



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:48 PM UTC

PDB ID : 3YPI / pdb_00003ypi
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

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

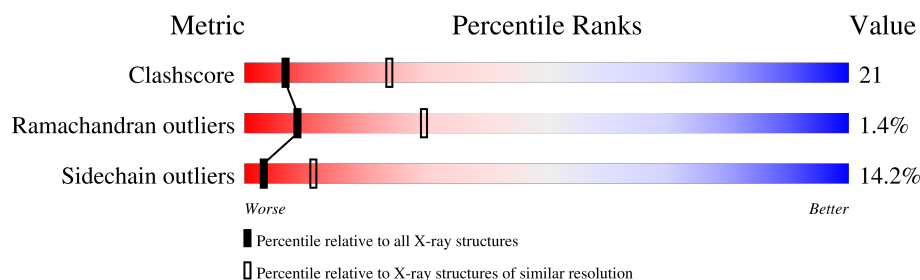
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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	A	247	43% 43% 12% .
1	B	247	44% 38% 15% .

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.

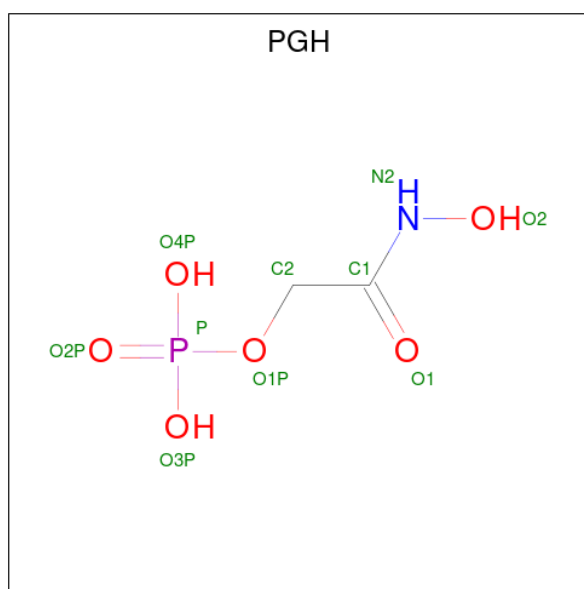
- Molecule 1 is a protein called TRIOSEPHOSPHATE ISOMERASE.

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 (CCD ID: 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		

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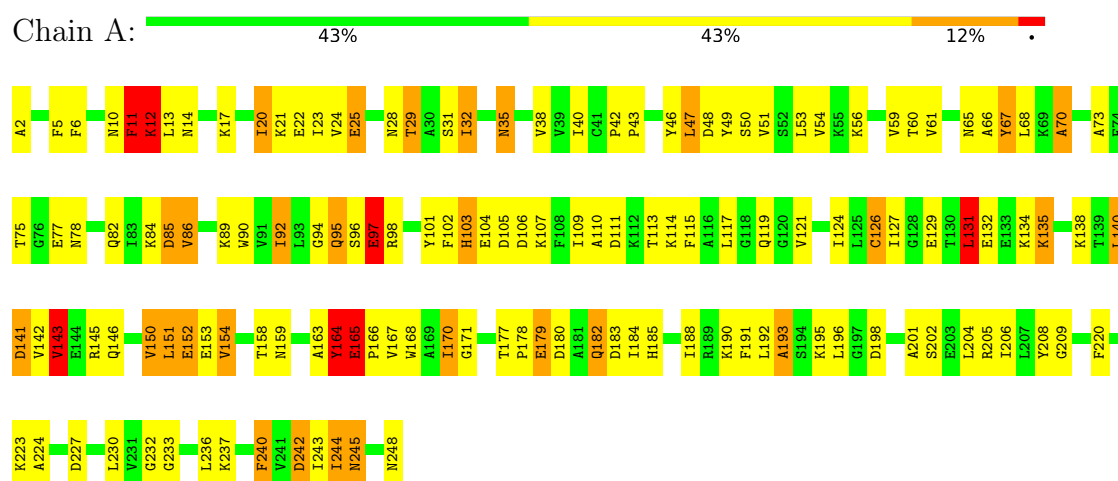
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

