WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 10:09 PM GMT

PDB ID	:	5CDM
Title	:	2.5A structure of QPT-1 with S.aureus DNA gyrase and DNA
Authors	:	Bax, B.D.; Srikannathasan, V.; Chan, P.F.
Deposited on	:	2015-07-04
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) 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 ⓘ

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.
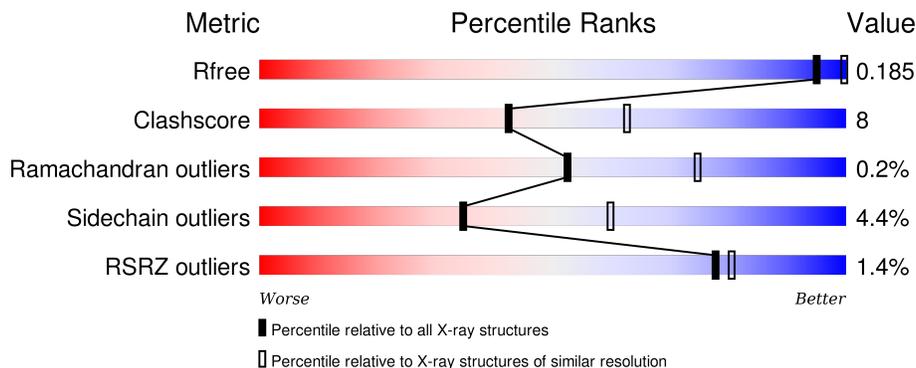
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	B	190	3% 78% 21% ••
1	D	190	3% 71% 27% •
2	A	482	% 78% 20% •
2	C	482	% 81% 18% •
3	E	8	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	8	75% 13% 13%
4	I	12	67% 33%
4	N	12	33% 50% 8% 8%

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 23019 atoms, of which 11161 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 B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	189	Total 2937	C 931	H 1455	N 260	O 282	S 9	0	2	0
1	D	190	Total 2953	C 937	H 1459	N 262	O 286	S 9	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	544	THR	-	linker	UNP P66937
B	545	GLY	-	linker	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	A	482	Total 7668	C 2373	H 3845	N 696	O 736	P 1	S 17	0	4	0
2	C	481	Total 7803	C 2406	H 3926	N 711	O 743	P 1	S 16	0	12	0

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP* CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	8	Total 256	C 78	H 90	N 33	O 47	P 8	0	0	0
3	F	7	Total 223	C 68	H 79	N 28	O 41	P 7	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP* CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	I	12	Total 375	C 116	H 134	N 43	O 71	P 11	0	0	0
4	N	11	Total 342	C 106	H 121	N 41	O 64	P 10	0	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mn 1	0	0
5	D	1	Total 1	Mn 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
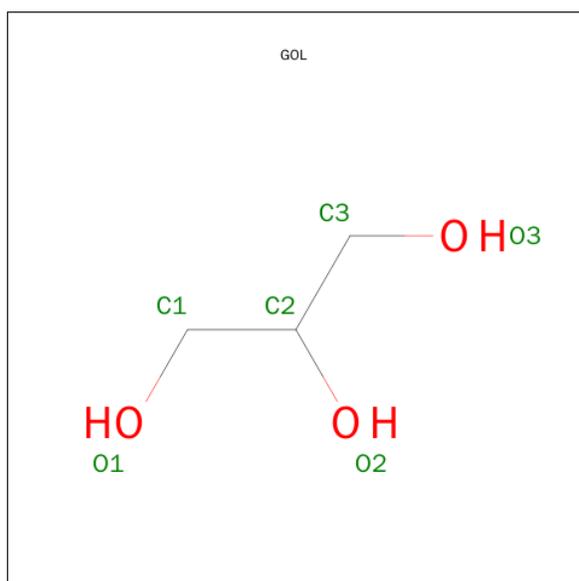
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 14	C 3	H 8	O 3	0	0
6	A	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
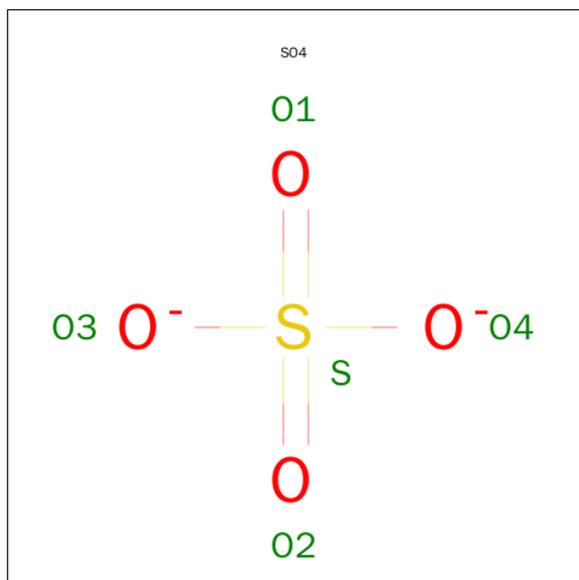
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	A	1	5	4	1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
8	A	1	1	1	0	0

