



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:23 PM GMT

PDB ID : 3YPI  
Title : ELECTROPHILIC CATALYSIS IN TRIOSEPHOSPHASE ISOMERASE:  
THE ROLE OF HISTIDINE-95  
Authors : Lolis, E.; Petsko, G.A.  
Deposited on : 1990-12-31  
Resolution : 2.80 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

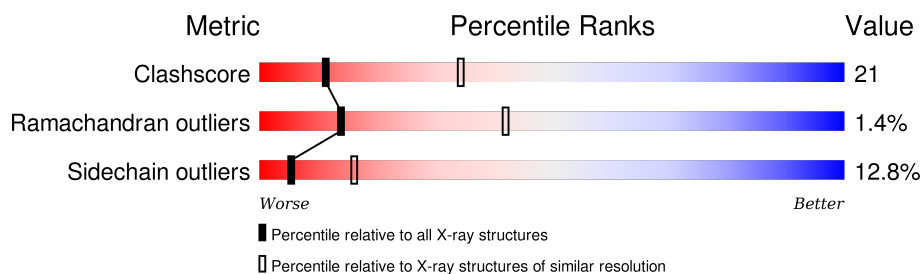
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	A	247	
1	B	247	

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
2	PGH	A	249	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3784 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.

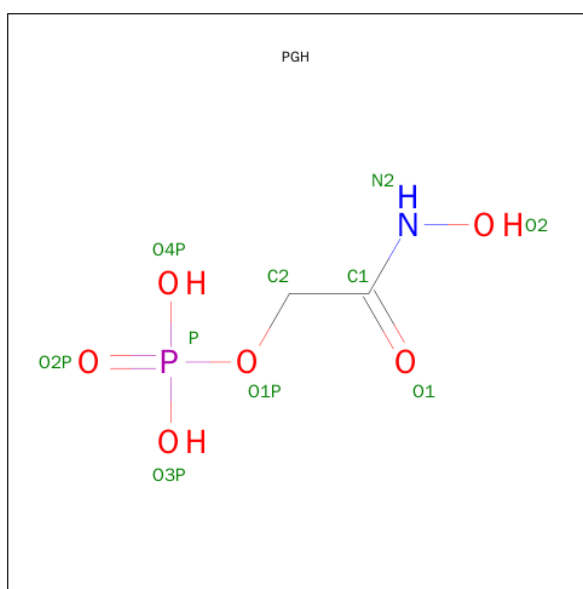
- Molecule 1 is a protein called TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1882	1195	319	366	2			
1	B	247	Total	C	N	O	S	0	0	0
			1882	1195	319	366	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLN	HIS	CONFLICT	UNP P00942
B	95	GLN	HIS	CONFLICT	UNP P00942

- Molecule 2 is PHOSPHOGLYCOLOHYDROXAMIC ACID (three-letter code: PGH) (formula: C<sub>2</sub>H<sub>6</sub>NO<sub>6</sub>P).



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

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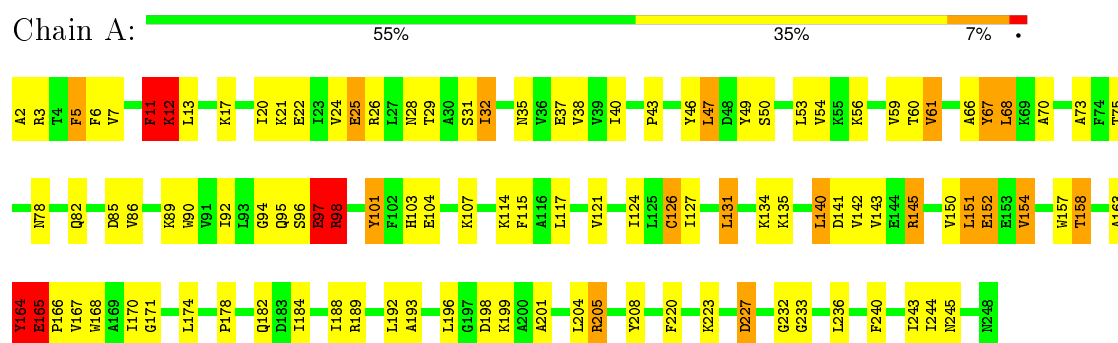
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

