



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:01 PM UTC

PDB ID : 5CDM / pdb\_00005cdm  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

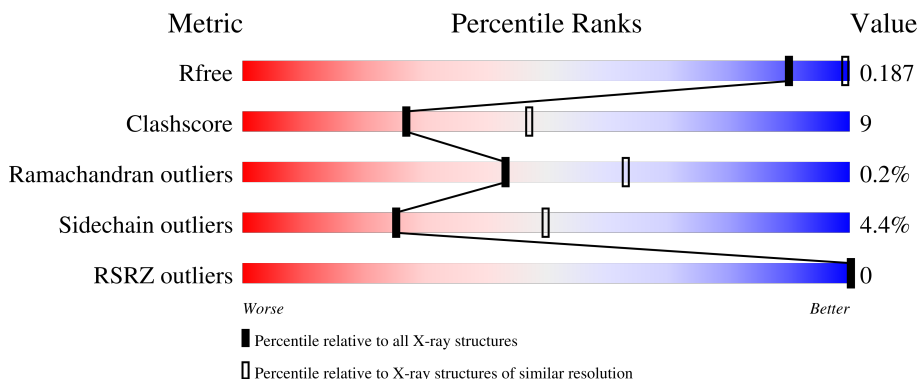
# 1 Overall quality at a glance i

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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	 75% 24% ..
1	D	190	 71% 27% .
2	A	482	 75% 23% .
2	C	482	 78% 20% .
3	E	8	 38% 62%

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Mol	Chain	Length	Quality of chain
3	F	8	 75% 12% 12%
4	I	12	 58% 42%
4	N	12	 33% 58% 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
			Total	C	H	N	O	S			
1	B	189	2937	931	1455	260	282	9	0	2	0
1	D	190	2953	937	1459	262	286	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
			Total	C	H	N	O	P	S			
2	A	482	7668	2373	3845	696	736	1	17	0	4	0
2	C	481	7803	2406	3926	711	743	1	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	
			Total	C	H	N	O				P
3	E	8	256	78	90	33	47	8	0	0	0
3	F	7	223	68	79	28	41	7	0	0	0

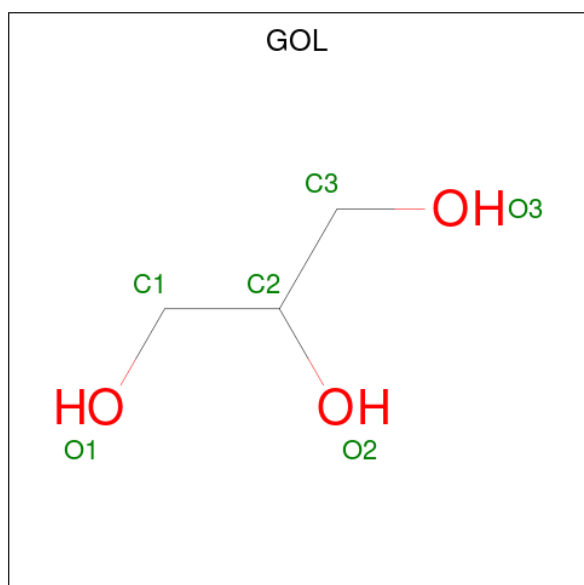
- Molecule 4 is a DNA chain called DNA (5'-D(P\*GP\*AP\*GP\*CP\*GP\*TP\*AP\*C\*GP\*GP\*CP\*CP\*GP\*TP\*AP\*CP\*GP\*CP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				P
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 (CCD ID: 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 (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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 (CCD ID: SO4) (formula: O<sub>4</sub>S).

