



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:10 PM UTC

PDB ID : 7TIM / pdb_00007tim
Title : STRUCTURE OF THE TRIOSEPHOSPHATE ISOMERASE-PHOSPHOGLYCOLOHYDROXAMATE COMPLEX: AN ANALOGUE OF THE INTERMEDIATE ON THE REACTION PATHWAY
Authors : Davenport, R.C.; Bash, P.A.; Seaton, B.A.; Karplus, M.; Petsko, G.A.; Ringe, D.
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 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)
Xtrriage (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

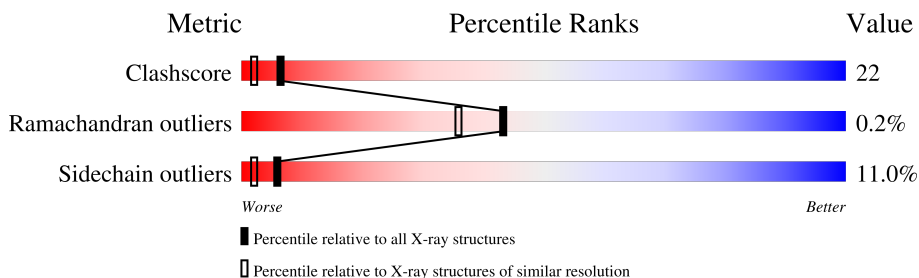
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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	
1	B	247	

2 Entry composition [i](#)

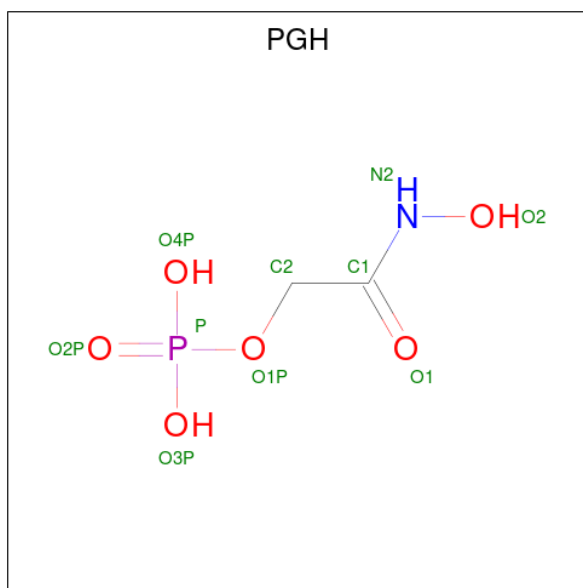
There are 3 unique types of molecules in this entry. The entry contains 4033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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

- 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

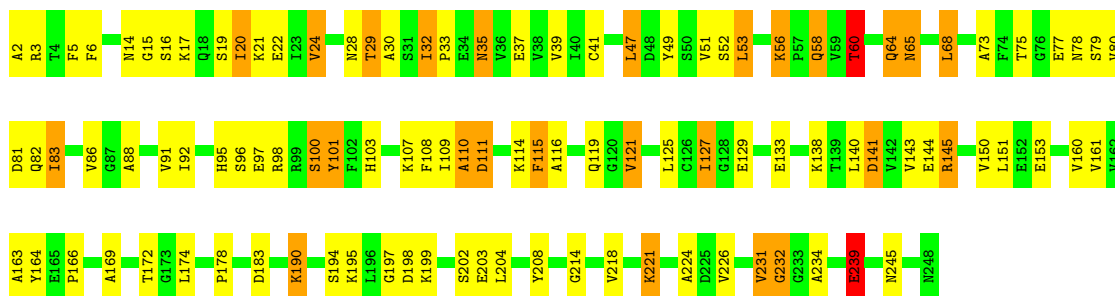
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

