Full wwPDB X-ray Structure Validation Report (i)

Jun 9, 2016 – 05:18 AM EDT

PDB ID	:	5IM3
Title	:	Crystal structure of the class I ribonucleotide reductase from Pseudomonas aeruginosa in complex with dATP
Authors	:	Johansson, R.; Logan, D.T.
Deposited on	:	2016-03-05
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

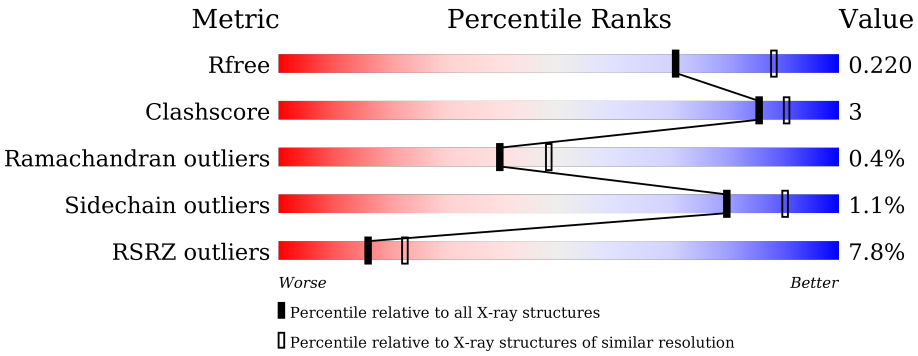
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	A	963	12% 84% 6% • 9%
1	B	963	2% 84% 5% 11%

2 Entry composition

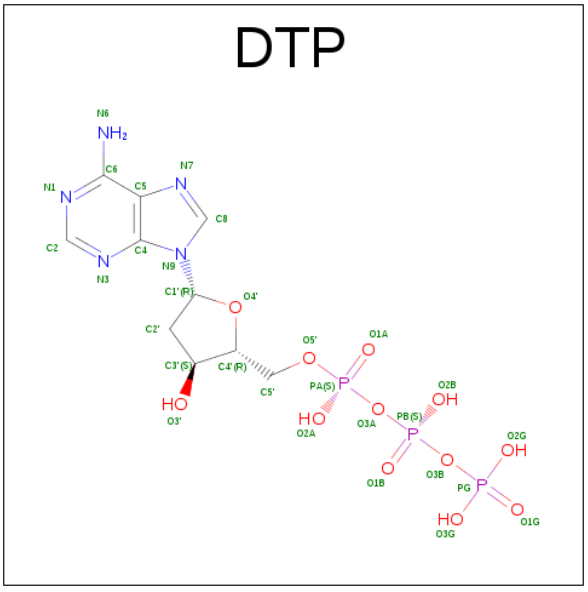
There are 4 unique types of molecules in this entry. The entry contains 14201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	874	Total	C	N	O	S	0	1	0
			6925	4389	1193	1315	28			
1	B	860	Total	C	N	O	S	0	1	0
			6838	4337	1177	1296	28			

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

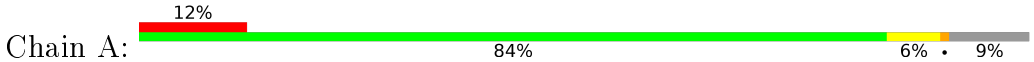
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	177	Total	O	0	0
			177	177		