3 Residue-property plots

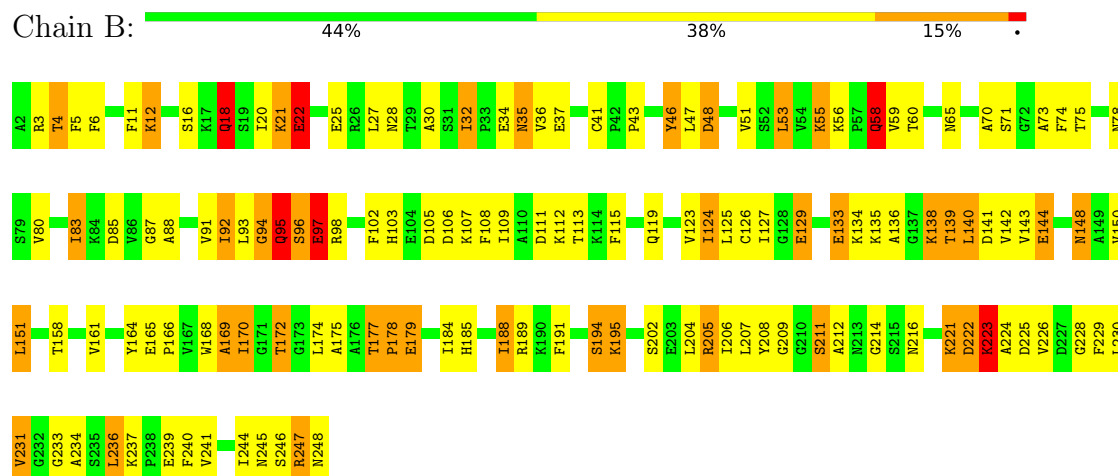
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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	1.98	9/1912 (0.5%)	2.29	94/2584 (3.6%)
1	B	2.01	13/1913 (0.7%)	2.35	73/2587 (2.8%)
All	All	1.99	22/3825 (0.6%)	2.32	167/5171 (3.2%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	GLU	C-N	-56.80	0.54	1.33
1	A	97	GLU	C-N	49.83	1.96	1.33
1	A	11	PHE	C-N	-45.27	0.70	1.33
1	B	94	GLY	C-N	36.35	1.84	1.33
1	A	12	LYS	C-N	14.73	1.54	1.33
1	A	164	TYR	C-N	13.14	1.51	1.33
1	B	12	LYS	C-N	12.21	1.49	1.33
1	B	11	PHE	C-N	10.09	1.47	1.33
1	B	103	HIS	CD2-NE2	-7.29	1.29	1.37
1	B	172	THR	CA-CB	7.07	1.65	1.53
1	A	185	HIS	CD2-NE2	-6.66	1.30	1.37
1	B	59	VAL	CA-CB	6.61	1.61	1.53
1	A	185	HIS	CG-ND1	-6.50	1.31	1.38
1	B	161	VAL	CA-CB	6.49	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	35	ASN	CA-CB	5.65	1.61	1.53
1	B	97	GLU	C-O	-5.55	1.17	1.24
1	B	185	HIS	CG-ND1	-5.28	1.32	1.38
1	A	103	HIS	CA-CB	5.24	1.61	1.53
1	A	35	ASN	CA-C	5.16	1.58	1.53
1	B	32	ILE	CA-CB	5.03	1.60	1.54
1	B	143	VAL	CA-CB	5.03	1.60	1.54