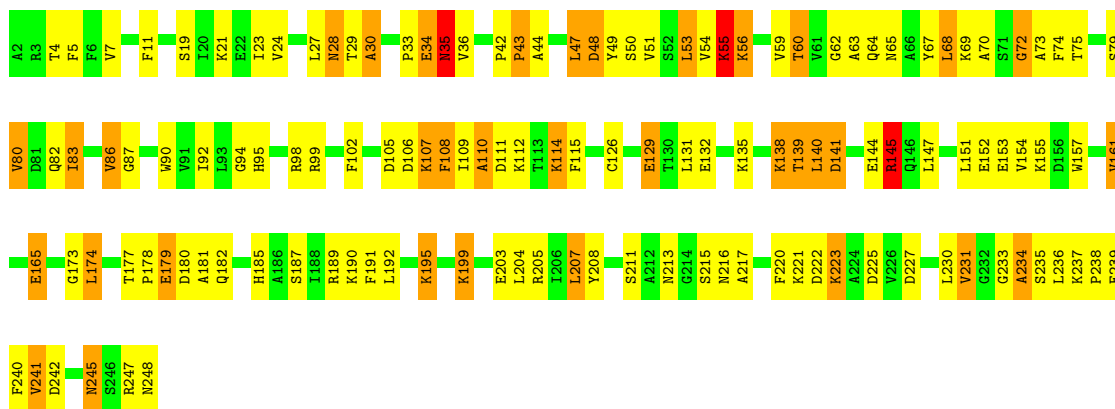
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A:  57% 32% 11%



- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B:  47% 38% 14%



4 Data and refinement statistics

Xtrriage (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	74.00Å 83.50Å 38.40Å 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.	Xtrriage
Total number of atoms	4033	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.16	0/1915	2.02	55/2590 (2.1%)
1	B	1.16	0/1915	2.03	59/2590 (2.3%)
All	All	1.16	0/3830	2.03	114/5180 (2.2%)

There are no bond length outliers.

