

Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 12:16 am GMT

PDB ID	:	1E3P
Title	:	tungstate derivative of Streptomyces antibioticus PNPase/GPSI enzyme
Authors	:	Symmons, M.F.; Jones, G.H.; Luisi, B.F.
Deposited on	:	2000-06-20
Resolution	:	2.50 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	4661 (2.50-2.50)		
Clashscore	141614	5346 (2.50-2.50)		
Ramachandran outliers	138981	5231 (2.50-2.50)		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559 (2.50-2.50)		

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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						
			9%						
1	А	757	68%	16%	•	15%			



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5080 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 Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	645	Total 4720	C 2954	N 834	0 913	S 19	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-16	ALA	-	expression tag	UNP A0A1S9NJJ0
А	-15	SER	-	expression tag	UNP A0A1S9NJJ0
А	-14	MET	-	expression tag	UNP A0A1S9NJJ0
А	-13	THR	-	expression tag	UNP A0A1S9NJJ0
А	-12	GLY	-	expression tag	UNP A0A1S9NJJ0
A	-11	GLY	-	expression tag	UNP A0A1S9NJJ0
А	-10	GLN	-	expression tag	UNP A0A1S9NJJ0
A	-9	GLN	-	expression tag	UNP A0A1S9NJJ0
А	-8	MET	-	expression tag	UNP A0A1S9NJJ0
А	-7	GLY	-	expression tag	UNP A0A1S9NJJ0
А	-6	ARG	-	expression tag	UNP A0A1S9NJJ0
А	-5	GLY	-	expression tag	UNP A0A1S9NJJ0
A	-4	SER	-	expression tag	UNP A0A1S9NJJ0
А	-3	GLY	-	expression tag	UNP A0A1S9NJJ0
A	-2	SER	-	expression tag	UNP A0A1S9NJJ0
А	-1	GLU	-	expression tag	UNP A0A1S9NJJ0
А	0	PHE	-	expression tag	UNP A0A1S9NJJ0
A	31	ARG	LYS	conflict	UNP A0A1S9NJJ0
А	323	ALA	SER	conflict	UNP A0A1S9NJJ0
А	327	SER	GLN	conflict	UNP A0A1S9NJJ0
А	335	ALA	LYS	conflict	UNP A0A1S9NJJ0
А	600	ARG	GLY	conflict	UNP A0A1S9NJJ0
A	601	GLN	LYS	conflict	UNP A0A1S9NJJ0
А	647	SER	MET	conflict	UNP A0A1S9NJJ0
А	654	ILE	TYR	conflict	UNP A0A1S9NJJ0
A	657	SER	THR	conflict	UNP A0A1S9NJJ0

There are 26 discrepancies between the modelled and reference sequences:



• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is TUNGSTATE(VI)ION (three-letter code: WO4) (formula: O_4W).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 5	0 4	\mathbf{W} 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	305	Total O 305 305	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Polyribonucleotide nucleotidyltransferase



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	H 3 2	Depositor	
Cell constants	130.83Å 130.83Å 328.73Å	Deperitor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Besolution (Å)	19.84 - 2.50	Depositor	
	19.84 - 2.50	EDS	
% Data completeness	$97.9\ (19.84 ext{-}2.50)$	Depositor	
(in resolution range)	98.4(19.84-2.50)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	0.08	Depositor	
$< I/\sigma(I) > 1$	$2.51 (at 2.50 \text{\AA})$	Xtriage	
Refinement program	CNS 0.9	Depositor	
B B.	0.213 , 0.247	Depositor	
It, Itfree	0.210 , 0.242	DCC	
R_{free} test set	3536 reflections $(4.98%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	46.9	Xtriage	
Anisotropy	0.193	Xtriage	
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , 55.5	EDS	
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	Xtriage	
	0.009 for $-1/3$ *h $+1/3$ *k $+1/3$ *l,-k, $8/3$ *h $+4/$		
	$3^{*}k+1/3^{*}l$		
Estimated twinning fraction	0.011 for $-2/3$ *h $-1/3$ *k $-1/3$ *l $-1/3$ *h $-2/3$ *k+	Xtriage	
C C	$\frac{1/3^{+}l, -4/3^{+}h + 4/3^{+}k + 1/3^{+}l}{1/2^{+}l, 1/2^{+}l, 1/2^{+}l, 4/2^{+}h, 9/2^{+}l}$	0	
	$0.012 \text{ IOF - II, I/3 \cdot II - I/3 \cdot K - I/3 \cdot I, -4/3 \cdot II - 8/3 \cdot K}$ + 1/2*1		
F F correlation	$\frac{+1/5}{0.94}$	EDS	
Total number of atoms	5080	wwPDR-VP	
$\Delta vorago B$ all atoms (λ^2)	50.0	wwPDR VP	
A monage D, an atoms (A)	0.0		

