



# Full wwPDB X-ray Structure Validation Report ⓘ

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)

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](mailto: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 ⓘ](#)) 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

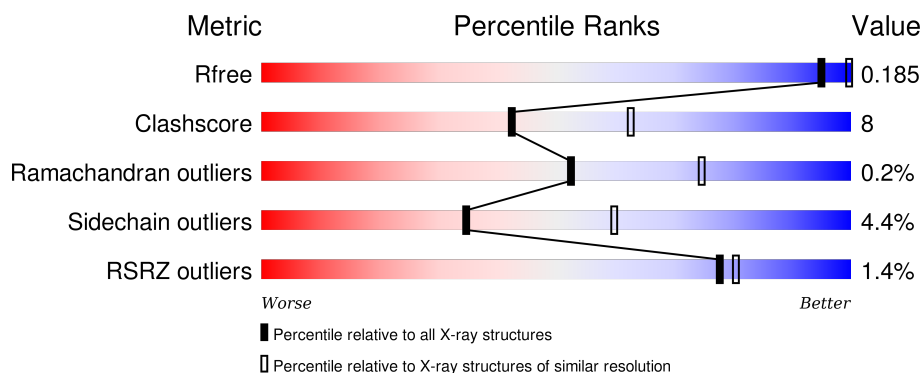
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	190	<div> <div>3%</div> <div>78%</div> <div>21%</div> <div>..</div> </div>
1	D	190	<div> <div>3%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>
2	A	482	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
2	C	482	<div> <div>%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
3	E	8	<div> <div>50%</div> <div>50%</div> </div>

*Continued on next page...*

*Continued from previous page...*

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 [i](#)

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	C	H	N	O	S	0	2	0
			2937	931	1455	260	282	9			
1	D	190	Total	C	H	N	O	S	0	4	0
			2953	937	1459	262	286	9			

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	C	H	N	O	P	S	0	4	0
			7668	2373	3845	696	736	1	17			
2	C	481	Total	C	H	N	O	P	S	0	12	0
			7803	2406	3926	711	743	1	16			

- 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	C	H	N	O	P	0	0	0
			256	78	90	33	47	8			
3	F	7	Total	C	H	N	O	P	0	0	0
			223	68	79	28	41	7			

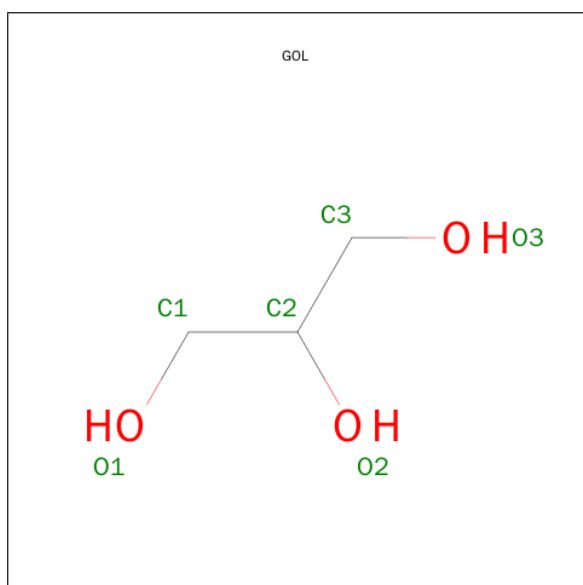
- Molecule 4 is a DNA chain called DNA (5'-D(P\*GP\*AP\*GP\*CP\*GP\*TP\*AP\*C\*GP\*GP\*CP\*CP\*GP\*TP\*AP\*CP\*GP\*CP\*TP\*T)-3').

