



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:30 PM UTC

PDB ID : 1AG1 / pdb_00001ag1
Title : MONOHYDROGEN PHOSPHATE BINDING TO TRYPANOSOMAL
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

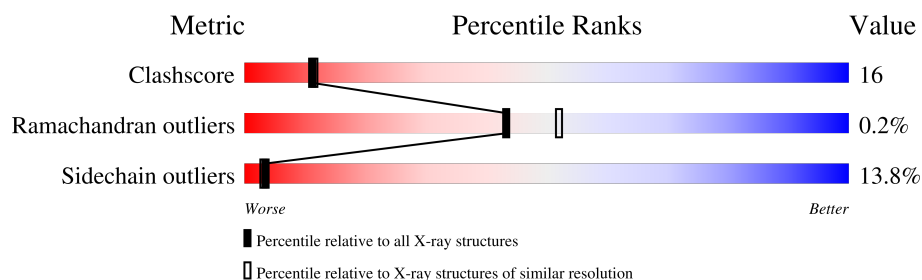
1 Overall quality at a glance

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	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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 $\leq 5\%$.

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 (CCD ID: PO4) (formula: O₄P).



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		

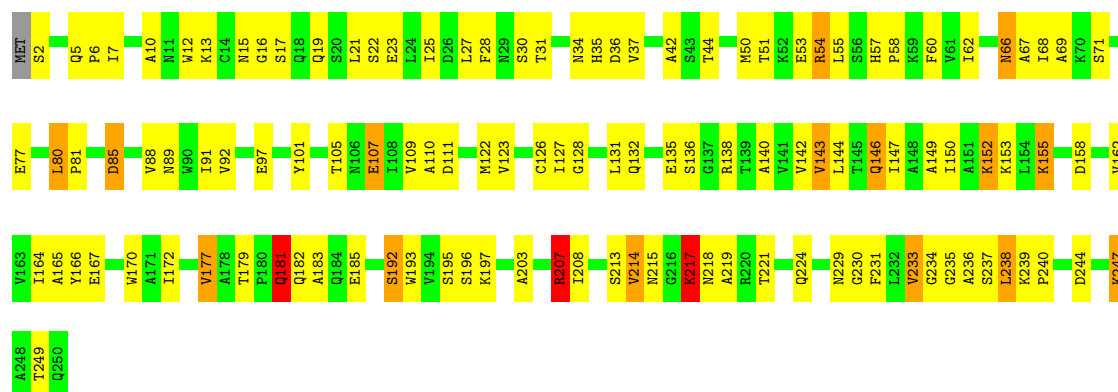
3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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.

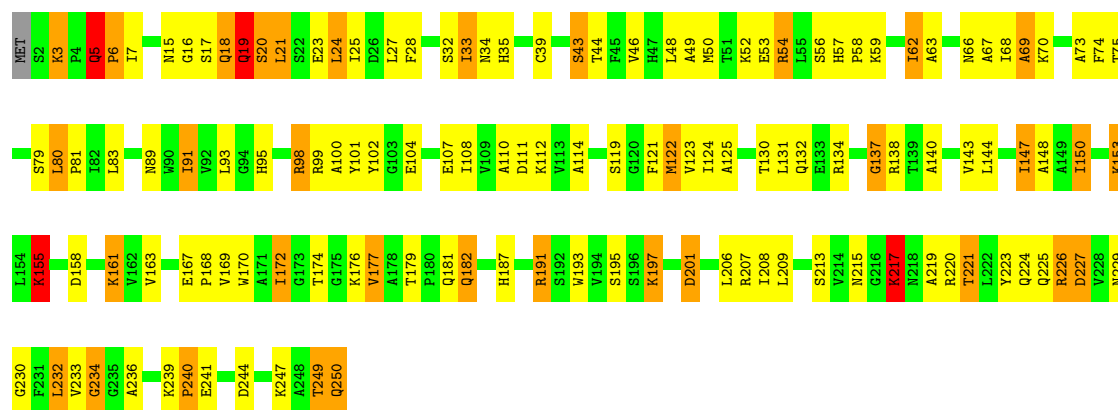
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain O: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain T: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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 5C	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 ²)	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	1.01	0/1917	2.04	61/2599 (2.3%)
1	T	0.98	0/1917	2.07	67/2599 (2.6%)
All	All	0.99	0/3834	2.05	128/5198 (2.5%)

There are no bond length outliers.