### 3 Residue-property plots

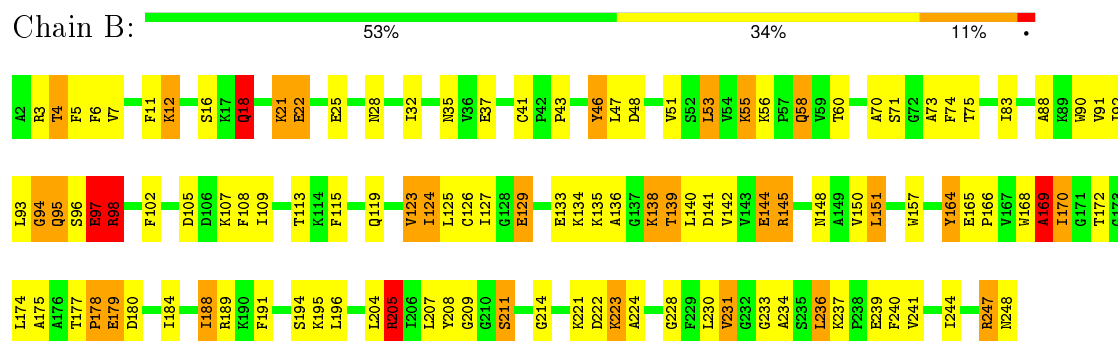
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.35Å 83.97Å 38.67Å 90.00° 99.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	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	1.33	5/1912 (0.3%)	1.84	46/2584 (1.8%)
1	B	1.38	5/1913 (0.3%)	1.92	43/2587 (1.7%)
All	All	1.36	10/3825 (0.3%)	1.88	89/5171 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	5
All	All	0	14

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	GLU	C-N	-34.73	0.54	1.34
1	A	11	PHE	C-N	-27.71	0.70	1.34
1	A	97	GLU	C-N	26.96	1.96	1.34
1	B	94	GLY	C-N	21.97	1.84	1.34
1	A	12	LYS	C-N	8.81	1.54	1.34
1	A	164	TYR	C-N	7.41	1.51	1.34
1	B	97	GLU	CD-OE2	7.33	1.33	1.25
1	B	12	LYS	C-N	6.76	1.49	1.34
1	B	11	PHE	C-N	5.98	1.47	1.34
1	A	165	GLU	C-N	-5.50	1.23	1.34