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	GLY	O-C-N	28.07	157.34	122.25
1	B	94	GLY	CA-C-N	-26.77	70.41	121.54
1	B	94	GLY	C-N-CA	-26.77	70.41	121.54
1	A	164	TYR	CA-C-N	15.11	139.47	122.85
1	A	164	TYR	C-N-CA	15.11	139.47	122.85
1	A	165	GLU	CA-C-N	-13.07	103.50	119.84
1	A	165	GLU	C-N-CA	-13.07	103.50	119.84
1	B	141	ASP	CA-CB-CG	12.49	125.09	112.60
1	A	164	TYR	O-C-N	-11.83	109.73	123.22
1	A	35	ASN	CA-CB-CG	10.65	123.25	112.60
1	A	12	LYS	O-C-N	10.60	136.69	122.59
1	A	97	GLU	CA-C-N	10.52	138.72	122.42
1	A	97	GLU	C-N-CA	10.52	138.72	122.42
1	A	12	LYS	CA-C-N	-9.59	103.23	121.54
1	A	12	LYS	C-N-CA	-9.59	103.23	121.54
1	B	177	THR	N-CA-C	9.46	120.48	109.60
1	A	146	GLN	OE1-CD-NE2	-9.23	113.37	122.60
1	A	77	GLU	N-CA-C	9.08	122.81	110.55
1	B	124	ILE	N-CA-C	-9.06	94.76	107.99
1	B	148	ASN	CA-CB-CG	9.06	121.66	112.60
1	A	111	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	183	ASP	CA-CB-CG	8.80	121.40	112.60
1	B	247	ARG	N-CA-C	-8.36	95.67	108.96
1	B	209	GLY	O-C-N	-8.18	114.15	122.82
1	B	18	GLN	OE1-CD-NE2	-8.13	114.47	122.60
1	B	170	ILE	CB-CG1-CD1	-7.87	97.27	113.80
1	B	103	HIS	CB-CG-CD2	-7.87	120.97	131.20
1	A	103	HIS	CA-CB-CG	7.79	121.59	113.80
1	B	35	ASN	CA-CB-CG	7.77	120.37	112.60
1	B	20	ILE	N-CA-C	-7.75	102.89	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	GLU	O-C-N	7.69	127.46	121.23
1	A	230	LEU	CA-C-O	7.62	129.38	120.70
1	B	103	HIS	CA-CB-CG	7.57	121.37	113.80
1	B	36	VAL	N-CA-C	-7.55	97.78	108.80
1	A	248	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	B	216	ASN	CA-CB-CG	7.41	120.01	112.60
1	B	106	ASP	N-CA-C	7.36	120.17	111.71
1	B	58	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	A	35	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	A	141	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	65	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	B	11	PHE	CA-CB-CG	7.10	120.90	113.80
1	B	189	ARG	NE-CZ-NH2	-7.10	112.81	119.20
1	B	12	LYS	CA-C-N	-7.07	111.55	122.16
1	B	12	LYS	C-N-CA	-7.07	111.55	122.16
1	A	152	GLU	CB-CG-CD	7.05	124.58	112.60
1	B	225	ASP	CA-CB-CG	-7.02	105.58	112.60
1	B	211	SER	N-CA-C	7.00	125.72	110.80
1	A	22	GLU	CA-CB-CG	6.94	127.98	114.10
1	A	182	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	129	GLU	CA-C-O	6.90	128.46	120.80
1	B	248	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	A	180	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	67	TYR	N-CA-CB	-6.71	100.51	110.85
