



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:13 AM GMT

PDB ID : 3HNE
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effectors
TTP and ATP
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on : 2009-05-31
Resolution : 3.11 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 (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

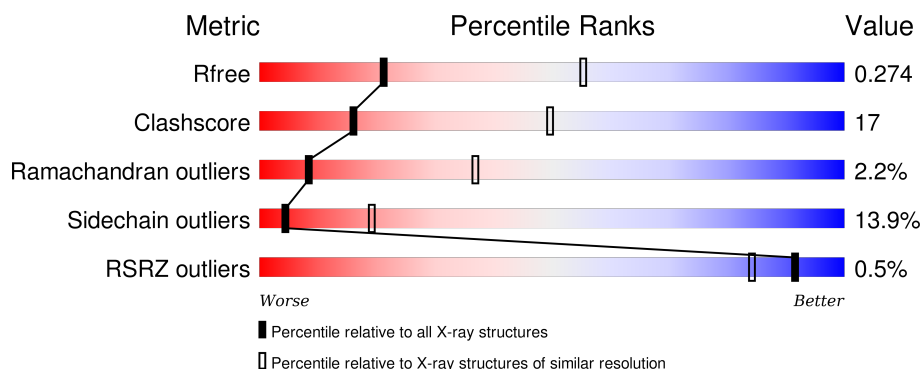
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	 61% 24% 5% • 10%
1	B	792	 51% 33% 8% 9%

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	813	-	-	-	X

2 Entry composition [i](#)

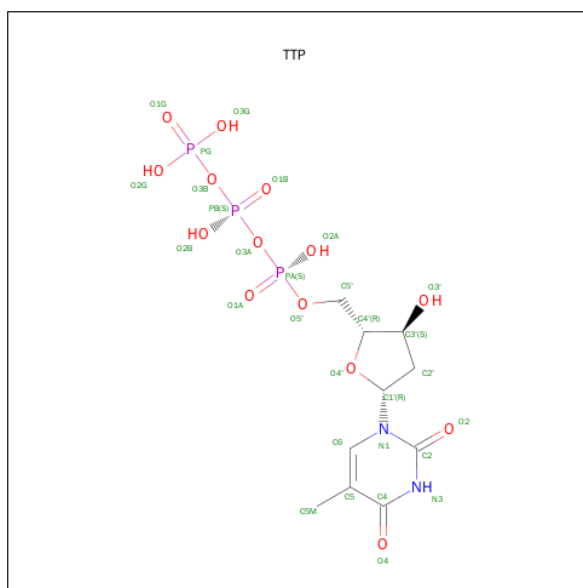
There are 6 unique types of molecules in this entry. The entry contains 11380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			5568	3557	927	1051	33			
1	B	724	Total	C	N	O	S	0	0	0
			5644	3593	955	1062	34			

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



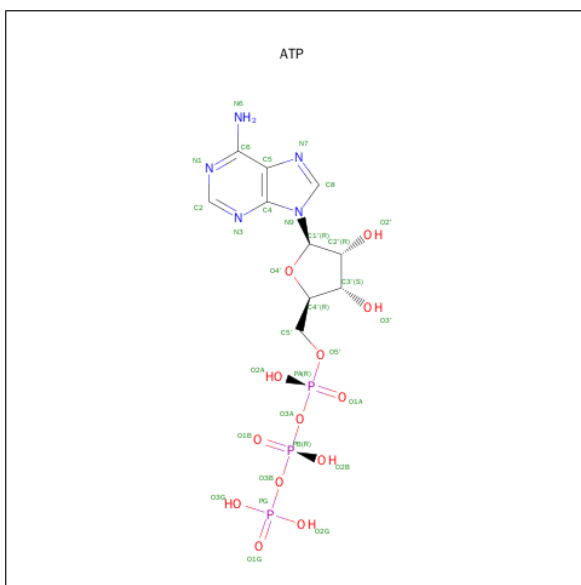
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Mg 3 3	0	0
3	A	1	Total Mg 1 1	0	0

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



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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

