



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 05:30 AM EDT

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 : unknown
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

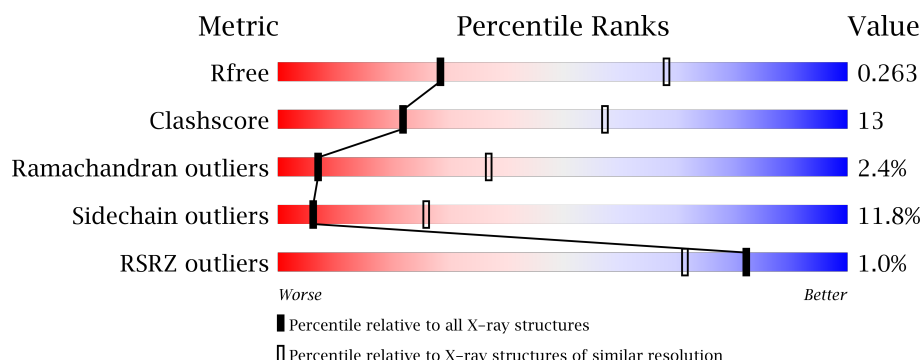
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (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 $\leq 5\%$. 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	A	792	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>28%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	792	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>27%</div> <div>5%</div> <div>7%</div> </div> </div>

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 [i](#)

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.

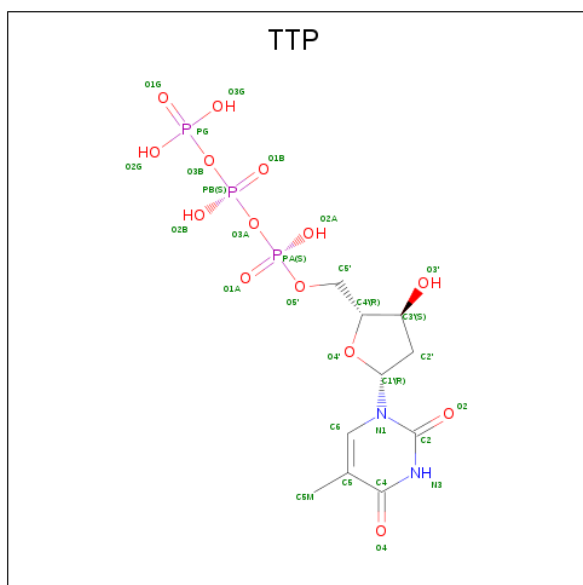
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

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: $C_{10}H_{17}N_2O_{14}P_3$).



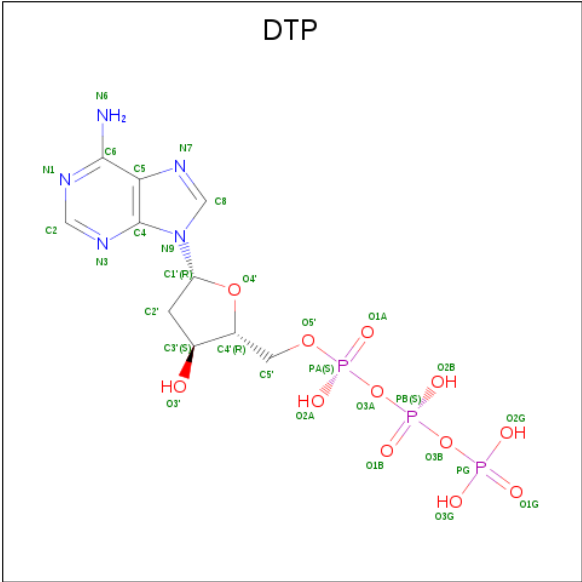
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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: C₁₀H₁₆N₅O₁₂P₃).