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

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

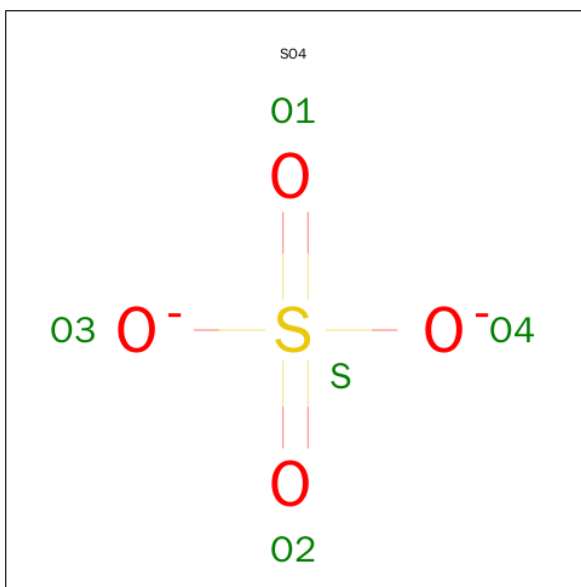
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

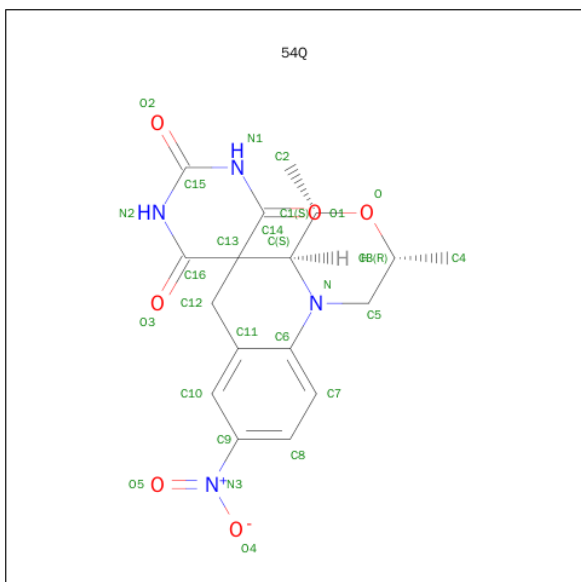


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		

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

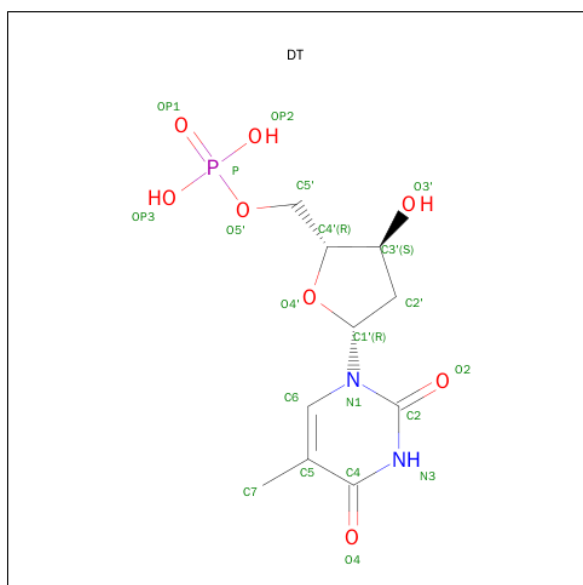
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

- 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<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	I	1	Total	C	H	N	O	
			45	17	18	4	6	
9	N	1	Total	C	H	N	O	
			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		
			8	6	2	0	1

- Molecule 11 is water.

