wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:13 AM 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 wwPDB X-ray Structure Validation Summary 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:

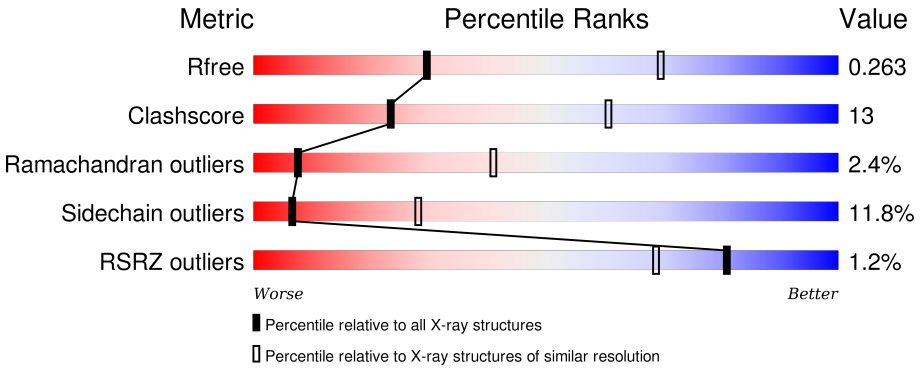
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	792	% 58% 28% • 10%
1	B	792	2% 61% 27% 5% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	806	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11549 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.

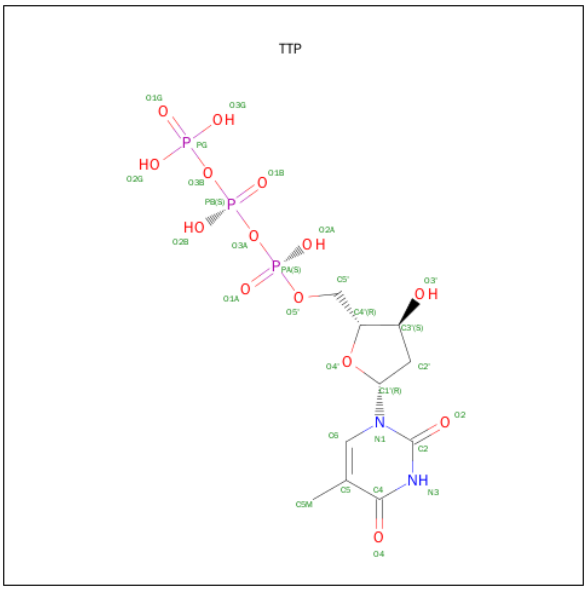
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

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).

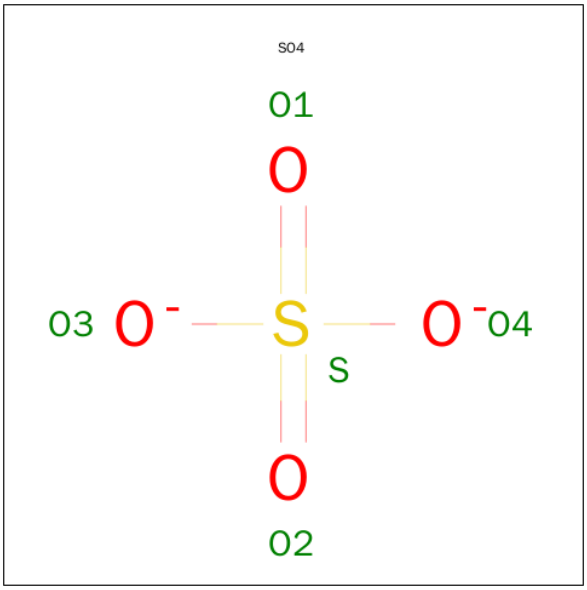
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



