



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:19 pm BST

PDB ID : 7TIM
Title : STRUCTURE OF THE TRIOSEPHOSPHATE ISOMERASE-PHOSPHOGL
YCOLOHYDROXAMATE COMPLEX: AN ANALOGUE OF THE INTER-
MEDIATE ON THE REACTION PATHWAY
Authors : Davenport, R.C.; Bash, P.A.; Seaton, B.A.; Karplus, M.; Petsko, G.A.; Ringe,
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Deposited on : 1991-04-23
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

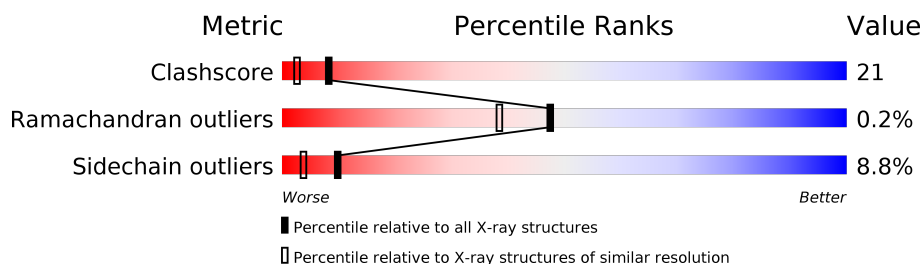
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 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	A	247	
1	B	247	

2 Entry composition [i](#)

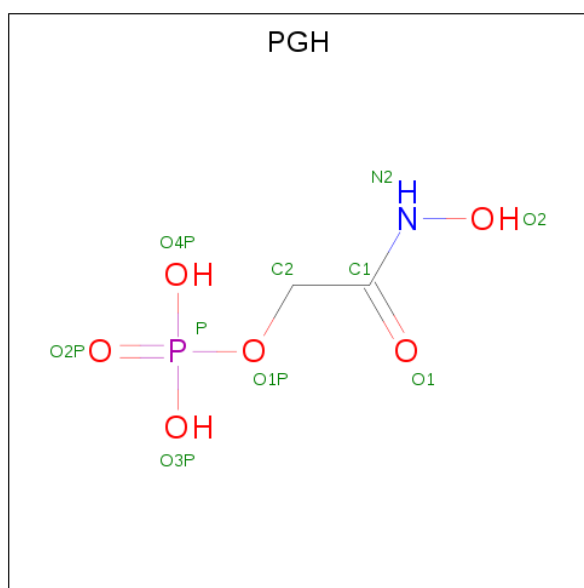
There are 3 unique types of molecules in this entry. The entry contains 4033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	A	247	Total	C	N	O	S	0	0	0
			1883	1196	320	365	2			
1	B	247	Total	C	N	O	S	0	0	0
			1883	1196	320	365	2			

- Molecule 2 is PHOSPHOGLYCOLOHYDROXAMIC ACID (three-letter code: PGH) (formula: $C_2H_6NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total 139	O 139	0	0
3	B	108	Total 108	O 108	0	0