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: SO4, WO4 $\,$

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	А	0.34	0/4785	0.61	0/6487	

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 (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	А	4720	0	4626	102	0
2	А	50	0	0	1	0
3	А	5	0	0	1	0
4	А	305	0	0	7	0
All	All	5080	0	4626	102	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 11.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:446:PRO:HB2	1:A:582:ILE:HD12	1.40	1.02	
1:A:349:ARG:HH22	1:A:460:GLY:HA3	1.30	0.96	
1:A:275:VAL:HG12	1:A:301:LEU:HD12	1.56	0.88	
1:A:275:VAL:HG11	1:A:302:ALA:HB2	1.65	0.78	
1:A:261:LEU:HD12	1:A:264:GLN:HE22	1.56	0.70	
1:A:667:PHE:HA	1:A:676:GLY:O	1.92	0.69	
1:A:55:LYS:H	1:A:55:LYS:HD3	1.58	0.69	
1:A:626:ALA:HB1	1:A:631:ALA:HB3	1.73	0.69	
1:A:575:MET:HB3	1:A:581:ARG:HH22	1.57	0.68	
1:A:308:PRO:O	1:A:311:GLU:HG2	1.95	0.66	
1:A:55:LYS:HG2	2:A:905:SO4:O3	1.96	0.65	
1:A:369:ARG:HD3	1:A:508:ASP:OD1	1.97	0.65	
1:A:275:VAL:HG12	1:A:301:LEU:CD1	2.24	0.65	
1:A:276:ARG:HB3	1:A:277:PRO:HD3	1.79	0.65	
1:A:349:ARG:NH2	1:A:460:GLY:HA3	2.07	0.65	
1:A:420:PRO:HA	1:A:424:GLU:OE1	1.96	0.65	
1:A:399:ARG:HD3	1:A:442:ARG:HG2	1.82	0.61	
1:A:629:GLY:N	1:A:630:PRO:HD2	2.16	0.61	
1:A:444:GLU:HA	1:A:703:GLN:HA	1.84	0.60	
1:A:626:ALA:CB	1:A:631:ALA:HB3	2.32	0.60	
1:A:424:GLU:HG3	4:A:2244:HOH:O	2.01	0.60	
1:A:493:ILE:HD13	1:A:517:GLY:HA2	1.83	0.60	
1:A:495:GLN:HE21	1:A:497:ILE:HD11	1.67	0.59	
1:A:58:LYS:HA	1:A:60:GLN:HE22	1.67	0.59	
1:A:580:PRO:C	1:A:581:ARG:HD2	2.23	0.58	
1:A:389:LEU:HD12	1:A:389:LEU:N	2.19	0.58	
1:A:100:ARG:HD3	4:A:2095:HOH:O	2.03	0.58	
1:A:28:ARG:HG2	1:A:29:LEU:HD13	1.86	0.57	
1:A:90:ARG:HD2	1:A:90:ARG:H	1.69	0.57	
1:A:575:MET:HB3	1:A:581:ARG:NH2	2.19	0.57	
1:A:111:LYS:HE2	1:A:259:VAL:CG2	2.35	0.57	
1:A:55:LYS:HD3	1:A:55:LYS:N	2.20	0.56	
1:A:90:ARG:H	1:A:90:ARG:CD	2.20	0.54	
1:A:541:GLY:HA3	4:A:2158:HOH:O	2.08	0.54	
1:A:399:ARG:NH2	1:A:440:PRO:O	2.40	0.53	
1:A:261:LEU:HD12	1:A:264:GLN:NE2	2.22	0.53	
1:A:334:ILE:HG13	1:A:495:GLN:HG2	1.91	0.53	
1:A:294:GLU:O	1:A:298:VAL:HG23	2.09	0.53	
1:A:55:LYS:H	1:A:55:LYS:CD	2.16	0.53	
1:A:611:GLY:O	1:A:612:ALA:HB2	2.09	0.53	
1:A:496:GLU:HA	1:A:501:THR:HA	1.90	0.53	
1:A:444:GLU:HB3	4:A:2296:HOH:O	2.07	0.53	