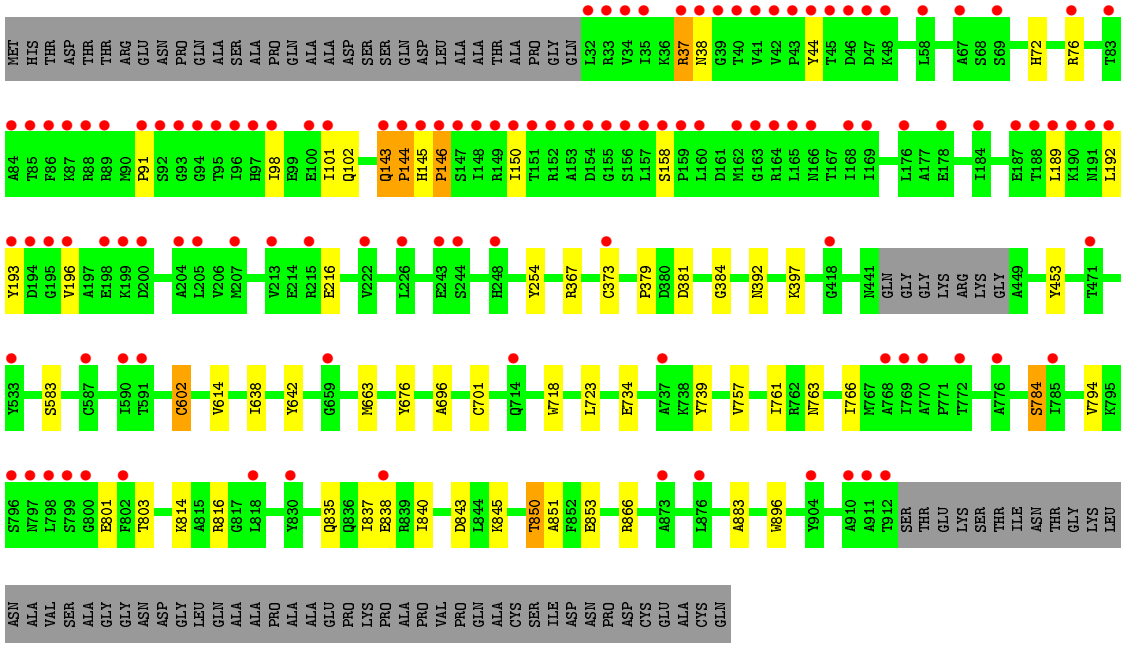
3 Residue-property plots (i)

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: Ribonucleoside-diphosphate reductase

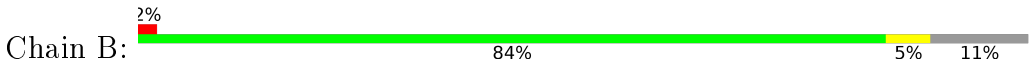
Chain A:

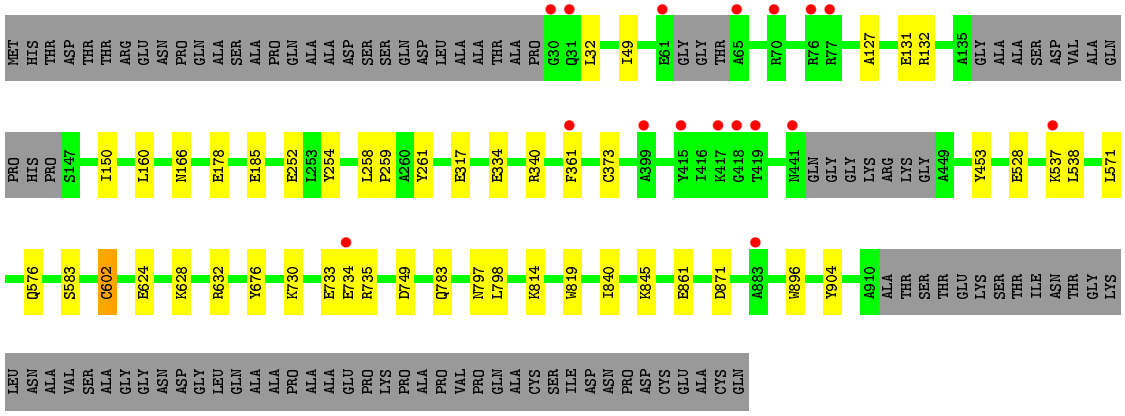




- Molecule 1: Ribonucleoside-diphosphate reductase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	267.46Å 62.58Å 173.76Å 90.00° 127.81° 90.00°	Depositor
Resolution (Å)	46.09 – 2.30 46.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.09-2.30) 99.0 (46.08-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_2328: ???)	Depositor
R, R_{free}	0.186 , 0.217 0.188 , 0.220	Depositor DCC
R_{free} test set	5059 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14201	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.25	0/7063	0.43	0/9573
1	B	0.27	0/6971	0.44	0/9441
All	All	0.26	0/14034	0.43	0/19014