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

*Continued on next page...*

*Continued from previous page...*

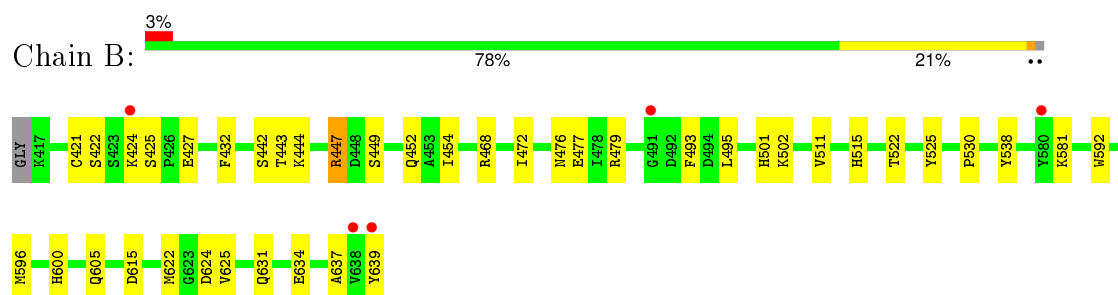
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	F	14	Total 14	O 14	0	0
11	N	21	Total 21	O 21	0	0



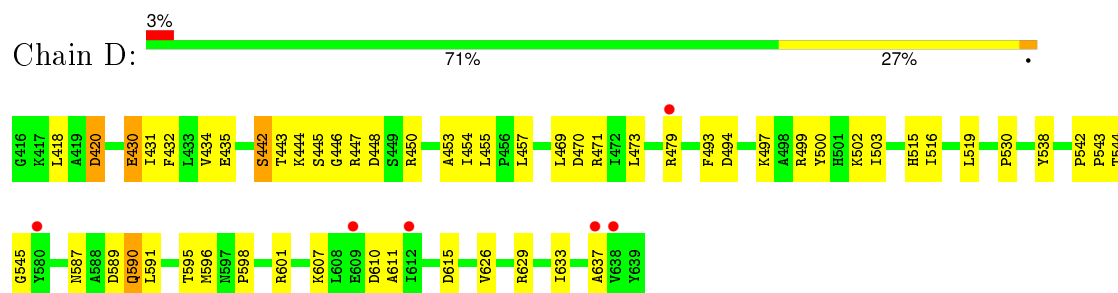
### 3 Residue-property plots [i](#)

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.

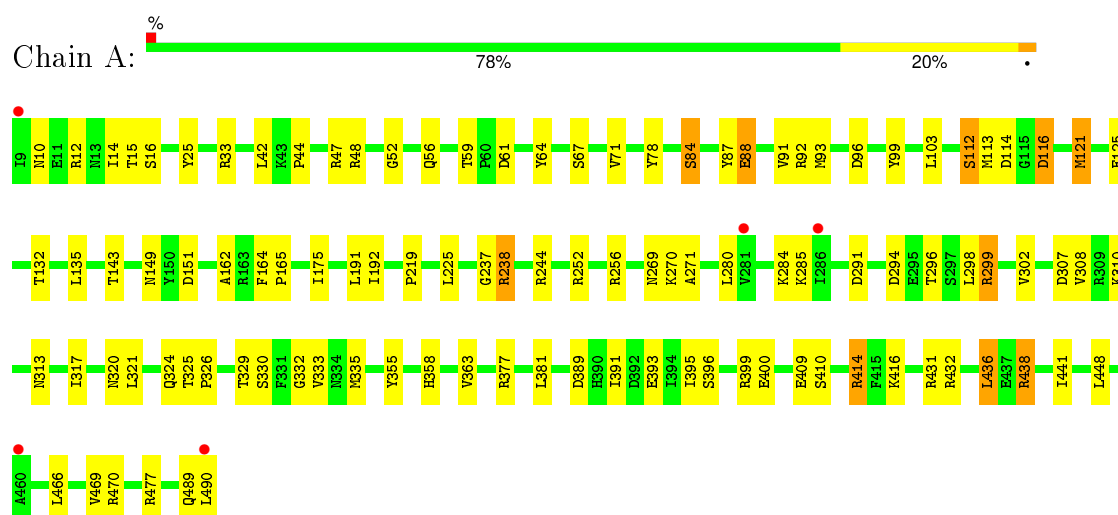
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B