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	233	VAL	N-CA-C	10.80	123.47	107.80
1	T	95	HIS	CA-CB-CG	-10.52	103.28	113.80
1	O	143	VAL	N-CA-CB	9.39	120.93	110.51
1	T	69	ALA	N-CA-C	8.92	121.09	111.36
1	O	54	ARG	N-CA-C	8.83	122.55	111.69
1	T	219	ALA	N-CA-C	8.07	120.80	111.11
1	O	30	SER	CB-CA-C	-8.02	94.88	110.11
1	O	183	ALA	N-CA-C	-7.74	102.79	111.07
1	O	231	PHE	N-CA-CB	-7.60	98.33	111.55
1	O	123	VAL	CB-CA-C	-7.48	99.44	110.81
1	O	207	ARG	CD-NE-CZ	7.47	134.86	124.40
1	T	123	VAL	N-CA-C	7.33	118.43	108.17
1	O	244	ASP	CA-CB-CG	-7.30	105.30	112.60
1	O	177	VAL	CB-CA-C	-7.23	98.86	110.28
1	T	16	GLY	N-CA-C	7.13	120.82	111.70
1	T	206	LEU	N-CA-C	7.09	120.52	109.96
1	O	166	TYR	CA-C-O	-6.98	112.39	120.49
1	T	217	LYS	N-CA-C	6.94	118.54	110.97
1	T	20	SER	CA-C-N	6.91	129.54	120.28
1	T	20	SER	C-N-CA	6.91	129.54	120.28
1	T	197	LYS	CA-C-N	-6.84	114.49	122.63
1	T	197	LYS	C-N-CA	-6.84	114.49	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	232	LEU	CA-C-O	-6.84	113.15	120.46
1	O	162	VAL	N-CA-C	6.82	118.88	108.71
1	O	122	MET	N-CA-C	-6.77	98.22	109.46
1	O	234	GLY	CA-C-N	6.75	127.61	119.99
1	O	234	GLY	C-N-CA	6.75	127.61	119.99
1	T	62	ILE	CB-CA-C	6.74	121.72	111.68
1	T	195	SER	N-CA-C	-6.70	103.45	111.69
1	T	197	LYS	N-CA-CB	-6.68	100.72	110.47
1	O	85	ASP	CA-C-O	6.67	127.64	120.10
1	T	155	LYS	CB-CA-C	6.64	120.73	109.50
1	O	233	VAL	N-CA-C	6.62	118.11	108.58
1	O	207	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	T	89	ASN	CA-CB-CG	-6.60	106.00	112.60
1	T	134	ARG	CA-CB-CG	-6.59	100.92	114.10
1	T	121	PHE	CA-CB-CG	6.56	120.36	113.80
1	T	80	LEU	CA-C-O	6.52	124.33	118.33
1	O	233	VAL	CA-C-O	6.44	127.98	120.71
1	T	21	LEU	N-CA-CB	6.41	119.54	110.12
1	O	123	VAL	N-CA-C	6.39	117.80	108.53
1	T	63	ALA	O-C-N	-6.36	115.41	123.24
1	O	101	TYR	CA-C-N	-6.35	110.95	122.50
1	O	101	TYR	C-N-CA	-6.35	110.95	122.50
1	O	51	THR	CB-CA-C	6.30	120.77	110.88
1	T	5	GLN	O-C-N	6.21	126.31	121.47
1	O	158	ASP	CA-CB-CG	-6.20	106.40	112.60
1	O	138	ARG	N-CA-C	6.18	120.44	113.02
1	T	191	ARG	NE-CZ-NH2	-6.17	113.65	119.20
1	T	100	ALA	CA-C-N	-6.14	112.60	122.24
1	T	100	ALA	C-N-CA	-6.14	112.60	122.24
1	T	17	SER	N-CA-CB	6.14	121.56	111.62
1	O	15	ASN	CB-CA-C	-6.13	97.00	110.67
1	T	125	ALA	CB-CA-C	-6.11	99.67	109.75
1	T	250	GLN	N-CA-CB	6.10	120.87	110.50
1	T	227	ASP	O-C-N	6.09	129.65	122.34
1	O	126	CYS	N-CA-C	6.09	119.17	109.24
1	O	235	GLY	N-CA-C	6.08	120.00	112.64
1	T	249	THR	CB-CA-C	-6.06	98.62	109.71
1	T	74	PHE	CA-CB-CG	-5.98	107.82	113.80
1	O	217	LYS	N-CA-CB	5.94	119.11	110.26
1	T	49	ALA	CA-C-N	5.93	128.55	120.54
1	T	49	ALA	C-N-CA	5.93	128.55	120.54
1	T	172	ILE	N-CA-C	5.92	116.91	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	137	GLY	N-CA-C	-5.88	105.45	115.08
1	T	221	THR	CB-CA-C	5.87	120.83	110.85
1	O	218	ASN	CA-C-N	5.86	128.45	120.54
1	O	218	ASN	C-N-CA	5.86	128.45	120.54
1	T	122	MET	N-CA-C	-5.83	99.22	108.73
1	O	181	GLN	CB-CG-CD	5.83	122.51	112.60
1	T	163	VAL	N-CA-C	-5.82	99.74	108.12
1	O	172	ILE	N-CA-C	5.80	115.96	107.37
1	O	207	ARG	CA-C-O	-5.79	114.12	120.43
1	T	19	GLN	N-CA-CB	5.78	118.69	110.13
1	O	55	LEU	CB-CA-C	-5.77	101.61	110.26
1	T	75	THR	CA-C-O	-5.72	114.62	120.80
1	T	101	TYR	CB-CA-C	-5.72	99.41	109.02
1	T	3	LYS	N-CA-C	-5.71	102.91	110.40
1	T	244	ASP	O-C-N	5.69	127.93	122.07
1	O	240	PRO	N-CA-CB	5.69	109.22	103.25
1	T	234	GLY	CA-C-N	5.67	126.40	119.99
1	T	234	GLY	C-N-CA	5.67	126.40	119.99
1	T	39	CYS	N-CA-CB	5.63	119.81	110.52
1	O	71	SER	N-CA-CB	5.60	118.36	110.36
1	T	111	ASP	N-CA-C	5.59	117.18	111.14
1	O	146	GLN	CA-C-N	5.57	127.68	120.56
1	O	146	GLN	C-N-CA	5.57	127.68	120.56
1	O	28	PHE	N-CA-C	5.54	118.03	111.33
1	O	101	TYR	CB-CA-C	-5.54	100.81	110.17
1	O	218	ASN	N-CA-C	5.54	120.04	113.28
1	T	15	ASN	CB-CA-C	-5.52	100.34	110.62
1	T	167	GLU	CB-CA-C	-5.50	103.42	111.01
1	O	66	ASN	CA-CB-CG	5.48	118.08	112.60
1	T	18	GLN	O-C-N	5.47	127.92	122.12
1	O	219	ALA	N-CA-C	5.46	117.67	111.11
1	T	240	PRO	N-CA-CB	5.45	108.75	103.51
1	T	43	SER	CB-CA-C	-5.43	100.24	110.51
1	O	138	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	T	56	SER	N-CA-C	5.33	120.64	113.72
1	O	214	VAL	CA-C-N	-5.32	113.54	123.01
1	O	214	VAL	C-N-CA	-5.32	113.54	123.01
1	T	62	ILE	N-CA-CB	5.32	120.84	110.95
1	T	140	ALA	N-CA-C	5.30	117.05	111.28
1	T	124	ILE	N-CA-CB	5.25	117.98	111.41
1	O	69	ALA	N-CA-C	5.23	117.06	111.36
1	O	165	ALA	CB-CA-C	-5.23	101.47	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	92	VAL	N-CA-C	-5.22	100.90	108.36
1	T	232	LEU	O-C-N	5.22	129.71	123.13
1	T	220	ARG	N-CA-C	5.21	117.36	111.11
1	O	34	ASN	CA-C-N	-5.21	113.73	123.05
1	O	34	ASN	C-N-CA	-5.21	113.73	123.05
1	O	42	ALA	O-C-N	-5.21	116.47	122.87
1	O	80	LEU	CA-C-O	5.20	123.42	118.63
1	O	17	SER	N-CA-C	-5.19	101.31	109.50
1	O	214	VAL	N-CA-C	5.17	115.57	108.12
1	O	22	SER	O-C-N	5.16	128.26	122.22
1	T	6	PRO	CB-CA-C	-5.14	103.48	111.40
1	O	229	ASN	N-CA-C	5.12	118.84	112.59
1	O	155	LYS	N-CA-C	-5.09	102.25	110.14
1	O	58	PRO	O-C-N	5.09	128.79	122.22
1	T	143	VAL	N-CA-C	5.09	115.81	110.62
1	T	163	VAL	CB-CA-C	-5.08	102.91	110.33
1	T	209	LEU	N-CA-C	5.08	118.39	110.32
1	O	42	ALA	CA-C-O	5.07	126.31	120.84
1	T	150	ILE	O-C-N	5.05	126.86	121.91
1	O	107	GLU	CB-CG-CD	5.04	121.17	112.60
1	T	73	ALA	CA-C-O	-5.03	116.15	122.63
1	T	191	ARG	CD-NE-CZ	5.01	131.41	124.40

