



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:02 AM UTC

PDB ID : 1TPH / pdb_00001tph
Title : 1.8 ANGSTROMS CRYSTAL STRUCTURE OF WILD TYPE CHICKEN
TRIOSEPHOSPHATE ISOMERASE-PHOSPHOGLYCOLOHYDROXAMA
TE COMPLEX
Authors : Zhang, Z.; Sugio, S.; Komives, E.A.; Liu, K.D.; Knowles, J.R.; Petsko, G.A.;
Ringe, D.
Deposited on : 1993-12-22
Resolution : 1.80 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

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

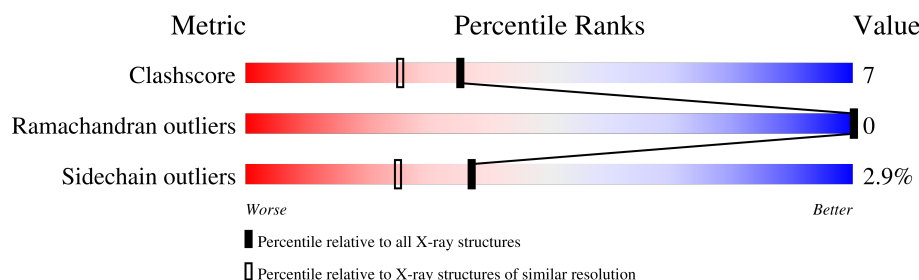
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 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	1	247	
1	2	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	1	250	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3981 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.

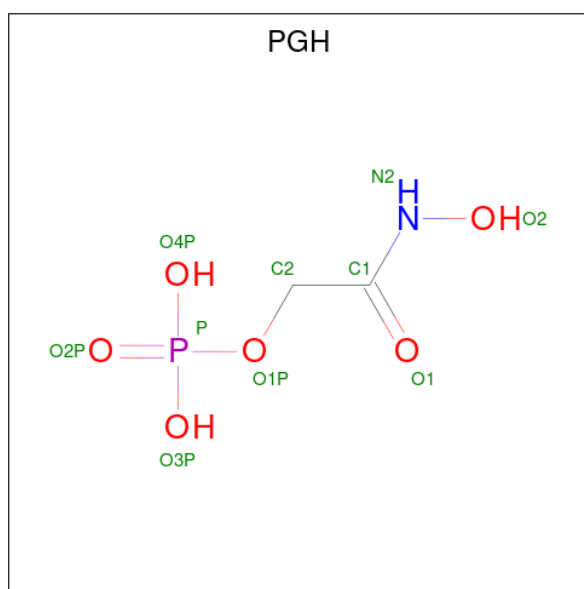
- Molecule 1 is a protein called TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	245	Total	C	N	O	S	0	0	0
			1856	1176	325	349	6			
1	2	245	Total	C	N	O	S	0	0	0
			1856	1176	325	349	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	194	THR	SER	conflict	UNP P00940
2	194	THR	SER	conflict	UNP P00940

- Molecule 2 is PHOSPHOGLYCOLOHYDROXAMIC ACID (CCD ID: PGH) (formula: $C_2H_6NO_6P$).



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

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

- Molecule 3 is water.

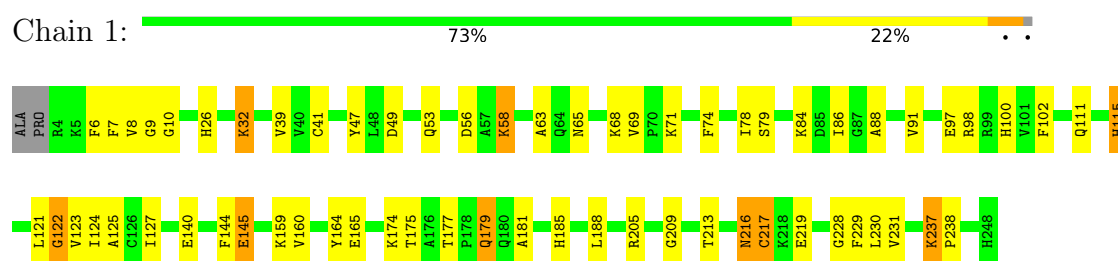
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	119	Total	O	0	0
			119	119		
3	2	130	Total	O	0	0
			130	130		