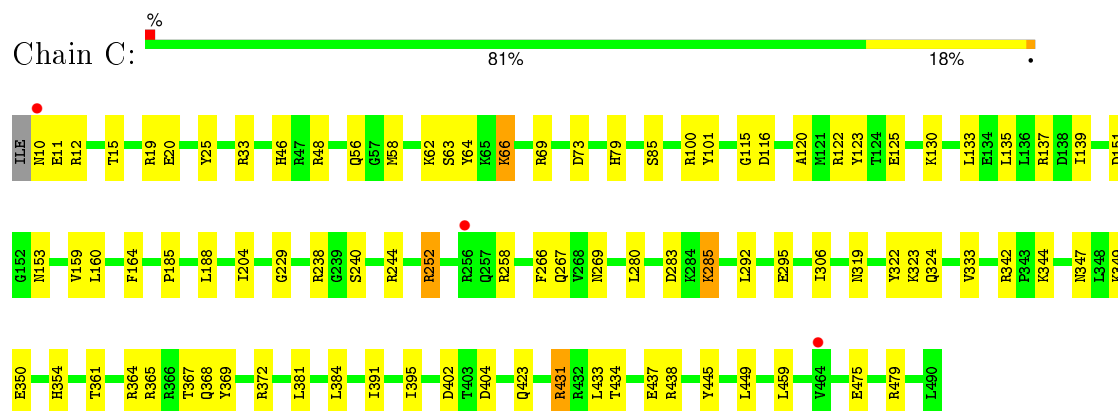
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B



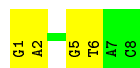
- Molecule 2: DNA gyrase subunit A



- Molecule 2: DNA gyrase subunit A



- 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')



- 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')



- 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')



- 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')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	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 <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	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 <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

*Continued on next page...*

*Continued from previous page...*

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.

