



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:58 PM GMT

PDB ID : 3HNF  
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effectors  
TTP and dATP  
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.  
Deposited on : 2009-05-31  
Resolution : 3.16 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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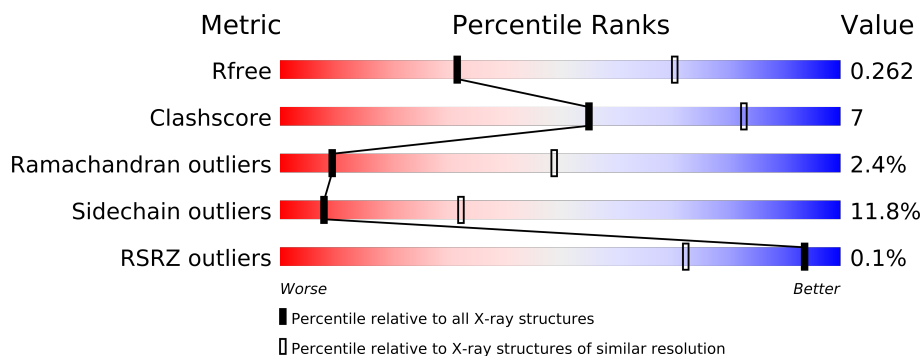
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 3.16 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))
$R_{free}$	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	792	
1	B	792	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	801	-	X
2	MG	B	802	-	X
4	SO4	B	806	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11549 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

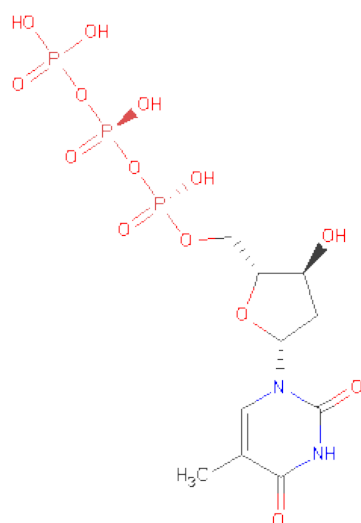
- Molecule 1 is a protein called Ribonucleoside-diphosphatereductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	6	0	0
			5596	3579	925	1059	33			
1	B	737	Total	C	N	O	S	0	0	0
			5795	3698	980	1083	34			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

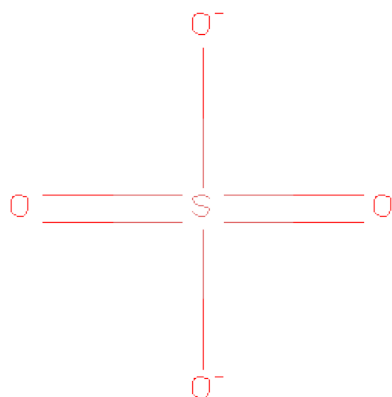
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>2</sub>O<sub>14</sub>P<sub>3</sub>).



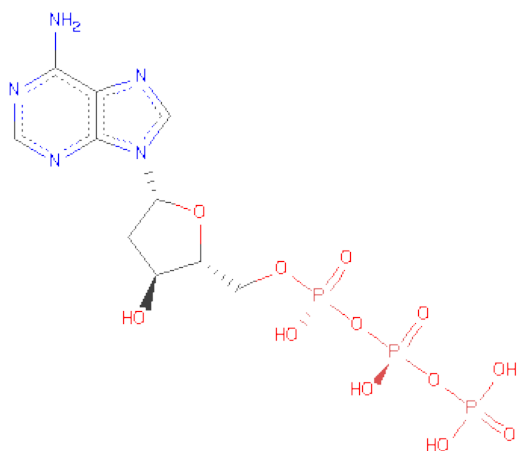
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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



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

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	30	10	5	12	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	22	Total	O	0	0
			22	22		
6	B	26	Total	O	0	0
			26	26		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.86Å 114.39Å 220.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.86 – 3.16 40.85 – 3.16	Depositor EDS
% Data completeness (in resolution range)	89.4 (40.86-3.16) 89.4 (40.85-3.16)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.260 0.188 , 0.262	Depositor DCC
$R_{free}$ test set	1335 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27352 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11549	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DTP, TTP, SO4