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CA-CB-CG	13.17	125.77	112.60
1	B	34	GLU	N-CA-C	-9.49	97.74	110.55
1	B	145	ARG	CD-NE-CZ	9.38	137.53	124.40
1	A	28	ASN	CA-CB-CG	9.10	121.70	112.60
1	A	22	GLU	CA-CB-CG	8.88	131.86	114.10
1	A	5	PHE	CA-CB-CG	8.54	122.34	113.80
1	B	28	ASN	CA-C-N	8.26	134.50	120.71
1	B	28	ASN	C-N-CA	8.26	134.50	120.71
1	B	48	ASP	CA-CB-CG	8.23	120.83	112.60
1	A	28	ASN	CA-C-N	8.00	131.66	120.29
1	A	28	ASN	C-N-CA	8.00	131.66	120.29
1	A	47	LEU	CA-C-N	7.55	130.62	120.65
1	A	47	LEU	C-N-CA	7.55	130.62	120.65
1	A	78	ASN	CA-CB-CG	7.47	120.07	112.60
1	B	205	ARG	NE-CZ-NH2	7.25	125.72	119.20
1	B	245	ASN	CA-CB-CG	7.15	119.75	112.60
1	A	32	ILE	CB-CA-C	7.11	116.30	109.33
1	B	56	LYS	CA-C-N	7.10	126.81	119.56
1	B	56	LYS	C-N-CA	7.10	126.81	119.56
1	A	161	VAL	CA-C-O	-7.06	113.14	120.27
1	B	247	ARG	NE-CZ-NH1	-6.93	114.56	121.50
1	B	157	TRP	CA-C-N	6.70	129.58	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	TRP	C-N-CA	6.70	129.58	120.54
1	A	29	THR	N-CA-C	6.67	118.63	111.36
1	A	231	VAL	N-CA-CB	-6.61	103.47	111.21
1	B	231	VAL	N-CA-CB	-6.61	103.06	110.99
1	A	183	ASP	O-C-N	6.56	129.63	122.15
1	B	220	PHE	CA-CB-CG	6.52	120.32	113.80
1	B	110	ALA	CA-C-O	6.41	127.30	120.70
1	B	36	VAL	N-CA-C	-6.38	99.34	109.17
1	B	211	SER	CA-C-O	-6.25	113.85	121.28
1	B	180	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	72	GLY	N-CA-C	6.21	119.33	110.46
1	B	63	ALA	CA-C-N	6.20	131.99	121.14
1	B	63	ALA	C-N-CA	6.20	131.99	121.14
1	A	14	ASN	CA-CB-CG	6.18	118.78	112.60
1	A	141	ASP	N-CA-C	-6.18	104.46	111.07
1	B	43	PRO	CA-C-O	-6.14	114.56	121.43
1	A	114	LYS	CA-C-O	6.11	127.23	120.63
1	A	98	ARG	CD-NE-CZ	-6.10	115.86	124.40
1	B	47	LEU	CA-C-N	6.08	128.74	120.54
1	B	47	LEU	C-N-CA	6.08	128.74	120.54
1	B	55	LYS	CA-C-O	6.08	125.52	118.77
1	A	197	GLY	CA-C-O	-6.06	117.38	122.29
1	B	223	LYS	CA-C-N	6.06	128.68	120.38
1	B	223	LYS	C-N-CA	6.06	128.68	120.38
1	B	129	GLU	CA-CB-CG	6.06	126.21	114.10
1	A	111	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	30	ALA	CA-C-O	6.05	127.96	121.55
1	A	115	PHE	CA-CB-CG	-6.03	107.77	113.80
1	A	163	ALA	N-CA-CB	6.02	119.99	110.84
1	B	102	PHE	CB-CA-C	6.02	120.89	110.72
1	B	165	GLU	O-C-N	6.01	126.43	121.44
1	B	108	PHE	CA-CB-CG	5.99	119.79	113.80
1	B	30	ALA	CA-C-O	5.94	128.04	121.56
1	A	56	LYS	CA-C-N	5.92	126.07	119.32
1	A	56	LYS	C-N-CA	5.92	126.07	119.32
1	B	5	PHE	CA-CB-CG	5.91	119.71	113.80
1	B	80	VAL	O-C-N	5.85	128.41	121.80
1	A	145	ARG	N-CA-C	-5.85	104.54	111.03
1	A	197	GLY	N-CA-C	-5.79	105.38	112.68
1	B	129	GLU	CB-CG-CD	5.77	122.41	112.60
1	B	231	VAL	N-CA-C	5.75	116.58	108.36
1	A	232	GLY	CA-C-N	5.72	126.44	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	GLY	C-N-CA	5.72	126.44	120.03
1	A	92	ILE	CA-C-O	-5.69	114.37	120.85
1	A	100	SER	O-C-N	5.68	128.70	122.11
1	A	103	HIS	CA-CB-CG	-5.62	108.18	113.80
1	B	161	VAL	CA-C-O	-5.58	114.53	120.39
1	A	127	ILE	CB-CG1-CD1	5.58	125.52	113.80
1	B	126	CYS	O-C-N	5.57	129.62	123.16
1	B	34	GLU	CA-CB-CG	5.54	125.18	114.10
1	A	239	GLU	CA-CB-CG	5.54	125.18	114.10
1	B	44	ALA	CA-C-N	5.50	127.92	120.38
1	B	44	ALA	C-N-CA	5.50	127.92	120.38
1	B	35	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	41	CYS	O-C-N	5.45	126.38	121.04
1	B	92	ILE	CA-C-O	-5.43	114.29	120.65
1	B	181	ALA	O-C-N	5.42	127.65	122.07
1	B	233	GLY	CA-C-N	5.39	128.05	120.28
1	B	233	GLY	C-N-CA	5.39	128.05	120.28
1	B	141	ASP	O-C-N	5.38	128.71	122.20
1	B	5	PHE	CB-CA-C	5.38	118.29	109.90
1	A	103	HIS	ND1-CE1-NE2	5.37	113.77	108.40
1	B	67	TYR	CA-C-O	-5.35	114.92	121.88
1	A	64	GLN	OE1-CD-NE2	5.33	127.93	122.60
1	A	24	VAL	O-C-N	5.32	127.03	121.87
1	B	59	VAL	N-CA-C	5.32	116.24	108.58
1	A	160	VAL	O-C-N	5.31	128.74	122.69
1	A	108	PHE	CA-CB-CG	5.31	119.11	113.80
1	B	227	ASP	O-C-N	5.30	128.96	122.34
1	B	139	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	29	THR	CA-C-N	5.27	128.71	120.75
1	A	29	THR	C-N-CA	5.27	128.71	120.75
1	A	101	TYR	CB-CA-C	-5.23	101.95	110.85
1	A	2	ALA	CB-CA-C	5.22	118.33	110.50
1	A	37	GLU	O-C-N	5.21	129.32	123.27
1	A	178	PRO	CA-C-N	5.21	127.21	120.44
1	A	178	PRO	C-N-CA	5.21	127.21	120.44
1	A	91	VAL	O-C-N	5.19	129.06	122.57
1	A	141	ASP	N-CA-CB	5.18	117.52	110.01
1	A	226	VAL	N-CA-CB	5.17	117.87	111.41
1	B	234	ALA	N-CA-C	5.17	117.65	111.71
1	B	75	THR	CA-CB-OG1	-5.17	101.85	109.60
1	B	247	ARG	CA-C-O	5.12	127.13	121.39
1	A	65	ASN	OD1-CG-ND2	-5.11	117.49	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	THR	N-CA-CB	-5.10	102.05	111.53
1	B	173	GLY	N-CA-C	-5.07	108.32	115.32
1	B	7	VAL	CB-CA-C	5.05	118.10	110.63
1	B	138	LYS	CB-CA-C	-5.03	100.90	109.65
1	A	110	ALA	CA-C-N	5.03	127.42	120.29
1	A	110	ALA	C-N-CA	5.03	127.42	120.29
1	A	208	TYR	N-CA-C	-5.02	101.97	109.95
1	B	114	LYS	CA-C-O	5.02	126.09	120.82

