GLY	5.7
1	A	107	LYS	5.4
1	B	130	GLY	5.3
1	B	171	LEU	5.2
1	B	212	ASP	5.1
1	A	441	SER	4.7
1	A	434	GLN	4.6
1	B	115	LEU	4.5
1	A	108	ILE	4.4
1	B	524	LYS	4.3
1	A	432	LEU	4.3
1	A	438	GLU	4.3
1	B	131	LYS	4.2
1	A	27	ILE	4.2
1	A	112	ARG	4.2
1	B	189	HIS	4.2
1	B	175	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	188	ASP	4.1
1	A	75	PHE	4.0
1	B	190	ASP	4.0
1	B	523	GLU	4.0
1	A	105	ARG	4.0
1	B	7	LEU	3.9
1	A	109	SER	3.9
1	A	440	GLU	3.8
1	A	28	ARG	3.7
1	B	111	GLU	3.7
1	B	443	LYS	3.6
1	B	448	ILE	3.5
1	B	5	ARG	3.4
1	B	420	GLN	3.4
1	B	447	ARG	3.4
1	A	73	GLY	3.4
1	A	442	GLU	3.4
1	B	109	SER	3.3
1	B	440	GLU	3.3
1	B	129	ASP	3.3
1	B	177	VAL	3.3
1	B	103	GLU	3.2
1	A	102	LYS	3.2
1	A	420	GLN	3.2
1	B	178	PRO	3.1
1	B	6	THR	3.1
1	A	427	GLU	3.1
1	B	428	ARG	3.1
1	A	101	ASP	3.1
1	B	101	ASP	3.1
1	B	174	ASP	3.0
1	A	437	ARG	3.0
1	B	126	ALA	3.0
1	B	431	LYS	2.9
1	A	319	ASN	2.9
1	A	83	ILE	2.9
1	B	416	LYS	2.9
1	A	296	GLU	2.8
1	A	106	LYS	2.8
1	B	201	LEU	2.7
1	B	438	GLU	2.7
1	B	439	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	176	PRO	2.7
1	B	427	GLU	2.7
1	A	29	GLY	2.6
1	B	432	LEU	2.6
1	B	113	LYS	2.5
1	B	185	ILE	2.5
1	B	449	ALA	2.5
1	A	74	ARG	2.5
1	B	127	GLU	2.5
1	B	116	ARG	2.5
1	A	429	VAL	2.5
1	A	103	GLU	2.5
1	A	81	ASN	2.4
1	A	436	LEU	2.4
1	A	418	TRP	2.3
1	B	8	VAL	2.3
1	A	448	ILE	2.3
1	B	102	LYS	2.3
1	B	402	LEU	2.2
1	B	19	GLN	2.2
1	A	446	ALA	2.2
1	B	187	HIS	2.1
1	B	11	GLY	2.1
1	B	193	TRP	2.1
1	A	274	LYS	2.1
1	A	365	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	CL	B	603	1/1	0.78	0.10	61,61,61,61	0
2	CL	A	605	1/1	0.94	0.07	63,63,63,63	0
2	CL	B	604	1/1	0.96	0.03	64,64,64,64	0
2	CL	B	606	1/1	0.97	0.06	58,58,58,58	0
2	CL	A	606	1/1	0.98	0.07	43,43,43,43	0
2	CL	A	603	1/1	0.98	0.17	33,33,33,33	0
2	CL	B	601	1/1	0.99	0.06	36,36,36,36	0
2	CL	B	602	1/1	0.99	0.07	38,38,38,38	0
2	CL	A	604	1/1	0.99	0.09	34,34,34,34	0
2	CL	A	602	1/1	0.99	0.14	30,30,30,30	0
2	CL	B	605	1/1	0.99	0.08	33,33,33,33	0
2	CL	A	601	1/1	0.99	0.10	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.