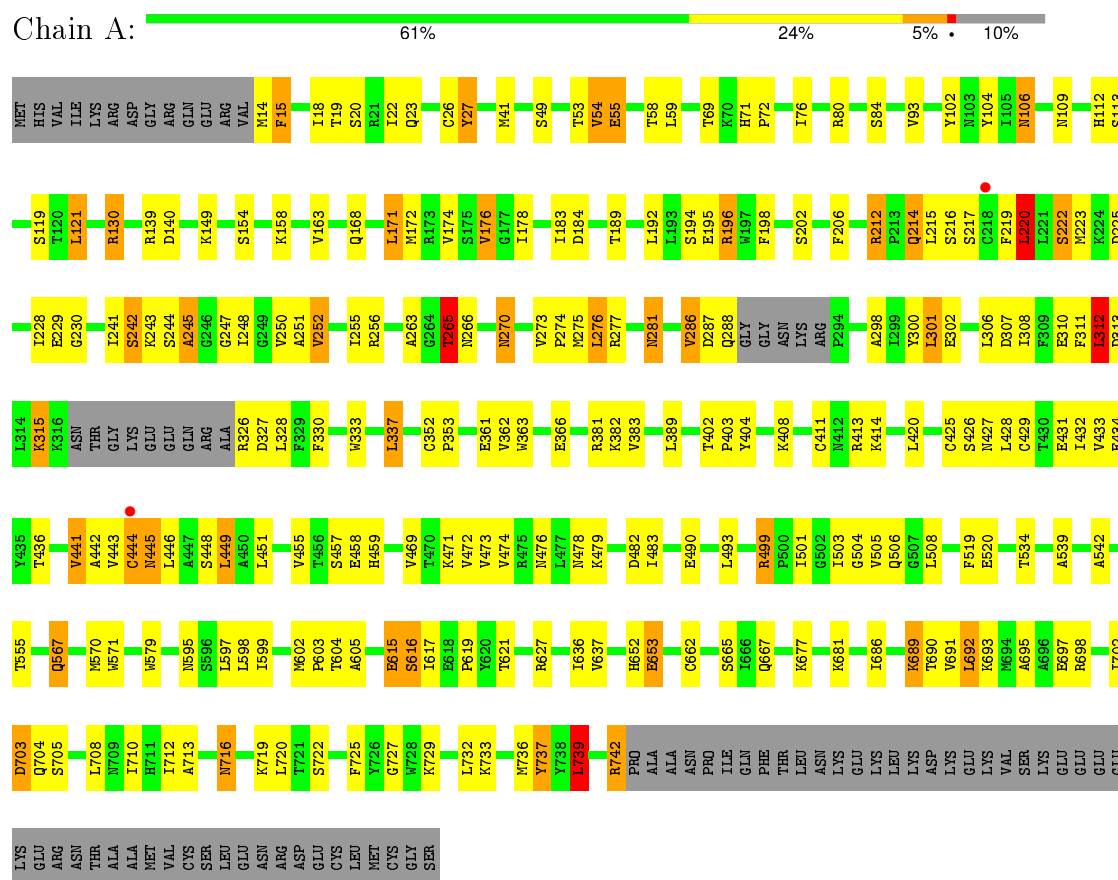
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	27	Total O 27 27	0	0
6	B	18	Total O 18 18	0	0