1	A	242	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	42	PRO	N-CA-C	6.71	118.89	110.70
1	A	23	ILE	N-CA-C	-6.68	105.24	111.45
1	B	48	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	165	GLU	N-CA-C	6.66	120.06	108.75
1	B	18	GLN	CA-C-O	-6.64	113.38	120.42
1	A	143	VAL	N-CA-CB	-6.60	102.22	110.47
1	A	105	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	92	ILE	N-CA-C	-6.54	100.25	108.89
1	A	182	GLN	CG-CD-NE2	6.51	126.17	116.40
1	B	175	ALA	O-C-N	6.49	131.31	123.13
1	A	95	GLN	O-C-N	6.47	130.22	122.85
1	A	102	PHE	N-CA-C	6.45	120.07	112.72
1	A	248	ASN	CA-CB-CG	6.44	119.04	112.60
1	B	106	ASP	CA-CB-CG	-6.40	106.20	112.60
1	A	202	SER	CA-CB-OG	-6.38	98.35	111.10
1	A	119	GLN	N-CA-C	6.33	121.00	113.16
1	B	245	ASN	OD1-CG-ND2	-6.28	116.32	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	GLN	CA-CB-CG	6.24	126.58	114.10
1	A	29	THR	N-CA-C	6.19	121.12	113.50
1	B	245	ASN	CA-CB-CG	6.19	118.79	112.60
1	B	35	ASN	CA-C-O	6.15	129.72	122.03
1	A	31	SER	N-CA-C	-6.14	97.28	108.02
1	A	65	ASN	CB-CG-ND2	6.12	125.58	116.40
1	B	96	SER	CA-C-O	-6.09	114.05	120.63
1	A	86	VAL	N-CA-CB	-6.07	98.31	111.05
1	A	20	ILE	N-CA-C	-6.06	104.59	110.72
1	A	191	PHE	N-CA-C	-6.06	104.36	110.97
1	A	183	ASP	CB-CA-C	-6.01	101.44	110.88
1	A	48	ASP	CA-C-N	6.00	128.24	120.44
1	A	48	ASP	C-N-CA	6.00	128.24	120.44
1	A	240	PHE	N-CA-C	-6.00	104.74	111.28
1	B	161	VAL	O-C-N	-5.98	116.90	123.18
1	A	150	VAL	CA-C-N	5.96	128.27	120.28
1	A	150	VAL	C-N-CA	5.96	128.27	120.28
1	B	194	SER	CA-CB-OG	5.96	123.01	111.10
1	A	29	THR	CA-CB-OG1	-5.95	100.67	109.60
1	A	113	THR	CA-C-O	-5.91	114.29	120.55
1	A	209	GLY	O-C-N	-5.84	118.11	123.42
1	B	18	GLN	CB-CG-CD	5.82	122.49	112.60
1	B	202	SER	CA-CB-OG	5.79	122.68	111.10
1	A	244	ILE	CA-CB-CG2	-5.77	100.70	110.50
1	A	245	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	190	LYS	CG-CD-CE	5.75	124.53	111.30
1	A	92	ILE	O-C-N	-5.74	116.40	122.83
1	A	95	GLN	CA-C-O	-5.72	115.06	121.81
1	B	138	LYS	CA-CB-CG	5.72	125.53	114.10
1	B	85	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	133	GLU	N-CA-C	-5.71	105.42	112.90
1	B	195	LYS	CG-CD-CE	5.67	124.34	111.30
1	B	18	GLN	CG-CD-NE2	5.66	124.89	116.40
1	A	159	ASN	CA-CB-CG	5.63	118.23	112.60
1	B	65	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	B	140	LEU	CA-C-O	-5.61	114.48	120.42
1	B	175	ALA	CB-CA-C	-5.60	101.66	110.79
1	A	85	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	12	LYS	CA-C-O	-5.55	112.57	120.51