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	0.59	1/5721 (0.0%)	0.70	1/7782 (0.0%)
1	B	0.57	0/5920	0.70	2/8035 (0.0%)
All	All	0.58	1/11641 (0.0%)	0.70	3/15817 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	CYS	CB-SG	-5.55	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	LEU	CA-CB-CG	7.19	131.84	115.30
1	B	449	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	508	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5596	0	7	31	0
1	B	5795	0	26	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	1	0
3	B	29	0	13	4	0
4	A	10	0	0	0	0
4	B	10	0	0	1	0
5	B	30	0	12	0	0
6	A	22	0	0	0	0
6	B	26	0	0	1	0
All	All	11549	0	71	77	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (77) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:PHE:C	1:A:220:LEU:CD2	2.30	1.00
1:B:416:ASN:OD1	1:B:561:VAL:CG2	2.09	1.00
1:A:443:VAL:CG1	1:A:444:CYS:N	2.29	0.94
1:A:220:LEU:N	1:A:220:LEU:CD2	2.30	0.92
1:A:219:PHE:O	1:A:220:LEU:CD2	2.30	0.78
1:B:490:GLU:N	1:B:490:GLU:OE1	2.18	0.76
1:B:260:SER:OG	1:B:352:CYS:SG	2.46	0.73
1:A:256:ARG:NH1	3:A:804:TTP:O3G	2.22	0.72
1:B:212:ARG:NH1	1:B:485:TYR:CE1	2.60	0.69
1:B:416:ASN:CG	1:B:561:VAL:CG2	2.61	0.68
1:A:243:LYS:NZ	3:B:803:TTP:O3A	2.31	0.63
1:B:644:ASP:OD1	1:B:644:ASP:N	2.33	0.61
1:B:478:ASN:OD1	1:B:595:ASN:ND2	2.37	0.58
1:B:695:ALA:O	1:B:699:GLY:N	2.38	0.56
1:B:431:GLU:OE2	1:B:431:GLU:N	2.39	0.55
1:B:547:ALA:O	1:B:551:GLY:N	2.39	0.55
1:B:561:VAL:O	1:B:563:LYS:N	2.39	0.55
1:B:130:ARG:CG	1:B:130:ARG:NH1	2.70	0.55
1:A:284:ARG:NH2	1:B:277:ARG:NH2	2.55	0.55
1:A:103:ASN:O	1:A:104:TYR:C	2.44	0.55
1:A:378:GLY:O	1:A:380:VAL:N	2.40	0.54
1:B:516:ARG:NH2	1:B:644:ASP:OD2	2.40	0.54
1:B:561:VAL:C	1:B:563:LYS:N	2.61	0.54
1:A:346:GLN:O	1:A:386:ALA:N	2.41	0.53
1:B:523:GLU:OE2	1:B:523:GLU:N	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:722:SER:O	1:A:726:TYR:N	2.43	0.52
1:A:170:MET:C	1:A:170:MET:SD	2.88	0.52
1:A:478:ASN:OD1	1:A:499:ARG:NH1	2.43	0.52
1:B:561:VAL:O	1:B:564:GLY:N	2.42	0.52
1:A:445:ASN:ND2	1:A:445:ASN:N	2.58	0.51
1:B:256:ARG:CD	3:B:803:TTP:H4'	2.41	0.51
1:B:224:LYS:O	1:B:225:ASP:CB	2.58	0.51
1:A:462:ASP:OD2	1:A:462:ASP:C	2.49	0.51
1:B:416:ASN:ND2	1:B:561:VAL:CG2	2.75	0.50
1:B:551:GLY:O	1:B:594:ARG:NH1	2.45	0.50
1:B:588:ILE:O	1:B:592:GLY:N	2.45	0.49
1:A:159:ILE:O	1:A:160:ASN:O	2.30	0.49
1:A:515:MET:O	1:A:516:ARG:CB	2.59	0.49
1:B:273:VAL:CB	1:B:274:PRO:CD	2.91	0.48
1:A:217:SER:O	1:A:217:SER:OG	2.30	0.48
1:A:243:LYS:CG	3:B:803:TTP:HM53	2.43	0.48
1:A:159:ILE:O	1:A:160:ASN:C	2.52	0.48
1:B:310:GLU:CD	1:B:310:GLU:N	2.67	0.48
1:B:109:ASN:O	1:B:111:LYS:N	2.46	0.48
1:B:330:PHE:CD2	1:B:330:PHE:N	2.81	0.48
1:B:256:ARG:NH1	3:B:803:TTP:H5'1	2.28	0.48
1:B:689:LYS:CG	4:B:809:SO4:O1	2.61	0.48
1:A:140:ASP:OD2	1:A:168:GLN:NE2	2.47	0.47
1:A:336:ASP:O	1:A:337:LEU:C	2.53	0.46
1:A:362:VAL:O	1:A:408:LYS:NZ	2.49	0.46
1:A:708:LEU:O	1:A:737:TYR:N	2.50	0.45
1:B:471:LYS:NZ	1:B:541:GLU:OE1	2.49	0.45
1:B:2:HIS:O	1:B:50:GLY:N	2.49	0.45
1:B:452:ASN:OD1	1:B:452:ASN:N	2.50	0.45
1:B:225:ASP:O	1:B:227:SER:N	2.49	0.45
1:B:654:GLU:O	1:B:658:GLN:N	2.49	0.45
1:B:553:TYR:O	1:B:554:GLU:C	2.56	0.44
1:B:137:TYR:OH	1:B:169:HIS:NE2	2.51	0.44
1:B:3:VAL:N	1:B:11:GLU:O	2.51	0.44
1:B:121:LEU:O	1:B:125:LEU:N	2.50	0.44
1:B:485:TYR:CD2	1:B:485:TYR:C	2.92	0.43
1:A:302:GLU:OE1	1:A:304:TRP:NE1	2.51	0.43
1:B:27:TYR:O	1:B:80:ARG:NH2	2.51	0.43
1:B:674:ASP:OD1	1:B:674:ASP:N	2.49	0.43
1:A:551:GLY:O	1:A:594:ARG:NH1	2.52	0.43
1:B:637:VAL:O	1:B:638:ASN:C	2.57	0.42
1:A:144:ASN:C	1:A:144:ASN:OD1	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:GLU:OE2	1:A:173:ARG:NE	2.53	0.42
1:A:603:PRO:O	1:A:604:THR:C	2.58	0.42
1:A:287:ASP:OD1	1:A:288:GLN:N	2.54	0.41
1:A:297:PHE:CD2	1:A:297:PHE:N	2.87	0.41
1:B:436:THR:N	6:B:801:HOH:O	2.52	0.41
1:B:674:ASP:O	1:B:678:GLN:N	2.53	0.41
1:B:258:THR:OG1	1:B:307:ASP:OD1	2.39	0.41
1:B:567:GLN:OE1	1:B:571:TRP:NE1	2.54	0.40
1:B:39:ILE:O	1:B:40:THR:C	2.57	0.40
1:B:149:LYS:CE	1:B:152:GLU:OE2	2.70	0.40