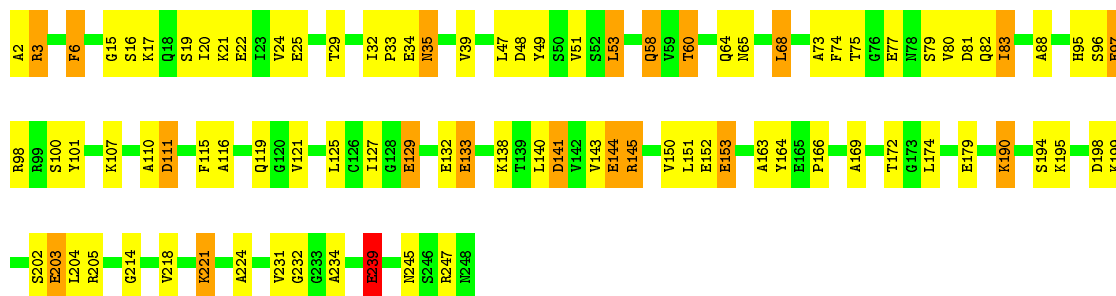
3 Residue-property plots

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

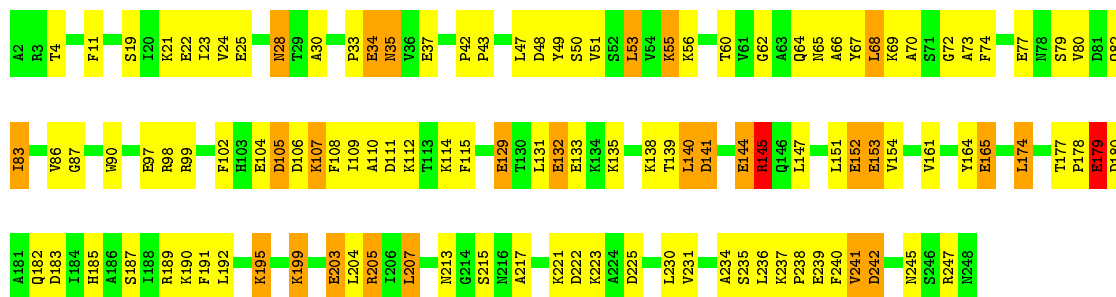
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.00 Å 83.50 Å 38.40 Å 90.00° 99.55° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4033	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: PGH

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	1.05	12/1915 (0.6%)	1.51	16/2590 (0.6%)
1	B	1.05	15/1915 (0.8%)	1.58	22/2590 (0.8%)
All	All	1.05	27/3830 (0.7%)	1.54	38/5180 (0.7%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	GLU	CD-OE1	7.49	1.33	1.25
1	A	132	GLU	CD-OE2	7.03	1.33	1.25
1	A	129	GLU	CD-OE2	6.84	1.33	1.25
1	A	25	GLU	CD-OE1	6.76	1.33	1.25
1	B	97	GLU	CD-OE2	6.63	1.32	1.25
1	A	133	GLU	CD-OE2	6.54	1.32	1.25
1	B	25	GLU	CD-OE2	6.47	1.32	1.25
1	A	153	GLU	CD-OE1	6.41	1.32	1.25
1	B	34	GLU	CD-OE1	6.37	1.32	1.25
1	A	34	GLU	CD-OE2	6.32	1.32	1.25
1	A	203	GLU	CD-OE1	6.32	1.32	1.25
1	B	22	GLU	CD-OE2	6.31	1.32	1.25
1	B	133	GLU	CD-OE1	6.30	1.32	1.25
1	A	144	GLU	CD-OE2	6.28	1.32	1.25
1	B	152	GLU	CD-OE1	6.24	1.32	1.25
1	B	37	GLU	CD-OE1	6.05	1.32	1.25
1	A	22	GLU	CD-OE1	6.02	1.32	1.25
1	B	104	GLU	CD-OE1	6.01	1.32	1.25
1	B	132	GLU	CD-OE2	6.00	1.32	1.25
1	B	179	GLU	CD-OE1	6.00	1.32	1.25
1	A	179	GLU	CD-OE1	5.98	1.32	1.25
1	B	203	GLU	CD-OE1	5.92	1.32	1.25
1	B	77	GLU	CD-OE1	5.85	1.32	1.25
1	B	153	GLU	CD-OE1	5.70	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	GLU	CD-OE2	-5.45	1.19	1.25
1	A	239	GLU	CD-OE1	5.21	1.31	1.25
1	B	144	GLU	CD-OE2	5.09	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ARG	NE-CZ-NH1	11.89	126.24	120.30
1	B	247	ARG	NE-CZ-NH1	-11.47	114.56	120.30
1	B	205	ARG	NE-CZ-NH2	10.85	125.72	120.30
1	B	145	ARG	CD-NE-CZ	9.95	137.53	123.60
1	B	141	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	A	22	GLU	CA-CB-CG	8.39	131.86	113.40
1	A	48	ASP	CB-CG-OD2	8.27	125.74	118.30
1	A	163	ALA	N-CA-CB	7.06	119.99	110.10
1	A	3	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	105	ASP	CB-CG-OD1	6.43	124.09	118.30
1	B	242	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	242	ASP	CB-CG-OD1	6.12	123.80	118.30
1	B	145	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	145	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	67	TYR	CB-CG-CD2	-5.94	117.43	121.00
1	A	111	ASP	CB-CG-OD1	5.92	123.62	118.30
1	B	141	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	129	GLU	CA-CB-CG	5.82	126.21	113.40
1	A	141	ASP	CA-CB-CG	5.62	125.77	113.40
1	A	98	ARG	CD-NE-CZ	-5.53	115.86	123.60
1	A	239	GLU	CG-CD-OE1	-5.53	107.25	118.30
1	A	74	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	A	2	ALA	CB-CA-C	5.49	118.33	110.10
1	B	205	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	105	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	B	34	GLU	CA-CB-CG	5.36	125.18	113.40
1	A	239	GLU	CA-CB-CG	5.35	125.18	113.40
1	A	98	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	102	PHE	CB-CA-C	5.25	120.89	110.40
1	B	165	GLU	CG-CD-OE2	5.19	128.68	118.30
1	B	183	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	A	247	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	180	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	28	ASN	C-N-CA	5.12	134.50	121.70
1	B	164	TYR	CB-CG-CD1	-5.10	117.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ALA	N-CA-CB	5.07	117.20	110.10
1	A	34	GLU	CG-CD-OE1	5.04	128.37	118.30
1	A	97	GLU	OE1-CD-OE2	5.00	129.30	123.30