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	A	1883	0	1892	63	0
1	B	1883	0	1892	105	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	166	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 22.

All (166) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:58:GLN:HE21	1.20	0.84
1:B:178:PRO:HB2	1:B:223:LYS:HE3	1.59	0.84
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:N	1:B:56:LYS:HD3	2.09	0.68
1:B:33:PRO:HD3	1:B:245:ASN:OD1	1.93	0.67
1:A:58:GLN:H	1:A:58:GLN:NE2	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:B:140:LEU:C	1:B:140:LEU:HD22	2.21	0.65
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:B:140:LEU:HD23	1:B:144:GLU:CD	2.23	0.64
1:A:79:SER:O	1:A:83:ILE:HG23	1.97	0.64
1:B:87:GLY:HA2	3:B:728:HOH:O	1.99	0.63
1:B:182:GLN:NE2	1:B:225:ASP:HB2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:HE21	1:A:58:GLN:N	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:B:21:LYS:HE3	1:B:53:LEU:HD21	1.92	0.50
1:B:80:VAL:HG22	1:B:115:PHE:HE2	1.77	0.50
1:B:237:LYS:HB3	1:B:238:PRO:HD2	1.92	0.50
1:B:21:LYS:HE2	1:B:53:LEU:CG	2.41	0.50
1:B:107:LYS:O	1:B:108:PHE:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:107:LYS:HZ2	1:A:110:ALA:HB3	1.77	0.49
1:A:190:LYS:HE3	3:A:706:HOH:O	2.12	0.49
1:A:49:TYR:O	1:A:52:SER:OG	2.21	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
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:N	1:B:11:PHE:CD1	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:6:PHE:C	1:A:6:PHE:CD1	2.92	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:A:145:ARG:NH1	3:A:797:HOH:O	2.13	0.47
1:B:72:GLY:HA3	1:B:74:PHE:CE2	2.49	0.47
1:B:151:LEU:O	1:B:154:VAL:O	2.31	0.47
1:B:138:LYS:O	1:B:139:THR:C	2.58	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:A:64:GLN:O	1:A:65:ASN:HB2	2.17	0.45
1:B:19:SER:O	1:B:23:ILE:HD13	2.16	0.45
1:B:21:LYS:HB2	1:B:49:TYR:OH	2.17	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:165:GLU:OE2	2:B:249:PGH:N2	2.51	0.44
1:B:213:ASN:OD1	1:B:215:SER:N	2.50	0.44
1:A:107:LYS:NZ	1:A:110:ALA:HB3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:208:TYR:CD1	1:B:208:TYR:C	2.96	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
1:B:68:LEU:C	1:B:68:LEU:HD23	2.43	0.42
1:B:174:LEU:N	1:B:174:LEU:HD13	2.34	0.42
1:A:151:LEU:HD13	1:A:195:LYS:HE2	2.01	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:21:LYS:CD	1:B:53:LEU:HD21	2.49	0.42
1:B:42:PRO:HB2	1:B:43:PRO:HD2	2.01	0.42
1:B:105:ASP:O	1:B:109:ILE:HD12	2.19	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:B:216:ASN:O	1:B:217:ALA:C	2.61	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:94:GLY:O	1:B:95:HIS:C	2.63	0.41
1:B:238:PRO:C	1:B:240:PHE:N	2.78	0.41
1:B:21:LYS:HA	1:B:53:LEU:CD2	2.50	0.41
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.50	0.41
1:A:80:VAL:CG2	1:A:115:PHE:CE2	3.03	0.41
1:A:21:LYS:HA	1:A:53:LEU:HD23	2.03	0.41
1:A:138:LYS:HG2	1:A:141:ASP:OD2	2.21	0.41
1:B:235:SER:HA	1:B:240:PHE:CD1	2.55	0.41
1:A:33:PRO:HB2	1:A:35:ASN:ND2	2.36	0.41
1:A:116:ALA:HB1	1:A:121:VAL:HG22	2.03	0.41
1:A:129:GLU:HB2	1:A:133:GLU:HB2	2.04	0.40
1:A:35:ASN:O	1:A:35:ASN:CG	2.64	0.40
1:B:28:ASN:OD1	1:B:56:LYS:HG2	2.21	0.40
1:B:191:PHE:CD2	1:B:192:LEU:HD23	2.57	0.40
1:B:230:LEU:HD12	1:B:230:LEU:HA	1.80	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 [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	245/247 (99%)	235 (96%)	10 (4%)	0	100	100
1	B	245/247 (99%)	232 (95%)	12 (5%)	1 (0%)	30	22
All	All	490/494 (99%)	467 (95%)	22 (4%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	ARG

