



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:22 PM GMT

PDB ID : 1AG1  
Title : MONOHYDROGEN PHOSPHATE BINDING TO TRYPA NOSOMAL  
TRIOSEPHOSPHATE ISOMERASE  
Authors : Verlinde, C.L.M.J.; Hol, W.G.J.  
Deposited on : 1997-03-28  
Resolution : 2.36 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

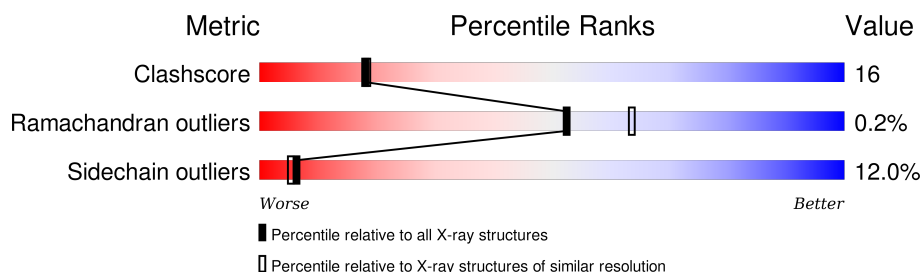
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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))
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	O	250	
1	T	250	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3927 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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			
1	T	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	T	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	100	Total	O	0	0
			100	100		

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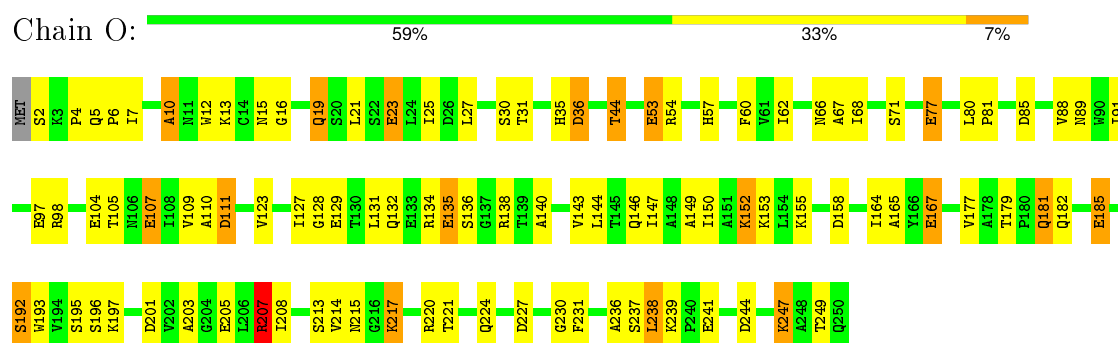
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	56	Total	O	0	0
			56	56		

### 3 Residue-property plots

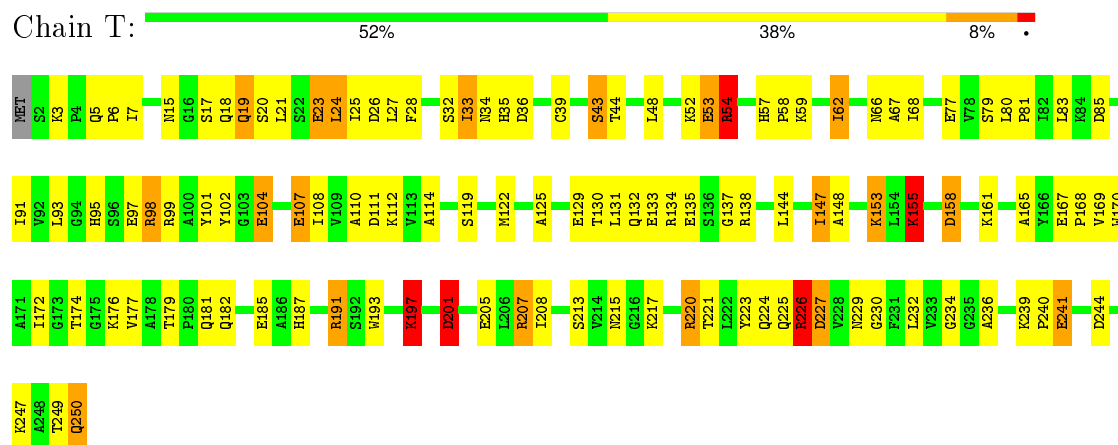
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE



#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.84Å 97.60Å 46.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.36	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.36)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 5-C	Depositor
R, $R_{free}$	0.150 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	O	0.89	11/1917 (0.6%)	1.64	28/2599 (1.1%)
1	T	0.87	13/1917 (0.7%)	1.64	34/2599 (1.3%)
All	All	0.88	24/3834 (0.6%)	1.64	62/5198 (1.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	77	GLU	CD-OE2	7.86	1.34	1.25
1	T	53	GLU	CD-OE2	7.75	1.34	1.25
1	T	77	GLU	CD-OE2	7.63	1.34	1.25
1	O	167	GLU	CD-OE1	7.40	1.33	1.25
1	O	104	GLU	CD-OE2	7.34	1.33	1.25
1	T	185	GLU	CD-OE1	6.85	1.33	1.25
1	O	23	GLU	CD-OE2	6.83	1.33	1.25
1	T	97	GLU	CD-OE2	6.79	1.33	1.25
1	T	23	GLU	CD-OE2	6.74	1.33	1.25
1	O	185	GLU	CD-OE2	6.66	1.32	1.25
1	T	133	GLU	CD-OE2	6.57	1.32	1.25
1	T	205	GLU	CD-OE2	6.42	1.32	1.25
1	T	107	GLU	CD-OE1	6.35	1.32	1.25
1	T	241	GLU	CD-OE1	6.24	1.32	1.25
1	T	167	GLU	CD-OE2	6.07	1.32	1.25
1	O	241	GLU	CD-OE2	6.05	1.32	1.25
1	O	53	GLU	CD-OE1	5.84	1.32	1.25
1	O	107	GLU	CD-OE2	5.77	1.32	1.25
1	T	104	GLU	CD-OE2	5.48	1.31	1.25
1	O	129	GLU	CD-OE2	5.48	1.31	1.25
1	T	135	GLU	CD-OE2	5.44	1.31	1.25
1	O	135	GLU	CD-OE1	5.42	1.31	1.25
1	O	205	GLU	CD-OE2	5.29	1.31	1.25
1	T	129	GLU	CD-OE1	5.20	1.31	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	207	ARG	NE-CZ-NH2	-14.09	113.26	120.30
1	T	191	ARG	NE-CZ-NH2	-13.31	113.65	120.30
1	O	134	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	T	26	ASP	CB-CG-OD1	9.35	126.72	118.30
1	O	207	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	O	244	ASP	CB-CG-OD1	-8.76	110.41	118.30
1	T	191	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	T	26	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	O	201	ASP	CB-CG-OD1	8.43	125.89	118.30
1	O	138	ARG	NE-CZ-NH1	-8.39	116.10	120.30
1	O	158	ASP	CB-CG-OD1	8.13	125.61	118.30
1	O	207	ARG	CD-NE-CZ	8.04	134.86	123.60
1	O	30	SER	CB-CA-C	-8.01	94.88	110.10
1	O	201	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	T	227	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	T	17	SER	N-CA-CB	7.37	121.56	110.50
1	T	201	ASP	CB-CG-OD1	7.29	124.86	118.30
1	T	111	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	T	125	ALA	CB-CA-C	-6.95	99.67	110.10
1	T	201	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	O	231	PHE	N-CA-CB	-6.82	98.33	110.60
1	O	158	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	O	15	ASN	CB-CA-C	-6.70	97.00	110.40
1	O	36	ASP	CB-CG-OD2	6.63	124.27	118.30
1	O	134	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	O	177	VAL	CB-CA-C	-6.60	98.86	111.40
1	O	220	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	T	85	ASP	CB-CG-OD1	6.44	124.09	118.30
1	O	123	VAL	CB-CA-C	-6.29	99.44	111.40
1	T	158	ASP	CB-CG-OD2	6.20	123.88	118.30
1	T	244	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	T	220	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	T	95	HIS	CA-CB-CG	-6.07	103.28	113.60
1	T	158	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	T	111	ASP	CB-CG-OD1	5.92	123.63	118.30
1	T	165	ALA	N-CA-CB	5.84	118.27	110.10
1	O	165	ALA	CB-CA-C	-5.75	101.47	110.10
1	T	250	GLN	N-CA-CB	5.71	120.87	110.60
1	T	134	ARG	CA-CB-CG	-5.67	100.92	113.40
1	T	85	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	O	227	ASP	CB-CG-OD1	5.65	123.39	118.30
1	O	111	ASP	CB-CG-OD2	-5.59	113.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	191	ARG	CD-NE-CZ	5.58	131.41	123.60
1	O	44	THR	CA-CB-CG2	-5.57	104.60	112.40
1	O	36	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	O	98	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	T	101	TYR	CB-CA-C	-5.50	99.41	110.40
1	T	197	LYS	N-CA-CB	-5.49	100.72	110.60
1	T	134	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	O	134	ARG	CD-NE-CZ	5.39	131.15	123.60
1	T	36	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	O	10	ALA	N-CA-CB	5.25	117.45	110.10
1	O	71	SER	N-CA-CB	5.24	118.36	110.50
1	T	43	SER	CB-CA-C	-5.19	100.24	110.10
1	T	226	ARG	CD-NE-CZ	5.17	130.84	123.60
1	T	155	LYS	CB-CA-C	5.16	120.73	110.40
1	O	227	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	T	39	CYS	N-CA-CB	5.12	119.81	110.60
1	T	62	ILE	CB-CA-C	5.06	121.72	111.60
1	T	54	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	T	15	ASN	CB-CA-C	-5.03	100.34	110.40
1	T	36	ASP	CB-CG-OD2	5.01	122.81	118.30