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	A	1883	0	1892	61	0
1	B	1883	0	1892	101	0
2	A	10	0	4	2	0
2	B	10	0	4	1	0
3	A	139	0	0	9	1
3	B	108	0	0	10	1
All	All	4033	0	3792	160	2

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 21.

All (160) 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:B:114:LYS:HE3	1:B:153:GLU:HB3	1.28	1.14
1:B:21:LYS:HE2	1:B:53:LEU:HD11	1.13	1.12
1:B:48:ASP:HB2	1:B:86:VAL:CG2	1.89	1.03
1:A:199:LYS:O	1:A:203:GLU:HG3	1.62	0.98
1:B:21:LYS:HE2	1:B:53:LEU:CD1	1.97	0.94
1:B:21:LYS:HE3	1:B:49:TYR:OH	1.67	0.93
1:B:48:ASP:HB2	1:B:86:VAL:HG21	1.49	0.92
1:A:239:GLU:HB3	3:A:812:HOH:O	1.69	0.90
1:A:81:ASP:OD1	1:A:119:GLN:NE2	2.09	0.85
1:A:58:GLN:HE21	1:A:58:GLN:H	1.20	0.84
1:B:178:PRO:HB2	1:B:223:LYS:HE3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:HE22	1:B:225:ASP:HB2	1.45	0.82
1:B:70:ALA:HB2	1:B:115:PHE:HZ	1.43	0.82
1:B:21:LYS:CE	1:B:53:LEU:HD11	2.07	0.79
1:A:24:VAL:HG11	1:A:53:LEU:HB3	1.65	0.78
1:B:48:ASP:HB2	1:B:86:VAL:HG22	1.65	0.77
1:A:68:LEU:HD12	1:A:111:ASP:HB3	1.68	0.76
1:B:60:THR:HG21	1:B:90:TRP:CD1	2.20	0.75
1:B:79:SER:O	1:B:83:ILE:HG23	1.87	0.75
1:A:77:GLU:OE2	3:A:820:HOH:O	2.04	0.74
1:A:198:ASP:O	1:A:202:SER:HB3	1.90	0.71
1:B:147:LEU:HD13	1:B:192:LEU:HD21	1.74	0.70
1:B:21:LYS:CE	1:B:53:LEU:HD21	2.22	0.70
1:A:214:GLY:N	1:A:239:GLU:OE2	2.24	0.69
1:A:16:SER:O	1:A:20:ILE:HG12	1.91	0.69
1:B:24:VAL:HG11	1:B:53:LEU:HB3	1.74	0.69
1:A:140:LEU:O	1:A:144:GLU:HG3	1.94	0.68
1:B:4:THR:HG23	1:B:35:ASN:O	1.94	0.68
1:B:56:LYS:HD3	1:B:56:LYS:N	2.09	0.68
1:B:33:PRO:HD3	1:B:245:ASN:OD1	1.93	0.67
1:A:58:GLN:NE2	1:A:58:GLN:H	1.92	0.67
1:B:129:GLU:HG3	1:B:139:THR:OG1	1.95	0.67
1:A:127:ILE:HD12	1:A:143:VAL:HB	1.77	0.67
1:B:48:ASP:CB	1:B:86:VAL:HG22	2.25	0.66
1:B:82:GLN:OE1	3:B:727:HOH:O	2.13	0.66
1:A:60:THR:HB	3:A:819:HOH:O	1.95	0.65
1:B:140:LEU:HD13	1:B:141:ASP:H	1.61	0.65
1:B:70:ALA:HB2	1:B:115:PHE:CZ	2.29	0.64
1:A:79:SER:O	1:A:83:ILE:HG23	1.97	0.64
1:B:182:GLN:NE2	1:B:225:ASP:HB2	2.14	0.63
1:B:87:GLY:HA2	3:B:728:HOH:O	1.99	0.63
1:B:28:ASN:O	1:B:56:LYS:HE2	2.00	0.62
1:B:131:LEU:O	1:B:135:LYS:HG3	1.99	0.62
1:B:199:LYS:O	1:B:203:GLU:HG3	2.00	0.62
1:A:231:VAL:CG1	1:A:234:ALA:HB3	2.30	0.61
1:B:114:LYS:NZ	1:B:153:GLU:OE1	2.30	0.61
1:A:96:SER:OG	3:A:666:HOH:O	2.09	0.61
1:A:145:ARG:HD3	3:A:797:HOH:O	2.00	0.61
1:B:140:LEU:HD22	1:B:140:LEU:C	2.21	0.60
1:B:60:THR:CG2	1:B:90:TRP:CD1	2.85	0.59
