



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:20 AM UTC

PDB ID : 1HTI / pdb_00001hti
Title : CRYSTAL STRUCTURE OF RECOMBINANT HUMAN TRIOSEPHOSPHATE ISOMERASE AT 2.8 ANGSTROMS RESOLUTION. TRIOSEPHOSPHATE ISOMERASE RELATED HUMAN GENETIC DISORDERS AND COMPARISON WITH THE TRYPA NOSOMAL ENZYME
Authors : Mande, S.C.; Hol, W.G.J.
Deposited on : 1994-10-12
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

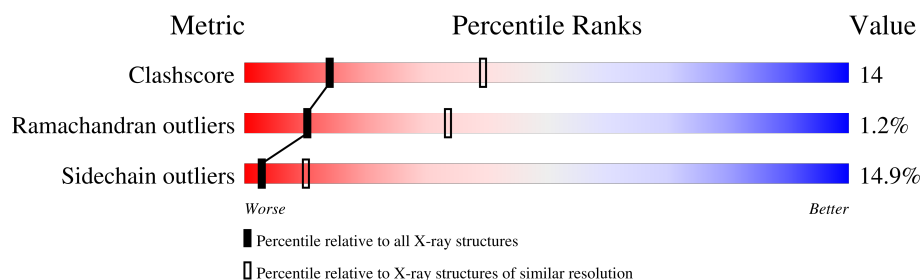
1 Overall quality at a glance

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	248	47% 33% 18% .
1	B	248	44% 41% 11% .

2 Entry composition [i](#)

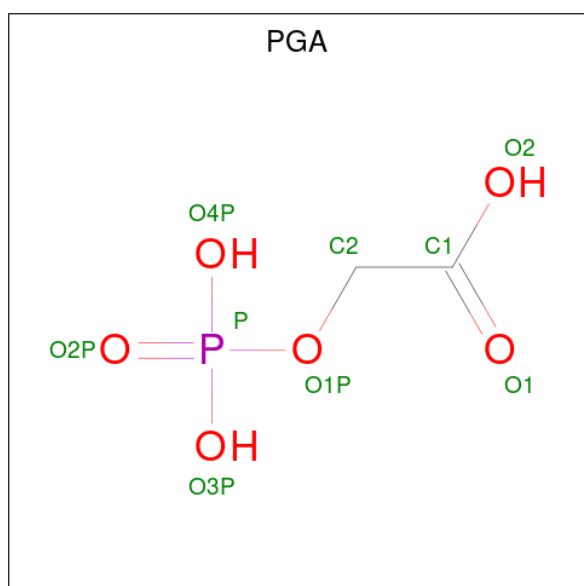
There are 2 unique types of molecules in this entry. The entry contains 3745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	248	Total	C	N	O	S	0	0	0
			1868	1181	324	356	7			
1	B	248	Total	C	N	O	S	0	0	0
			1868	1181	324	356	7			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (CCD ID: PGA) (formula: $C_2H_5O_6P$).



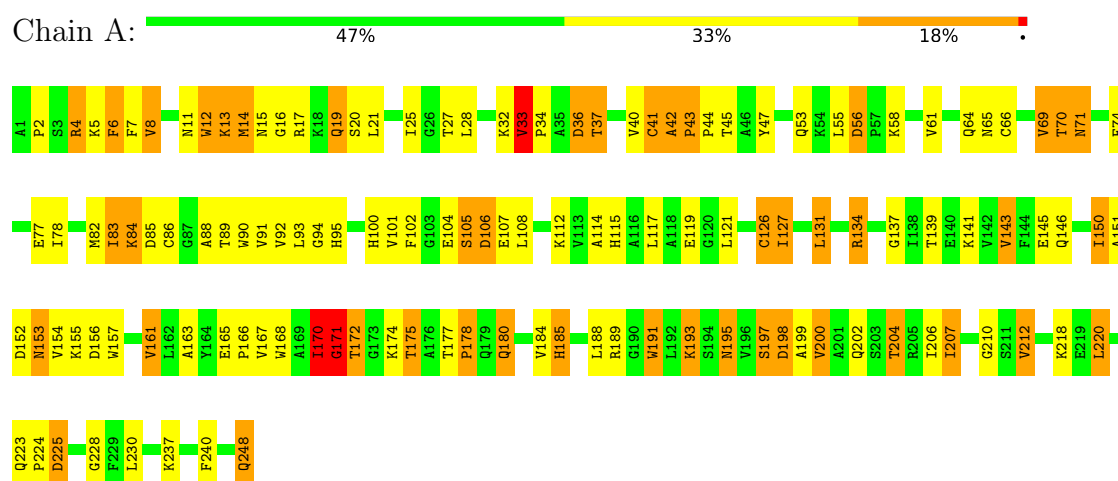
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