All (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
1:B:631:GLN:NE2	1:B:634:GLU:OE1	2.23	0.71
1:D:587:ASN:ND2	1:D:590:GLN:OE1	2.25	0.69
1:D:420:ASP:OD2	1:D:499:ARG:NH1	2.26	0.68
1:D:470:ASP:OD2	11:D:801:HOH:O	2.12	0.67
2:C:344:LYS:NZ	2:C:350:GLU:OE1	2.27	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:2019:DT:O4	3:F:2:DA:N1	2.29	0.66
1:B:477:GLU:OE1	6:B:1002:GOL:O1	2.11	0.66
2:C:437:GLU:OE2	11:C:501:HOH:O	2.13	0.65
2:A:299:ARG:NH2	1:D:446:GLY:O	2.30	0.65
2:C:354:HIS:O	11:C:502:HOH:O	2.15	0.65
2:A:321:LEU:O	2:A:325:THR:OG1	2.10	0.64
2:C:445:TYR:CE2	2:C:449:LEU:HD11	2.34	0.63
2:C:115:GLY:HA3	2:C:269:ASN:ND2	2.14	0.63
2:C:283:ASP:HB2	2:C:285:LYS:CD	2.29	0.62
2:A:116:ASP:N	2:A:116:ASP:OD1	2.32	0.62
2:A:114:ASP:O	2:A:269:ASN:ND2	2.32	0.62
2:C:64:TYR:HB3	2:C:125:GLU:HB3	1.79	0.62
2:A:12:ARG:HH12	2:A:16:SER:HB3	1.65	0.62
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.30	0.61
1:D:430:GLU:HB3	1:D:502:LYS:HB2	1.83	0.61
2:C:66:LYS:HE3	2:C:125:GLU:HG3	1.81	0.61
4:N:2019:DT:HO3'	10:N:2101[A]:DT:P	2.25	0.60
2:A:64:TYR:HB3	2:A:125:GLU:HB3	1.84	0.60
1:B:447:ARG:HG2	1:B:454:ILE:HD11	1.83	0.60
1:B:476:ASN:OD1	1:B:479:ARG:NH2	2.35	0.59
4:N:2016:DC:H2''	4:N:2017:DG:H5'	1.85	0.59
2:C:292:LEU:CD1	2:C:306:ILE:HG12	2.34	0.58
1:B:605:GLN:N	2:A:10:ASN:O	2.36	0.58
4:N:2019:DT:O3'	10:N:2101[A]:DT:P	2.62	0.57
2:C:324:GLN:NE2	11:C:506:HOH:O	2.37	0.57
1:D:470:ASP:OD1	1:D:471:ARG:N	2.38	0.57
1:B:624:ASP:OD1	1:B:625:VAL:N	2.38	0.57
1:D:469:LEU:HG	1:D:473:LEU:HD11	1.86	0.56
1:D:443:THR:HG23	1:D:596:MET:SD	2.46	0.56
2:A:299:ARG:HH11	2:A:299:ARG:HG3	1.71	0.56
1:B:501:HIS:ND1	11:B:1103:HOH:O	2.33	0.56
2:A:298:LEU:HB2	2:A:299:ARG:NH1	2.22	0.54
2:A:256:ARG:HG2	2:A:310:LYS:HB2	1.90	0.54
1:D:448:ASP:OD1	1:D:450[B]:ARG:HG3	2.07	0.53
1:D:633:ILE:O	1:D:637:ALA:HB2	2.08	0.53
1:B:443:THR:HG22	1:B:454:ILE:HD11	1.91	0.53
2:A:92:ARG:NH2	3:E:6:DT:OP2	2.42	0.53
2:C:475:GLU:OE2	2:C:479:ARG:NH2	2.42	0.52
2:A:112:SER:HB2	2:A:116:ASP:OD1	2.09	0.52
1:D:479[B]:ARG:HG3	1:D:479[B]:ARG:HH11	1.75	0.52
1:D:607:LYS:HE3	2:C:11:GLU:CB	2.40	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:ARG:HD3	1:D:454:ILE:HD12	1.92	0.52
1:B:493:PHE:CE1	1:B:530:PRO:HB2	2.45	0.52
1:B:592:TRP:HA	1:B:596:MET:HB2	1.90	0.51
2:A:363:VAL:HG21	2:A:469:VAL:HG22	1.92	0.51
4:N:2012:DC:C2	9:N:2102:54Q:H12	2.45	0.51
2:C:15:THR:O	2:C:19:ARG:HG3	2.09	0.51
2:C:283:ASP:HB2	2:C:285:LYS:HD3	1.92	0.51
1:D:515:HIS:HB2	2:C:25:TYR:CD1	2.45	0.51
2:A:135:LEU:HD23	2:A:162:ALA:HA	1.93	0.51
1:B:476:ASN:N	6:B:1002:GOL:O2	2.30	0.51
1:D:447:ARG:HD3	1:D:454:ILE:CD1	2.42	0.50
2:A:355:TYR:O	2:A:358:HIS:HB3	2.11	0.50
2:A:103:LEU:HB3	2:A:132:THR:OG1	2.12	0.50