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

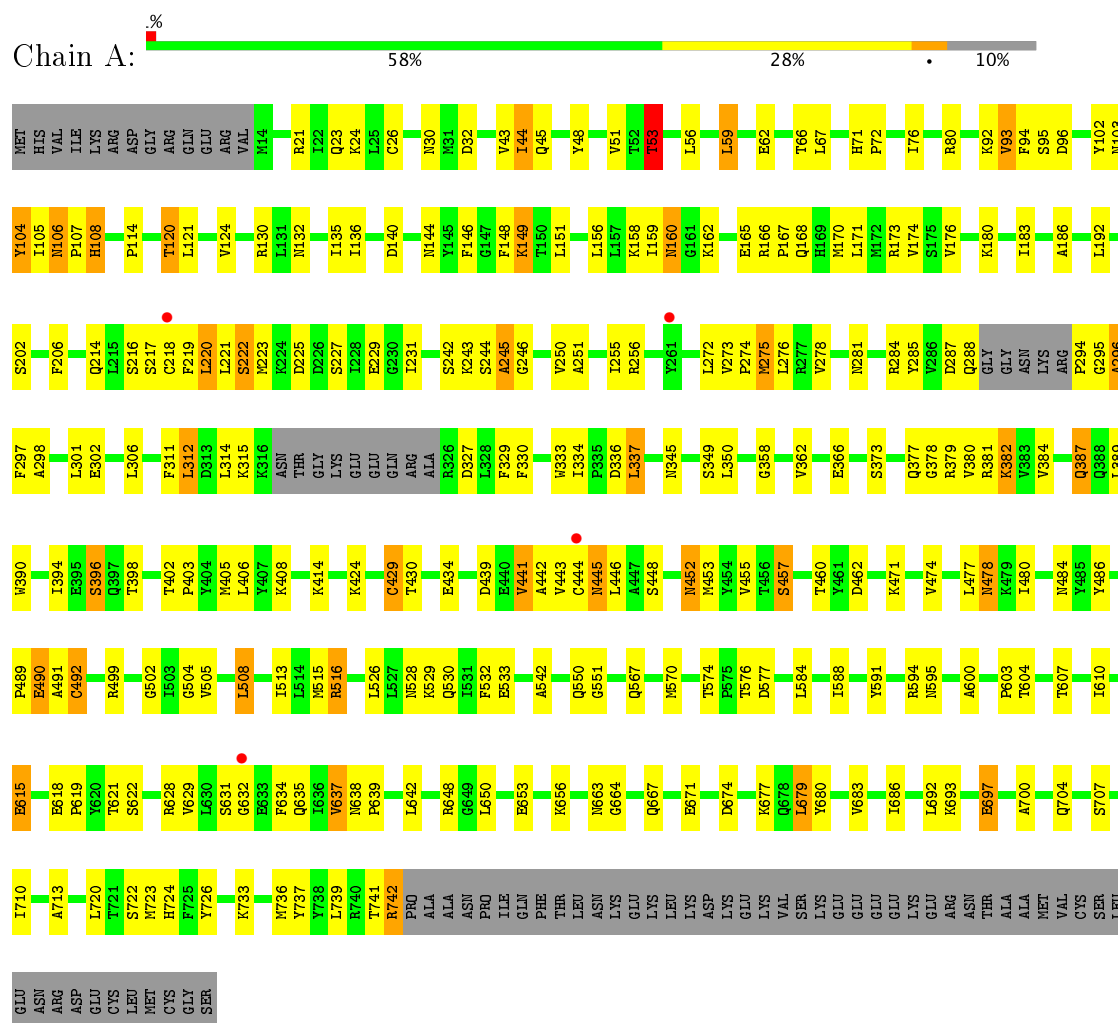
- Molecule 6 is water.

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

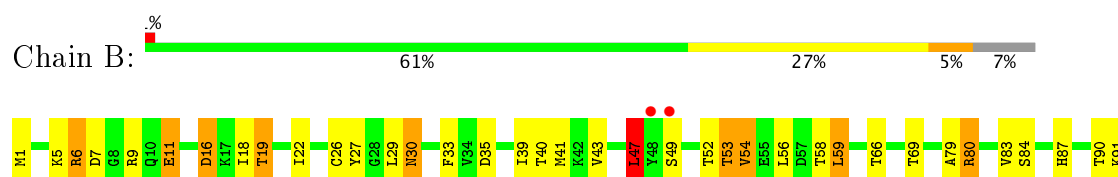
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