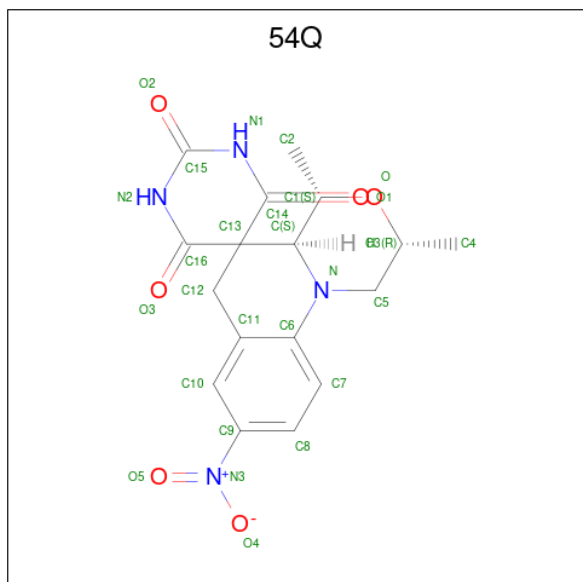


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

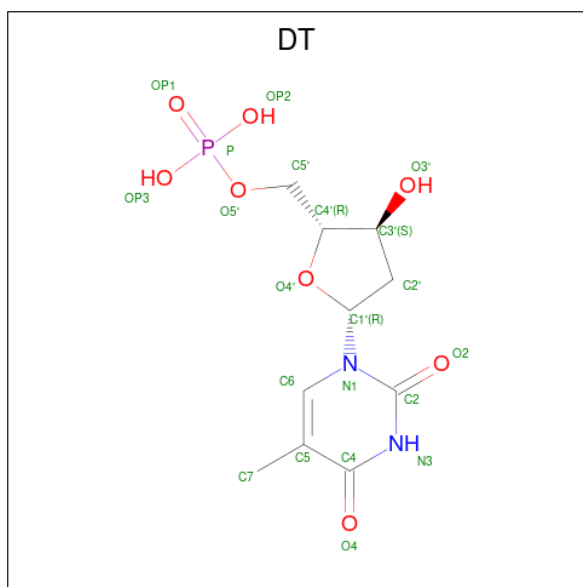
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

- 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 (CCD ID: 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	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 (CCD ID: DT) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>8</sub>P).



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		
11	F	14	Total	O	0	0
			14	14		

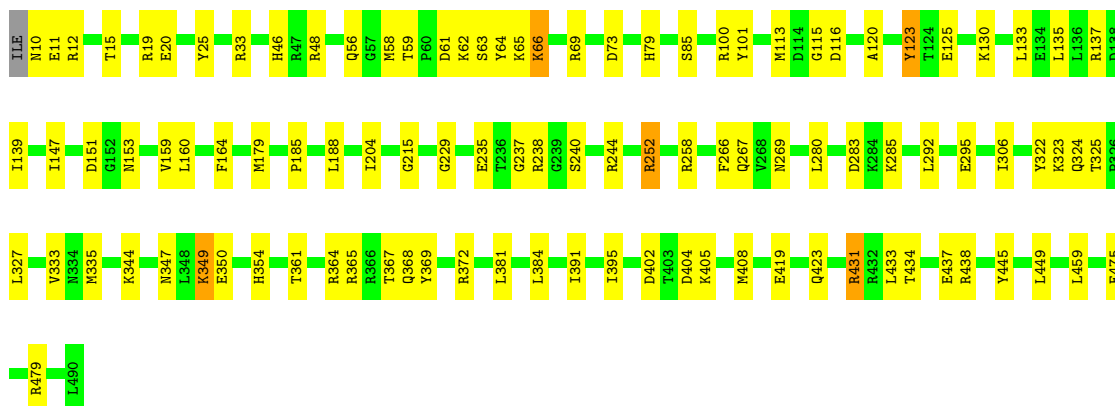
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
11	N	21	Total	O	0	0
			21	21		

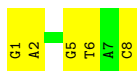


Chain C:  78% 20%



- 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:  38% 62%



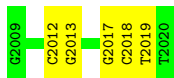
- Molecule 3: DNA (5'-D(P\*GP\*AP\*GP\*CP\*GP\*TP\*AP\*C\*GP\*GP\*CP\*CP\*GP\*TP\*AP\*CP\*GP\*CP\*TP\*T)-3')

Chain F:  75% 12% 12%



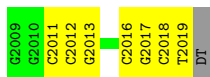
- Molecule 4: DNA (5'-D(P\*GP\*AP\*GP\*CP\*GP\*TP\*AP\*C\*GP\*GP\*CP\*CP\*GP\*TP\*AP\*CP\*GP\*CP\*TP\*T)-3')