1	A	182	GLN	CB-CG-CD	5.55	122.03	112.60
1	A	90	TRP	CG-CD2-CE3	5.47	139.37	133.90
1	B	144	GLU	CA-CB-CG	5.46	125.02	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	ARG	O-C-N	5.46	129.40	123.13
1	B	129	GLU	CA-CB-CG	5.45	125.00	114.10
1	B	111	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	244	ILE	CA-CB-CG1	5.39	119.57	110.40
1	A	190	LYS	CB-CG-CD	5.38	123.69	111.30
1	A	109	ILE	CA-C-N	5.38	127.44	120.44
1	A	109	ILE	C-N-CA	5.38	127.44	120.44
1	B	223	LYS	N-CA-C	-5.38	99.75	108.52
1	B	179	GLU	CA-C-O	-5.37	115.17	120.80
1	A	177	THR	N-CA-C	-5.35	103.19	110.36
1	A	10	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	170	ILE	CA-C-O	5.32	127.43	120.78
1	B	30	ALA	N-CA-C	5.31	117.55	110.53
1	A	106	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	237	LYS	O-C-N	-5.30	116.85	121.35
1	A	90	TRP	CE2-CD2-CG	-5.28	100.86	107.20
1	A	2	ALA	CA-C-O	-5.28	111.83	120.80
1	A	165	GLU	CA-C-O	5.27	127.08	121.28
1	A	179	GLU	CA-C-O	-5.27	112.97	120.51
1	A	70	ALA	N-CA-C	5.25	119.31	113.01
1	A	121	VAL	N-CA-CB	-5.23	101.22	110.95
1	B	87	GLY	CA-C-O	5.23	124.61	118.96
1	B	36	VAL	O-C-N	-5.23	117.25	123.00
1	A	132	GLU	CB-CG-CD	5.22	121.48	112.60
1	A	95	GLN	OE1-CD-NE2	5.22	127.82	122.60
1	B	22	GLU	N-CA-CB	-5.21	102.51	110.07
1	B	212	ALA	O-C-N	-5.21	116.86	123.01
1	B	34	GLU	N-CA-C	-5.21	102.77	110.48
1	B	83	ILE	N-CA-C	-5.21	105.63	110.53
1	B	78	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	158	THR	CA-CB-OG1	-5.19	101.82	109.60
1	B	170	ILE	CB-CA-C	-5.18	102.79	111.29
1	A	35	ASN	N-CA-CB	-5.18	104.40	110.35
1	A	51	VAL	O-C-N	-5.18	116.64	121.87
1	B	97	GLU	CA-C-O	5.17	127.91	120.51
1	B	226	VAL	N-CA-C	-5.17	99.23	107.15
1	B	189	ARG	CA-CB-CG	-5.16	103.78	114.10
1	A	168	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	A	224	ALA	N-CA-C	5.14	116.97	111.36
1	A	193	ALA	N-CA-C	-5.13	103.71	111.56
1	A	240	PHE	CA-C-O	-5.12	115.12	120.55
1	A	114	LYS	N-CA-C	5.09	117.73	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	SER	CA-C-O	5.09	125.82	120.42
1	A	146	GLN	CG-CD-NE2	5.07	124.00	116.40
1	A	110	ALA	N-CA-C	5.06	116.48	111.07
1	B	229	PHE	CA-C-O	-5.06	115.19	121.06
1	A	206	ILE	CA-C-O	5.05	127.26	120.69
1	B	206	ILE	O-C-N	-5.05	117.81	123.26
1	B	112	LYS	CA-CB-CG	5.03	124.16	114.10
1	A	131	LEU	CA-C-O	-5.03	114.57	120.20
1	A	126	CYS	CA-C-O	5.01	126.77	121.11
1	B	103	HIS	CB-CG-ND1	5.01	130.22	122.70
1	B	80	VAL	N-CA-CB	-5.00	103.73	110.54