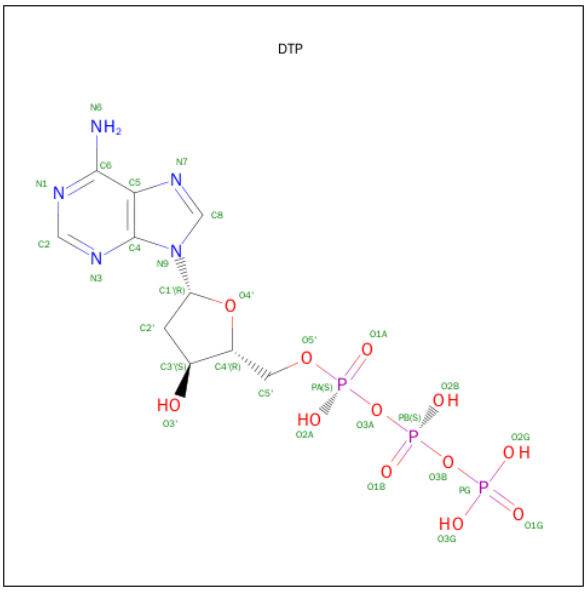
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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: $C_{10}H_{16}N_5O_{12}P_3$).



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

- Molecule 6 is water.

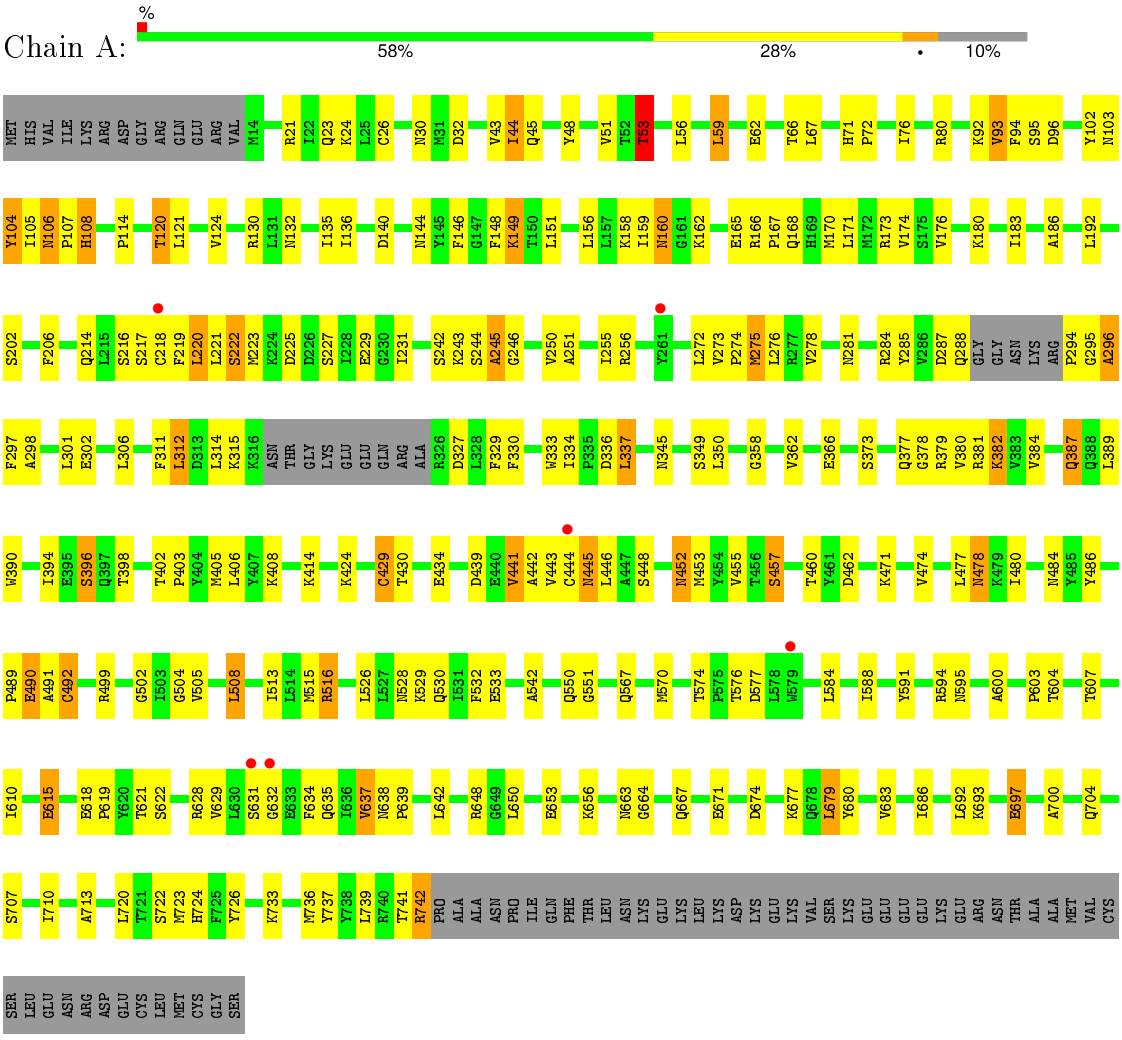
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	22	Total	O	0	0
			22	22		
6	B	26	Total	O	0	0
			26	26		