L739	V629	F519	S373	ASN	V92
R740	LEU	Q525	Q377	R292	V93
T741	SER	Q632	L389	A298	V97
R742	G635	I531	E395	I299	M98
PRO	I536	T534	S396	Y300	N106
ALA	M637	I535	E399	L301	P107
ASN	M638	Y536	L406	E302	H108
PRO	L642	L540	Y407	P303	N109
GLN	R643	E541	K408	I308	G110
PHE	D644	A542	S415	F309	K111
THR	R648	A547	M416	E310	H112
LEU	M655	G551	Q418	F311	S113
ASN	M659	P552	S426	L312	P114
LYS	I660	Y553	V561	D313	M115
LEU	G664	E554	S562	L314	L121
ASP	Q667	K563	T430	K315	V124
LYS	D674	G564	E431	K316	L125
LYS	D675	L566	V441	K317	D129
LYS	L676	M567	A442	T318	R130
GLU	K677	D569	V443	G319	I135
GLU	Q678	M570	K444	E321	I136
GLU	L679	V583	M445	R322	R139
GLU	R680	L584	I446	Q323	D140
LYS	K681	I588	A447	R324	G147
GLU	T682	I593	S448	Q325	F148
ARG	V683	R594	L449	A325	K149
ASN	M684	N595	I452	R326	L150
THR	E685	S596	V455	L337	L151
ALA	K689	P601	K471	F338	E152
ALA	L692	M602	N478	V342	R153
NET	L695	S606	K479	T344	S154
VAL	A695	T607	I481	N345	Y155
SER	G699	I610	Y485	Q346	L156
LEU	I702	E615	E490	L359	L157
GLU	L708	E618	L493	V362	N160
ASN	M709	P619	S494	K363	R166
ASP	I710	Y620	T621	G364	P167
GLU	H711	S622	R627	E365	Q168
GLY	A713	R628	R516	E366	H169
GLY	E714	M723		F367	L171
SER	P715	M736		GLY	M172
				GLY	R173
					V174
					I187
					L192
					T199

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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 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	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	29
1	B	731/792 (92%)	639 (87%)	79 (11%)	13 (2%)	10	45
All	All	1440/1584 (91%)	1272 (88%)	133 (9%)	35 (2%)	7	37

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 ⓘ

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	30
1	B	617/693 (89%)	538 (87%)	79 (13%)	5	22
All	All	1214/1386 (88%)	1071 (88%)	143 (12%)	6	26

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	22,30,30	0.69	0	25,47,47	2.13	4 (16%)
4	SO4	A	807	-	4,4,4	0.21	0	6,6,6	0.19	0
4	SO4	A	808	-	4,4,4	0.17	0	6,6,6	0.30	0
3	TTP	B	803	2	22,30,30	0.63	0	25,47,47	1.81	3 (12%)
5	DTP	B	805	-	26,32,32	0.98	1 (3%)	26,50,50	1.81	3 (11%)
4	SO4	B	806	-	4,4,4	0.23	0	6,6,6	0.44	0
4	SO4	B	809	-	4,4,4	0.22	0	6,6,6	0.18	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 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	TTP	C5-C4-N3	-7.00	117.52	125.24
5	B	805	DTP	N3-C2-N1	-6.87	122.87	128.86
3	B	803	TTP	C5-C4-N3	-5.97	118.66	125.24
3	B	803	TTP	C5-C6-N1	-3.40	118.47	122.15
3	A	804	TTP	C5-C6-N1	-3.38	118.49	122.15

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 [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, 95th 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%)	-0.36	4 (0%) 89 83	45, 63, 85, 123	2 (0%)
1	B	737/792 (93%)	-0.27	11 (1%) 74 60	38, 58, 94, 110	0
All	All	1452/1584 (91%)	-0.31	15 (1%) 82 71	38, 61, 91, 123	2 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	5.4
1	A	218	CYS	4.6
1	B	49	SER	3.1
1	A	632	GLY	3.0
1	B	675	ASP	2.7

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, 95th 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(\AA^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 [i](#)

There are no such residues in this entry.