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	O	1883	0	1917	50	0
1	T	1883	0	1917	71	0
2	T	5	0	0	0	0
3	O	100	0	0	3	0
3	T	56	0	0	7	0
All	All	3927	0	3834	119	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 16.

All (119) 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:T:132:GLN:HE22	1:T:138:ARG:NH2	1.62	0.97
1:O:179:THR:H	1:O:182:GLN:HE21	1.00	0.95
1:O:179:THR:H	1:O:182:GLN:NE2	1.71	0.89
1:T:132:GLN:HE22	1:T:138:ARG:HH21	1.17	0.85
1:T:226:ARG:O	1:T:226:ARG:HD2	1.82	0.79
1:T:179:THR:H	1:T:182:GLN:NE2	1.81	0.78
1:T:5:GLN:HE21	1:T:207:ARG:HH12	1.31	0.78
1:O:85:ASP:OD2	1:T:18:GLN:HG3	1.86	0.75
1:T:172:ILE:O	1:T:174:THR:HG23	1.87	0.74
1:T:54:ARG:HH11	1:T:54:ARG:HB2	1.53	0.73
1:T:80:LEU:HB2	1:T:81:PRO:HD3	1.73	0.71
1:O:10:ALA:HB1	1:O:237:SER:HB2	1.73	0.70
1:T:57:HIS:ND1	1:T:58:PRO:HD2	2.07	0.69
3:O:659:HOH:O	1:T:44:THR:HG22	1.91	0.69
1:O:132:GLN:OE1	1:O:132:GLN:N	2.25	0.69
1:T:27:LEU:CD2	1:T:240:PRO:HB3	2.23	0.68
1:T:5:GLN:NE2	3:T:676:HOH:O	2.26	0.67
1:T:191:ARG:HD2	1:T:227:ASP:OD1	1.96	0.66
1:O:193:TRP:CE2	1:O:197:LYS:HG3	2.31	0.66
1:T:54:ARG:HH11	1:T:54:ARG:CB	2.08	0.66
1:T:67:ALA:O	1:T:112:LYS:HE2	1.96	0.65
1:T:132:GLN:NE2	1:T:138:ARG:HH21	1.92	0.65
1:O:217:LYS:HD2	1:O:217:LYS:N	2.12	0.65
1:T:33:ILE:HG13	1:T:59:LYS:HD2	1.79	0.65
1:O:149:ALA:HA	1:O:152:LYS:HE2	1.80	0.64
1:T:24:LEU:HD12	1:T:28:PHE:CZ	2.33	0.64
1:T:110:ALA:HB1	1:T:153:LYS:HD3	1.80	0.63
1:O:13:LYS:NZ	1:O:97:GLU:OE2	2.26	0.61
1:T:34:ASN:N	1:T:34:ASN:OD1	2.27	0.61
1:T:35:HIS:NE2	1:T:249:THR:O	2.35	0.60
1:O:192:SER:O	1:O:196:SER:HB3	2.01	0.60
1:T:27:LEU:HD22	1:T:240:PRO:HB3	1.84	0.59
1:T:20:SER:O	1:T:23:GLU:HB2	2.02	0.59
1:T:226:ARG:HD2	1:T:226:ARG:C	2.22	0.59
1:O:181:GLN:H	1:O:181:GLN:CD	2.03	0.59
1:T:19:GLN:NE2	3:T:739:HOH:O	2.34	0.59
1:O:62:ILE:HD11	1:O:88:VAL:HG22	1.85	0.59
1:T:54:ARG:NH1	1:T:54:ARG:HB2	2.17	0.59
1:O:44:THR:HG23	3:O:606:HOH:O	2.01	0.59
1:T:215:ASN:OD1	1:T:217:LYS:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:193:TRP:CZ2	1:O:197:LYS:HG3	2.37	0.58
1:T:99:ARG:HD3	3:T:611:HOH:O	2.03	0.58
1:T:177:VAL:HG22	1:T:213:SER:HB2	1.85	0.58
1:T:24:LEU:O	1:T:27:LEU:HB3	2.04	0.57
1:T:130:THR:HA	1:T:169:VAL:HB	1.86	0.57
1:T:155:LYS:O	1:T:158:ASP:HB2	2.05	0.57
1:T:27:LEU:HD21	1:T:240:PRO:HB3	1.86	0.56
1:O:31:THR:O	1:O:57:HIS:NE2	2.35	0.56
1:T:155:LYS:O	1:T:158:ASP:N	2.39	0.55
1:O:21:LEU:O	1:O:25:ILE:HG12	2.06	0.55
1:O:57:HIS:HB3	1:O:60:PHE:HD1	1.71	0.55
1:O:131:LEU:O	1:O:135:GLU:HG2	2.06	0.54
1:T:187:HIS:CE1	1:T:208:ILE:HG22	2.42	0.54
1:T:201:ASP:N	1:T:201:ASP:OD1	2.41	0.54
1:O:144:LEU:HA	1:O:147:ILE:HG22	1.89	0.53
1:O:128:GLY:HA3	1:O:167:GLU:O	2.08	0.53
1:O:181:GLN:O	1:O:185:GLU:HG3	2.08	0.52
1:O:57:HIS:HB3	1:O:60:PHE:CD1	2.45	0.52
1:O:127:ILE:HB	1:O:146:GLN:OE1	2.10	0.52
1:T:122:MET:HE3	1:T:161:LYS:O	2.10	0.52
1:O:12:TRP:CD1	1:O:238:LEU:HD13	2.45	0.52