3 Residue-property plots

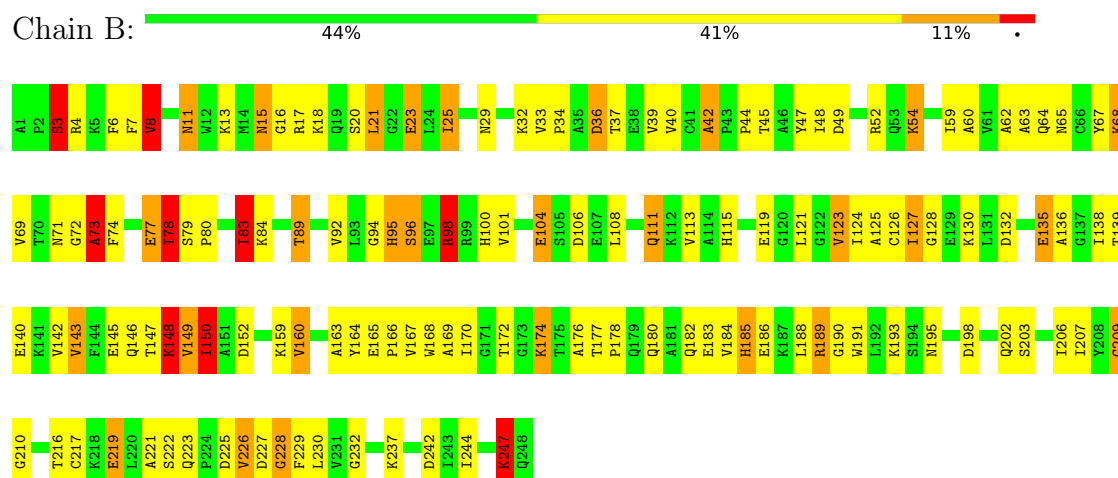
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.81Å 75.39Å 92.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	85.5 (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3745	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: PGA

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	1.32	15/1903 (0.8%)	2.35	108/2577 (4.2%)
1	B	1.27	8/1903 (0.4%)	2.25	93/2577 (3.6%)
All	All	1.30	23/3806 (0.6%)	2.30	201/5154 (3.9%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	PRO	CA-C	8.32	1.56	1.51
1	A	33	VAL	CA-CB	7.39	1.63	1.54
1	A	115	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	115	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	185	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	185	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	92	VAL	CA-CB	6.40	1.61	1.54
1	B	95	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	127	ILE	CA-CB	6.14	1.65	1.55
1	B	8	VAL	CA-CB	6.08	1.62	1.54
1	A	8	VAL	CA-CB	6.03	1.62	1.54
1	A	95	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	150	ILE	CA-CB	5.59	1.61	1.54
1	A	195	ASN	CA-CB	-5.42	1.46	1.53
1	A	146	GLN	N-CA	-5.41	1.40	1.46
1	B	185	HIS	CG-ND1	-5.40	1.32	1.38
1	A	170	ILE	CA-CB	5.39	1.60	1.54
1	B	150	ILE	CA-CB	5.30	1.60	1.54
1	A	204	THR	CA-CB	5.27	1.61	1.53
1	A	166	PRO	CA-CB	-5.25	1.48	1.53
1	A	100	HIS	CD2-NE2	-5.20	1.32	1.37
1	A	78	ILE	CA-CB	5.07	1.63	1.55
1	B	100	HIS	CD2-NE2	-5.05	1.32	1.37