There are no symmetry-related clashes.

## 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	A	709/792 (90%)	633 (89%)	54 (8%)	22 (3%)	7	40
1	B	731/792 (92%)	639 (87%)	79 (11%)	13 (2%)	13	58
All	All	1440/1584 (91%)	1272 (88%)	133 (9%)	35 (2%)	9	49

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	296	ALA
1	A	327	ASP
1	A	379	ARG
1	B	110	GLY
1	B	225	ASP
1	B	713	ALA
1	A	104	TYR
1	A	162	LYS
1	A	218	CYS

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Mol	Chain	Res	Type
1	A	245	ALA
1	A	246	GLY
1	A	345	ASN
1	A	516	ARG
1	B	327	ASP
1	A	180	LYS
1	A	457	SER
1	A	653	GLU
1	A	663	ASN
1	A	713	ALA
1	B	6	ARG
1	B	226	ASP
1	B	345	ASN
1	B	516	ARG
1	B	562	SER
1	A	53	THR
1	A	737	TYR
1	B	7	ASP
1	B	601	PRO
1	A	285	TYR
1	A	312	LEU
1	B	267	GLY
1	B	493	LEU
1	A	106	ASN
1	A	44	ILE

### 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	A	597/693 (86%)	533 (89%)	64 (11%)	10	38
1	B	617/693 (89%)	538 (87%)	79 (13%)	6	27
All	All	1214/1386 (88%)	1071 (88%)	143 (12%)	8	32