- Molecule 9 is (2R,4S,4aS)-2,4-dimethyl-8-nitro-1,2,4,4a-tetrahydro-2'H,6H-spiro[1,4-oxazino [4,3-a]quinoline-5,5'-pyrimidine]-2',4',6'(1'H,3'H)-trione (three-letter code: 54Q) (formula: $C_{17}H_{18}N_4O_6$).

54Q

O2

O

N1

H

N

C15

C2

O

N2 HN

C1(S) O1 O

C13

C14

C(S)

HB(R)

C4

C16

N

O

O3 C12

C5

C11 C6

C10

C7

C9

C8

O5 O

N⁺ N3

O⁻

O4
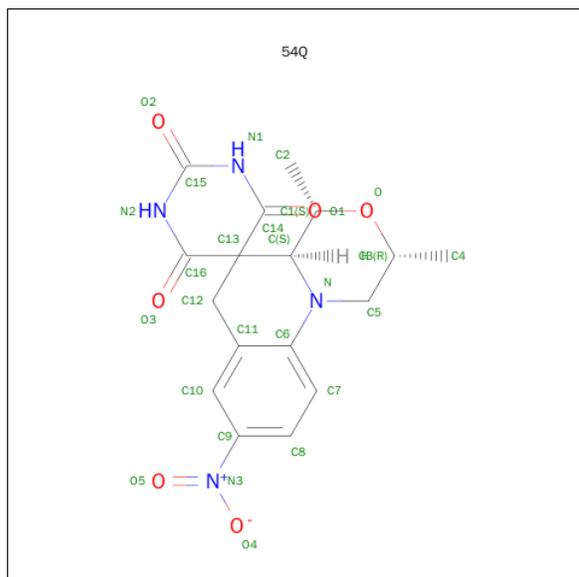
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	I	1	Total	C	H	N	O	0	0
			45	17	18	4	6		
9	N	1	Total	C	H	N	O	0	0
			45	17	18	4	6		

- Molecule 10 is THYMIDINE-5'-MONOPHOSPHATE (three-letter code: DT) (formula: $C_{10}H_{15}N_2O_8P$).
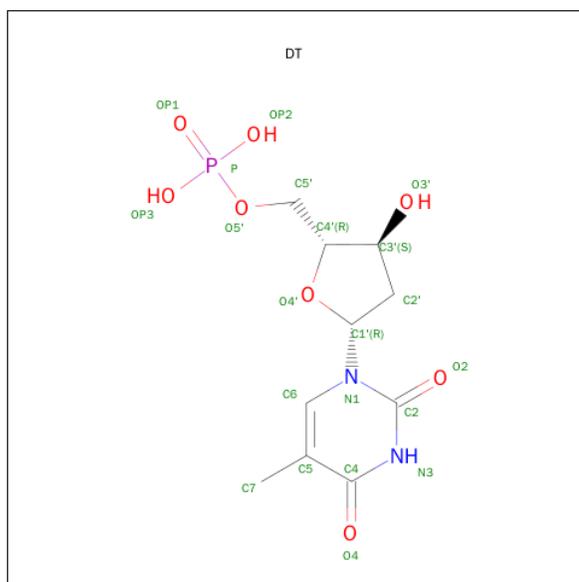
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	N	1	Total	O	P	0	1
			8	6	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	35	Total	O	0	0
			35	35		
11	A	113	Total	O	0	0
			113	113		
11	D	25	Total	O	0	0
			25	25		
11	C	102	Total	O	0	0
			102	102		
11	E	13	Total	O	0	0
			13	13		
11	I	5	Total	O	0	0
			5	5		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	F	14	Total O 14 14		0	0
11	N	21	Total O 21 21		0	0