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	GLY	O-C-N	21.65	157.34	122.70
1	B	94	GLY	C-N-CA	-20.52	70.41	121.70
1	B	94	GLY	CA-C-N	-19.48	74.36	117.20
1	B	189	ARG	NE-CZ-NH2	-14.97	112.81	120.30
1	B	205	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	B	205	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	98	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	A	168	TRP	CD1-CG-CD2	8.88	113.40	106.30
1	B	90	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	A	12	LYS	O-C-N	8.75	136.69	122.70
1	A	90	TRP	CD1-CG-CD2	8.55	113.14	106.30
1	A	101	TYR	CB-CG-CD2	-8.53	115.88	121.00
1	A	164	TYR	O-C-N	-8.11	109.73	122.70
1	A	90	TRP	CE2-CD2-CG	-8.04	100.86	107.30
1	A	168	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	B	90	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	A	26	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	12	LYS	C-N-CA	-7.39	103.23	121.70
1	A	157	TRP	CD1-CG-CD2	7.32	112.15	106.30
1	B	189	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	164	TYR	C-N-CA	7.11	139.47	121.70
1	B	145	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	98	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	97	GLU	CA-C-N	-6.83	102.17	117.20
1	A	227	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	97	GLU	C-N-CA	6.81	138.72	121.70
1	A	152	GLU	OE1-CD-OE2	-6.74	115.22	123.30
1	A	157	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	B	168	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	A	22	GLU	CA-CB-CG	6.63	127.98	113.40
1	B	123	VAL	CG1-CB-CG2	-6.63	100.29	110.90
1	A	165	GLU	CA-C-N	-6.55	98.76	117.10
1	A	68	LEU	CA-CB-CG	6.48	130.19	115.30
1	A	67	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	B	97	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	B	168	TRP	CD1-CG-CD2	6.32	111.36	106.30
1	A	189	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	B	157	TRP	CE2-CD2-CG	-6.25	102.30	107.30
1	A	126	CYS	CA-C-N	-6.22	103.51	117.20
1	B	157	TRP	CD1-CG-CD2	6.17	111.24	106.30
1	B	90	TRP	CG-CD1-NE1	-6.09	104.00	110.10
1	A	90	TRP	CG-CD2-CE3	6.08	139.37	133.90
1	B	124	ILE	N-CA-C	-6.01	94.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	VAL	N-CA-CB	-6.00	98.31	111.50
1	B	18	GLN	CA-CB-CG	5.99	126.58	113.40
1	A	145	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	174	LEU	CA-C-N	-5.96	104.08	117.20
1	B	170	ILE	CB-CG1-CD1	-5.94	97.27	113.90
1	A	168	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	B	247	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	61	VAL	CG1-CB-CG2	-5.81	101.60	110.90
1	A	101	TYR	CB-CG-CD1	5.76	124.45	121.00
1	A	3	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	26	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	247	ARG	N-CA-C	-5.68	95.67	111.00
1	B	209	GLY	CA-C-N	5.68	127.55	116.20
1	B	247	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	175	ALA	CB-CA-C	-5.62	101.66	110.10
1	A	67	TYR	N-CA-CB	-5.61	100.51	110.60
1	B	90	TRP	CB-CG-CD1	-5.53	119.82	127.00
1	B	138	LYS	CA-CB-CG	5.51	125.53	113.40
1	B	211	SER	N-CA-C	5.45	125.72	111.00
1	A	131	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	175	ALA	N-CA-CB	5.40	117.66	110.10
1	B	175	ALA	O-C-N	5.38	131.31	122.70
1	A	86	VAL	CB-CA-C	5.38	121.62	111.40
1	B	7	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	B	209	GLY	O-C-N	-5.32	114.15	123.20
1	B	141	ASP	CA-CB-CG	5.31	125.09	113.40
1	B	164	TYR	CB-CG-CD2	-5.29	117.82	121.00
1	A	5	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	B	144	GLU	CA-CB-CG	5.28	125.02	113.40
1	B	142	VAL	CA-CB-CG2	-5.28	102.98	110.90
1	B	129	GLU	CA-CB-CG	5.27	125.00	113.40
1	A	158	THR	CA-CB-CG2	-5.21	105.11	112.40
1	B	97	GLU	CG-CD-OE1	5.19	128.67	118.30
1	B	98	ARG	CG-CD-NE	5.17	122.65	111.80
1	A	121	VAL	CA-CB-CG2	-5.15	103.18	110.90
1	A	164	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	B	196	LEU	CA-CB-CG	5.14	127.11	115.30
1	B	204	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	2	ALA	N-CA-C	-5.10	97.22	111.00
1	A	244	ILE	CA-CB-CG2	-5.10	100.70	110.90
1	A	165	GLU	C-N-CD	5.10	139.11	128.40
1	A	31	SER	N-CA-C	-5.08	97.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	189	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	7	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	B	169	ALA	CB-CA-C	-5.01	102.59	110.10

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	TYR	Sidechain
1	A	11	PHE	Mainchain
1	A	164	TYR	Sidechain,Mainchain
1	A	165	GLU	Mainchain
1	A	208	TYR	Sidechain
1	A	5	PHE	Sidechain
1	A	6	PHE	Sidechain
1	A	67	TYR	Sidechain
1	B	102	PHE	Sidechain
1	B	164	TYR	Sidechain
1	B	208	TYR	Sidechain
1	B	46	TYR	Sidechain
1	B	97	GLU	Mainchain

## 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	1882	0	1890	90	0
1	B	1882	0	1889	90	0
2	A	10	0	4	6	0
2	B	10	0	4	0	0
All	All	3784	0	3787	156	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 21.