Chain I:  58% 42%



- 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:  33% 58% 8%



## 4 Data and refinement statistics i

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 36.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (36.78-2.50) 95.3 (36.78-2.50)	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)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.163 , 0.192 0.166 , 0.187	Depositor DCC
$R_{free}$ test set	3409 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 21.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.213 for h,-h-k,-l	Xtrriage
Reported twinning fraction	0.220 for h,-h-k,-l	Depositor
Outliers	0 of 67361 reflections	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	23019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 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: 54Q, PTR, NA, MN, SO4, GOL

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	0.59	0/1513	0.81	2/2043 (0.1%)
1	D	0.55	0/1534	0.84	4/2072 (0.2%)
2	A	0.59	0/3866	0.81	5/5212 (0.1%)
2	C	0.62	0/3952	0.80	2/5320 (0.0%)
3	E	0.51	0/186	0.52	0/285
3	F	0.53	0/161	0.56	0/246
4	I	0.51	0/269	0.57	0/414
4	N	0.56	0/247	0.62	0/380
All	All	0.59	0/11728	0.79	13/15972 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	455	LEU	CA-C-N	-6.40	113.36	120.14
1	D	455	LEU	C-N-CA	-6.40	113.36	120.14
1	B	455	LEU	CA-C-N	-6.12	113.97	120.03
1	B	455	LEU	C-N-CA	-6.12	113.97	120.03
2	C	215	GLY	CA-C-N	5.99	125.95	119.78
2	C	215	GLY	C-N-CA	5.99	125.95	119.78
1	D	541	GLN	CA-C-N	-5.52	114.70	120.38
1	D	541	GLN	C-N-CA	-5.52	114.70	120.38
2	A	156	GLU	CA-C-N	-5.45	114.36	120.14
2	A	156	GLU	C-N-CA	-5.45	114.36	120.14
2	A	112	SER	N-CA-C	5.18	116.85	109.14
2	A	221	ALA	CB-CA-C	-5.13	110.67	116.63
2	A	116	ASP	N-CA-C	-5.11	103.86	110.19

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	31	0
1	D	1494	1459	1442	35	0
2	A	3823	3845	3831	69	2
2	C	3877	3926	3872	66	2
3	E	166	90	90	4	0
3	F	144	79	79	1	0
4	I	241	134	134	5	0
4	N	221	121	122	10	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	208	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 9.