3 Residue-property plots ⓘ

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 B,DNA gyrase subunit B
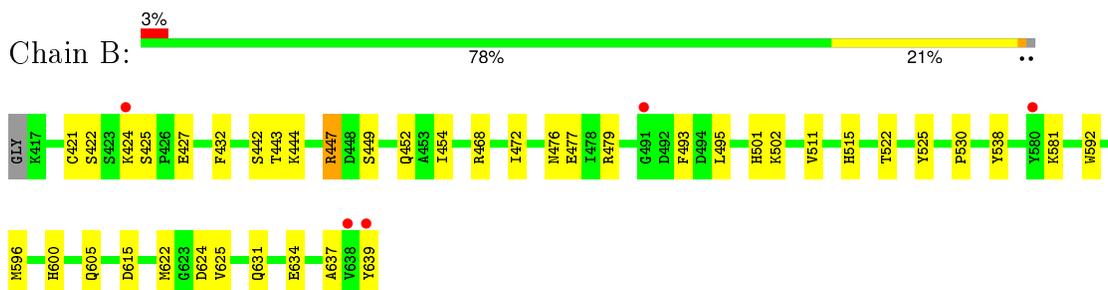
• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B
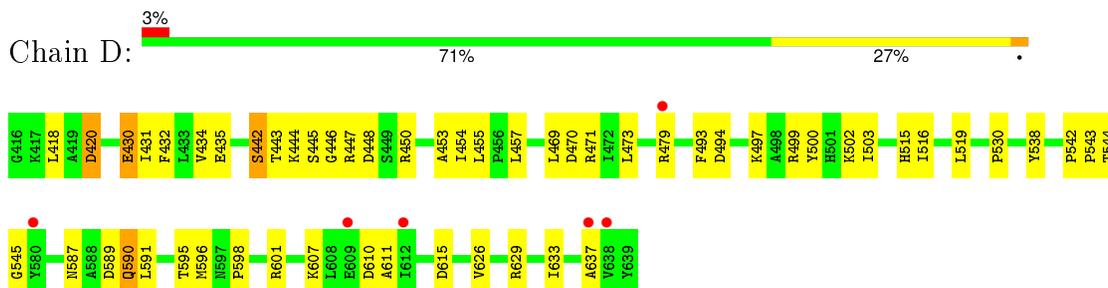
• Molecule 2: DNA gyrase subunit A
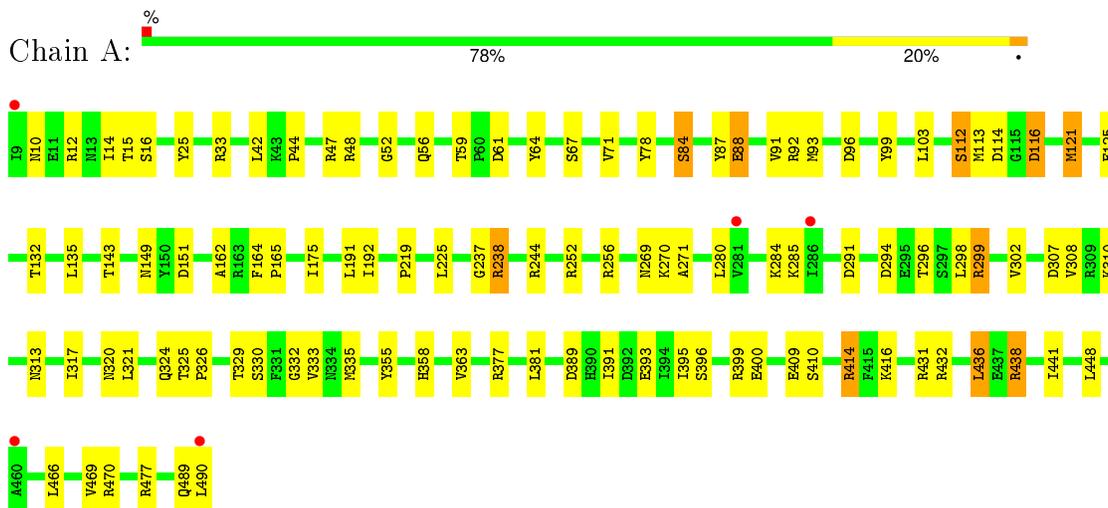
• Molecule 2: DNA gyrase subunit A
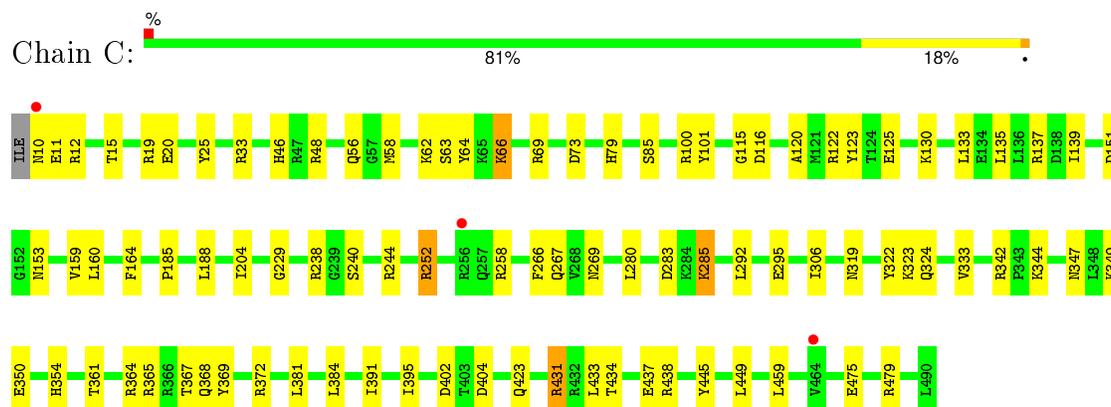
Chain C:

• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP *GP*CP*TP*T)-3')

Chain E:

• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP *GP*CP*TP*T)-3')

Chain F:

• Molecule 4: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP *GP*CP*TP*T)-3')

Chain I:

• Molecule 4: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP *GP*CP*TP*T)-3')

Chain N:
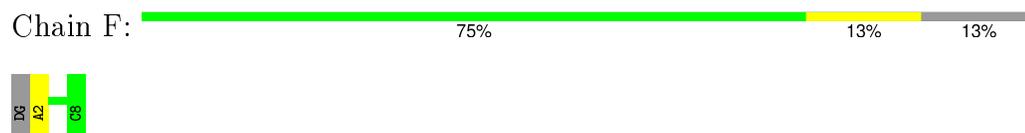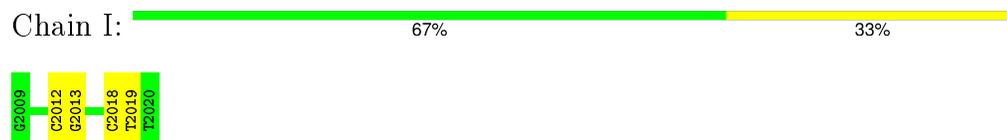
4   Data and refinement statistics (i)

| Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	93.88Å 93.88Å 412.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.78 – 2.50 36.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (36.78-2.50) 95.3 (36.79-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.163 , 0.192 0.163 , 0.185	Depositor DCC
R_{free} test set	3409 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.6	EDS
Estimated twinning fraction	0.220 for h,-h-k,-l 0.213 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.220 for h,-h-k,-l	Depositor
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.21$	Xtriage
Outliers	0 of 67361 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23019	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NA, MN, 54Q, SO4, 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	B	0.44	0/1513	0.54	0/2043
1	D	0.42	0/1534	0.56	0/2072
2	A	0.44	0/3866	0.57	0/5212
2	C	0.46	0/3952	0.56	0/5320
3	E	0.98	0/186	0.86	0/285
3	F	1.09	0/161	0.91	0/246
4	I	1.09	0/269	0.94	0/414
4	N	1.12	1/247 (0.4%)	0.97	0/380
All	All	0.52	1/11728 (0.0%)	0.60	0/15972

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	2013	DG	C3'-O3'	-5.77	1.36	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1482	1455	1449	28	0
1	D	1494	1459	1442	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3823	3845	3831	61	2
2	C	3877	3926	3872	56	2
3	E	166	90	90	3	0
3	F	144	79	79	1	0
4	I	241	134	134	4	0
4	N	221	121	122	9	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	8	8	0	0
6	B	6	8	7	2	0
7	A	5	0	0	0	0
8	A	1	0	0	0	0
9	I	27	18	18	3	0
9	N	27	18	18	4	0
10	N	8	0	0	3	0
11	A	113	0	0	1	0
11	B	35	0	0	1	0
11	C	102	0	0	5	0
11	D	25	0	0	1	0
11	E	13	0	0	0	0
11	F	14	0	0	0	0
11	I	5	0	0	0	0
11	N	21	0	0	0	0
All	All	11858	11161	11070	188	2

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 8.

The worst 5 of 188 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:525:TYR:OH	1:B:615:ASP:OD1	1.92	0.87
1:B:425:SER:OG	1:B:427:GLU:OE1	1.94	0.86
2:C:204:ILE:O	2:C:349:LYS:NZ	2.09	0.85
2:A:252:ARG:NH1	2:A:308:VAL:O	2.16	0.78
2:A:389:ASP:OD1	2:A:438:ARG:NH2	2.18	0.77

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:416:LYS:NZ	2:C:322:TYR:O[1_545]	2.11	0.09
2:A:409:GLU:OE1	2:C:323:LYS:NZ[1_545]	2.16	0.04

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	B	189/190 (100%)	185 (98%)	4 (2%)	0	100	100
1	D	192/190 (101%)	189 (98%)	3 (2%)	0	100	100
2	A	483/482 (100%)	470 (97%)	12 (2%)	1 (0%)	52	75
2	C	490/482 (102%)	470 (96%)	19 (4%)	1 (0%)	52	75
All	All	1354/1344 (101%)	1314 (97%)	38 (3%)	2 (0%)	52	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	33	ARG
2	A	33	ARG

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	B	155/158 (98%)	149 (96%)	6 (4%)	39	66
1	D	156/158 (99%)	146 (94%)	10 (6%)	22	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	412/416 (99%)	394 (96%)	18 (4%)	35	60
2	C	421/416 (101%)	404 (96%)	17 (4%)	38	64
All	All	1144/1148 (100%)	1093 (96%)	51 (4%)	35	59

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	490	LEU
1	D	445	SER
2	C	342[B]	ARG
1	D	420	ASP
1	D	457	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	501	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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	#$|Z| > 2$
2	PTR	A	123	2,4	13,16,17	1.20	1 (7%)	19,22,24	0.65	1 (5%)
2	PTR	C	123	2,4	13,16,17	1.29	1 (7%)	19,22,24	0.77	1 (5%)

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	PTR	A	123	2,4	-	0/9/11/13	0/1/1/1
2	PTR	C	123	2,4	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	123	PTR	OH-CZ	-4.11	1.30	1.40
2	A	123	PTR	OH-CZ	-4.04	1.31	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	123	PTR	O-C-CA	-2.47	119.10	125.72
2	A	123	PTR	O-C-CA	-2.28	119.61	125.72