All (156) 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:11:PHE:C	1:A:12:LYS:CA	1.93	1.37
1:A:11:PHE:CA	1:A:12:LYS:N	1.89	1.32
1:B:94:GLY:N	1:B:95:GLN:N	1.80	1.30
1:A:11:PHE:O	1:A:12:LYS:N	1.69	1.24
1:B:93:LEU:C	1:B:95:GLN:N	1.92	1.20
1:A:97:GLU:C	1:A:98:ARG:N	1.96	1.18
1:A:95:GLN:OE1	1:B:75:THR:OG1	1.69	1.09
1:A:95:GLN:HG2	1:A:97:GLU:H	1.17	1.06
1:A:97:GLU:CD	1:B:73:ALA:HB1	1.77	1.04
1:A:94:GLY:C	1:A:95:GLN:N	2.12	1.03
1:B:94:GLY:CA	1:B:95:GLN:N	2.04	0.99
1:B:95:GLN:OE1	1:B:95:GLN:HA	1.56	0.99
1:A:75:THR:OG1	1:B:97:GLU:OE1	1.81	0.97
1:A:97:GLU:HG2	1:B:73:ALA:O	1.66	0.96
1:B:93:LEU:O	1:B:95:GLN:N	1.99	0.94
1:A:171:GLY:CA	2:A:249:PGH:O3P	2.14	0.94
1:A:171:GLY:HA2	2:A:249:PGH:O3P	1.66	0.93
1:B:95:GLN:HA	1:B:126:CYS:SG	2.10	0.92
1:B:83:ILE:HG23	1:B:88:ALA:HB3	1.53	0.89
1:B:56:LYS:HG3	1:B:58:GLN:HE22	1.38	0.87
1:A:75:THR:CB	1:B:97:GLU:OE1	2.22	0.86
1:A:95:GLN:NE2	1:A:97:GLU:HB2	1.92	0.83
1:A:95:GLN:CD	1:B:75:THR:OG1	2.15	0.83
1:A:171:GLY:N	2:A:249:PGH:O3P	2.12	0.82
1:A:97:GLU:OE2	1:B:73:ALA:HB1	1.78	0.82
1:B:92:ILE:HG22	1:B:95:GLN:HB2	1.63	0.81
1:A:11:PHE:C	1:A:12:LYS:N	0.70	0.75
1:A:11:PHE:O	1:A:12:LYS:CA	2.21	0.75
1:A:24:VAL:HG21	1:A:53:LEU:HB3	1.70	0.72
1:A:73:ALA:HA	1:B:12:LYS:HD3	1.69	0.72
1:A:75:THR:HB	1:B:97:GLU:OE1	1.91	0.71
1:B:56:LYS:HG3	1:B:58:GLN:NE2	2.07	0.69
1:A:97:GLU:HG2	1:B:73:ALA:C	2.13	0.68
1:A:193:ALA:HA	1:A:201:ALA:HB2	1.76	0.68
1:A:97:GLU:CG	1:B:73:ALA:O	2.42	0.66
1:A:95:GLN:OE1	1:B:75:THR:CB	2.43	0.66
1:A:95:GLN:HG2	1:A:97:GLU:N	2.01	0.66
1:B:95:GLN:HA	1:B:126:CYS:HB2	1.78	0.65
1:B:32:ILE:HD11	1:B:56:LYS:HG2	1.78	0.65
1:B:95:GLN:HA	1:B:126:CYS:CB	2.27	0.65
1:A:11:PHE:C	1:A:12:LYS:CB	2.64	0.65
1:A:165:GLU:O	1:A:166:PRO:C	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:O	1:A:167:VAL:N	2.31	0.63
1:A:95:GLN:CG	1:A:96:SER:N	2.62	0.62
1:A:97:GLU:OE1	1:B:73:ALA:HB1	1.99	0.62
1:A:205:ARG:HG3	1:A:227:ASP:HB3	1.83	0.61
1:B:144:GLU:O	1:B:148:ASN:HB2	2.01	0.60
1:B:92:ILE:CG2	1:B:95:GLN:HB2	2.29	0.59
1:A:13:LEU:O	1:B:71:SER:HA	2.02	0.59
1:B:70:ALA:HB2	1:B:115:PHE:HZ	1.67	0.59
1:A:165:GLU:HB3	1:A:170:ILE:HD11	1.85	0.59
1:B:113:THR:HG23	1:B:123:VAL:HG11	1.85	0.59
1:B:32:ILE:HG22	1:B:244:ILE:HD11	1.84	0.58
1:B:32:ILE:HG22	1:B:244:ILE:CD1	2.33	0.57
1:B:25:GLU:HA	1:B:28:ASN:HB2	1.85	0.57