All (208) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:321:LEU:O	2:A:325:THR:OG1	2.10	0.70
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
4:I:2019:DT:O4	3:F:2:DA:N1	2.29	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
1:B:447:ARG:HB3	1:B:596:MET:HE1	1.79	0.64
2:C:58:MET:HE2	2:C:58:MET:HA	1.78	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:OD1	2:A:116:ASP:N	2.32	0.62
2:A:114:ASP:O	2:A:269:ASN:ND2	2.32	0.62
2:A:12:ARG:HH12	2:A:16:SER:HB3	1.65	0.62
2:C:64:TYR:HB3	2:C:125:GLU:HB3	1.79	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
2:C:408:MET:HE1	2:C:419:GLU:HG2	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
1:B:605:GLN:N	2:A:10:ASN:O	2.36	0.58
2:C:292:LEU:CD1	2:C:306:ILE:HG12	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:237:GLY:HA2	2:C:335:MET:HE2	1.88	0.55
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
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
2:C:369:TYR:C	2:C:369:TYR:CD1	2.88	0.51
2:A:83:ASP:HB2	2:A:121:MET:HE1	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:A:58:MET:HA	2:A:58:MET:HE2	1.93	0.51
1:B:477:GLU:OE1	6:B:1002:GOL:O1	2.11	0.51
2:A:135:LEU:HD23	2:A:162:ALA:HA	1.93	0.51
1:D:515:HIS:HB2	2:C:25:TYR:CD1	2.45	0.51
2:C:283:ASP:HB2	2:C:285:LYS:HD3	1.92	0.51
1:B:476:ASN:N	6:B:1002:GOL:O2	2.30	0.51
2:A:355:TYR:O	2:A:358:HIS:HB3	2.11	0.50
1:D:447:ARG:HD3	1:D:454:ILE:CD1	2.42	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:A:466:LEU:HD23	2:A:470:ARG:NH2	2.27	0.49
2:C:137:ARG:NH2	11:C:512:HOH:O	2.44	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:12:ARG:HH22	2:C:20:GLU:CD	2.21	0.49
2:C:101:TYR:CZ	2:C:188:LEU:HB2	2.47	0.49
2:A:381:LEU:HD22	2:A:441:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:2102:54Q:H3	9:N:2102:54Q:C14	2.42	0.48
2:A:149:ASN:ND2	2:A:151:ASP:OD1	2.47	0.48
2:A:329:THR:HG22	2:A:330:SER:N	2.29	0.48
2:A:395:ILE:O	2:A:399:ARG:HG3	2.13	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:237:GLY:HA2	2:A:335:MET:HE2	1.95	0.47
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
2:A:71:VAL:HG11	2:A:121:MET:HE1	1.95	0.47
2:C:10:ASN:CG	2:C:11:GLU:H	2.22	0.47
9:I:2101:54Q:C14	9:I:2101:54Q:H3	2.45	0.47
1:B:427:GLU:H	1:B:427:GLU:CD	2.22	0.47
1:D:420:ASP:OD1	1:D:500:TYR:OH	2.25	0.47
2:C:116:ASP:OD1	2:C:116:ASP:N	2.48	0.47
2:A:291:ASP:HB3	2:A:307:ASP:HB2	1.95	0.47
4:N:2012:DC:H1'	9:N:2102:54Q:O5	2.15	0.47
1:D:434:VAL:HG12	1:D:435:GLU:N	2.30	0.47
4:I:2018:DC:H2''	4:I:2019:DT:H71	1.96	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
2:C:475:GLU:CD	2:C:479:ARG:HH21	2.23	0.46
1:D:494:ASP:CG	1:D:497:LYS:HG3	2.40	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:59:THR:OG1	2:C:61:ASP:OD1	2.31	0.46
1:D:516:ILE:HA	1:D:519:LEU:HD12	1.97	0.46
2:C:252:ARG:HD3	2:C:258:ARG:HB3	1.98	0.46
2:A:192:ILE:HD13	2:A:477:ARG:HB2	1.98	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
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:431[B]:ARG:C	2:C:433:LEU:H	2.23	0.45
2:C:381:LEU:HD23	2:C:384:LEU:HD12	1.98	0.45