3 Residue-property plots

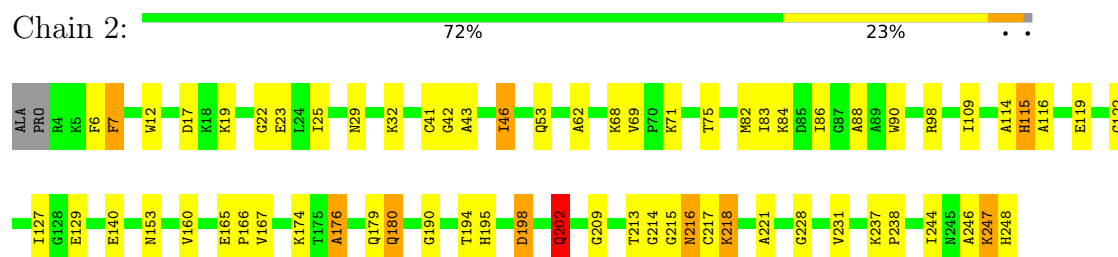
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



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	136.40Å 74.00Å 57.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3981	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	1	1.31	2/1891 (0.1%)	1.96	55/2552 (2.2%)
1	2	1.33	3/1891 (0.2%)	2.03	58/2552 (2.3%)
All	All	1.32	5/3782 (0.1%)	1.99	113/5104 (2.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	216	ASN	CA-CB	11.05	1.71	1.53
1	2	41	CYS	CA-C	5.30	1.59	1.52
1	1	97	GLU	CD-OE2	5.28	1.35	1.25
1	1	164	TYR	CA-CB	5.25	1.59	1.53
1	2	69	VAL	N-CA	5.09	1.51	1.46