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6925	0	6870	43	0
1	B	6838	0	6789	26	0
2	A	120	0	48	14	0
2	B	60	0	24	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	79	0	0	3	0
4	B	177	0	0	4	0
All	All	14201	0	13731	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (77) 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)
2:B:1002:DTP:H5'1	2:B:1002:DTP:H8	1.49	0.93
2:A:1001:DTP:H5'2	2:A:1001:DTP:H8	1.54	0.88
1:B:749:ASP:O	4:B:1101:HOH:O	2.00	0.78
1:A:397:LYS:NZ	2:A:1004:DTP:O1A	2.18	0.73
1:B:840:ILE:O	1:B:845:LYS:NZ	2.23	0.70
1:B:334:GLU:HG2	1:B:340:ARG:HG3	1.74	0.69
1:B:528:GLU:OE2	4:B:1102:HOH:O	2.11	0.69
1:A:734:GLU:OE2	4:A:1101:HOH:O	2.12	0.68
2:A:1002:DTP:C5'	2:A:1002:DTP:H8	2.23	0.67
1:A:44:TYR:CE1	2:A:1001:DTP:H2	2.31	0.65
1:A:837:ILE:HD11	1:A:840:ILE:HD12	1.77	0.65
1:A:835:GLN:O	4:A:1102:HOH:O	2.14	0.65
1:B:334:GLU:OE2	1:B:632:ARG:NH2	2.29	0.63
1:A:150:ILE:N	1:A:158:SER:O	2.32	0.61
1:A:373[B]:CYS:HB3	1:A:602:CYS:SG	2.40	0.61
1:A:866:ARG:NH2	4:A:1104:HOH:O	2.26	0.61
1:A:801:GLU:N	1:A:801:GLU:OE2	2.34	0.60
1:B:861:GLU:OE2	4:B:1103:HOH:O	2.16	0.59
2:A:1002:DTP:H8	2:A:1002:DTP:H5'2	1.84	0.59
1:A:840:ILE:O	1:A:845:LYS:NZ	2.38	0.57
1:A:102:GLN:OE1	2:A:1001:DTP:O3'	2.21	0.57
1:B:132:ARG:NH2	4:B:1109:HOH:O	2.36	0.57
1:B:797:ASN:OD1	1:B:798:LEU:N	2.36	0.56
1:A:216:GLU:OE1	1:A:814:LYS:NZ	2.24	0.55
1:A:101:ILE:HD13	2:A:1001:DTP:N3	2.22	0.55
1:B:166:ASN:ND2	1:B:185:GLU:OE2	2.40	0.55
1:B:49:ILE:HG12	2:B:1001:DTP:H2'1	1.88	0.55
1:A:837:ILE:HD11	1:A:840:ILE:CD1	2.40	0.52
1:B:571:LEU:HD22	1:B:734:GLU:OE1	2.11	0.51
1:A:794:VAL:HG12	1:A:803:THR:HG22	1.94	0.50
1:A:44:TYR:CD1	2:A:1001:DTP:H2	2.46	0.50
1:A:816:ARG:NH2	1:A:843:ASP:OD2	2.45	0.50
1:B:730:LYS:HE2	1:B:734:GLU:OE2	2.12	0.49
1:A:143:GLN:H	1:A:144:PRO:CD	2.25	0.49
1:B:814:LYS:HE2	1:B:819:TRP:CD1	2.48	0.49
1:A:367:ARG:NH1	1:A:642:TYR:OH	2.46	0.48
2:A:1002:DTP:H8	2:A:1002:DTP:H5'1	1.95	0.48
2:B:1002:DTP:C5'	2:B:1002:DTP:H8	2.34	0.47