1:A:24:VAL:HG11	1:A:53:LEU:CB	2.32	0.59
1:B:140:LEU:HD23	1:B:144:GLU:CD	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD13	1:B:108:PHE:CE1	2.38	0.59
1:B:60:THR:CG2	1:B:90:TRP:HD1	2.15	0.59
1:A:83:ILE:HG13	1:A:88:ALA:HB3	1.85	0.59
1:A:97:GLU:OE2	1:B:73:ALA:HB1	2.03	0.59
1:B:238:PRO:O	1:B:241:VAL:HG23	2.03	0.59
1:A:218:VAL:O	1:A:221:LYS:HB3	2.02	0.58
1:B:55:LYS:HE3	1:B:55:LYS:HA	1.85	0.58
1:A:15:GLY:HA3	1:A:20:ILE:HD11	1.84	0.58
1:B:140:LEU:HD22	1:B:141:ASP:N	2.18	0.58
1:A:100:SER:OG	1:A:101:TYR:N	2.36	0.58
1:B:138:LYS:HG2	3:B:822:HOH:O	2.03	0.58
1:A:24:VAL:CG1	1:A:53:LEU:HB3	2.34	0.58
1:A:58:GLN:N	1:A:58:GLN:HE21	1.97	0.58
1:B:114:LYS:HE3	1:B:153:GLU:CB	2.19	0.56
1:B:138:LYS:O	1:B:141:ASP:HB2	2.05	0.56
1:B:83:ILE:O	1:B:86:VAL:HG12	2.06	0.55
1:B:177:THR:HB	1:B:179:GLU:OE2	2.06	0.55
1:B:48:ASP:CB	1:B:86:VAL:CG2	2.73	0.55
1:A:68:LEU:HD12	1:A:111:ASP:CB	2.36	0.55
1:B:140:LEU:HD13	1:B:141:ASP:N	2.22	0.55
1:B:80:VAL:HG22	1:B:115:PHE:CE2	2.41	0.55
1:A:33:PRO:HD3	1:A:245:ASN:ND2	2.22	0.54
1:B:108:PHE:CE2	1:B:112:LYS:HE3	2.42	0.54
1:B:187:SER:O	1:B:190:LYS:HB2	2.09	0.53
1:A:79:SER:HB3	1:A:82:GLN:HG3	1.92	0.52
1:B:189:ARG:NE	1:B:225:ASP:OD1	2.41	0.52
1:B:30:ALA:HB2	3:B:770:HOH:O	2.10	0.51
1:B:11:PHE:HD1	1:B:11:PHE:N	2.08	0.51
1:B:47:LEU:O	1:B:51:VAL:HG23	2.11	0.50
1:A:166:PRO:HG2	1:A:169:ALA:HB3	1.93	0.50
1:B:223:LYS:HE2	3:B:783:HOH:O	2.11	0.50
1:A:107:LYS:HZ2	1:A:110:ALA:HB3	1.76	0.50
1:B:21:LYS:HE3	1:B:53:LEU:HD21	1.92	0.50
1:B:237:LYS:HB3	1:B:238:PRO:HD2	1.92	0.50
1:B:80:VAL:HG22	1:B:115:PHE:HE2	1.77	0.50
1:B:21:LYS:HE2	1:B:53:LEU:CG	2.41	0.50
1:B:107:LYS:NZ	1:B:111:ASP:OD1	2.43	0.50
1:A:75:THR:O	1:B:98:ARG:HD2	2.12	0.49
1:A:190:LYS:HE3	3:A:706:HOH:O	2.12	0.49
1:A:232:GLY:N	2:A:249:PGH:H21	2.28	0.49
1:A:107:LYS:HE2	1:A:153:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD21	1:A:150:VAL:HG21	1.95	0.48
1:B:73:ALA:HB3	3:B:644:HOH:O	2.13	0.48
1:B:11:PHE:CD1	1:B:11:PHE:N	2.81	0.48
1:B:135:LYS:HE3	3:B:799:HOH:O	2.13	0.48
1:B:60:THR:HG21	1:B:90:TRP:NE1	2.28	0.48
1:A:172:THR:HA	3:A:781:HOH:O	2.13	0.47
1:A:164:TYR:CE2	1:A:166:PRO:HD3	2.50	0.47
1:A:3:ARG:HD3	1:A:202:SER:O	2.14	0.47
1:B:151:LEU:O	1:B:154:VAL:O	2.31	0.47
1:B:72:GLY:HA3	1:B:74:PHE:CE2	2.49	0.47
1:A:145:ARG:NH1	3:A:797:HOH:O	2.13	0.47
1:B:28:ASN:HA	1:B:56:LYS:HG2	1.97	0.46
1:B:191:PHE:O	1:B:195:LYS:HG2	2.15	0.46