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	198	ASP	CA-CB-CG	-11.20	101.40	112.60
1	2	41	CYS	O-C-N	10.33	135.46	123.27
1	2	216	ASN	CA-CB-CG	-9.72	102.88	112.60
1	2	215	GLY	CA-C-N	9.59	142.06	121.64
1	2	215	GLY	C-N-CA	9.59	142.06	121.64
1	2	109	ILE	CA-C-N	9.12	130.06	119.94
1	2	109	ILE	C-N-CA	9.12	130.06	119.94
1	1	68	LYS	N-CA-C	8.98	122.96	112.72
1	2	41	CYS	CA-C-O	-8.82	110.61	120.32
1	2	216	ASN	CB-CA-C	-8.50	94.05	110.11
1	2	217	CYS	N-CA-C	8.49	120.54	111.28
1	2	216	ASN	N-CA-C	8.22	123.87	112.45
1	2	129	GLU	CB-CG-CD	7.79	125.85	112.60
1	2	22	GLY	N-CA-C	-7.59	103.69	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	63	ALA	CA-C-O	-7.24	113.27	121.81
1	1	39	VAL	O-C-N	7.12	130.40	123.14
1	1	69	VAL	CB-CA-C	6.99	117.44	109.89
1	2	90	TRP	O-C-N	6.99	131.77	122.96
1	2	180	GLN	CA-C-O	-6.99	113.01	120.42
1	2	244	ILE	O-C-N	6.95	128.61	121.87
1	2	217	CYS	O-C-N	6.92	129.46	122.12
1	2	68	LYS	N-CA-C	6.90	121.41	112.92
1	2	214	GLY	N-CA-C	-6.85	104.27	113.24
1	2	231	VAL	O-C-N	6.84	130.63	123.03
1	1	10	GLY	CA-C-O	-6.83	114.33	120.75
1	1	91	VAL	O-C-N	6.82	130.62	123.05
1	2	98	ARG	CD-NE-CZ	-6.79	114.89	124.40
1	2	167	VAL	O-C-N	6.74	128.41	121.87
1	1	145	GLU	CB-CG-CD	6.73	124.05	112.60
1	2	43	ALA	O-C-N	6.70	129.32	121.21
1	1	160	VAL	O-C-N	6.68	129.95	123.14
1	2	216	ASN	CB-CG-ND2	6.67	126.41	116.40
1	2	215	GLY	N-CA-C	6.65	121.29	112.77
1	2	160	VAL	O-C-N	6.62	130.33	123.18
1	1	217	CYS	N-CA-C	6.61	118.56	111.36
1	2	179	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	1	121	LEU	O-C-N	6.49	130.21	122.94
1	1	125	ALA	O-C-N	6.45	130.56	123.27
1	1	74	PHE	CA-CB-CG	-6.41	107.39	113.80
1	1	115	HIS	ND1-CG-CD2	6.35	112.45	106.10
1	1	122	GLY	N-CA-C	-6.23	101.39	112.54
1	2	69	VAL	CA-C-N	6.20	125.77	119.19
1	2	69	VAL	C-N-CA	6.20	125.77	119.19
1	2	115	HIS	CA-CB-CG	-6.20	107.60	113.80
1	1	39	VAL	CA-C-O	-6.16	113.70	120.72
1	1	231	VAL	CA-C-O	-6.15	113.99	120.57
1	1	26	HIS	O-C-N	6.12	128.38	122.07
1	1	125	ALA	CA-C-O	-6.11	113.77	120.43
1	1	9	GLY	CA-C-N	-6.07	117.09	122.73
1	1	9	GLY	C-N-CA	-6.07	117.09	122.73
1	1	100	HIS	CA-CB-CG	-6.06	107.74	113.80
1	2	202	GLN	CB-CG-CD	6.02	122.84	112.60
1	2	166	PRO	CA-C-O	6.02	127.67	121.23
1	1	53	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	1	102	PHE	CA-CB-CG	-6.00	107.80	113.80
1	2	23	GLU	CB-CG-CD	5.99	122.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	84	LYS	N-CA-CB	5.93	118.93	110.16
1	2	176	ALA	CA-C-O	-5.88	115.15	121.56
1	2	82	MET	O-C-N	5.85	129.84	122.23
1	1	175	THR	CA-C-O	-5.83	115.37	121.55
1	1	6	PHE	O-C-N	5.74	130.07	122.95
1	2	17	ASP	N-CA-C	-5.74	100.59	109.14
1	1	205	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	1	123	VAL	O-C-N	5.64	129.14	123.10
1	1	8	VAL	O-C-N	5.63	129.17	123.20
1	1	231	VAL	N-CA-C	5.58	116.34	108.36
1	1	181	ALA	CA-C-O	5.55	126.65	120.82
1	2	23	GLU	CA-C-N	5.55	127.72	120.28
1	2	23	GLU	C-N-CA	5.55	127.72	120.28
1	2	53	GLN	CA-C-O	-5.47	113.67	119.97
1	2	75	THR	O-C-N	5.45	129.60	123.06
1	2	231	VAL	N-CA-C	5.44	116.14	108.36
1	1	229	PHE	O-C-N	5.42	129.73	123.17
1	1	185	HIS	ND1-CE1-NE2	5.41	113.81	108.40
1	2	29	ASN	O-C-N	5.41	128.55	122.22
1	1	177	THR	CA-C-N	5.38	125.20	119.28
1	1	177	THR	C-N-CA	5.38	125.20	119.28
1	2	122	GLY	N-CA-C	-5.38	102.91	112.54
1	2	180	GLN	O-C-N	5.38	128.28	122.15
1	2	69	VAL	CA-C-O	-5.35	114.54	121.13
1	1	219	GLU	CB-CG-CD	5.35	121.69	112.60
1	1	98	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	2	12	TRP	O-C-N	5.31	129.79	122.46
1	1	124	ILE	N-CA-C	-5.31	99.51	107.37
1	1	41	CYS	CA-C-O	-5.27	114.64	120.38
1	2	116	ALA	O-C-N	5.25	127.69	122.12
1	2	116	ALA	CA-C-O	-5.24	115.00	120.55
1	2	218	LYS	CA-C-O	-5.24	115.32	120.82
1	1	111	GLN	CG-CD-NE2	5.22	124.23	116.40
1	2	53	GLN	O-C-N	5.21	128.68	122.27
1	1	69	VAL	N-CA-C	-5.21	103.12	109.01
1	1	231	VAL	O-C-N	5.20	128.81	123.03
1	1	179	GLN	OE1-CD-NE2	-5.20	117.41	122.60
1	2	179	GLN	CG-CD-NE2	5.19	124.19	116.40
1	2	127	ILE	CA-C-O	-5.17	116.51	121.63
1	1	97	GLU	CA-C-O	-5.16	114.03	119.97
1	1	97	GLU	O-C-N	5.15	128.61	122.27
1	1	47	TYR	CA-C-O	-5.12	113.54	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	166	PRO	CB-CA-C	5.10	118.06	111.64
1	1	97	GLU	CG-CD-OE1	5.09	130.12	118.40
1	1	174	LYS	CA-C-O	-5.09	116.06	122.63
1	2	140	GLU	CA-CB-CG	5.09	124.28	114.10
1	1	53	GLN	CB-CG-CD	5.09	121.25	112.60
1	1	79	SER	CA-C-N	5.08	125.11	119.32
1	1	79	SER	C-N-CA	5.08	125.11	119.32
1	2	246	ALA	N-CA-C	5.08	117.55	111.71
1	2	176	ALA	N-CA-C	-5.07	103.34	110.50
1	1	115	HIS	CA-CB-CG	-5.06	108.74	113.80
1	1	65	ASN	CA-CB-CG	5.02	117.62	112.60
1	1	88	ALA	N-CA-C	-5.02	103.06	110.48
1	1	49	ASP	O-C-N	5.00	127.22	122.07
1	2	7	PHE	CA-CB-CG	5.00	118.80	113.80
1	2	25	ILE	O-C-N	5.00	126.98	121.83