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	THR	N-CA-C	11.46	123.77	111.28
1	A	36	ASP	CA-CB-CG	11.18	123.78	112.60
1	A	198	ASP	CA-CB-CG	10.31	122.91	112.60
1	A	153	ASN	CA-CB-CG	-9.91	102.69	112.60
1	B	132	ASP	CA-CB-CG	9.90	122.50	112.60
1	B	15	ASN	OD1-CG-ND2	-9.49	113.11	122.60
1	A	43	PRO	N-CA-C	9.29	119.39	110.47
1	B	124	ILE	N-CA-C	-8.17	95.01	106.53
1	B	15	ASN	CA-CB-CG	8.14	120.74	112.60
1	B	36	ASP	CA-CB-CG	8.07	120.67	112.60
1	A	61	VAL	CA-CB-CG2	-8.00	96.80	110.40
1	B	67	TYR	CA-C-N	7.97	131.76	120.28
1	B	67	TYR	C-N-CA	7.97	131.76	120.28
1	A	139	THR	CA-CB-OG1	-7.96	97.66	109.60
1	A	19	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	A	71	ASN	OD1-CG-ND2	-7.91	114.69	122.60
1	A	178	PRO	N-CA-C	-7.80	102.69	113.53
1	A	101	VAL	N-CA-C	-7.78	103.33	111.58
1	B	71	ASN	CA-CB-CG	7.67	120.27	112.60
1	B	6	PHE	CA-CB-CG	7.53	121.33	113.80
1	A	237	LYS	CA-C-N	7.52	127.69	119.87
1	A	237	LYS	C-N-CA	7.52	127.69	119.87
1	B	176	ALA	N-CA-C	-7.49	97.78	109.25
1	A	134	ARG	O-C-N	7.48	130.16	122.09
1	B	95	HIS	CB-CG-CD2	-7.41	121.57	131.20
1	A	37	THR	N-CA-C	7.32	121.58	109.95
1	A	12	TRP	CG-CD2-CE3	7.28	141.18	133.90
1	B	113	VAL	O-C-N	7.19	129.13	121.94
1	B	145	GLU	N-CA-C	-7.14	103.43	111.07
1	A	150	ILE	N-CA-C	-7.14	103.82	110.53
1	A	69	VAL	N-CA-CB	-7.11	102.57	112.52
1	B	72	GLY	CA-C-O	7.06	129.11	121.56
1	A	74	PHE	CA-CB-CG	-7.04	106.76	113.80
1	B	139	THR	N-CA-C	-7.00	103.59	111.07
1	A	43	PRO	O-C-N	-6.97	118.10	121.31
1	B	54	LYS	N-CA-C	6.93	118.62	111.14
1	A	56	ASP	CA-C-N	6.91	126.61	119.56
1	A	56	ASP	C-N-CA	6.91	126.61	119.56
1	B	45	THR	CA-CB-OG1	-6.88	99.29	109.60
1	A	139	THR	CA-CB-CG2	6.84	122.13	110.50
1	A	210	GLY	N-CA-C	-6.79	104.64	112.79
1	A	230	LEU	N-CA-C	-6.78	94.07	107.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	LYS	N-CA-C	-6.76	103.69	112.68
1	B	73	ALA	O-C-N	-6.74	113.63	122.59
1	A	70	THR	CB-CA-C	-6.71	98.41	110.70
1	A	41	CYS	CA-CB-SG	-6.70	99.00	114.40
1	B	149	VAL	N-CA-C	6.63	116.78	110.42
1	A	197	SER	N-CA-CB	-6.62	101.50	111.56
1	B	68	LYS	CB-CA-C	-6.57	98.47	110.63
1	B	68	LYS	N-CA-C	6.53	119.22	111.71
1	B	143	VAL	N-CA-C	-6.52	104.50	110.82
1	A	180	GLN	OE1-CD-NE2	-6.51	116.08	122.60
1	A	86	CYS	CA-CB-SG	-6.49	99.47	114.40
1	A	95	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	A	156	ASP	CA-C-O	6.47	128.72	120.57
1	A	82	MET	CA-C-O	-6.46	114.04	120.82
1	B	195	ASN	CB-CG-ND2	6.45	126.07	116.40
1	B	237	LYS	CA-C-N	6.45	126.14	119.56
1	B	237	LYS	C-N-CA	6.45	126.14	119.56
1	B	16	GLY	N-CA-C	6.44	120.81	112.18
1	A	248	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	A	115	HIS	N-CA-C	6.42	118.36	111.36
1	B	230	LEU	CA-C-O	6.39	127.19	120.54
1	A	102	PHE	CA-CB-CG	-6.38	107.42	113.80
1	B	37	THR	N-CA-CB	-6.35	100.68	110.85
1	B	219	GLU	N-CA-C	-6.34	104.45	111.36
1	A	40	VAL	CG1-CB-CG2	-6.33	96.88	110.80
1	B	64	GLN	N-CA-C	6.31	120.71	112.89