1:A:127:ILE:HD12	1:A:143:VAL:HG13	1.87	0.57
1:B:95:GLN:NE2	1:B:165:GLU:CD	2.59	0.56
1:A:24:VAL:CG2	1:A:53:LEU:HD23	2.36	0.56
1:A:11:PHE:CB	1:A:12:LYS:N	2.65	0.55
1:B:16:SER:HA	1:B:46:TYR:OH	2.06	0.55
1:A:232:GLY:HA3	2:A:249:PGH:H21	1.88	0.55
1:B:21:LYS:HA	1:B:53:LEU:HD11	1.88	0.54
1:A:95:GLN:OE1	1:B:75:THR:CG2	2.56	0.53
1:A:178:PRO:HA	1:A:220:PHE:CE2	2.42	0.53
1:B:58:GLN:H	1:B:58:GLN:NE2	2.07	0.52
1:A:70:ALA:HB2	1:A:115:PHE:HZ	1.75	0.52
1:A:97:GLU:CD	1:B:73:ALA:CB	2.65	0.52
1:A:240:PHE:HA	1:A:243:ILE:HD12	1.92	0.52
1:B:91:VAL:HG13	1:B:93:LEU:HG	1.92	0.51
1:B:47:LEU:HD21	1:B:83:ILE:HG13	1.92	0.51
1:B:5:PHE:CE1	1:B:228:GLY:HA2	2.46	0.51
1:B:125:LEU:HD21	1:B:150:VAL:HG21	1.93	0.50
1:B:4:THR:HB	1:B:205:ARG:NH2	2.25	0.50
1:B:18:GLN:O	1:B:22:GLU:HB2	2.12	0.50
1:B:191:PHE:O	1:B:194:SER:HB3	2.12	0.50
1:B:32:ILE:HD11	1:B:56:LYS:CG	2.42	0.50
1:B:95:GLN:CA	1:B:126:CYS:SG	2.94	0.50
1:A:11:PHE:N	1:A:12:LYS:N	2.55	0.49
1:A:32:ILE:HA	1:A:245:ASN:HD21	1.76	0.49
1:A:95:GLN:OE1	1:B:75:THR:HG21	2.13	0.49
1:B:127:ILE:HD11	1:B:188:ILE:HD12	1.94	0.49
1:A:21:LYS:O	1:A:25:GLU:HB2	2.13	0.48
1:A:24:VAL:CG2	1:A:53:LEU:HB3	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:CYS:SG	1:A:163:ALA:HB3	2.52	0.48
1:A:43:PRO:HG2	1:A:46:TYR:HD2	1.78	0.48
1:B:233:GLY:O	1:B:236:LEU:HD22	2.14	0.48
1:B:214:GLY:HA3	1:B:239:GLU:HB2	1.96	0.48
1:A:60:THR:OG1	1:A:89:LYS:HG3	2.14	0.47
1:B:21:LYS:NZ	1:B:25:GLU:OE2	2.47	0.47
1:B:135:LYS:HG3	1:B:136:ALA:N	2.29	0.47
1:A:95:GLN:NE2	1:B:75:THR:OG1	2.48	0.47
1:B:47:LEU:O	1:B:51:VAL:HG23	2.15	0.47
1:A:20:ILE:HB	1:A:49:TYR:HE2	1.79	0.47
1:A:47:LEU:HD23	1:A:61:VAL:HG12	1.98	0.46
1:A:192:LEU:HD13	1:A:204:LEU:CD1	2.46	0.46
1:A:131:LEU:O	1:A:135:LYS:HG2	2.16	0.46
1:A:143:VAL:HG11	1:A:188:ILE:HG12	1.96	0.46
1:A:97:GLU:HG2	1:B:74:PHE:HA	1.96	0.46
1:A:38:VAL:HG12	1:A:59:VAL:HG13	1.96	0.46
1:B:95:GLN:NE2	1:B:230:LEU:HD23	2.31	0.46
1:A:178:PRO:HB2	1:A:223:LYS:HE2	1.97	0.46
1:B:170:ILE:O	1:B:172:THR:HG23	2.15	0.46
1:B:177:THR:HA	1:B:178:PRO:HD2	1.70	0.45
1:B:129:GLU:HB2	1:B:133:GLU:HB2	1.98	0.45
1:A:107:LYS:HD2	1:A:107:LYS:HA	1.47	0.45
1:A:11:PHE:O	1:A:12:LYS:C	2.55	0.45
1:B:93:LEU:HD12	1:B:123:VAL:HG13	1.97	0.45
1:B:21:LYS:HA	1:B:53:LEU:CD1	2.47	0.45
1:A:151:LEU:HD11	1:A:196:LEU:HD21	1.99	0.45
1:A:95:GLN:HG3	1:A:96:SER:N	2.31	0.45