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	C	123	PTR	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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

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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	$\#|Z| > 2$
7	SO4	A	501	-	4,4,4	0.42	0	6,6,6	0.26	0
6	GOL	A	503	-	5,5,5	0.42	0	5,5,5	0.83	0
6	GOL	B	1002	-	5,5,5	1.09	1 (20%)	5,5,5	1.01	0
9	54Q	I	2101	-	26,30,30	0.63	0	35,47,47	0.69	1 (2%)
10	DT	N	2101[A]	-	0,3,22	0.00	-	0,3,33	0.00	-
10	DT	N	2101[B]	-	0,3,22	0.00	-	0,3,33	0.00	-
9	54Q	N	2102	-	26,30,30	0.79	1 (3%)	35,47,47	0.70	1 (2%)

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
7	SO4	A	501	-	-	0/0/0/0	0/0/0/0
6	GOL	A	503	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1002	-	-	0/4/4/4	0/0/0/0
9	54Q	I	2101	-	-	0/4/55/55	0/4/4/4
10	DT	N	2101[A]	-	-	0/0/0/22	0/0/0/2
10	DT	N	2101[B]	-	-	0/0/0/22	0/0/0/2
9	54Q	N	2102	-	-	0/4/55/55	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1002	GOL	O2-C2	-2.38	1.36	1.43
9	N	2102	54Q	C-N	2.50	1.49	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	2101	54Q	C5-N-C6	2.21	124.28	118.83
9	N	2102	54Q	C5-N-C6	2.30	124.49	118.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1002	GOL	2	0
9	I	2101	54Q	3	0
10	N	2101[A]	DT	2	0
10	N	2101[B]	DT	1	0
9	N	2102	54Q	4	0

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	B	189/190 (99%)	0.21	5 (2%)	59	63	35, 55, 76, 103	0
1	D	190/190 (100%)	0.34	6 (3%)	51	56	38, 59, 83, 97	0
2	A	481/482 (99%)	-0.04	5 (1%)	84	86	30, 46, 71, 95	0
2	C	480/482 (99%)	-0.16	3 (0%)	90	91	26, 45, 66, 82	0
3	E	8/8 (100%)	0.14	0	100	100	34, 39, 48, 59	0
3	F	7/8 (87%)	-0.02	0	100	100	35, 37, 54, 83	0
4	I	12/12 (100%)	-0.17	0	100	100	39, 45, 76, 98	0
4	N	11/12 (91%)	-0.12	0	100	100	35, 39, 51, 52	0
All	All	1378/1384 (99%)	0.01	19 (1%)	78	80	26, 48, 74, 103	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	638	VAL	3.7
1	B	580	TYR	3.6
1	D	609	GLU	3.5
2	A	490	LEU	3.3
1	B	491	GLY	3.0

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

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, 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	LLDF	B-factors($\text{\AA}^2$)	Q<0.9
2	PTR	C	123	16/17	0.97	0.17	-	36,46,56,58	0
2	PTR	A	123	16/17	0.98	0.17	-	31,38,43,44	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, 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	LLDF	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	A	501	5/5	0.90	0.18	1.20	61,61,67,74	0
6	GOL	A	503	6/6	0.92	0.17	0.68	29,48,67,70	0
5	MN	B	1001	1/1	0.98	0.14	-0.10	43,43,43,43	0
9	54Q	N	2102	27/27	0.94	0.14	-0.56	27,35,43,50	0
6	GOL	B	1002	6/6	0.86	0.14	-0.80	40,48,53,54	0
9	54Q	I	2101	27/27	0.92	0.14	-0.98	29,36,43,50	0
5	MN	D	701	1/1	0.99	0.15	-1.46	38,38,38,38	0
8	NA	A	502	1/1	0.98	0.09	-2.44	41,41,41,41	0
10	DT	N	2101[B]	4/21	0.91	0.19	-	26,31,33,38	4
10	DT	N	2101[A]	4/21	0.91	0.19	-	23,29,33,42	4

6.5 Other polymers (i)

There are no such residues in this entry.