1	A	43	PRO	N-CA-CB	-6.30	99.66	103.19
1	B	101	VAL	N-CA-C	-6.29	106.67	112.96
1	B	45	THR	O-C-N	-6.28	114.87	122.22
1	A	53	GLN	CA-C-O	-6.28	113.90	120.55
1	A	161	VAL	N-CA-C	-6.27	99.17	108.45
1	B	45	THR	N-CA-C	6.23	118.87	111.71
1	B	195	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	A	14	MET	N-CA-C	-6.19	96.58	107.73
1	A	36	ASP	N-CA-C	-6.19	105.22	112.89
1	A	106	ASP	N-CA-C	6.16	118.00	111.28
1	B	3	SER	N-CA-C	6.16	123.93	110.80
1	B	217	CYS	CA-CB-SG	6.14	128.52	114.40
1	B	104	GLU	CB-CA-C	-6.07	101.42	110.16
1	A	65	ASN	CA-C-O	-6.06	114.33	121.06
1	A	61	VAL	CB-CA-C	6.04	119.83	111.49
1	A	184	VAL	N-CA-C	-6.02	104.54	113.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	LYS	O-C-N	6.02	130.72	122.41
1	A	131	LEU	O-C-N	6.02	128.27	122.07
1	B	77	GLU	CA-C-N	6.01	132.49	122.57
1	B	77	GLU	C-N-CA	6.01	132.49	122.57
1	B	237	LYS	CB-CG-CD	-5.99	97.52	111.30
1	B	32	LYS	CA-C-N	-5.98	116.81	123.02
1	B	32	LYS	C-N-CA	-5.98	116.81	123.02
1	B	189	ARG	N-CA-C	-5.97	104.85	111.36
1	A	42	ALA	CA-C-N	5.96	124.01	119.66
1	A	42	ALA	C-N-CA	5.96	124.01	119.66
1	A	185	HIS	CA-CB-CG	-5.94	107.86	113.80
1	B	148	LYS	O-C-N	5.93	128.18	122.07
1	B	142	VAL	N-CA-C	5.90	120.30	112.04
1	B	210	GLY	N-CA-C	-5.84	102.90	110.38
1	A	27	THR	O-C-N	5.84	128.08	122.07
1	A	198	ASP	N-CA-CB	5.83	119.90	110.40
1	A	115	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	A	6	PHE	CA-CB-CG	5.80	119.60	113.80
1	B	23	GLU	CB-CG-CD	5.79	122.45	112.60
1	B	242	ASP	CA-C-O	-5.79	114.74	120.82
1	B	59	ILE	N-CA-C	-5.79	99.41	107.80
1	B	217	CYS	O-C-N	-5.79	115.99	122.12
1	A	92	VAL	N-CA-C	-5.77	99.56	107.99
1	B	135	GLU	N-CA-C	-5.77	104.68	110.97
1	B	25	ILE	CB-CG1-CD1	5.75	125.88	113.80
1	A	82	MET	N-CA-C	-5.75	104.92	111.07
1	B	11	ASN	CA-CB-CG	5.74	118.34	112.60
1	A	61	VAL	CA-CB-CG1	5.70	120.09	110.40
1	B	152	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	226	VAL	N-CA-C	-5.68	98.96	107.37
1	B	229	PHE	N-CA-C	5.67	118.02	109.23
1	A	64	GLN	CG-CD-NE2	-5.67	107.89	116.40
1	B	145	GLU	CB-CG-CD	5.67	122.23	112.60
1	A	185	HIS	CB-CG-CD2	-5.67	123.84	131.20
1	A	43	PRO	CA-C-O	-5.66	116.82	120.90
1	A	78	ILE	CB-CG1-CD1	-5.66	101.92	113.80
1	A	85	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	29	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	117	LEU	O-C-N	-5.59	116.32	122.07
1	B	77	GLU	CB-CG-CD	5.57	122.07	112.60
1	A	180	GLN	CA-CB-CG	5.56	125.22	114.10
1	B	71	ASN	OD1-CG-ND2	-5.55	117.05	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	134	ARG	N-CA-C	-5.51	105.19	111.14
1	A	105	SER	O-C-N	-5.50	116.37	122.86
1	A	61	VAL	N-CA-CB	-5.50	101.36	111.91
1	B	209	GLY	CA-C-O	5.48	125.90	120.75
1	B	83	ILE	CA-C-N	5.47	127.56	120.44
1	B	83	ILE	C-N-CA	5.47	127.56	120.44
1	A	126	CYS	N-CA-C	5.47	118.73	109.76
1	A	206	ILE	N-CA-C	-5.47	96.88	106.61
1	A	137	GLY	CA-C-N	5.45	129.86	121.19
1	A	137	GLY	C-N-CA	5.45	129.86	121.19