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	94	0
1	B	1882	0	1889	93	0
2	A	10	0	4	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	4	0	0
All	All	3784	0	3787	162	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 (162) 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	1.40
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:B:93:LEU:C	1:B:95:GLN:N	1.92	1.25
1:A:11:PHE:O	1:A:12:LYS:N	1.69	1.24
1:A:97:GLU:C	1:A:98:ARG:N	1.96	1.23
1:A:97:GLU:CD	1:B:73:ALA:HB1	1.77	1.09
1:A:95:GLN:OE1	1:B:75:THR:OG1	1.69	1.09
1:A:94:GLY:C	1:A:95:GLN:N	2.12	1.08
1:A:95:GLN:HG2	1:A:97:GLU:H	1.17	1.06
1:B:94:GLY:CA	1:B:95:GLN:N	2.04	0.99
1:B:95:GLN:HA	1:B:95:GLN:OE1	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:A:95:GLN:CD	1:B:75:THR:OG1	2.15	0.88
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:171:GLY:N	2:A:249:PGH:O3P	2.12	0.82
1:A:95:GLN:CD	1:B:75:THR:HG1	1.88	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	0.80
1:A:11:PHE:O	1:A:12:LYS:CA	2.21	0.75
1:A:97:GLU:HG2	1:B:73:ALA:C	2.13	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:HB	1:B:97:GLU:OE1	1.91	0.71
1:A:11:PHE:C	1:A:12:LYS:CB	2.64	0.69
1:A:165:GLU:O	1:A:166:PRO:C	2.27	0.69
1:B:56:LYS:HG3	1:B:58:GLN:NE2	2.07	0.69
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:97:GLU:CD	1:B:73:ALA:CB	2.65	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:165:GLU:O	1:A:167:VAL:N	2.31	0.63
1:B:168:TRP:CD1	1:B:168:TRP:H	2.17	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:B:95:GLN:NE2	1:B:165:GLU:CD	2.59	0.61
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: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:A:12:LYS:NZ	1:A:97:GLU:OE1	2.34	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:NE2	1:B:58:GLN:H	2.07	0.52
1:A:70:ALA:HB2	1:A:115:PHE:HZ	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:11:PHE:O	1:A:12:LYS:C	2.55	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
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:214:GLY:HA3	1:B:239:GLU:HB2	1.96	0.48
1:B:233:GLY:O	1:B:236:LEU:HD22	2.14	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:20:ILE:HB	1:A:49:TYR:HE2	1.79	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: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:107:LYS:HZ1	1:A:153:GLU:CD	2.23	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:38:VAL:HG12	1:A:59:VAL:HG13	1.96	0.46
1:A:97:GLU:HG2	1:B:74:PHE:HA	1.96	0.46
1:A:178:PRO:HB2	1:A:223:LYS:HE2	1.97	0.46
1:B:95:GLN:NE2	1:B:230:LEU:HD23	2.31	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:A:97:GLU:CG	1:B:73:ALA:C	2.88	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:151:LEU:HD11	1:A:196:LEU:HD21	1.99	0.45
1:B:21:LYS:HA	1:B:53:LEU:CD1	2.47	0.45
1:B:93:LEU:HD12	1:B:123:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:GLN:HE22	1:B:43:PRO:HG2	1.82	0.44
1:A:95:GLN:HG2	1:A:96:SER:N	2.30	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:A:142:VAL:O	1:A:145:ARG:HB3	2.19	0.43
1:B:47:LEU:CD2	1:B:83:ILE:HG13	2.49	0.43
1:A:66:ALA:HA	1:A:78:ASN:HB2	2.00	0.42
1:B:151:LEU:CD2	1:B:195:LYS:HG3	2.49	0.42
1:A:40:ILE:HD11	1:A:61:VAL:HG22	2.01	0.42
1:A:82:GLN:NE2	1:B:43:PRO:HG2	2.34	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: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:11:PHE:C	1:A:12:LYS:C	2.82	0.42
1:A:171:GLY:CA	2:A:249:PGH:P	3.08	0.41
1:A:50:SER:O	1:A:54:VAL:HG13	2.21	0.41
1:B:231:VAL:HG21	1:B:240:PHE:CE1	2.54	0.41
1:B:241:VAL:O	1:B:244:ILE:HG13	2.20	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:A:92:ILE:HA	1:A:124:ILE:HB	2.02	0.41
1:A:150:VAL:O	1:A:154:VAL:HG23	2.20	0.41
1:B:3:ARG:NH2	1:B:224:ALA:O	2.53	0.41
1:A:95:GLN:HE21	1:A:97:GLU:HB2	1.79	0.41
1:A:17:LYS:NZ	1:B:48:ASP:OD1	2.51	0.41
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.50	0.41
1:A:117:LEU:HD12	1:A:154:VAL:HG11	2.02	0.41
1:B:107:LYS:HA	1:B:107:LYS:HD2	1.79	0.41
1:B:179:GLU:OE2	1:B:223:LYS:NZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LYS:HG3	1:B:247:ARG:HD3	2.03	0.41
1:B:6:PHE:CD1	1:B:37:GLU:HB3	2.56	0.41
1:B:221:LYS:HZ3	1:B:222:ASP:CG	2.29	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:12:LYS:C	1:A:14:ASN:N	2.78	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 [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	A	243/247 (98%)	225 (93%)	17 (7%)	1 (0%)	30	60
1	B	245/247 (99%)	221 (90%)	18 (7%)	6 (2%)	4	17
All	All	488/494 (99%)	446 (91%)	35 (7%)	7 (1%)	9	30