	, and pagetti	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:26:THR:HG22	1:A:246:LEU:HD11	1.90	0.52		
1:A:461:SER:HA	3:A:911:WO4:O1	2.08	0.52		
1:A:10:ALA:HB1	1:A:238:VAL:HG12	1.91	0.52		
1:A:382:MET:HB2	1:A:384:ARG:HG2	1.91	0.51		
1:A:212:LEU:HD23	4:A:2173:HOH:O	2.10	0.51		
1:A:407:PRO:HB2	1:A:409:TYR:CE2	2.45	0.51		
1:A:178:GLU:HG3	4:A:2141:HOH:O	2.10	0.50		
1:A:271:LEU:HD21	1:A:321:TYR:HA	1.94	0.49		
1:A:446:PRO:HB2	1:A:582:ILE:CD1	2.26	0.49		
1:A:700:GLY:H	1:A:703:GLN:CB	2.25	0.49		
1:A:523:VAL:HG22	1:A:533:LEU:HD13	1.94	0.49		
1:A:90:ARG:HD2	1:A:90:ARG:N	2.28	0.49		
1:A:291:ARG:NH2	1:A:341:ASP:HA	2.27	0.48		
1:A:443:GLU:OE1	1:A:443:GLU:N	2.45	0.48		
1:A:580:PRO:HB3	1:A:626:ALA:O	2.13	0.48		
1:A:133:TYR:C	1:A:133:TYR:CD1	2.87	0.48		
1:A:107:ARG:HB3	1:A:108:PRO:HD3	1.95	0.48		
1:A:6:HIS:CD2	1:A:250:ALA:HB2	2.49	0.47		
1:A:107:ARG:HB3	1:A:108:PRO:CD	2.45	0.46		
1:A:291:ARG:O	1:A:295:LEU:HB2	2.15	0.46		
1:A:463:SER:O	1:A:466:SER:HB3	2.15	0.46		
1:A:427:HIS:HB3	1:A:463:SER:HB3	1.97	0.46		
1:A:345:VAL:HG23	1:A:346:THR:HG23	1.96	0.46		
1:A:340:ILE:HG12	1:A:340:ILE:O	2.16	0.46		
1:A:369:ARG:HD3	1:A:508:ASP:CG	2.36	0.46		
1:A:580:PRO:HB3	1:A:627:ALA:HA	1.97	0.46		
1:A:297:ARG:HH11	1:A:297:ARG:HD2	1.60	0.45		
1:A:314:GLU:H	1:A:314:GLU:CD	2.19	0.45		
1:A:371:GLU:HB2	1:A:459:ASN:HB3	1.98	0.45		
1:A:278:GLU:CD	1:A:278:GLU:H	2.20	0.45		
1:A:349:ARG:HH11	1:A:510:LEU:HD23	1.82	0.45		
1:A:388:GLN:C	1:A:389:LEU:HD12	2.38	0.44		
1:A:349:ARG:NH1	1:A:510:LEU:HD23	2.33	0.44		
1:A:322:ARG:NE	1:A:322:ARG:HA	2.33	0.44		
1:A:285:ILE:HD12	1:A:291:ARG:HA	2.00	0.43		
1:A:301:LEU:HD13	1:A:301:LEU:O	2.19	0.43		
1:A:399:ARG:CD	1:A:442:ARG:HG2	2.46	0.43		
1:A:299:LYS:HG2	1:A:321:TYR:CZ	2.53	0.43		
1:A:612:ALA:O	1:A:614:ILE:N	2.51	0.43		
1:A:302:ALA:C	1:A:304:GLU:H	2.22	0.42		
1:A:333:VAL:O	1:A:337:LYS:HA	2.20	0.42		