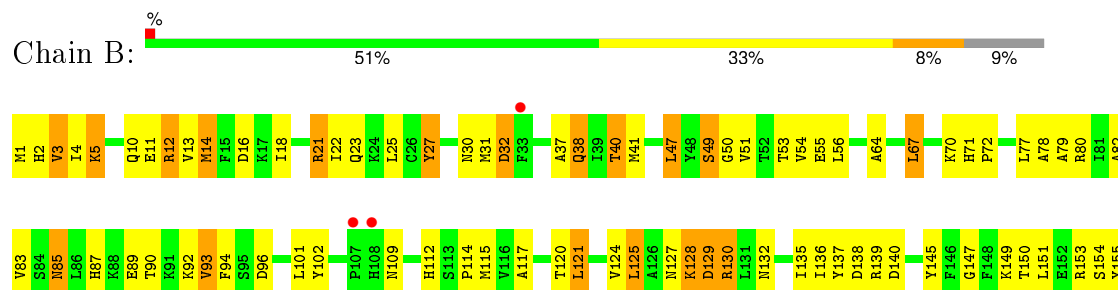
3 Residue-property plots

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



• Molecule 1: Ribonucleoside-diphosphate reductase large subunit



ASP	E685	P601	L503	K414	K315	V250	LYS	I159
LYS	I686	M602	G504	S415	K316	A251	GLU	K162
GLU	S687	P603	V505	N416	T317	V252	LYS	K166
VAL	K688	T607	G507	Q417	GLY	C254	GLY	R166
SER	K689	T690	L508	Q418	LYS	R255	LYS	H169
LYS	V691	L610	P512	N419	GLU	R256	GLU	M170
GLU	L692	L611	P515	L420	GLN	A257	LYS	M170
GLU		G612	N515	N426	GLY	T258	GLY	M170
GLU	A695	N613	N516	S427	R324	G259	GLY	L171
GLU	A696	N614	P517	N427	A325	S260	GLY	M172
LYS	E697	H614	P518	S428	R326	Y261	GLY	R173
GLU	R698	E615	P518	I432	D327	I262	GLY	V174
ARG	G699	S616	P518	I432	D327	I262	GLY	S175
ASN	A700	I617	E523	D439	F330	G264	GLY	V176
THR	F701	E618	A524	E440	N333	N265	GLY	T265
ALA	I702	P619	P525	V441	N333	N266	GLY	I187
ALA	D703	Y620	P525	A442	N333	N266	GLY	E188
MET	Q704	T621	N528	V443	L337	N270	GLY	E195
VAL	S705	S622	K529	C444	Q346	G271	GLY	R196
CYS	Q706	H623	P532	N445	D347	L272	GLY	T199
SER	S707	T624	P533	L446	A447	P274	GLY	S202
LEU	L708	Y625	P533	A447	A447	R277	GLY	P203
GLU		T626	P537	S448	G352	N275	GLY	
ASN	Y717	ARG	G538	L451	P353	L276	GLY	
ARG	G718	VAL	A539	L451	N354	R277	GLY	
ASP	K719	LEU	L540	Y454	L359	N281	GLY	
CYS	M723	SER	E541	S457	V362	T282	GLY	
LEU	R724	GLY	A542	Y461	E366	A283	GLY	
MET		GLU	S543	Y461	F367	R284	GLY	
CYS	G727	P634	C544	K464	E368	Y285	GLY	
GLY	Q730	Q635	D545	K464	E368	V286	GLY	
SER		L645	L546	E468	Y374	D287	GLY	
	T734	H651	G551	K471	Y374	Q288	GLY	
	G735	H652	P552	K471	R379	G289	GLY	
	M736	E653	V553	V474	R379	ASN	GLY	
	Y737	E654	P554	V474	R379	LYS	GLY	
	Y738	P655	T555	R475	V383	ARG	GLY	
	L739	M655	P560	N476	V383	PRO	GLY	
	R740	K656	V561	L477	A386	L221	GLY	
	T741	N657	V561	L477	A386	G295	GLY	
	R742	Q658	L566	D482	L389	A296	GLY	
	PRO	I659	Q567	I483	L389	P297	GLY	
	ALA	I660	Y568	N484	I393	A298	GLY	
	ALA	A661	D569	Y485	I394	L299	GLY	
	ASN		P570	E490	E395	Y300	GLY	
	PRO		G664	A491	S396	E302	GLY	
	ILE			A491	Q397	P303	GLY	
	GLN			C492	Q397		GLY	
	PHE	D674	V573	L493	P403		GLY	
	THR	D675	T574	L493	P403		GLY	
	LEU	L676	T575	R497	Y404		GLY	
	ASN	K677	T576	N405	F309		GLY	
	LYS	Q678	K587	R498	E310		GLY	
	GLU	L679		R499	F311		GLY	
	LYS			P500	L312		GLY	
	LEU	V683	R594	I501	D408		GLY	
	LYS	W684	L598	G502	S410		GLY	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.15Å 114.37Å 222.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 3.11 44.07 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.5 (44.07-3.11) 88.5 (44.07-3.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.275 0.188 , 0.274	Depositor DCC
R_{free} test set	1440 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 28684 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11380	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, TTP, SO4, ATP

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	0.74	3/5696 (0.1%)	0.78	4/7749 (0.1%)
1	B	0.71	2/5767 (0.0%)	0.80	1/7840 (0.0%)
All	All	0.72	5/11463 (0.0%)	0.79	5/15589 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	615	GLU	CB-CG	6.68	1.64	1.52
1	B	218	CYS	CB-SG	-6.52	1.71	1.82
1	A	662	CYS	CB-SG	-6.20	1.71	1.82
1	A	615	GLU	CG-CD	5.86	1.60	1.51
1	B	365	GLU	CB-CG	5.49	1.62	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	LEU	CA-CB-CG	7.33	132.16	115.30
1	A	312	LEU	CA-CB-CG	6.74	130.81	115.30
1	A	220	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	739	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	221	LEU	CA-CB-CG	5.14	127.13	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	5568	0	5368	166	0
1	B	5644	0	5448	208	0
2	A	29	0	13	1	0
2	B	29	0	13	4	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	15	0	0	2	0
4	B	15	0	0	1	0
5	B	31	0	12	3	0
6	A	27	0	0	3	0
6	B	18	0	0	3	0
All	All	11380	0	10854	374	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 17.