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	45	GLN
1	A	53	THR
1	A	59	LEU
1	A	62	GLU
1	A	66	THR
1	A	67	LEU
1	A	93	VAL
1	A	95	SER
1	A	108	HIS
1	A	120	THR
1	A	121	LEU
1	A	130	ARG
1	A	149	LYS
1	A	158	LYS
1	A	171	LEU
1	A	176	VAL
1	A	192	LEU
1	A	214	GLN
1	A	220	LEU
1	A	221	LEU
1	A	222	SER
1	A	225	ASP
1	A	242	SER
1	A	250	VAL
1	A	272	LEU
1	A	275	MET
1	A	276	LEU
1	A	301	LEU
1	A	312	LEU
1	A	337	LEU
1	A	382	LYS
1	A	387	GLN
1	A	389	LEU
1	A	396	SER
1	A	429	CYS
1	A	441	VAL
1	A	445	ASN
1	A	452	ASN
1	A	455	VAL
1	A	457	SER
1	A	460	THR
1	A	478	ASN

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Mol	Chain	Res	Type
1	A	490	GLU
1	A	505	VAL
1	A	508	LEU
1	A	550	GLN
1	A	574	THR
1	A	577	ASP
1	A	591	TYR
1	A	615	GLU
1	A	631	SER
1	A	635	GLN
1	A	637	VAL
1	A	648	ARG
1	A	656	LYS
1	A	674	ASP
1	A	679	LEU
1	A	692	LEU
1	A	693	LYS
1	A	697	GLU
1	A	739	LEU
1	A	741	THR
1	A	742	ARG
1	B	9	ARG
1	B	11	GLU
1	B	16	ASP
1	B	19	THR
1	B	30	ASN
1	B	35	ASP
1	B	41	MET
1	B	47	LEU
1	B	53	THR
1	B	54	VAL
1	B	58	THR
1	B	59	LEU
1	B	66	THR
1	B	69	THR
1	B	80	ARG
1	B	84	SER
1	B	93	VAL
1	B	106	ASN
1	B	113	SER
1	B	121	LEU
1	B	129	ASP

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Mol	Chain	Res	Type
1	B	130	ARG
1	B	149	LYS
1	B	154	SER
1	B	171	LEU
1	B	187	ILE
1	B	192	LEU
1	B	217	SER
1	B	256	ARG
1	B	265	THR
1	B	266	ASN
1	B	273	VAL
1	B	276	LEU
1	B	281	ASN
1	B	301	LEU
1	B	310	GLU
1	B	312	LEU
1	B	313	ASP
1	B	326	ARG
1	B	327	ASP
1	B	337	LEU
1	B	349	SER
1	B	359	LEU
1	B	389	LEU
1	B	396	SER
1	B	431	GLU
1	B	444	CYS
1	B	445	ASN
1	B	446	LEU
1	B	449	LEU
1	B	455	VAL
1	B	464	LYS
1	B	471	LYS
1	B	493	LEU
1	B	508	LEU
1	B	516	ARG
1	B	541	GLU
1	B	554	GLU
1	B	561	VAL
1	B	570	MET
1	B	583	VAL
1	B	602	MET
1	B	606	SER