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	53	0
1	T	1883	0	1917	73	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	124	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 (124) 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:5:GLN:HE21	1:T:207:ARG:HH12	1.31	0.78
1:T:179:THR:H	1:T:182:GLN:NE2	1.81	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:O:21:LEU:HB2	1:O:50:MET:HE1	1.77	0.66
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:N	1:O:217:LYS:HD2	2.12	0.65
1:T:33:ILE:HG13	1:T:59:LYS:HD2	1.79	0.65
1:O:13:LYS:NZ	1:O:97:GLU:OE2	2.26	0.64
1:T:226:ARG:HD2	1:T:226:ARG:C	2.22	0.64
1:O:149:ALA:HA	1:O:152:LYS:HE2	1.80	0.64
1:O:181:GLN:H	1:O:181:GLN:CD	2.03	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:T:34:ASN:OD1	1:T:34:ASN:N	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:19:GLN:NE2	3:T:739:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:ILE:HD11	1:O:88:VAL:HG22	1.85	0.59
1:T:54:ARG:HB2	1:T:54:ARG:NH1	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
1:T:21:LEU:HB2	1:T:50:MET:HE1	1.85	0.58
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:122:MET:HE3	1:T:161:LYS:O	2.07	0.54
1:T:201:ASP:N	1:T:201:ASP:OD1	2.41	0.54
1:O:128:GLY:HA3	1:O:167:GLU:O	2.08	0.53
1:O:144:LEU:HA	1:O:147:ILE:HG22	1.89	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: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:19:GLN:OE1	1:O:23:GLU:OE2	2.31	0.48
1:O:149:ALA:HA	1:O:152:LYS:CE	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3:LYS:NZ	1:T:225:GLN:O	2.38	0.46
1:T:193:TRP:CZ2	1:T:197:LYS:HG2	2.51	0.46
1:T:249:THR:O	1:T:249:THR:OG1	2.32	0.46
1:O:66:ASN:O	1:O:67:ALA:HB2	2.16	0.46
1:T:5:GLN:O	1:T:207:ARG:NH1	2.43	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:O:247:LYS:HZ3	1:O:247:LYS:HG2	1.48	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:O:89:ASN:ND2	3:O:682:HOH:O	2.50	0.44
1:T:236:ALA:HA	1:T:239:LYS:HD2	2.00	0.44
1:T:7:ILE:O	1:T:230:GLY:HA3	2.18	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:O:35:HIS:HE1	1:O:249:THR:OG1	2.02	0.43
1:T:20:SER:HA	3:T:739:HOH:O	2.19	0.43
1:T:69:ALA:C	1:T:70:LYS:HG3	2.44	0.43
1:T:108:ILE:O	1:T:112:LYS:HG3	2.19	0.43
1:O:170:TRP:CD1	1:O:170:TRP:H	2.36	0.42
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:83:LEU:HA	1:T:83:LEU:HD23	1.76	0.42
1:T:104:GLU:OE2	3:T:641:HOH:O	2.22	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:T:170:TRP:CD1	1:T:170:TRP:H	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:181:GLN:CD	1:O:181:GLN:N	2.77	0.40
1:T:177:VAL:H	1:T:177:VAL:HG23	1.54	0.40