The worst 5 of 374 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:445:ASN:C	1:A:446:LEU:HD23	1.34	1.44
1:A:445:ASN:O	1:A:446:LEU:HD23	1.50	1.11
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.18	1.01
1:A:443:VAL:HG12	1:A:444:CYS:H	1.23	0.99
1:A:445:ASN:C	1:A:446:LEU:CD2	2.30	0.98

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	710/792 (90%)	636 (90%)	61 (9%)	13 (2%)	11	43
1	B	716/792 (90%)	616 (86%)	82 (12%)	18 (2%)	7	33
All	All	1426/1584 (90%)	1252 (88%)	143 (10%)	31 (2%)	8	37

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	B	130	ARG
1	B	288	GLN
1	B	316	LYS
1	B	327	ASP

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	586/693 (85%)	523 (89%)	63 (11%)	8	31
1	B	593/693 (86%)	492 (83%)	101 (17%)	2	11
All	All	1179/1386 (85%)	1015 (86%)	164 (14%)	4	19

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	LEU
1	B	154	SER
1	B	678	GLN
1	B	54	VAL
1	B	109	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	567	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	23	GLN
1	B	652	HIS
1	A	595	ASN
1	A	716	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	TTP	A	806	3	21,30,30	0.53	0	31,47,47	2.02	6 (19%)
4	SO4	A	808	-	4,4,4	0.14	0	6,6,6	0.31	0
4	SO4	A	809	-	4,4,4	0.17	0	6,6,6	0.30	0
4	SO4	A	812	-	4,4,4	0.18	0	6,6,6	0.57	0
2	TTP	B	805	3	21,30,30	0.58	0	31,47,47	2.04	4 (12%)
5	ATP	B	807	3	24,33,33	1.39	2 (8%)	31,52,52	2.27	8 (25%)
4	SO4	B	810	-	4,4,4	0.20	0	6,6,6	0.26	0
4	SO4	B	811	-	4,4,4	0.18	0	6,6,6	0.57	0
4	SO4	B	813	-	4,4,4	0.32	0	6,6,6	0.41	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	TTP	A	806	3	-	0/18/34/34	0/2/2/2
4	SO4	A	808	-	-	0/0/0/0	0/0/0/0
4	SO4	A	809	-	-	0/0/0/0	0/0/0/0
4	SO4	A	812	-	-	0/0/0/0	0/0/0/0
2	TTP	B	805	3	-	0/18/34/34	0/2/2/2
5	ATP	B	807	3	-	0/18/38/38	0/3/3/3
4	SO4	B	810	-	-	0/0/0/0	0/0/0/0
4	SO4	B	811	-	-	0/0/0/0	0/0/0/0
4	SO4	B	813	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	807	ATP	C5-C4	3.24	1.47	1.40
5	B	807	ATP	O4'-C1'	4.95	1.47	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	805	TTP	C5-C4-N3	-5.62	118.88	125.14
2	A	806	TTP	C5-C4-N3	-5.57	118.94	125.14
5	B	807	ATP	PA-O3A-PB	-5.36	117.67	132.73
5	B	807	ATP	N3-C2-N1	-5.27	124.86	128.89
2	A	806	TTP	PB-O3A-PA	-4.92	118.92	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	806	TTP	1	0
4	A	809	SO4	1	0
4	A	812	SO4	1	0
2	B	805	TTP	4	0
5	B	807	ATP	3	0
4	B	810	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%)	-0.46	2 (0%) 94 89	46, 61, 81, 110	2 (0%)
1	B	724/792 (91%)	-0.41	5 (0%) 89 79	46, 65, 94, 126	0
All	All	1439/1584 (90%)	-0.43	7 (0%) 91 84	46, 63, 90, 126	2 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	6.6
1	A	218	CYS	6.3
1	B	107	PRO	2.6
1	B	676	LEU	2.3
1	B	659	ILE	2.2

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	813	5/5	0.93	0.27	2.20	70,70,72,72	0
4	SO4	A	812	5/5	0.96	0.21	0.04	83,83,85,86	0
4	SO4	B	810	5/5	0.97	0.13	-0.52	79,79,80,81	0
2	TTP	A	806	29/29	0.96	0.14	-1.04	59,63,74,75	0
2	TTP	B	805	29/29	0.97	0.13	-1.06	72,75,83,85	0
5	ATP	B	807	31/31	0.91	0.15	-1.57	65,69,76,76	0
3	MG	B	804	1/1	0.93	0.12	-	47,47,47,47	0
3	MG	B	802	1/1	0.96	0.10	-	62,62,62,62	0
4	SO4	B	811	5/5	0.94	0.13	-	99,100,100,100	0
4	SO4	A	809	5/5	0.89	0.13	-	127,127,127,127	0
3	MG	A	801	1/1	0.98	0.20	-	56,56,56,56	0
3	MG	B	803	1/1	0.94	0.19	-	42,42,42,42	0
4	SO4	A	808	5/5	0.94	0.16	-	86,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.