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	A	200/200 (100%)	181 (90%)	19 (10%)	8	3
1	B	200/200 (100%)	175 (88%)	25 (12%)	4	1
All	All	400/400 (100%)	356 (89%)	44 (11%)	6	2

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	20	ILE
1	A	29	THR
1	A	35	ASN
1	A	53	LEU
1	A	56	LYS
1	A	58	GLN
1	A	60	THR
1	A	68	LEU
1	A	83	ILE
1	A	86	VAL
1	A	109	ILE
1	A	121	VAL
1	A	174	LEU
1	A	190	LYS
1	A	194	SER
1	A	204	LEU
1	A	221	LYS
1	A	239	GLU
1	B	27	LEU
1	B	29	THR
1	B	34	GLU
1	B	35	ASN
1	B	53	LEU
1	B	54	VAL
1	B	55	LYS
1	B	60	THR
1	B	68	LEU
1	B	69	LYS
1	B	83	ILE
1	B	86	VAL
1	B	107	LYS
1	B	140	LEU
1	B	152	GLU
1	B	155	LYS
1	B	174	LEU
1	B	179	GLU
1	B	195	LYS
1	B	199	LYS
1	B	204	LEU
1	B	207	LEU
1	B	236	LEU
1	B	241	VAL

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Mol	Chain	Res	Type
1	B	248	ASN

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	18	GLN
1	A	35	ASN
1	A	58	GLN
1	A	245	ASN
1	B	35	ASN
1	B	103	HIS
1	B	148	ASN

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	1.36	1 (11%)	10,12,12	1.17	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	1.53	1 (11%)	10,12,12	2.09	5 (50%)

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	-	-	5/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	249	PGH	P-O3P	-3.49	1.41	1.54
2	A	249	PGH	P-O3P	-2.95	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	2.63	117.66	107.80
2	B	249	PGH	C2-C1-N2	-2.54	112.03	116.41
2	A	249	PGH	O3P-P-O1P	-2.12	101.13	106.67
2	B	249	PGH	O1P-P-O2P	-2.09	100.80	106.44

There are no chirality outliers.

All (9) 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-O3P
2	A	249	PGH	C2-O1P-P-O4P
2	B	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	A	249	PGH	2	0
2	B	249	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.