1:A:38:ASN:OD1	1:A:38:ASN:N	2.48	0.46
1:A:37:ARG:HG2	1:A:98:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:ARG:NH2	1:B:896:TRP:O	2.49	0.46
1:A:381:ASP:HB2	2:A:1005:DTP:O1A	2.15	0.45
1:A:453:TYR:CG	1:A:583:SER:HB2	2.51	0.45
1:A:381:ASP:CB	2:A:1005:DTP:O1A	2.65	0.45
1:A:143:GLN:N	1:A:144:PRO:CD	2.79	0.45
1:A:189:LEU:HA	1:A:192:LEU:HD13	1.97	0.45
1:A:850:THR:CG2	1:A:851:ALA:N	2.79	0.45
1:A:763:ASN:HB2	1:A:766:ILE:HD13	1.99	0.45
1:A:850:THR:H	1:A:853:GLU:HG3	1.82	0.45
1:B:150:ILE:HD11	1:B:160:LEU:HG	1.99	0.45
1:B:261:TYR:OH	1:B:317:GLU:OE2	2.32	0.45
2:A:1002:DTP:C5'	2:A:1002:DTP:C8	2.94	0.45
2:A:1002:DTP:C8	2:A:1002:DTP:H5'1	2.48	0.44
1:B:373[B]:CYS:HB3	1:B:602:CYS:SG	2.58	0.44
1:A:663:MET:HA	1:A:784:SER:HA	2.00	0.44
1:B:453:TYR:CG	1:B:583:SER:HB2	2.54	0.43
1:B:178:GLU:HG2	1:B:814:LYS:HZ3	1.84	0.43
1:B:537:LYS:HG3	1:B:538:LEU:N	2.34	0.43
1:A:144:PRO:O	1:A:145:HIS:CG	2.71	0.43
1:A:72:HIS:CE1	1:A:76:ARG:HH11	2.36	0.43
1:A:143:GLN:H	1:A:144:PRO:HD3	1.85	0.42
1:A:145:HIS:HB3	1:A:146:PRO:HA	2.00	0.42
1:A:193:TYR:O	1:A:196:VAL:HG23	2.19	0.42
1:B:537:LYS:HG3	1:B:538:LEU:H	1.83	0.42
1:A:723:LEU:HD21	1:A:757:VAL:HG11	2.00	0.42
1:A:718:TRP:CD1	1:A:761:ILE:HD11	2.55	0.42
1:B:871:ASP:N	1:B:871:ASP:OD1	2.48	0.42
1:B:571:LEU:O	1:B:576:GLN:NE2	2.52	0.41
1:A:838:GLU:CD	1:A:838:GLU:H	2.23	0.41
1:A:701:CYS:SG	1:A:761:ILE:HG22	2.61	0.41
1:A:739:TYR:HB3	1:A:896:TRP:CH2	2.55	0.41
1:A:381:ASP:HA	2:A:1005:DTP:O1A	2.21	0.41
1:A:696:ALA:HB1	1:A:766:ILE:HG21	2.03	0.40
1:B:624:GLU:O	1:B:628:LYS:HG2	2.21	0.40
1:B:127:ALA:O	1:B:131:GLU:HG2	2.21	0.40
1:B:258:LEU:HB3	1:B:259:PRO:HD3	2.04	0.40
1:A:379:PRO:HG2	1:A:384:GLY:HA3	2.03	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	871/963 (90%)	839 (96%)	25 (3%)	7 (1%)	24 27
1	B	853/963 (89%)	830 (97%)	23 (3%)	0	100 100
All	All	1724/1926 (90%)	1669 (97%)	48 (3%)	7 (0%)	39 48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	146	PRO
1	A	614	VAL
1	A	883	ALA
1	A	784	SER
1	A	144	PRO
1	A	143	GLN