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	1	1856	0	1863	27	0
1	2	1856	0	1863	30	0
2	1	10	0	4	0	0
2	2	10	0	4	1	0
3	1	119	0	0	2	0
3	2	130	0	0	4	0
All	All	3981	0	3734	55	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 7.

All (55) 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)
1:1:32:LYS:CE	1:1:32:LYS:H	1.91	0.84
1:1:32:LYS:H	1:1:32:LYS:HE3	1.45	0.82
1:1:145:GLU:HG3	3:1:481:HOH:O	1.84	0.77
1:1:216:ASN:C	1:1:216:ASN:HD22	1.94	0.75
1:2:176:ALA:HB1	1:2:180:GLN:HG3	1.72	0.72
1:1:32:LYS:H	1:1:32:LYS:CD	2.06	0.69
1:2:202:GLN:HA	1:2:202:GLN:HE21	1.58	0.69
1:2:198:ASP:O	1:2:202:GLN:HG2	1.95	0.67
1:2:190:GLY:O	1:2:194:THR:HG23	1.98	0.62
1:2:247:LYS:C	1:2:248:HIS:HD2	2.08	0.62
1:1:32:LYS:HE3	1:1:32:LYS:N	2.13	0.60
1:1:32:LYS:O	1:1:32:LYS:HD2	2.02	0.60
1:2:32:LYS:O	1:2:32:LYS:HD3	2.01	0.59
1:1:213:THR:H	1:1:216:ASN:HD21	1.50	0.59
1:2:247:LYS:C	1:2:248:HIS:CD2	2.82	0.58
1:1:140:GLU:HG2	1:1:144:PHE:CE2	2.39	0.56
1:1:115:HIS:HD2	3:1:459:HOH:O	1.89	0.56
1:2:174:LYS:O	1:2:174:LYS:HG3	2.07	0.53
1:1:179:GLN:NE2	1:1:179:GLN:H	2.07	0.53
1:2:7:PHE:O	1:2:228:GLY:HA3	2.09	0.52
1:1:7:PHE:O	1:1:228:GLY:HA3	2.10	0.52
1:1:32:LYS:H	1:1:32:LYS:HD2	1.74	0.51
1:2:19:LYS:HE2	3:2:544:HOH:O	2.08	0.51
1:2:213:THR:H	1:2:216:ASN:HB2	1.76	0.51
1:1:213:THR:H	1:1:216:ASN:ND2	2.09	0.50
1:1:237:LYS:HB3	1:1:238:PRO:HD2	1.94	0.50
1:1:78:ILE:HD12	1:2:46:ILE:HD11	1.93	0.49
1:1:32:LYS:N	1:1:32:LYS:HD2	2.28	0.49
1:1:32:LYS:CD	1:1:32:LYS:N	2.72	0.48
1:2:84:LYS:HD2	1:2:119:GLU:O	2.14	0.47
1:1:78:ILE:HG21	1:2:46:ILE:HG13	1.95	0.47
1:2:237:LYS:HB3	1:2:238:PRO:HD2	1.97	0.46
1:1:56:ASP:OD1	1:1:58:LYS:HB2	2.15	0.46
1:1:216:ASN:C	1:1:216:ASN:ND2	2.68	0.46
1:1:216:ASN:HD22	1:1:217:CYS:N	2.12	0.46
1:2:165:GLU:OE2	2:2:250:PGH:N2	2.49	0.45
1:2:165:GLU:OE2	1:2:209:GLY:HA3	2.18	0.44
1:2:180:GLN:HE21	1:2:180:GLN:HB3	1.37	0.44
1:2:247:LYS:HE2	3:2:369:HOH:O	2.18	0.43
1:2:46:ILE:HG22	1:2:46:ILE:O	2.18	0.43
1:1:122:GLY:HA2	1:1:159:LYS:HB3	1.98	0.43
1:2:6:PHE:CE1	1:2:228:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:115:HIS:HD2	3:2:461:HOH:O	2.02	0.43
1:1:165:GLU:OE2	1:1:209:GLY:HA3	2.18	0.42
1:2:194:THR:OG1	1:2:195:HIS:ND1	2.52	0.42
1:2:221:ALA:O	1:2:247:LYS:NZ	2.50	0.42
1:1:230:LEU:HD12	1:1:230:LEU:HA	1.83	0.42
1:2:247:LYS:O	1:2:248:HIS:CD2	2.73	0.41
1:2:218:LYS:HE2	3:2:412:HOH:O	2.20	0.41
1:2:202:GLN:HA	1:2:202:GLN:NE2	2.32	0.41
1:1:32:LYS:HD2	1:1:32:LYS:C	2.46	0.41
1:2:42:GLY:HA2	1:2:62:ALA:O	2.21	0.41
1:2:83:ILE:HG23	1:2:88:ALA:HB3	2.03	0.40
1:2:114:ALA:HB2	1:2:153:ASN:HB3	2.01	0.40
1:1:127:ILE:HD11	1:1:188:LEU:HD11	2.04	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	1	243/247 (98%)	236 (97%)	7 (3%)	0	100	100
1	2	243/247 (98%)	235 (97%)	8 (3%)	0	100	100
All	All	486/494 (98%)	471 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	191/192 (100%)	185 (97%)	6 (3%)	35	23
1	2	191/192 (100%)	186 (97%)	5 (3%)	40	28
All	All	382/384 (100%)	371 (97%)	11 (3%)	37	25