1:A:95:GLN:HG3	1:A:96:SER:H	1.82	0.45
1:A:140:LEU:HD13	1:A:140:LEU:HA	1.81	0.45
1:A:95:GLN:HG2	1:A:96:SER:N	2.30	0.44
1:A:82:GLN:HE22	1:B:43:PRO:HG2	1.82	0.44
1:B:113:THR:HG23	1:B:123:VAL:HG21	1.99	0.44
1:A:98:ARG:HB3	1:A:104:GLU:HG3	1.99	0.44
1:A:164:TYR:OH	1:A:184:ILE:HD13	2.19	0.43
1:B:92:ILE:HA	1:B:124:ILE:HB	2.00	0.43
1:A:96:SER:CB	1:A:170:ILE:HD12	2.48	0.43
1:B:184:ILE:O	1:B:188:ILE:HG12	2.18	0.43
1:B:94:GLY:HA2	1:B:109:ILE:HD13	2.00	0.43
1:A:205:ARG:HA	1:A:227:ASP:OD2	2.17	0.43
1:A:11:PHE:O	1:A:12:LYS:CB	2.63	0.43
1:B:47:LEU:CD2	1:B:83:ILE:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:O	1:A:145:ARG:HB3	2.19	0.43
1:B:151:LEU:CD2	1:B:195:LYS:HG3	2.49	0.42
1:A:66:ALA:HA	1:A:78:ASN:HB2	2.00	0.42
1:A:40:ILE:HD11	1:A:61:VAL:HG22	2.01	0.42
1:A:233:GLY:H	2:A:249:PGH:P	2.42	0.42
1:B:53:LEU:O	1:B:55:LYS:HD2	2.19	0.42
1:A:82:GLN:NE2	1:B:43:PRO:HG2	2.34	0.42
1:B:105:ASP:OD1	1:B:108:PHE:HB2	2.19	0.42
1:B:115:PHE:O	1:B:119:GLN:HG2	2.19	0.42
1:A:12:LYS:NZ	1:A:97:GLU:OE1	2.34	0.42
1:A:171:GLY:CA	2:A:249:PGH:P	3.08	0.41
1:B:241:VAL:O	1:B:244:ILE:HG13	2.20	0.41
1:B:231:VAL:HG21	1:B:240:PHE:CE1	2.54	0.41
1:A:50:SER:O	1:A:54:VAL:HG13	2.21	0.41
1:B:166:PRO:HG2	1:B:169:ALA:HB3	2.00	0.41
1:B:41:CYS:SG	1:B:92:ILE:HD11	2.61	0.41
1:B:231:VAL:HG11	1:B:234:ALA:HB3	2.02	0.41
1:B:3:ARG:NH2	1:B:224:ALA:O	2.53	0.41
1:A:150:VAL:O	1:A:154:VAL:HG23	2.20	0.41
1:A:92:ILE:HA	1:A:124:ILE:HB	2.02	0.41
1:A:95:GLN:HE21	1:A:97:GLU:HB2	1.79	0.41
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.50	0.41
1:A:17:LYS:NZ	1:B:48:ASP:OD1	2.51	0.41
1:A:97:GLU:CG	1:B:73:ALA:C	2.88	0.41
1:A:117:LEU:HD12	1:A:154:VAL:HG11	2.02	0.41
1:B:221:LYS:HG3	1:B:247:ARG:HD3	2.03	0.41
1:B:107:LYS:HD2	1:B:107:LYS:HA	1.79	0.41
1:B:179:GLU:OE2	1:B:223:LYS:NZ	2.50	0.41
1:B:6:PHE:CD1	1:B:37:GLU:HB3	2.56	0.41
1:B:129:GLU:HG3	1:B:139:THR:HA	2.03	0.40
1:A:28:ASN:HA	1:A:56:LYS:HD3	2.04	0.40
1:A:97:GLU:OE1	1:B:73:ALA:CA	2.69	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	A	243/247 (98%)	225 (93%)	17 (7%)	1 (0%)	39	74
1	B	245/247 (99%)	221 (90%)	18 (7%)	6 (2%)	7	25
All	All	488/494 (99%)	446 (91%)	35 (7%)	7 (1%)	14	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	GLN
1	B	98	ARG
1	B	211	SER
1	A	12	LYS
1	B	169	ALA
1	B	178	PRO
1	B	139	THR