2:A:270:LYS:NZ	2:A:294:ASP:OD2	2.41	0.50
1:D:443:THR:HG22	1:D:454:ILE:CD1	2.42	0.50
2:C:137:ARG:NH2	11:C:512:HOH:O	2.44	0.49
2:A:466:LEU:HD23	2:A:470:ARG:NH2	2.27	0.49
4:N:2017:DG:H1'	4:N:2018:DC:H5'	1.94	0.49
1:D:442:SER:HB3	1:D:591:LEU:HD12	1.93	0.49
1:D:444:LYS:HA	1:D:447:ARG:HG2	1.93	0.49
2:C:283:ASP:HB2	2:C:285:LYS:HD2	1.93	0.49
2:A:44:PRO:O	2:A:48:ARG:HG3	2.11	0.49
2:A:59:THR:OG1	2:A:61:ASP:OD1	2.22	0.49
2:C:101:TYR:CZ	2:C:188:LEU:HB2	2.47	0.49
2:A:237:GLY:HA2	2:A:335:MET:HE2	1.96	0.48
9:N:2102:54Q:C14	9:N:2102:54Q:H3	2.42	0.48
2:A:381:LEU:HD22	2:A:441:ILE:HG23	1.96	0.48
2:A:149:ASN:ND2	2:A:151:ASP:OD1	2.47	0.48
2:A:395:ILE:O	2:A:399:ARG:HG3	2.13	0.48
2:A:329:THR:HG22	2:A:330:SER:N	2.29	0.48
2:C:367:THR:HG22	2:C:459:LEU:HD11	1.96	0.48
1:B:511:VAL:HB	2:A:25:TYR:HA	1.96	0.48
2:C:151:ASP:OD1	2:C:153:ASN:HB2	2.13	0.48
2:A:377:ARG:CG	2:A:448:LEU:HD11	2.45	0.47
2:A:320:ASN:O	2:A:324:GLN:HG3	2.14	0.47
9:I:2101:54Q:C14	9:I:2101:54Q:H3	2.45	0.47
2:C:116:ASP:OD1	2:C:116:ASP:N	2.48	0.47
4:N:2012:DC:H1'	9:N:2102:54Q:O5	2.15	0.47
2:A:291:ASP:HB3	2:A:307:ASP:HB2	1.95	0.47
4:I:2018:DC:H2''	4:I:2019:DT:H71	1.96	0.47
1:D:434:VAL:HG12	1:D:435:GLU:N	2.30	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:369:TYR:C	2:C:369:TYR:CD1	2.88	0.47
2:A:164:PHE:HB2	2:A:165:PRO:HD2	1.97	0.47
1:B:443:THR:O	1:B:447:ARG:HG2	2.15	0.46
4:I:2012:DC:C2	9:I:2101:54Q:H12	2.50	0.46
2:A:48:ARG:HD3	2:A:78:TYR:CB	2.45	0.46
2:C:252:ARG:HD3	2:C:258:ARG:HB3	1.98	0.46
1:D:516:ILE:HA	1:D:519:LEU:HD12	1.97	0.46
1:D:420:ASP:OD1	1:D:500:TYR:OH	2.25	0.46
2:A:410:SER:O	2:A:414:ARG:HG3	2.16	0.46
1:D:598:PRO:HA	1:D:601:ARG:HG2	1.97	0.46
2:A:192:ILE:HD13	2:A:477:ARG:HB2	1.98	0.46
1:B:444:LYS:HA	1:B:454:ILE:CD1	2.46	0.45
2:A:332:GLY:O	11:A:601:HOH:O	2.20	0.45
2:C:381:LEU:HD23	2:C:384:LEU:HD12	1.98	0.45
4:N:2013:DG:C2	9:N:2102:54Q:H15	2.51	0.45
1:B:502:LYS:HG2	1:B:538:TYR:CE1	2.52	0.45
2:C:159:VAL:HG22	2:C:160:LEU:N	2.31	0.45
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.51	0.45
1:B:637:ALA:HB1	1:B:639:TYR:CE2	2.51	0.45
1:B:515:HIS:CD2	2:A:25:TYR:CD2	3.05	0.45
2:A:84:SER:O	2:A:88:GLU:HB2	2.17	0.45
1:D:542:PRO:HB2	1:D:543:PRO:HD2	1.99	0.45
4:I:2013:DG:C2	9:I:2101:54Q:H15	2.52	0.45
1:D:503:ILE:HD12	1:D:503:ILE:N	2.32	0.45
2:C:115:GLY:HA3	2:C:269:ASN:HD21	1.79	0.44
2:A:296:THR:HG23	2:A:302:VAL:HA	1.99	0.44
1:D:544:THR:HG22	1:D:545:GLY:N	2.32	0.44
3:E:1:DG:H2'	3:E:2:DA:C4	2.53	0.44
2:C:12:ARG:HH22	2:C:20:GLU:CD	2.21	0.44
2:A:87:TYR:O	2:A:91:VAL:HG23	2.17	0.44
2:C:364:ARG:O	2:C:368:GLN:HG3	2.18	0.44
2:A:313:ASN:O	2:A:317:ILE:HG13	2.18	0.44
2:C:280:LEU:HD23	2:C:285:LYS:HE2	2.00	0.43
2:C:347:ASN:ND2	2:C:350:GLU:OE2	2.51	0.43