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Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:58:LYS:HA	1:A:60:GLN:NE2	2.33	0.42	
1:A:279:LEU:HG	1:A:328:LEU:HD12	2.02	0.42	
1:A:461:SER:CB	1:A:489:ALA:HB2	2.50	0.42	
1:A:278:GLU:CD	1:A:278:GLU:N	2.73	0.42	
1:A:25:GLU:HG2	1:A:26:THR:N	2.35	0.42	
1:A:161:VAL:HA	1:A:169:VAL:O	2.20	0.42	
1:A:491:GLY:HA3	1:A:509:ILE:HG21	2.01	0.41	
1:A:111:LYS:HE2	1:A:259:VAL:HG21	2.02	0.41	
1:A:517:GLY:HA3	4:A:2268:HOH:O	2.21	0.41	
1:A:349:ARG:HH22	1:A:460:GLY:CA	2.16	0.41	
1:A:435:ILE:O	1:A:438:VAL:HG22	2.21	0.41	
1:A:111:LYS:HE2	1:A:259:VAL:HG22	2.02	0.41	
1:A:66:LEU:HD12	1:A:118:ILE:O	2.21	0.41	
1:A:363:GLY:HA3	1:A:477:ALA:HB2	2.02	0.41	
1:A:521:PHE:CZ	1:A:550:ALA:HB1	2.56	0.41	
1:A:629:GLY:N	1:A:630:PRO:CD	2.81	0.41	
1:A:205:ALA:HB2	1:A:531:THR:HA	2.02	0.40	
1:A:402:HIS:HA	1:A:451:GLN:O	2.21	0.40	
1:A:40:TYR:HA	1:A:45:THR:O	2.21	0.40	

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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	А	631/757~(83%)	577 (91%)	44 (7%)	10 (2%)	9 17	

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	459	ASN
1	А	461	SER



Continueu from pretious puye								
Mol	Chain	\mathbf{Res}	Type					
1	А	612	ALA					
1	А	605	GLN					
1	А	633	GLU					
1	А	702	GLY					
1	А	498	ASN					
1	А	713	ASP					
1	А	611	GLY					
1	А	701	VAL					

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5.3.2Protein 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	А	463/597 (78%)	453~(98%)	10 (2%)	52 77		

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	ASN
1	А	20	ARG
1	А	29	LEU
1	А	55	LYS
1	А	59	ASP
1	А	90	ARG
1	А	132	LEU
1	А	384	ARG
1	А	520	ASP
1	А	581	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	3	ASN
1	А	6	HIS
1	А	60	GLN



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Mol	Chain	Res	Type
1	А	211	GLN
1	А	264	GLN
1	А	388	GLN
1	А	495	GLN
1	А	578	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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).