1	B	13	LYS	CB-CG-CD	5.45	123.82	111.30
1	A	191	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	A	70	THR	CA-CB-OG1	-5.43	101.45	109.60
1	B	183	GLU	O-C-N	5.42	127.67	122.03
1	B	115	HIS	CA-CB-CG	-5.41	108.39	113.80
1	B	190	GLY	CA-C-O	-5.39	115.20	120.75
1	B	52	ARG	CA-C-O	-5.39	114.71	120.42
1	B	42	ALA	O-C-N	-5.38	115.13	121.32
1	A	77	GLU	N-CA-C	5.38	118.49	110.52
1	A	90	TRP	O-C-N	-5.38	116.62	123.24
1	A	198	ASP	CB-CA-C	-5.37	98.77	109.99
1	A	225	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	96	SER	N-CA-C	5.37	122.23	110.80
1	A	15	ASN	O-C-N	5.34	130.66	123.34
1	B	29	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	175	THR	N-CA-C	5.28	117.78	108.75
1	A	223	GLN	CA-C-N	5.28	126.44	119.84
1	A	223	GLN	C-N-CA	5.28	126.44	119.84
1	B	89	THR	N-CA-CB	-5.28	102.37	110.44
1	B	168	TRP	CE2-CD2-CG	-5.28	100.87	107.20
1	B	168	TRP	N-CA-C	5.26	118.48	111.75
1	A	13	LYS	O-C-N	-5.25	115.61	122.59
1	B	48	ILE	CB-CG1-CD1	-5.25	102.78	113.80
1	A	143	VAL	N-CA-CB	-5.25	101.27	110.77
1	A	121	LEU	N-CA-C	-5.24	101.73	110.17
1	A	70	THR	N-CA-CB	5.24	118.00	110.20
1	B	111	GLN	CA-CB-CG	-5.23	103.63	114.10
1	B	163	ALA	CB-CA-C	-5.23	102.72	110.62
1	B	49	ASP	N-CA-C	5.20	116.76	111.14
1	B	45	THR	CA-CB-CG2	5.20	119.34	110.50
1	B	49	ASP	CA-CB-CG	5.20	117.80	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LEU	N-CA-CB	-5.20	102.47	110.42
1	A	19	GLN	CG-CD-NE2	5.20	124.19	116.40
1	B	98	ARG	CD-NE-CZ	5.18	131.66	124.40
1	A	212	VAL	CA-CB-CG1	-5.17	101.61	110.40
1	A	127	ILE	CA-C-O	-5.17	115.80	121.28
1	A	191	TRP	CB-CG-CD1	-5.15	119.18	126.90
1	A	171	GLY	CA-C-N	5.15	127.18	120.28
1	A	171	GLY	C-N-CA	5.15	127.18	120.28
1	B	183	GLU	CA-C-N	5.14	127.72	120.42
1	B	183	GLU	C-N-CA	5.14	127.72	120.42
1	B	227	ASP	N-CA-C	5.14	118.69	112.93
1	B	228	GLY	CA-C-O	-5.13	117.03	122.01
1	A	83	ILE	N-CA-C	5.13	115.34	110.42
1	B	104	GLU	N-CA-CB	5.13	117.61	109.51
1	A	204	THR	CA-C-O	5.12	126.70	120.81
1	A	69	VAL	CA-C-O	-5.12	116.45	121.67
1	A	104	GLU	CA-CB-CG	-5.12	103.87	114.10
1	A	174	LYS	CB-CG-CD	5.11	123.06	111.30
1	A	207	ILE	N-CA-C	5.10	115.65	108.36
1	B	65	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	B	45	THR	N-CA-CB	-5.09	102.38	110.22
1	B	37	THR	N-CA-C	5.08	118.03	109.95
1	A	91	VAL	CA-CB-CG2	5.08	119.03	110.40
1	A	191	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	A	91	VAL	N-CA-C	-5.06	101.19	108.48
1	A	134	ARG	CA-C-N	5.06	127.32	120.44
1	A	134	ARG	C-N-CA	5.06	127.32	120.44
1	A	43	PRO	CA-C-N	5.03	126.12	119.84
1	A	43	PRO	C-N-CA	5.03	126.12	119.84
1	B	195	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	89	THR	N-CA-CB	-5.02	103.32	110.80
1	A	40	VAL	O-C-N	-5.02	117.76	123.18
1	B	78	ILE	N-CA-CB	-5.01	104.06	112.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1879	50	0
1	B	1868	0	1879	60	0
2	B	9	0	2	3	0
All	All	3745	0	3760	107	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 14.