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.

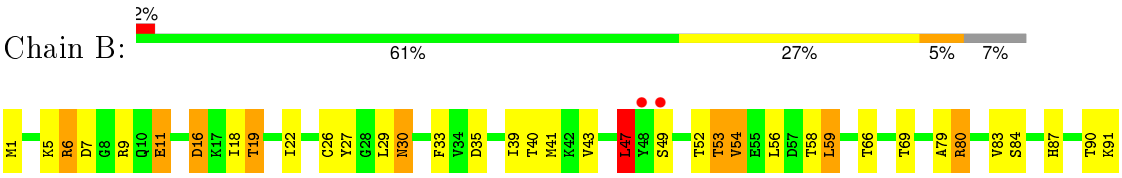
- Molecule 1: Ribonucleoside-diphosphate reductase large subunit

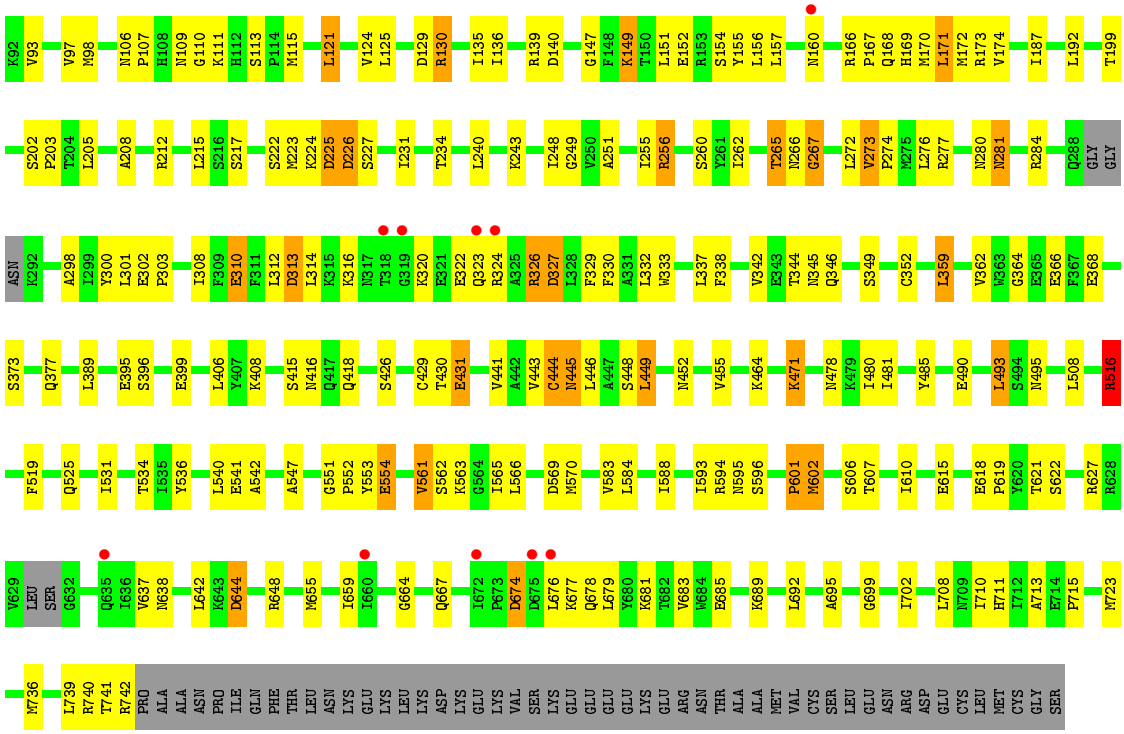
Chain A:



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit

Chain B:




K92 V93 V97 N98 N106 P107 H108 N109 G110 K111 H112 S113 P114 M115 L121 V124 L125 D129 R130 I135 I136 R139 D140 G147 F148 K149 T150 L151 E152 R153 S154 Y155 L156 L157 N160 R166 P167 Q168 H169 M170 L171 M172 R173 V174 I187 L192 T199
S202 P203 T204 L205 A208 R212 L215 S216 S217 S222 M223 K224 D225 D226 S227 I231 T224 L240 K243 I248 G249 V250 A251 I255 R256 S260 Y261 I262 T265 N266 G267 L272 V273 P274 N275 L276 R277 N280 M281 R284 Q288 GLY GLY
ASN K292 A298 I299 Y300 L301 E302 P303 I308 F309 E310 F311 L312 D313 L314 K315 K316 N317 T318 G319 K320 E321 E322 Q323 R324 A325 R326 D327 L328 F329 F330 A331 L332 W333 L337 F338 V342 E343 T344 N345 Q346 S349 C352 L359 V362 W363 G364 E365 E366 F367 E368
S373 Q377 L389 E395 S396 E399 L406 Y407 K408 S415 N416 Q417 Q418 S426 C429 T430 E431 V441 A442 V443 C444 N445 L446 A447 S448 L449 N452 V455 K464 K471 N478 K479 I480 I481 Y485 E490 L493 S494 N495 L508 R516
F519 Q525 I531 T534 I535 Y536 L540 E541 A542 A547 G551 P552 Y553 E554 V561 S562 K563 G564 I565 L566 D569 M570 V583 L584 I588 I593 R594 N595 S596 P601 M602 S606 T607 I610 E615 E618 P619 Y620 T621 S622 R627 R628
V629 LEU SER G632 Q635 I636 V637 N638 L642 K643 D644 R648 W655 I659 I660 G664 Q667 I672 P673 D674 D675 L676 K677 Q678 L679 Y680 K681 T682 V683 W684 E685 K689 L692 A695 G699 I702 L708 N709 I710 H711 I712 A713 E714 P715 M723
M736 L739 R740 T741 R742 PRO ALA ALA ASN PRO ILE GLN PHE THR LEU ASN LYS GLU LYS LEU LYS ASP LYS GLU LYS VAL SER LYS GLU GLU GLU GLU GLU LYS GLU ARG ASN THR ALA ALA MET VAL CYS SER LEU GLU ASN ARG ASP GLU CYS LEU MET CYS GLY SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.30 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.260 0.185 , 0.263	Depositor DCC
R_{free} test set	1335 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	63.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	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^2)	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.*

[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, 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(^{o})	Ideal(^{o})
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 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	5596	0	5436	151	0
1	B	5795	0	5687	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	3	0
3	B	29	0	13	7	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
5	B	30	0	12	1	0
6	A	22	0	0	0	0
6	B	26	0	0	1	0
All	All	11549	0	11161	301	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 13.