1:T:66:ASN:ND2	3:T:657:HOH:O	2.42	0.51
1:O:80:LEU:HB2	1:O:81:PRO:HD3	1.94	0.49
1:T:66:ASN:O	1:T:67:ALA:HB2	2.12	0.49
1:O:16:GLY:HA3	1:O:21:LEU:HD11	1.93	0.49
1:O:149:ALA:HA	1:O:152:LYS:CE	2.43	0.48
1:O:19:GLN:OE1	1:O:23:GLU:OE2	2.31	0.48
1:O:236:ALA:HA	1:O:239:LYS:HD2	1.96	0.48
1:T:114:ALA:HB2	1:T:153:LYS:HB3	1.96	0.48
1:O:5:GLN:OE1	1:O:207:ARG:NH2	2.47	0.48
1:O:179:THR:N	1:O:182:GLN:NE2	2.53	0.47
1:O:7:ILE:O	1:O:230:GLY:HA3	2.14	0.47
1:T:168:PRO:HB2	1:T:170:TRP:CE2	2.49	0.47
1:T:98:ARG:HA	1:T:102:TYR:HD2	1.80	0.47
1:T:91:ILE:HG12	1:T:93:LEU:HG	1.97	0.47
1:T:57:HIS:ND1	1:T:58:PRO:CD	2.77	0.47
1:O:164:ILE:O	1:O:208:ILE:HA	2.14	0.46
1:T:5:GLN:HE21	1:T:207:ARG:NH1	2.06	0.46
1:T:249:THR:OG1	1:T:249:THR:O	2.32	0.46
1:T:193:TRP:CZ2	1:T:197:LYS:HG2	2.51	0.46
1:T:5:GLN:O	1:T:207:ARG:NH1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:ASN:O	1:O:67:ALA:HB2	2.16	0.46
1:T:21:LEU:O	1:T:25:ILE:HG13	2.16	0.46
1:T:137:GLY:HA2	3:T:694:HOH:O	2.16	0.46
1:T:43:SER:OG	1:T:48:LEU:HD23	2.16	0.45
1:O:105:THR:O	1:O:109:VAL:HG23	2.16	0.45
1:O:140:ALA:O	1:O:144:LEU:HG	2.15	0.45
1:O:77:GLU:HG3	1:T:102:TYR:OH	2.17	0.45
1:T:6:PRO:HA	1:T:229:ASN:O	2.17	0.45
1:O:6:PRO:HD2	1:O:36:ASP:O	2.16	0.45
1:T:48:LEU:O	1:T:52:LYS:HB3	2.16	0.45
1:T:179:THR:N	1:T:182:GLN:NE2	2.59	0.45
1:O:215:ASN:OD1	1:O:217:LYS:N	2.45	0.44
1:O:68:ILE:HD13	1:O:77:GLU:CB	2.47	0.44
1:T:236:ALA:HA	1:T:239:LYS:HD2	2.00	0.44
1:O:89:ASN:ND2	3:O:682:HOH:O	2.50	0.44
1:T:7:ILE:O	1:T:230:GLY:HA3	2.18	0.44
1:O:247:LYS:HG2	1:O:247:LYS:HZ3	1.55	0.44
1:T:68:ILE:HD13	1:T:68:ILE:HG21	1.81	0.44
1:O:195:SER:HA	1:O:203:ALA:HB2	2.00	0.43
1:O:110:ALA:CB	1:O:150:ILE:HA	2.49	0.43
1:T:20:SER:HA	3:T:739:HOH:O	2.19	0.43
1:O:35:HIS:HE1	1:O:249:THR:OG1	2.02	0.43
1:T:108:ILE:O	1:T:112:LYS:HG3	2.19	0.43
1:T:3:LYS:NZ	1:T:225:GLN:O	2.38	0.43
1:O:62:ILE:CD1	1:O:88:VAL:HG22	2.49	0.42
1:T:79:SER:HB2	1:T:81:PRO:HD2	2.01	0.42
1:T:104:GLU:OE2	3:T:641:HOH:O	2.22	0.42
1:T:83:LEU:HA	1:T:83:LEU:HD23	1.76	0.42
1:O:131:LEU:HB3	1:O:132:GLN:OE1	2.20	0.42
1:O:7:ILE:HD11	1:O:207:ARG:CZ	2.49	0.41
1:T:147:ILE:CG2	1:T:148:ALA:N	2.82	0.41
1:O:68:ILE:HD13	1:O:77:GLU:HB3	2.02	0.41
1:T:223:TYR:HE2	1:T:250:GLN:OXT	2.02	0.41
1:T:144:LEU:HA	1:T:144:LEU:HD23	1.69	0.41
1:O:111:ASP:OD1	1:O:153:LYS:NZ	2.45	0.41
1:T:215:ASN:HB2	1:T:241:GLU:OE2	2.21	0.41
1:T:177:VAL:H	1:T:177:VAL:HG23	1.54	0.40
1:T:122:MET:HA	1:T:122:MET:HE3	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	O	247/250 (99%)	238 (96%)	9 (4%)	0	100	100
1	T	247/250 (99%)	237 (96%)	9 (4%)	1 (0%)	39	46
All	All	494/500 (99%)	475 (96%)	18 (4%)	1 (0%)	52	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	234	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	O	196/197 (100%)	174 (89%)	22 (11%)	7	7
1	T	196/197 (100%)	171 (87%)	25 (13%)	5	5
All	All	392/394 (100%)	345 (88%)	47 (12%)	6	5