All (107) 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:6:PHE:HB3	1:A:37:THR:HG22	1.49	0.94
1:A:25:ILE:HG23	1:A:55:LEU:HD13	1.56	0.88
1:B:169:ALA:HA	1:B:174:LYS:O	1.92	0.68
1:A:11:ASN:HA	1:A:42:ALA:HB3	1.76	0.67
1:B:8:VAL:HG13	1:B:39:VAL:HG12	1.77	0.67
1:A:193:LYS:HB3	1:A:193:LYS:NZ	2.11	0.64
1:A:34:PRO:HG3	1:A:248:GLN:HE21	1.64	0.62
1:B:11:ASN:HA	1:B:42:ALA:HB3	1.82	0.61
1:B:33:VAL:HG22	1:B:244:ILE:HG21	1.83	0.61
1:A:150:ILE:O	1:A:154:VAL:HG23	2.01	0.61
1:B:182:GLN:NE2	1:B:186:GLU:HB2	2.16	0.60
1:A:163:ALA:HA	1:A:207:ILE:O	2.02	0.60
1:A:5:LYS:HG3	1:A:36:ASP:O	2.03	0.58
1:B:106:ASP:HB3	1:B:149:VAL:HG11	1.84	0.58
1:A:178:PRO:HB3	1:A:220:LEU:HG	1.86	0.58
1:B:98:ARG:HB3	1:B:104:GLU:HG3	1.85	0.57
1:B:232:GLY:HA3	2:B:549:PGA:P	2.45	0.57
1:A:177:THR:H	1:A:180:GLN:HG2	1.70	0.56
1:B:125:ALA:HB1	1:B:150:ILE:HG12	1.87	0.56
1:A:191:TRP:O	1:A:195:ASN:HB2	2.06	0.56
1:B:182:GLN:HE21	1:B:186:GLU:HB2	1.72	0.55
1:A:13:LYS:O	1:A:44:PRO:HG3	2.06	0.55
1:A:17:ARG:HA	1:A:47:TYR:OH	2.05	0.55
1:A:7:PHE:O	1:A:228:GLY:HA3	2.06	0.55
1:A:14:MET:HE2	1:B:74:PHE:HD2	1.74	0.53
1:A:185:HIS:HB3	1:A:225:ASP:HB2	1.90	0.53
1:B:80:PRO:HB2	1:B:119:GLU:HG3	1.89	0.53
1:B:34:PRO:HB2	1:B:36:ASP:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ALA:HB1	1:B:247:LYS:HB2	1.90	0.53
1:A:4:ARG:HH21	1:A:189:ARG:NH2	2.07	0.52
1:A:94:GLY:O	1:A:126:CYS:HB2	2.09	0.52
1:A:200:VAL:HG12	1:A:204:THR:OG1	2.10	0.52
1:A:21:LEU:O	1:A:25:ILE:HG13	2.10	0.52
1:A:28:LEU:HD21	1:A:240:PHE:HD2	1.75	0.52
1:A:4:ARG:NH2	1:A:189:ARG:CZ	2.72	0.52
1:B:95:HIS:O	1:B:98:ARG:HB2	2.10	0.52
1:B:79:SER:O	1:B:83:ILE:HG13	2.09	0.52
1:B:164:TYR:CE2	1:B:184:VAL:HG21	2.45	0.52
1:B:127:ILE:HG22	1:B:146:GLN:HB3	1.93	0.51
1:B:223:GLN:HA	1:B:223:GLN:OE1	2.11	0.51
1:A:131:LEU:HA	1:A:168:TRP:HB2	1.91	0.51
1:B:17:ARG:O	1:B:21:LEU:HB2	2.10	0.51
1:B:7:PHE:HD2	1:B:207:ILE:HD13	1.75	0.50
1:B:39:VAL:HG11	1:B:244:ILE:HD13	1.92	0.50
1:B:128:GLY:HA3	1:B:165:GLU:O	2.11	0.50
1:A:93:LEU:HD22	1:A:112:LYS:HD2	1.93	0.50
1:A:25:ILE:HG23	1:A:55:LEU:CD1	2.35	0.50
1:B:172:THR:HB	1:B:174:LYS:HB2	1.92	0.50
1:A:71:ASN:OD1	1:B:15:ASN:HA	2.11	0.50
1:B:7:PHE:O	1:B:228:GLY:HA3	2.11	0.49
1:B:165:GLU:HA	1:B:209:GLY:O	2.12	0.49
1:A:33:VAL:HG23	1:A:34:PRO:O	2.13	0.49
1:B:44:PRO:HG2	1:B:47:TYR:HD2	1.78	0.49
1:B:166:PRO:HD2	1:B:209:GLY:O	2.12	0.48
1:B:177:THR:H	1:B:180:GLN:NE2	2.11	0.48
1:A:66:CYS:O	1:A:112:LYS:HD3	2.13	0.48
1:A:66:CYS:SG	1:A:93:LEU:HD21	2.54	0.47