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	736/800 (92%)	729 (99%)	7 (1%)	82 91
1	B	728/800 (91%)	719 (99%)	9 (1%)	78 89
All	All	1464/1600 (92%)	1448 (99%)	16 (1%)	80 90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	254	TYR
1	A	392	ASN
1	A	602	CYS
1	A	638	ILE
1	A	676	TYR
1	A	850	THR
1	B	32	LEU
1	B	252	GLU
1	B	254	TYR
1	B	361	PHE
1	B	602	CYS
1	B	676	TYR
1	B	733	GLU
1	B	783	GLN
1	B	904	TYR

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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
2	DTP	A	1001	3	25,32,32	0.63	0	26,50,50	0.67	0
2	DTP	A	1002	3	25,32,32	0.76	0	26,50,50	0.73	0
2	DTP	A	1004	-	25,32,32	0.53	0	26,50,50	0.50	0
2	DTP	A	1005	-	25,32,32	0.62	0	26,50,50	0.48	0
2	DTP	B	1001	3	25,32,32	0.70	0	26,50,50	0.65	0
2	DTP	B	1002	3	25,32,32	0.72	0	26,50,50	0.71	1 (3%)

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	DTP	A	1001	3	-	0/18/34/34	0/3/3/3
2	DTP	A	1002	3	-	0/18/34/34	0/3/3/3
2	DTP	A	1004	-	-	0/18/34/34	0/3/3/3
2	DTP	A	1005	-	-	0/18/34/34	0/3/3/3
2	DTP	B	1001	3	-	0/18/34/34	0/3/3/3
2	DTP	B	1002	3	-	0/18/34/34	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1002	DTP	O5'-PA-O1A	2.02	117.48	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	DTP	5	0
2	A	1002	DTP	5	0
2	A	1004	DTP	1	0
2	A	1005	DTP	3	0
2	B	1001	DTP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	DTP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	874/963 (90%)	0.71	119 (13%) 4 6	37, 62, 112, 154	0
1	B	860/963 (89%)	0.12	17 (1%) 68 75	27, 46, 86, 130	0
All	All	1734/1926 (90%)	0.42	136 (7%) 16 22	27, 54, 103, 154	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	GLY	11.0
1	A	150	ILE	8.4
1	A	155	GLY	8.2
1	B	65	ALA	7.7
1	A	86	PHE	7.7
1	A	911	ALA	7.6
1	A	32	LEU	7.4
1	A	153	ALA	7.2
1	A	43	PRO	7.0
1	A	44	TYR	7.0
1	A	33	ARG	6.7
1	A	34	VAL	6.7
1	A	157	LEU	6.4
1	B	61	GLU	6.3
1	A	148	ILE	6.2
1	A	145	HIS	5.8
1	A	146	PRO	5.8
1	A	147	SER	5.7
1	B	418	GLY	5.6
1	A	797	ASN	5.6
1	A	92	SER	5.5
1	A	912	THR	5.5
1	A	154	ASP	5.5
1	A	42	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	88	ARG	5.2
1	A	95	THR	5.1
1	A	184	ILE	5.1
1	A	156	SER	4.9
1	A	796	SER	4.8
1	A	193	TYR	4.8
1	A	45	THR	4.7
1	A	144	PRO	4.6
1	A	151	THR	4.5