The worst 5 of 301 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:A:219:PHE:C	1:A:220:LEU:HD23	1.40	1.42
1:A:443:VAL:HG12	1:A:444:CYS:N	1.67	1.10
1:A:220:LEU:N	1:A:220:LEU:HD23	1.48	1.09
1:B:416:ASN:OD1	1:B:561:VAL:CG2	2.09	1.00
1:A:219:PHE:C	1:A:220:LEU:CD2	2.30	0.99

There are no symmetry-related clashes.

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	A	709/792 (90%)	633 (89%)	54 (8%)	22 (3%)	5 32
1	B	731/792 (92%)	639 (87%)	79 (11%)	13 (2%)	11 49
All	All	1440/1584 (91%)	1272 (88%)	133 (9%)	35 (2%)	7 41

5 of 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

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	A	597/693 (86%)	533 (89%)	64 (11%)	8	32
1	B	617/693 (89%)	538 (87%)	79 (13%)	5	24
All	All	1214/1386 (88%)	1071 (88%)	143 (12%)	6	28

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	ARG
1	B	93	VAL
1	B	644	ASP
1	B	16	ASP
1	B	53	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	HIS
1	B	106	ASN
1	B	459	HIS
1	A	595	ASN
1	A	652	HIS

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 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	21,30,30	0.61	0	31,47,47	2.00	5 (16%)
4	SO4	A	807	-	4,4,4	0.09	0	6,6,6	0.16	0
4	SO4	A	808	-	4,4,4	0.17	0	6,6,6	0.37	0
3	TTP	B	803	2	21,30,30	0.51	0	31,47,47	1.97	4 (12%)
5	DTP	B	805	-	24,32,32	0.95	1 (4%)	32,50,50	1.85	5 (15%)
4	SO4	B	806	-	4,4,4	0.14	0	6,6,6	0.34	0
4	SO4	B	809	-	4,4,4	0.25	0	6,6,6	0.16	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	-	0/18/34/34	0/2/2/2
4	SO4	A	807	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	808	-	-	0/0/0/0	0/0/0/0
3	TTP	B	803	2	-	0/18/34/34	0/2/2/2
5	DTP	B	805	-	-	0/18/34/34	0/3/3/3
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	805	DTP	C5-C4	3.14	1.47	1.40

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	805	DTP	N3-C2-N1	-7.86	122.87	128.89
3	A	804	TTP	C5-C4-N3	-6.84	117.52	125.14
3	B	803	TTP	C5-C4-N3	-5.82	118.66	125.14
3	B	803	TTP	PB-O3A-PA	-5.59	117.03	132.73
3	B	803	TTP	PB-O3B-PG	-3.61	120.57	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	TTP	3	0
4	A	808	SO4	1	0
3	B	803	TTP	7	0
5	B	805	DTP	1	0
4	B	809	SO4	1	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	715/792 (90%)	-0.34	6 (0%)	87	79	45, 63, 85, 123	2 (0%)
1	B	737/792 (93%)	-0.25	12 (1%)	74	61	38, 58, 94, 110	0
All	All	1452/1584 (91%)	-0.29	18 (1%)	81	69	38, 61, 91, 123	2 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	5.5
1	A	218	CYS	4.8
1	B	49	SER	3.2
1	A	632	GLY	3.1
1	B	675	ASP	2.8

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^{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
4	SO4	B	806	5/5	0.91	0.50	4.26	101,102,102,102	0
4	SO4	A	807	5/5	0.97	0.20	1.09	91,91,91,91	0
4	SO4	A	808	5/5	0.93	0.19	-0.06	76,76,77,78	0
3	TTP	A	804	29/29	0.95	0.14	-0.88	58,60,66,67	0
5	DTP	B	805	30/30	0.96	0.17	-1.19	83,84,88,89	0
3	TTP	B	803	29/29	0.98	0.12	-1.37	54,57,66,67	0
4	SO4	B	809	5/5	0.97	0.10	-	74,75,75,75	0
2	MG	A	801	1/1	0.96	0.17	-	46,46,46,46	0
2	MG	B	802	1/1	0.94	0.17	-	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.