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	O	247/250 (99%)	238 (96%)	9 (4%)	0	100	100
1	T	247/250 (99%)	237 (96%)	9 (4%)	1 (0%)	30	34
All	All	494/500 (99%)	475 (96%)	18 (4%)	1 (0%)	43	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	234	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	196/197 (100%)	172 (88%)	24 (12%)	5	4
1	T	196/197 (100%)	166 (85%)	30 (15%)	3	2
All	All	392/394 (100%)	338 (86%)	54 (14%)	3	3

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	2	SER
1	O	27	LEU
1	O	37	VAL
1	O	53	GLU
1	O	54	ARG
1	O	91	ILE
1	O	107	GLU
1	O	136	SER
1	O	142	VAL
1	O	143	VAL
1	O	152	LYS
1	O	155	LYS
1	O	177	VAL
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	233	VAL
1	O	238	LEU
1	O	247	LYS
1	T	5	GLN
1	T	19	GLN
1	T	24	LEU
1	T	32	SER
1	T	33	ILE
1	T	46	VAL
1	T	53	GLU
1	T	54	ARG

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Mol	Chain	Res	Type
1	T	62	ILE
1	T	91	ILE
1	T	98	ARG
1	T	107	GLU
1	T	119	SER
1	T	131	LEU
1	T	147	ILE
1	T	150	ILE
1	T	153	LYS
1	T	155	LYS
1	T	161	LYS
1	T	176	LYS
1	T	177	VAL
1	T	181	GLN
1	T	182	GLN
1	T	201	ASP
1	T	217	LYS
1	T	221	THR
1	T	224	GLN
1	T	226	ARG
1	T	232	LEU
1	T	247	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	19	GLN
1	O	35	HIS
1	O	89	ASN
1	O	181	GLN
1	O	182	GLN
1	O	225	GLN
1	T	5	GLN
1	T	19	GLN
1	T	66	ASN
1	T	132	GLN
1	T	182	GLN
1	T	224	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 oligosaccharides 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	2.08	2 (50%)	6,6,6	1.06	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	600	PO4	P-O1	3.16	1.57	1.50
2	T	600	PO4	P-O4	2.63	1.62	1.54

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.