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	32	LYS
1	1	58	LYS
1	1	71	LYS
1	1	86	ILE
1	1	216	ASN
1	1	237	LYS
1	2	46	ILE
1	2	71	LYS
1	2	86	ILE
1	2	202	GLN
1	2	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	1	53	GLN
1	1	111	GLN
1	1	115	HIS
1	1	179	GLN
1	1	202	GLN
1	1	216	ASN
1	2	100	HIS
1	2	111	GLN
1	2	115	HIS
1	2	202	GLN
1	2	223	GLN
1	2	248	HIS

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 oligosaccharides 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	1	250	-	9,9,9	2.95	5 (55%)	10,12,12	2.86	5 (50%)
2	PGH	2	250	-	9,9,9	2.94	4 (44%)	10,12,12	1.43	2 (20%)

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	1	250	-	-	2/8/8/8	-
2	PGH	2	250	-	-	1/8/8/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	250	PGH	P-O4P	6.40	1.78	1.54
2	1	250	PGH	P-O1P	4.90	1.75	1.60
2	1	250	PGH	P-O2P	4.25	1.63	1.50
2	1	250	PGH	P-O3P	4.07	1.69	1.54
2	2	250	PGH	P-O1P	3.98	1.72	1.60
2	1	250	PGH	P-O4P	3.24	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	250	PGH	O1P-C2	-2.71	1.40	1.43
2	2	250	PGH	O1P-C2	2.43	1.45	1.43
2	2	250	PGH	P-O3P	2.39	1.63	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	250	PGH	O1-C1-N2	6.36	131.08	123.27
2	1	250	PGH	O4P-P-O1P	3.59	116.03	106.67
2	1	250	PGH	O3P-P-O2P	-2.82	99.83	110.83
2	2	250	PGH	O1-C1-N2	2.60	126.47	123.27
2	1	250	PGH	C2-C1-N2	-2.49	112.12	116.41
2	1	250	PGH	O3P-P-O1P	-2.43	100.33	106.67
2	2	250	PGH	O2-N2-C1	-2.28	116.42	119.79

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	250	PGH	C2-O1P-P-O3P
2	2	250	PGH	O1-C1-C2-O1P
2	1	250	PGH	O1-C1-C2-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	250	PGH	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

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.