2:C:120:ALA:HB3	2:C:123:PTR:HD1	2.00	0.43
4:N:2019:DT:O3'	10:N:2101[B]:DT:P	2.77	0.43
2:C:391:ILE:O	2:C:395:ILE:HG12	2.18	0.43
2:C:100:ARG:HB2	2:C:185:PRO:HB2	2.00	0.43
2:A:396:SER:O	2:A:400:GLU:HG3	2.19	0.43
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.54	0.43
2:C:434:THR:O	2:C:438:ARG:HD3	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LYS:HG3	1:B:454:ILE:HD12	2.00	0.43
2:A:225:LEU:HD21	2:A:244:ARG:HD2	2.00	0.43
2:C:229:GLY:HA3	2:C:240:SER:O	2.19	0.43
2:A:67:SER:O	2:A:71:VAL:HG23	2.19	0.43
2:C:135:LEU:HG	2:C:164:PHE:CE1	2.54	0.43
1:D:431:ILE:HA	1:D:453:ALA:O	2.19	0.42
1:D:610:ASP:OD1	1:D:611:ALA:N	2.53	0.42
2:A:325:THR:HB	2:A:326:PRO:CD	2.49	0.42
2:C:135:LEU:HG	2:C:164:PHE:HE1	1.84	0.42
2:A:52:GLY:O	2:A:56:GLN:HG3	2.19	0.42
2:C:238[A]:ARG:HA	2:C:333:VAL:O	2.20	0.42
2:C:10:ASN:CG	2:C:11:GLU:H	2.22	0.42
1:B:493:PHE:HE1	1:B:495:LEU:HB2	1.85	0.42
2:C:266:PHE:O	2:C:267:GLN:HB2	2.19	0.42
2:C:283:ASP:CB	2:C:285:LYS:HD2	2.49	0.42
2:C:361:THR:O	2:C:365:ARG:HG3	2.19	0.42
2:A:48:ARG:HD3	2:A:78:TYR:HB3	2.00	0.42
2:C:130:LYS:HA	2:C:133:LEU:HD12	2.01	0.42
2:C:475:GLU:CD	2:C:479:ARG:HH21	2.23	0.42
2:A:87:TYR:CD1	2:A:121:MET:HB3	2.55	0.42
2:C:56:GLN:NE2	2:C:73:ASP:HB3	2.34	0.42
2:C:238[B]:ARG:HA	2:C:333:VAL:O	2.20	0.42
2:A:436:LEU:HB3	2:C:402:ASP:O	2.20	0.41
1:D:494:ASP:CG	1:D:497:LYS:HG3	2.40	0.41
1:B:421:CYS:HA	1:B:449:SER:O	2.20	0.41
1:D:432:PHE:CE2	1:D:596:MET:HE3	2.55	0.41
2:C:368:GLN:O	2:C:372:ARG:HG3	2.20	0.41
2:A:175:ILE:HD12	3:E:5:DG:C2	2.56	0.41
1:B:522:THR:OG1	1:B:622:MET:HG3	2.20	0.41
2:A:280:LEU:HD22	2:A:285:LYS:HB2	2.03	0.41
1:B:427:GLU:CD	1:B:427:GLU:H	2.22	0.41
2:A:14:ILE:HG23	2:A:15:THR:N	2.35	0.41
2:A:96:ASP:O	2:A:219:PRO:HB2	2.20	0.41
1:D:434:VAL:HG23	1:D:454:ILE:HG23	2.02	0.41
2:C:100:ARG:HG3	2:C:101:TYR:CE2	2.56	0.41
1:B:468:ARG:O	1:B:472:ILE:HG13	2.21	0.41
2:C:58:MET:CE	2:C:58:MET:HA	2.51	0.41
2:A:93:MET:HG2	2:A:99:TYR:CZ	2.55	0.41
2:C:280:LEU:HD23	2:C:285:LYS:NZ	2.36	0.41
4:N:2011:DC:C5	4:N:2012:DC:N4	2.89	0.41
1:B:432:PHE:HE1	1:B:452:GLN:HG2	1.84	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:48:ARG:NH1	2:C:79:HIS:ND1	2.65	0.41
2:A:325:THR:HB	2:A:326:PRO:HD2	2.03	0.41
2:C:431[B]:ARG:C	2:C:433:LEU:H	2.23	0.41
2:C:46:HIS:ND1	11:C:505:HOH:O	2.37	0.41
2:A:42:LEU:HD13	2:A:47:ARG:HA	2.02	0.41
2:A:431:ARG:HB2	2:C:404:ASP:OD2	2.20	0.40
2:A:299:ARG:NH1	2:A:299:ARG:HG3	2.35	0.40
1:B:624:ASP:OD1	1:B:625:VAL:HG23	2.21	0.40
2:A:269:ASN:OD1	2:A:271:ALA:N	2.54	0.40
1:D:626:VAL:O	1:D:629:ARG:HB3	2.21	0.40
2:A:432:ARG:HH11	2:A:432:ARG:HG3	1.87	0.40
1:D:443:THR:HG22	1:D:454:ILE:HD13	2.03	0.40
2:A:238:ARG:HA	2:A:333:VAL:O	2.22	0.40