### 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%)	177 (88%)	23 (12%)	7	21
1	B	200/200 (100%)	172 (86%)	28 (14%)	4	13
All	All	400/400 (100%)	349 (87%)	51 (13%)	5	16

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	29	THR
1	A	32	ILE
1	A	35	ASN
1	A	47	LEU

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Mol	Chain	Res	Type
1	A	68	LEU
1	A	85	ASP
1	A	97	GLU
1	A	98	ARG
1	A	103	HIS
1	A	114	LYS
1	A	134	LYS
1	A	140	LEU
1	A	141	ASP
1	A	151	LEU
1	A	152	GLU
1	A	154	VAL
1	A	158	THR
1	A	182	GLN
1	A	198	ASP
1	A	199	LYS
1	A	205	ARG
1	A	236	LEU
1	B	4	THR
1	B	18	GLN
1	B	21	LYS
1	B	22	GLU
1	B	35	ASN
1	B	53	LEU
1	B	55	LYS
1	B	58	GLN
1	B	60	THR
1	B	96	SER
1	B	98	ARG
1	B	134	LYS
1	B	138	LYS
1	B	140	LEU
1	B	145	ARG
1	B	151	LEU
1	B	174	LEU
1	B	179	GLU
1	B	180	ASP
1	B	188	ILE
1	B	205	ARG
1	B	207	LEU
1	B	222	ASP
1	B	223	LYS

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Mol	Chain	Res	Type
1	B	231	VAL
1	B	236	LEU
1	B	237	LYS
1	B	248	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	245	ASN
1	A	248	ASN
1	B	58	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](#)

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	A	249	-	9,9,9	1.40	1 (11%)	10,12,12	1.25	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PGH	B	249	-	9,9,9	1.61	2 (22%)	10,12,12	3.25	4 (40%)

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	A	249	-	-	0/8/8/8	0/0/0/0
2	PGH	B	249	-	-	0/8/8/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	249	PGH	P-O2P	-2.22	1.43	1.51
2	B	249	PGH	C1-N2	2.15	1.34	1.32
2	B	249	PGH	O1P-C2	3.04	1.45	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	PGH	C2-C1-N2	-6.42	104.93	116.21
2	B	249	PGH	O4P-P-O1P	-4.50	93.61	106.56
2	A	249	PGH	O1P-P-O2P	-2.36	101.13	107.14
2	B	249	PGH	O4P-P-O3P	2.74	117.80	107.38
2	B	249	PGH	O2-N2-C1	5.78	128.30	119.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	249	PGH	6	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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