Mal	Turne	Chain	Dec	Tiple	B	ond leng	\mathbf{gths}	Bond angles		gles
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SO4	А	901	-	4,4,4	0.28	0	6,6,6	0.06	0
2	SO4	А	904	-	4,4,4	0.29	0	6,6,6	0.06	0
2	SO4	А	903	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	А	908	-	4,4,4	0.26	0	6,6,6	0.04	0
2	SO4	A	906	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	А	905	-	4,4,4	0.28	0	6,6,6	0.06	0
2	SO4	A	909	-	4,4,4	0.27	0	6,6,6	0.21	0
3	WO4	А	911	-	2,4,4	0.54	0	-		
2	SO4	A	910	-	4,4,4	0.28	0	6,6,6	0.09	0



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	B	ond ang	gles
MOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	SO4	А	902	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	А	907	-	4,4,4	0.24	0	6,6,6	0.14	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	905	SO4	1	0
3	А	911	WO4	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, 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	645/757~(85%)	0.31	65 (10%) 7 6	26, 45, 100, 100	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	585	VAL	8.0
1	А	710	ALA	7.2
1	А	713	ASP	6.9
1	А	707	VAL	6.9
1	А	664	PHE	6.5
1	А	606	ILE	6.0
1	А	608	GLU	6.0
1	А	632	ALA	5.8
1	А	666	ALA	5.6
1	А	3	ASN	5.6
1	А	714	SER	5.4
1	А	677	LEU	5.4
1	А	705	VAL	5.4
1	А	630	PRO	5.3
1	А	634	ALA	5.3
1	А	497	ILE	5.3
1	А	715	ARG	5.3
1	А	498	ASN	5.2
1	А	614	ILE	5.2
1	А	712	ILE	5.0
1	А	663	THR	4.9
1	А	286	ALA	4.9
1	А	716	GLY	4.7
1	А	706	GLN	4.6
1	А	678	LEU	4.6
1	А	627	ALA	4.6
1	А	289	GLN	4.4



1E3P

Mol	Chain	Res	Type	RSRZ
1	А	665	GLY	4.3
1	А	499	GLY	4.3
1	А	623	TYR	4.1
1	А	676	GLY	4.1
1	А	657	SER	4.0
1	А	671	LEU	4.0
1	А	297	ARG	4.0
1	А	709	ILE	3.8
1	А	290	ASP	3.8
1	А	670	LEU	3.6
1	А	711	GLU	3.6
1	А	675	ASP	3.6
1	А	660	LYS	3.5
1	А	610	THR	3.4
1	А	607	GLN	3.3
1	А	667	PHE	3.1
1	А	708	GLU	3.1
1	А	717	LYS	3.1
1	А	609	ASP	3.0
1	А	604	ASN	3.0
1	А	500	GLU	2.8
1	А	4	GLU	2.8
1	А	631	ALA	2.8
1	А	192	GLU	2.7
1	А	85	PHE	2.7
1	А	584	THR	2.7
1	А	416	ARG	2.6
1	А	611	GLY	2.6
1	А	679	HIS	2.6
1	А	311	GLU	2.6
1	А	287	GLY	2.6
1	А	60	GLN	2.5
1	А	704	LYS	2.2
1	А	605	GLN	2.2
1	А	699	LEU	2.1
1	А	661	THR	2.1
1	А	63	PHE	2.1
1	А	308	PRO	2.0

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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 monosaccharides 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. 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	B-factors(Å ²)	Q < 0.9
2	SO4	А	903	5/5	0.81	0.24	$57,\!57,\!59,\!61$	5
2	SO4	А	905	5/5	0.86	0.27	$66,\!66,\!67,\!68$	5
2	SO4	А	909	5/5	0.86	0.29	36,38,41,41	5
2	SO4	А	904	5/5	0.88	0.27	49,50,52,52	5
2	SO4	А	910	5/5	0.88	0.18	54,57,57,58	5
2	SO4	А	902	5/5	0.91	0.22	43,43,44,44	5
2	SO4	А	901	5/5	0.92	0.31	59,60,61,61	5
2	SO4	А	907	5/5	0.92	0.24	44,45,46,47	5
3	WO4	А	911	5/5	0.93	0.16	72,73,73,74	5
2	SO4	А	908	5/5	0.96	0.13	$54,\!55,\!55,\!55$	5
2	SO4	А	906	5/5	0.97	0.11	53,53,53,54	5

6.5 Other polymers (i)

There are no such residues in this entry.