1:B:148:LYS:HG2	1:B:191:TRP:CZ2	2.50	0.47
1:A:177:THR:N	1:A:180:GLN:HG2	2.30	0.47
1:A:193:LYS:HB3	1:A:193:LYS:HZ2	1.80	0.46
1:B:7:PHE:CD2	1:B:207:ILE:HD13	2.50	0.46
1:B:63:ALA:CB	1:B:83:ILE:HD13	2.45	0.46
1:B:42:ALA:HA	1:B:62:ALA:O	2.16	0.46
1:B:182:GLN:OE1	1:B:223:GLN:HB3	2.16	0.46
1:A:143:VAL:CG1	1:A:188:LEU:HD11	2.46	0.45
1:B:98:ARG:HH11	1:B:98:ARG:HG3	1.82	0.45
1:A:165:GLU:O	1:A:167:VAL:HG23	2.17	0.45
1:B:40:VAL:HG13	1:B:60:ALA:HB3	1.99	0.45
1:B:94:GLY:C	1:B:126:CYS:HB2	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:HG13	1:B:39:VAL:CG1	2.45	0.45
1:B:25:ILE:HG21	1:B:54:LYS:HB3	1.99	0.45
1:A:170:ILE:HG13	1:A:171:GLY:N	2.32	0.44
1:B:69:VAL:HG21	1:B:74:PHE:HE2	1.81	0.44
1:A:197:SER:HB3	1:A:200:VAL:HG23	2.00	0.44
1:B:94:GLY:O	1:B:126:CYS:HB2	2.18	0.44
1:A:134:ARG:HD3	1:A:168:TRP:CD1	2.53	0.44
1:B:77:GLU:O	1:B:78:ILE:HD13	2.18	0.44
1:A:32:LYS:HA	1:A:58:LYS:NZ	2.33	0.44
1:B:123:VAL:HG22	1:B:160:VAL:HB	1.99	0.44
1:B:148:LYS:HG2	1:B:191:TRP:HZ2	1.83	0.43
1:A:13:LYS:HD3	1:B:73:ALA:HA	2.00	0.43
1:B:130:LYS:HA	1:B:167:VAL:HB	2.00	0.43
1:A:83:ILE:HG22	1:A:88:ALA:HB3	2.01	0.43
1:A:168:TRP:O	1:A:172:THR:HG21	2.18	0.43
1:B:193:LYS:HD2	1:B:198:ASP:OD1	2.19	0.43
1:B:136:ALA:HB3	1:B:138:ILE:HG12	2.00	0.43
1:A:12:TRP:CD1	1:A:12:TRP:N	2.84	0.43
1:B:185:HIS:HD1	1:B:226:VAL:HA	1.83	0.43
1:B:68:LYS:HG2	1:B:111:GLN:HB3	2.00	0.42
1:B:170:ILE:HA	2:B:549:PGA:O2P	2.20	0.42
1:A:6:PHE:HD2	1:A:37:THR:CG2	2.33	0.42
1:A:114:ALA:HB2	1:A:153:ASN:HB3	2.01	0.42
1:A:2:PRO:HG3	1:A:4:ARG:NH1	2.35	0.42
1:A:16:GLY:C	1:A:17:ARG:HH11	2.27	0.42
1:A:41:CYS:O	1:A:43:PRO:HD3	2.21	0.41
1:A:151:ALA:HA	1:A:157:TRP:CZ2	2.56	0.41
1:B:172:THR:C	1:B:174:LYS:H	2.28	0.41
1:B:18:LYS:HG3	1:B:47:TYR:CE1	2.56	0.41
1:B:189:ARG:HH21	1:B:225:ASP:HA	1.86	0.41
1:B:207:ILE:HD13	1:B:207:ILE:HG21	1.81	0.41
1:B:7:PHE:HB3	1:B:207:ILE:HG21	2.03	0.40
1:A:197:SER:OG	1:A:199:ALA:HB3	2.21	0.40
1:A:4:ARG:HH21	1:A:189:ARG:CZ	2.34	0.40
1:B:80:PRO:HA	1:B:121:LEU:HD11	2.03	0.40
1:B:232:GLY:HA3	2:B:549:PGA:O1P	2.21	0.40
1:A:84:LYS:HB3	1:A:84:LYS:HE2	1.83	0.40
1:B:80:PRO:O	1:B:83:ILE:N	2.55	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	246/248 (99%)	224 (91%)	20 (8%)	2 (1%)	16	44
1	B	246/248 (99%)	221 (90%)	21 (8%)	4 (2%)	7	27
All	All	492/496 (99%)	445 (90%)	41 (8%)	6 (1%)	10	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	ALA
1	A	45	THR
1	A	171	GLY
1	B	3	SER
1	B	4	ARG
1	B	96	SER