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Mol	Chain	Res	Type
1	B	615	GLU
1	B	621	THR
1	B	622	SER
1	B	627	ARG
1	B	642	LEU
1	B	644	ASP
1	B	655	MET
1	B	674	ASP
1	B	679	LEU
1	B	685	GLU
1	B	692	LEU
1	B	708	LEU
1	B	723	MET
1	B	739	LEU
1	B	740	ARG
1	B	742	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 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	$\# Z  > 2$
3	TTP	A	804	2	30,30,30	1.57	4 (13%)	42,47,47	3.02	8 (19%)
4	SO4	A	807	-	4,4,4	0.08	0	6,6,6	0.16	0
4	SO4	A	808	-	4,4,4	0.15	0	6,6,6	0.36	0
3	TTP	B	803	2	30,30,30	1.33	3 (10%)	42,47,47	2.53	7 (16%)
5	DTP	B	805	-	32,32,32	1.13	4 (12%)	50,50,50	1.75	7 (14%)
4	SO4	B	806	-	4,4,4	0.14	0	6,6,6	0.35	0
4	SO4	B	809	-	4,4,4	0.25	0	6,6,6	0.15	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
3	TTP	A	804	2	-	0/19/34/34	0/2/2/2
4	SO4	A	807	-	-	0/0/0/0	0/0/0/0
4	SO4	A	808	-	-	0/0/0/0	0/0/0/0
3	TTP	B	803	2	-	0/19/34/34	0/2/2/2
5	DTP	B	805	-	-	0/20/34/34	0/1/3/3
4	SO4	B	806	-	-	0/0/0/0	0/0/0/0
4	SO4	B	809	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	TTP	C2-N1	5.63	1.44	1.38
3	B	803	TTP	C2-N1	5.22	1.44	1.38
3	B	803	TTP	C4-C5	3.36	1.50	1.42
3	A	804	TTP	C4-C5	3.20	1.49	1.42
5	B	805	DTP	C5-C4	3.14	1.47	1.40
3	A	804	TTP	C4-N3	-3.01	1.32	1.37
3	A	804	TTP	PB-O3A	2.52	1.64	1.59
3	B	803	TTP	C4-N3	-2.40	1.33	1.37
5	B	805	DTP	C4-N9	-2.33	1.34	1.37
5	B	805	DTP	PA-O3A	2.32	1.64	1.59
5	B	805	DTP	PB-O3A	2.01	1.63	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	TTP	C6-N1-C2	-14.73	118.22	122.41
3	B	803	TTP	C6-N1-C2	-9.97	119.57	122.41
3	A	804	TTP	N3-C2-N1	9.91	124.25	115.97
3	B	803	TTP	N3-C2-N1	9.26	123.70	115.97
5	B	805	DTP	N3-C2-N1	-6.98	122.87	128.71
5	B	805	DTP	N3-C4-N9	5.55	135.45	125.43
3	B	803	TTP	PB-O3A-PA	-5.00	117.03	131.68
3	B	803	TTP	PB-O3B-PG	-3.79	120.57	131.68
5	B	805	DTP	C5-C4-N3	-3.38	118.33	125.70
5	B	805	DTP	C4-C5-N7	-3.30	106.70	109.52
3	B	803	TTP	C5-C6-N1	-3.21	118.47	121.59
3	A	804	TTP	C5-C6-N1	-3.19	118.49	121.59
3	B	803	TTP	C4-N3-C2	-3.05	119.12	125.39
3	A	804	TTP	O4'-C1'-N1	3.03	113.37	107.68
5	B	805	DTP	O4'-C1'-N9	2.80	112.94	107.68
5	B	805	DTP	C2-N3-C4	2.74	121.81	114.01
3	A	804	TTP	C6-C5-C4	2.64	121.51	115.11
3	A	804	TTP	C4-N3-C2	-2.62	120.01	125.39
3	A	804	TTP	PB-O3B-PG	-2.56	124.19	131.68
3	A	804	TTP	PB-O3A-PA	-2.22	125.18	131.68
3	B	803	TTP	C6-C5-C4	2.21	120.47	115.11
5	B	805	DTP	PB-O3B-PG	-2.06	125.63	131.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	A	715/792 (90%)	-0.27	2 (0%) 91 56	45, 63, 85, 123	2 (0%)
1	B	737/792 (93%)	-0.23	0 100 100	38, 58, 94, 110	0
All	All	1452/1584 (91%)	-0.25	2 (0%) 93 72	38, 61, 91, 123	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	4.2
1	A	218	CYS	3.4

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	B	806	5/5	0.41	4.09	101,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	802	1/1	0.20	3.39	48,48,48,48	0
2	MG	A	801	1/1	0.18	2.40	46,46,46,46	0
4	SO4	A	807	5/5	0.19	1.03	91,91,91,91	0
4	SO4	A	808	5/5	0.19	0.74	76,76,77,78	0
3	TTP	A	804	29/29	0.14	-0.71	58,60,66,67	0
5	DTP	B	805	30/30	0.18	-0.79	83,84,88,89	0
3	TTP	B	803	29/29	0.12	-1.13	54,57,66,67	0
4	SO4	B	809	5/5	0.10	-5.80	74,75,75,75	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.