1	A	149	ARG	4.5
1	A	89	ARG	4.4
1	B	537	LYS	4.4
1	A	41	VAL	4.3
1	A	194	ASP	4.3
1	A	198	GLU	4.3
1	A	91	PRO	4.2
1	A	93	GLY	4.2
1	A	35	ILE	4.1
1	A	40	THR	4.0
1	A	800	GLY	4.0
1	A	189	LEU	3.9
1	A	76	ARG	3.9
1	B	30	GLY	3.8
1	A	152	ARG	3.8
1	A	798	LEU	3.6
1	A	38	ASN	3.5
1	A	168	ILE	3.5
1	A	162	MET	3.4
1	B	883	ALA	3.4
1	A	770	ALA	3.4
1	A	37	ARG	3.3
1	A	96	ILE	3.3
1	A	176	LEU	3.3
1	A	87	LYS	3.3
1	A	196	VAL	3.3
1	A	159	PRO	3.3
1	A	205	LEU	3.2
1	A	97	HIS	3.2
1	A	243	GLU	3.1
1	A	191	ASN	3.1
1	A	160	LEU	3.0
1	A	169	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	76	ARG	3.0
1	A	67	ALA	2.9
1	A	69	SER	2.9
1	A	94	GLY	2.9
1	A	876	LEU	2.8
1	A	590	ILE	2.8
1	A	471	THR	2.8
1	A	587	CYS	2.8
1	A	199	LYS	2.8
1	B	399	ALA	2.7
1	B	734	GLU	2.7
1	A	910	ALA	2.7
1	B	31	GLN	2.7
1	A	84	ALA	2.7
1	A	799	SER	2.7
1	A	39	GLY	2.7
1	A	46	ASP	2.6
1	A	164	ARG	2.6
1	A	166	ASN	2.6
1	A	373[A]	CYS	2.6
1	A	188	THR	2.6
1	A	818	LEU	2.6
1	A	163	GLY	2.6
1	A	100	GLU	2.5
1	B	70	ARG	2.5
1	A	192	LEU	2.5
1	A	207	MET	2.5
1	A	904	TYR	2.5
1	B	419	THR	2.5
1	A	48	LYS	2.4
1	A	768	ALA	2.4
1	A	85	THR	2.4
1	A	533	TYR	2.4
1	B	361	PHE	2.4
1	B	415	TYR	2.4
1	A	215	ARG	2.4
1	A	776	ALA	2.3
1	A	222	VAL	2.3
1	A	226	LEU	2.3
1	A	204	ALA	2.2
1	A	47	ASP	2.2
1	A	213	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	772	THR	2.2
1	A	785	ILE	2.2
1	A	244	SER	2.2
1	A	98	ILE	2.2
1	B	441	ASN	2.2
1	A	143	GLN	2.2
1	B	417	LYS	2.1
1	B	77	ARG	2.1
1	A	83	THR	2.1
1	A	873	ALA	2.1
1	A	838	GLU	2.1
1	A	101	ILE	2.1
1	A	190	LYS	2.1
1	A	248	HIS	2.1
1	A	802	PHE	2.1
1	A	659	GLY	2.1
1	A	769	ILE	2.1
1	A	158	SER	2.1
1	A	591	THR	2.1
1	A	830	TYR	2.1
1	A	58	LEU	2.1
1	A	200	ASP	2.1
1	A	714	GLN	2.1
1	A	178	GLU	2.1
1	A	165	LEU	2.0
1	A	737	ALA	2.0
1	A	187	GLU	2.0
1	A	195	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	DTP	A	1004	30/30	0.96	0.13	-0.36	39,49,83,85	0
2	DTP	A	1005	30/30	0.94	0.12	-0.46	41,44,74,79	0
2	DTP	A	1002	30/30	0.91	0.14	-0.65	61,70,79,82	0
2	DTP	B	1001	30/30	0.94	0.11	-0.95	53,62,70,71	0
2	DTP	A	1001	30/30	0.88	0.19	-0.96	85,94,104,105	0
2	DTP	B	1002	30/30	0.95	0.10	-1.22	53,58,65,66	0
3	MG	A	1003	1/1	0.80	0.08	-	81,81,81,81	1
3	MG	B	1003	1/1	0.90	0.17	-	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.