1:B:502:LYS:HG2	1:B:538:TYR:CE1	2.52	0.45
4:N:2013:DG:C2	9:N:2102:54Q:H15	2.51	0.45
2:C:159:VAL:HG22	2:C:160:LEU:N	2.31	0.45
1:B:637:ALA:HB1	1:B:639:TYR:CE2	2.51	0.45
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:503:ILE:N	1:D:503:ILE:HD12	2.32	0.45
2:C:325:THR:C	2:C:327:LEU:H	2.25	0.45
4:I:2013:DG:C2	9:I:2101:54Q:H15	2.52	0.45
2:A:296:THR:HG23	2:A:302:VAL:HA	1.99	0.44
2:C:115:GLY:HA3	2:C:269:ASN:HD21	1.79	0.44
1:D:544:THR:HG22	1:D:545:GLY:N	2.32	0.44
1:B:435:GLU:OE2	3:E:8:DC:O3'	2.29	0.44
3:E:1:DG:H2'	3:E:2:DA:C4	2.53	0.44
2:A:87:TYR:O	2:A:91:VAL:HG23	2.17	0.44
2:A:313:ASN:O	2:A:317:ILE:HG13	2.18	0.44
2:C:113:MET:C	2:C:115:GLY:H	2.26	0.44
2:C:364:ARG:O	2:C:368:GLN:HG3	2.18	0.44
2:C:280:LEU:HD23	2:C:285:LYS:HE2	2.00	0.43
2:C:120:ALA:HB3	2:C:123:PTR:HD1	2.00	0.43
2:C:347:ASN:ND2	2:C:350:GLU:OE2	2.51	0.43
2:C:391:ILE:O	2:C:395:ILE:HG12	2.18	0.43
4:N:2019:DT:O3'	10:N:2101[B]:DT:P	2.77	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:100:ARG:HB2	2:C:185:PRO:HB2	2.00	0.43
2:C:434:THR:O	2:C:438:ARG:HD3	2.19	0.43
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:C:408:MET:HE3	2:C:408:MET:HB3	1.92	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:A:179:MET:C	4:N:2017:DG:H4'	2.44	0.42
2:C:238[A]:ARG:HA	2:C:333:VAL:O	2.20	0.42
1:B:493:PHE:HE1	1:B:495:LEU:HB2	1.85	0.42
1:B:639:TYR:CD1	2:A:27[A]:MET:HE1	2.54	0.42
2:C:266:PHE:O	2:C:267:GLN:HB2	2.19	0.42
2:A:201:ASN:C	2:A:203:ASP:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:431[B]:ARG:C	2:C:433:LEU:N	2.78	0.42
2:C:238[B]:ARG:HA	2:C:333:VAL:O	2.20	0.42
1:B:421:CYS:HA	1:B:449:SER:O	2.20	0.41
2:A:436:LEU:HB3	2:C:402:ASP:O	2.20	0.41
2:C:408:MET:HE1	2:C:419:GLU:CG	2.48	0.41
2:C:179:MET:C	4:I:2017:DG:H4'	2.45	0.41
2:C:368:GLN:O	2:C:372:ARG:HG3	2.20	0.41
1:B:522:THR:OG1	1:B:622:MET:HG3	2.20	0.41
2:A:175:ILE:HD12	3:E:5:DG:C2	2.56	0.41
2:A:280:LEU:HD22	2:A:285:LYS:HB2	2.03	0.41
2:A:408:MET:HE3	2:A:408:MET:HB3	1.98	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:B:468:ARG:O	1:B:472:ILE:HG13	2.21	0.41
2:A:93:MET:HG2	2:A:99:TYR:CZ	2.55	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:432:PHE:HE1	1:B:452:GLN:HG2	1.84	0.41
2:C:56:GLN:OE1	2:C:65:LYS:NZ	2.49	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
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:A:42:LEU:HD13	2:A:47:ARG:HA	2.02	0.41
2:A:138:ASP:CG	2:A:366:ARG:HD3	2.46	0.41
2:C:46:HIS:ND1	11:C:505:HOH:O	2.37	0.41
2:A:431:ARG:HB2	2:C:404:ASP:OD2	2.20	0.40
2:A:299:ARG:HG3	2:A:299:ARG:NH1	2.35	0.40
1:D:447:ARG:HB3	1:D:596:MET:HE1	2.04	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
2:A:432:ARG:HH11	2:A:432:ARG:HG3	1.87	0.40
1:D:626:VAL:O	1:D:629:ARG:HB3	2.21	0.40
2:A:238:ARG:HA	2:A:333:VAL:O	2.22	0.40
1:D:443:THR:HG22	1:D:454:ILE:HD13	2.03	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 [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%)	43	63
2	C	490/482 (102%)	470 (96%)	19 (4%)	1 (0%)	43	63
All	All	1354/1344 (101%)	1314 (97%)	38 (3%)	2 (0%)	43	68