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	2	SER
1	O	4	PRO
1	O	19	GLN
1	O	27	LEU
1	O	53	GLU

*Continued on next page...*

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Mol	Chain	Res	Type
1	O	54	ARG
1	O	91	ILE
1	O	107	GLU
1	O	136	SER
1	O	143	VAL
1	O	152	LYS
1	O	155	LYS
1	O	181	GLN
1	O	192	SER
1	O	207	ARG
1	O	213	SER
1	O	214	VAL
1	O	217	LYS
1	O	221	THR
1	O	224	GLN
1	O	238	LEU
1	O	247	LYS
1	T	19	GLN
1	T	24	LEU
1	T	32	SER
1	T	33	ILE
1	T	53	GLU
1	T	54	ARG
1	T	62	ILE
1	T	98	ARG
1	T	107	GLU
1	T	119	SER
1	T	131	LEU
1	T	147	ILE
1	T	153	LYS
1	T	155	LYS
1	T	176	LYS
1	T	181	GLN
1	T	197	LYS
1	T	201	ASP
1	T	207	ARG
1	T	220	ARG
1	T	221	THR
1	T	224	GLN
1	T	226	ARG
1	T	232	LEU
1	T	247	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	19	GLN
1	O	35	HIS
1	O	89	ASN
1	O	182	GLN
1	T	5	GLN
1	T	19	GLN
1	T	66	ASN
1	T	132	GLN
1	T	182	GLN

### 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](#)

1 ligand is 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	T	600	-	4,4,4	1.49	1 (25%)	6,6,6	0.29	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	PO4	T	600	-	-	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)
2	T	600	PO4	P-O4	2.48	1.62	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.