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	195/195 (100%)	167 (86%)	28 (14%)	3	11
1	B	195/195 (100%)	165 (85%)	30 (15%)	2	10
All	All	390/390 (100%)	332 (85%)	58 (15%)	3	10

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	8	VAL
1	A	19	GLN
1	A	20	SER
1	A	33	VAL
1	A	56	ASP
1	A	69	VAL
1	A	70	THR
1	A	84	LYS
1	A	105	SER
1	A	106	ASP
1	A	107	GLU
1	A	108	LEU
1	A	119	GLU
1	A	127	ILE
1	A	141	LYS
1	A	145	GLU
1	A	161	VAL
1	A	170	ILE
1	A	175	THR
1	A	193	LYS
1	A	198	ASP
1	A	200	VAL
1	A	202	GLN
1	A	212	VAL
1	A	218	LYS
1	A	220	LEU
1	A	224	PRO
1	B	3	SER
1	B	8	VAL
1	B	20	SER
1	B	21	LEU
1	B	23	GLU
1	B	78	ILE
1	B	83	ILE
1	B	84	LYS
1	B	89	THR
1	B	98	ARG
1	B	108	LEU
1	B	123	VAL
1	B	127	ILE
1	B	135	GLU
1	B	140	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	143	VAL
1	B	147	THR
1	B	148	LYS
1	B	150	ILE
1	B	159	LYS
1	B	160	VAL
1	B	174	LYS
1	B	178	PRO
1	B	202	GLN
1	B	203	SER
1	B	206	ILE
1	B	216	THR
1	B	219	GLU
1	B	222	SER
1	B	247	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	65	ASN
1	A	95	HIS
1	A	195	ASN
1	A	248	GLN
1	B	19	GLN
1	B	111	GLN
1	B	180	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

1 ligand is 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	PGA	B	549	-	8,8,8	1.95	1 (12%)	10,11,11	3.62	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	PGA	B	549	-	-	3/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	549	PGA	O1-C1	4.61	1.37	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	549	PGA	O1P-C2-C1	-7.80	98.78	110.54
2	B	549	PGA	O2-C1-O1	-6.52	106.55	123.33
2	B	549	PGA	O2-C1-C2	3.09	128.24	113.66
2	B	549	PGA	O3P-P-O1P	-2.33	100.59	106.67
2	B	549	PGA	O4P-P-O2P	2.13	119.15	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	549	PGA	O2-C1-C2-O1P
2	B	549	PGA	O1-C1-C2-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	549	PGA	C2-O1P-P-O2P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	549	PGA	3	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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.