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%)	171 (86%)	29 (14%)	3	11
1	B	200/200 (100%)	172 (86%)	28 (14%)	3	12
All	All	400/400 (100%)	343 (86%)	57 (14%)	3	11

All (57) 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
1	A	68	LEU
1	A	84	LYS
1	A	85	ASP
1	A	86	VAL
1	A	97	GLU
1	A	103	HIS
1	A	131	LEU
1	A	134	LYS
1	A	135	LYS
1	A	138	LYS
1	A	140	LEU
1	A	141	ASP
1	A	143	VAL
1	A	151	LEU
1	A	152	GLU
1	A	154	VAL
1	A	158	THR
1	A	179	GLU
1	A	182	GLN
1	A	195	LYS
1	A	198	ASP
1	A	236	LEU

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Mol	Chain	Res	Type
1	A	242	ASP
1	A	244	ILE
1	B	4	THR
1	B	18	GLN
1	B	21	LYS
1	B	22	GLU
1	B	27	LEU
1	B	35	ASN
1	B	53	LEU
1	B	55	LYS
1	B	58	GLN
1	B	60	THR
1	B	95	GLN
1	B	96	SER
1	B	134	LYS
1	B	138	LYS
1	B	140	LEU
1	B	142	VAL
1	B	151	LEU
1	B	174	LEU
1	B	188	ILE
1	B	204	LEU
1	B	205	ARG
1	B	207	LEU
1	B	221	LYS
1	B	222	ASP
1	B	223	LYS
1	B	231	VAL
1	B	236	LEU
1	B	237	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	119	GLN
1	A	245	ASN
1	B	58	GLN
1	B	64	GLN
1	B	78	ASN
1	B	82	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](#)

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	1.31	1 (11%)	10,12,12	1.19	0
2	PGH	B	249	-	9,9,9	1.40	2 (22%)	10,12,12	3.35	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	-	-	4/8/8/8	-
2	PGH	B	249	-	-	3/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	249	PGH	C1-N2	2.23	1.34	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	249	PGH	P-O2P	-2.12	1.43	1.50
2	B	249	PGH	P-O1P	2.10	1.66	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	PGH	C2-C1-N2	-6.67	104.93	116.41
2	B	249	PGH	O2-N2-C1	5.76	128.30	119.79
2	B	249	PGH	O4P-P-O1P	-5.01	93.61	106.67
2	B	249	PGH	O4P-P-O3P	2.67	117.80	107.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	249	PGH	N2-C1-C2-O1P
2	A	249	PGH	C2-O1P-P-O2P
2	A	249	PGH	C2-O1P-P-O3P
2	A	249	PGH	C2-O1P-P-O4P
2	B	249	PGH	N2-C1-C2-O1P
2	B	249	PGH	C2-C1-N2-O2
2	B	249	PGH	O1-C1-C2-O1P

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

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Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	94:GLY	C	95:GLN	N	2.12
1	A	97:GLU	C	98:ARG	N	1.96
1	B	94:GLY	C	95:GLN	N	1.84
1	A	11:PHE	C	12:LYS	N	0.70
1	B	97:GLU	C	98:ARG	N	0.54

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.