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

### 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	
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 ⓘ

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
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

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	422	SER
1	B	424	LYS
1	B	442	SER
1	B	447	ARG
1	B	581	LYS
1	B	600	HIS
2	A	84	SER
2	A	88	GLU
2	A	112	SER
2	A	113	MET
2	A	116	ASP
2	A	121	MET
2	A	143	THR
2	A	191	LEU
2	A	238	ARG
2	A	284	LYS
2	A	299	ARG
2	A	391	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	393	GLU
2	A	414	ARG
2	A	436	LEU
2	A	438	ARG
2	A	489	GLN
2	A	490	LEU
1	D	418	LEU
1	D	420	ASP
1	D	430	GLU
1	D	442	SER
1	D	445	SER
1	D	457	LEU
1	D	589	ASP
1	D	590	GLN
1	D	595	THR
1	D	615	ASP
2	C	62	LYS
2	C	63	SER
2	C	66	LYS
2	C	69	ARG
2	C	85	SER
2	C	122	ARG
2	C	139	ILE
2	C	244	ARG
2	C	252	ARG
2	C	285	LYS
2	C	295	GLU
2	C	319	ASN
2	C	342[A]	ARG
2	C	342[B]	ARG
2	C	423	GLN
2	C	431[A]	ARG
2	C	431[B]	ARG

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 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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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(°)	Ideal(°)
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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	D	479[A]	ARG	2.8
2	A	9	ILE	2.5
2	A	460	ALA	2.5
1	B	424	LYS	2.4
1	D	612	ILE	2.4
2	C	256	ARG	2.3
1	B	638	VAL	2.3
2	A	286	ILE	2.3
2	C	10	ASN	2.2
1	D	580	TYR	2.2
1	D	637	ALA	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	281	VAL	2.1
1	B	639	TYR	2.1
2	C	464	VAL	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<sup>th</sup> 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 <sup>2</sup> )	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, 95<sup>th</sup> 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 <sup>2</sup> )	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.