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%)	144 (93%)	11 (7%)	13	29
1	D	156/158 (99%)	148 (95%)	8 (5%)	21	43
2	A	412/416 (99%)	395 (96%)	17 (4%)	27	53
2	C	421/416 (101%)	405 (96%)	16 (4%)	29	56
All	All	1144/1148 (100%)	1092 (96%)	52 (4%)	25	49

All (52) 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	450[A]	ARG
1	B	450[B]	ARG
1	B	451[A]	THR
1	B	451[B]	THR
1	B	581	LYS
1	B	600	HIS
1	B	638	VAL
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	385	ARG
2	A	391	ILE
2	A	393	GLU
2	A	436	LEU
2	A	438	ARG
2	A	490	LEU
1	D	418	LEU
1	D	430	GLU
1	D	442	SER
1	D	445	SER
1	D	457	LEU

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Mol	Chain	Res	Type
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	139	ILE
2	C	147	ILE
2	C	235	GLU
2	C	244	ARG
2	C	252	ARG
2	C	295	GLU
2	C	349	LYS
2	C	405	LYS
2	C	423	GLN
2	C	431[A]	ARG
2	C	431[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	501	HIS
2	A	56	GLN
2	A	187	ASN
1	D	600	HIS

### 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
2	PTR	C	123	4,2	15,16,17	1.31	1 (6%)	17,22,24	0.56	0
2	PTR	A	123	4,2	15,16,17	1.22	1 (6%)	17,22,24	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	C	123	4,2	-	2/10/11/13	0/1/1/1
2	PTR	A	123	4,2	-	0/10/11/13	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	-4.37	1.30	1.40
2	A	123	PTR	OH-CZ	-4.30	1.31	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	123	PTR	CZ-OH-P-O1P
2	C	123	PTR	CZ-OH-P-O3P

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 oligosaccharides in this entry.

## 5.6 Ligand geometry

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	0.48	0	6,6,6	0.30	0
9	54Q	I	2101	-	29,30,30	0.67	0	37,47,47	0.65	0
9	54Q	N	2102	-	29,30,30	0.80	0	37,47,47	0.65	0
10	DT	N	2101[B]	-	0,3,22	-	-	0,3,33	-	-
10	DT	N	2101[A]	-	0,3,22	-	-	0,3,33	-	-
6	GOL	B	1002	-	5,5,5	1.07	1 (20%)	5,5,5	1.18	1 (20%)
6	GOL	A	503	-	5,5,5	0.42	0	5,5,5	0.88	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
6	GOL	A	503	-	-	4/4/4/4	-
9	54Q	N	2102	-	-	0/2/55/55	0/4/4/4
6	GOL	B	1002	-	-	2/4/4/4	-
9	54Q	I	2101	-	-	0/2/55/55	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1002	GOL	O2-C2	-2.36	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1002	GOL	O2-C2-C1	-2.13	100.34	109.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1002	GOL	C1-C2-C3-O3
6	B	1002	GOL	O2-C2-C3-O3
6	A	503	GOL	O1-C1-C2-C3
6	A	503	GOL	C1-C2-C3-O3
6	A	503	GOL	O1-C1-C2-O2
6	A	503	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

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

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.51	0 100 100	30, 59, 82, 112	1 (0%)
1	D	190/190 (100%)	-1.47	0 100 100	37, 63, 90, 102	2 (1%)
2	A	481/482 (99%)	-1.61	0 100 100	23, 50, 77, 103	2 (0%)
2	C	480/482 (99%)	-1.62	0 100 100	24, 48, 72, 94	7 (1%)
3	E	8/8 (100%)	-1.97	0 100 100	35, 42, 52, 62	0
3	F	7/8 (87%)	-1.92	0 100 100	37, 39, 56, 88	0
4	I	12/12 (100%)	-1.86	0 100 100	41, 47, 81, 106	0
4	N	11/12 (91%)	-2.09	0 100 100	37, 40, 54, 55	0
All	All	1378/1384 (99%)	-1.59	0 100 100	23, 53, 81, 112	12 (0%)

There are no RSRZ outliers to report.

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	PTR	A	123	16/17	1.00	0.03	31,38,43,44	0
2	PTR	C	123	16/17	1.00	0.03	36,46,56,58	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
7	SO4	A	501	5/5	0.98	0.04	61,61,67,74	0
6	GOL	B	1002	6/6	0.99	0.04	40,48,53,54	0
10	DT	N	2101[A]	4/21	0.99	0.06	23,29,33,42	4
10	DT	N	2101[B]	4/21	0.99	0.06	26,31,33,38	4
5	MN	D	701	1/1	1.00	0.01	38,38,38,38	0
8	NA	A	502	1/1	1.00	0.01	41,41,41,41	0
9	54Q	I	2101	27/27	1.00	0.03	29,36,43,50	0
9	54Q	N	2102	27/27	1.00	0.02	27,35,43,50	0
5	MN	B	1001	1/1	1.00	0.00	43,43,43,43	0
6	GOL	A	503	6/6	1.00	0.03	29,48,67,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.