1:B:132:GLU:HG2	3:B:816:HOH:O	2.15	0.46
1:A:39:VAL:HA	1:A:60:THR:O	2.14	0.46
1:B:161:VAL:HG12	1:B:207:LEU:HD22	1.98	0.45
1:B:107:LYS:O	1:B:110:ALA:HB3	2.16	0.45
1:B:107:LYS:O	1:B:108:PHE:C	2.55	0.45
1:A:64:GLN:O	1:A:65:ASN:HB2	2.17	0.45
1:B:21:LYS:HB2	1:B:49:TYR:OH	2.17	0.45
1:B:19:SER:O	1:B:23:ILE:HD13	2.16	0.45
1:A:47:LEU:O	1:A:51:VAL:HG23	2.16	0.45
1:A:3:ARG:NH2	1:A:224:ALA:O	2.50	0.45
1:A:33:PRO:HB2	1:A:35:ASN:HD22	1.82	0.45
1:B:21:LYS:HE3	1:B:49:TYR:CZ	2.49	0.45
1:A:17:LYS:HA	1:A:49:TYR:CE2	2.53	0.44
1:B:185:HIS:N	1:B:185:HIS:CD2	2.85	0.44
1:B:213:ASN:OD1	1:B:215:SER:N	2.50	0.44
1:B:165:GLU:OE2	2:B:249:PGH:N2	2.51	0.44
1:B:21:LYS:HD3	1:B:53:LEU:HD21	2.00	0.44
1:A:95:HIS:ND1	1:A:96:SER:N	2.66	0.43
1:B:21:LYS:HA	1:B:53:LEU:HD21	1.99	0.43
1:A:232:GLY:H	2:A:249:PGH:H21	1.83	0.43
1:B:99:ARG:CZ	1:B:109:ILE:HD13	2.48	0.43
1:A:107:LYS:NZ	1:A:110:ALA:HB3	2.33	0.43
1:A:6:PHE:CD1	1:A:6:PHE:C	2.92	0.43
1:B:47:LEU:O	1:B:50:SER:HB2	2.19	0.43
1:B:64:GLN:O	1:B:65:ASN:HB2	2.18	0.43
1:A:32:ILE:HA	1:A:245:ASN:HD21	1.84	0.43
1:B:106:ASP:OD2	1:B:145:ARG:NH2	2.51	0.43
1:B:107:LYS:O	1:B:110:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD13	1:B:174:LEU:N	2.34	0.42
1:A:151:LEU:HD13	1:A:195:LYS:HE2	2.01	0.42
1:B:140:LEU:CD2	1:B:140:LEU:C	2.88	0.42
1:B:62:GLY:HA2	1:B:90:TRP:O	2.19	0.42
1:A:17:LYS:HE2	3:B:829:HOH:O	2.18	0.42
1:B:105:ASP:O	1:B:109:ILE:HD12	2.19	0.42
1:B:138:LYS:O	1:B:139:THR:C	2.58	0.42
1:B:42:PRO:HB2	1:B:43:PRO:HD2	2.01	0.42
1:B:21:LYS:CD	1:B:53:LEU:HD21	2.49	0.42
1:B:217:ALA:HB3	3:B:741:HOH:O	2.20	0.42
1:B:221:LYS:HE3	1:B:222:ASP:OD2	2.20	0.42
1:A:73:ALA:HB3	3:A:657:HOH:O	2.18	0.42
1:A:33:PRO:CD	1:A:245:ASN:ND2	2.83	0.41
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.50	0.41
1:B:21:LYS:HA	1:B:53:LEU:CD2	2.50	0.41
1:A:80:VAL:CG2	1:A:115:PHE:CE2	3.03	0.41
1:A:138:LYS:HG2	1:A:141:ASP:OD2	2.21	0.41
1:A:21:LYS:HA	1:A:53:LEU:HD23	2.03	0.41
1:B:235:SER:HA	1:B:240:PHE:CD1	2.55	0.41
1:A:116:ALA:HB1	1:A:121:VAL:HG22	2.03	0.41
1:A:33:PRO:HB2	1:A:35:ASN:ND2	2.36	0.41
1:A:129:GLU:HB2	1:A:133:GLU:HB2	2.04	0.40
1:B:191:PHE:CD2	1:B:192:LEU:HD23	2.57	0.40
1:B:230:LEU:HA	1:B:230:LEU:HD12	1.80	0.40
1:B:28:ASN:OD1	1:B:56:LYS:HG2	2.21	0.40
1:B:239:GLU:O	1:B:242:ASP:HB2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:672:HOH:O	3:A:701:HOH:O[1_554]	1.88	0.32
3:B:747:HOH:O	3:B:795:HOH:O[1_556]	2.05	0.15

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	A	245/247 (99%)	235 (96%)	10 (4%)	0	100	100
1	B	245/247 (99%)	232 (95%)	12 (5%)	1 (0%)	34	24
All	All	490/494 (99%)	467 (95%)	22 (4%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	ARG

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	200/200 (100%)	184 (92%)	16 (8%)	12	5
1	B	200/200 (100%)	181 (90%)	19 (10%)	8	3
All	All	400/400 (100%)	365 (91%)	35 (9%)	10	4

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	19	SER
1	A	29	THR
1	A	35	ASN
1	A	53	LEU
1	A	58	GLN
1	A	60	THR
1	A	68	LEU
1	A	83	ILE
1	A	174	LEU
1	A	190	LYS

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Mol	Chain	Res	Type
1	A	194	SER
1	A	204	LEU
1	A	205	ARG
1	A	221	LYS
1	A	239	GLU
1	B	34	GLU
1	B	35	ASN
1	B	53	LEU
1	B	55	LYS
1	B	68	LEU
1	B	69	LYS
1	B	83	ILE
1	B	107	LYS
1	B	140	LEU
1	B	152	GLU
1	B	174	LEU
1	B	179	GLU
1	B	195	LYS
1	B	199	LYS
1	B	204	LEU
1	B	205	ARG
1	B	207	LEU
1	B	236	LEU
1	B	241	VAL

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	35	ASN
1	A	58	GLN
1	A	159	ASN
1	A	245	ASN
1	B	35	ASN
1	B	82	GLN
1	B	103	HIS
1	B	248	ASN

5.3.3 RNA ⓘ

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](#)

2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PGH	B	249	-	9,9,9	1.57	1 (11%)	10,12,12	2.08	5 (50%)
2	PGH	A	249	-	9,9,9	1.36	1 (11%)	10,12,12	1.16	1 (10%)

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	PGH	B	249	-	-	5/8/8/8	-
2	PGH	A	249	-	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	249	PGH	P-O3P	-3.37	1.41	1.54
2	A	249	PGH	P-O3P	-2.85	1.43	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	PGH	O2-N2-C1	3.75	125.34	119.79
2	B	249	PGH	O1-C1-N2	2.83	126.75	123.27
2	B	249	PGH	O4P-P-O3P	2.62	117.66	107.64
2	B	249	PGH	C2-C1-N2	-2.50	112.03	116.37
2	A	249	PGH	O3P-P-O1P	-2.11	101.13	106.73
2	B	249	PGH	O1P-P-O2P	-2.02	100.80	106.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	249	PGH	C2-O1P-P-O4P
2	A	249	PGH	N2-C1-C2-O1P
2	A	249	PGH	C2-O1P-P-O3P
2	A	249	PGH	C2-O1P-P-O4P
2	A	249	PGH	C2-O1P-P-O2P
2	B	249	PGH	C2-O1P-P-O3P
2	B	249	PGH	N2-C1-C2-O1P
2	B	249	PGH	C2-O1P-P-O2P
2	B	249	PGH	O1-C1-C2-O1P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	249	PGH	1	0
2	A	249	PGH	2	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 ⓘ

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.