



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:54 PM GMT

PDB ID : 1HTI
Title : CRYSTAL STRUCTURE OF RECOMBINANT HUMAN TRIOSEPHOSPHATE ISOMERASE AT 2.8 ANGSTROMS RESOLUTION. TRIOSEPHOSPHATE ISOMERASE RELATED HUMAN GENETIC DISORDERS AND COMPARISON WITH THE TRYPANOSOMAL 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

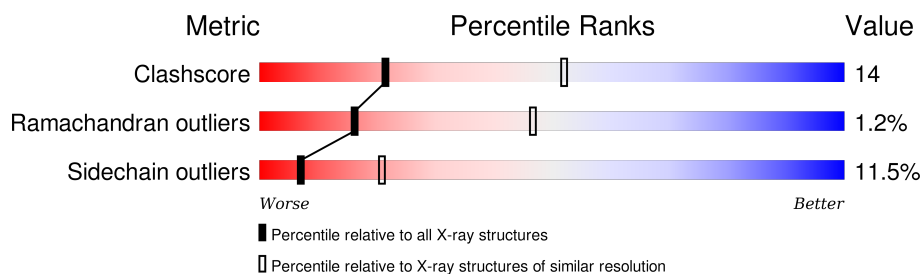
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	
1	B	248	

2 Entry composition [i](#)

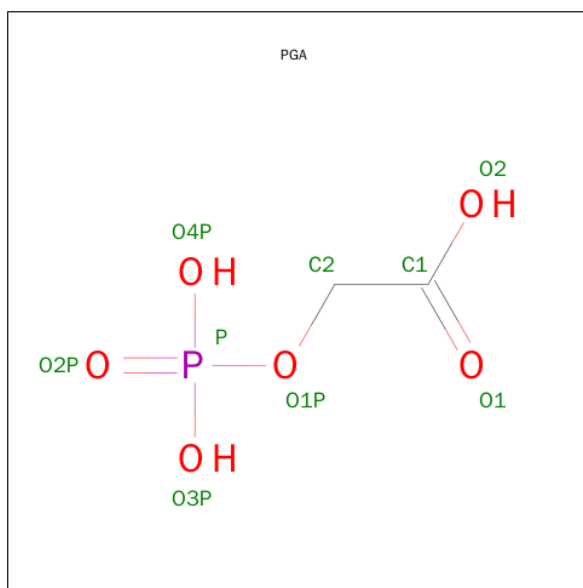
There are 2 unique types of molecules in this entry. The entry contains 3745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUGAR (2-PHOSPHOGLYCOLIC ACID) (three-letter code: PGA) (formula: $C_2H_5O_6P$).



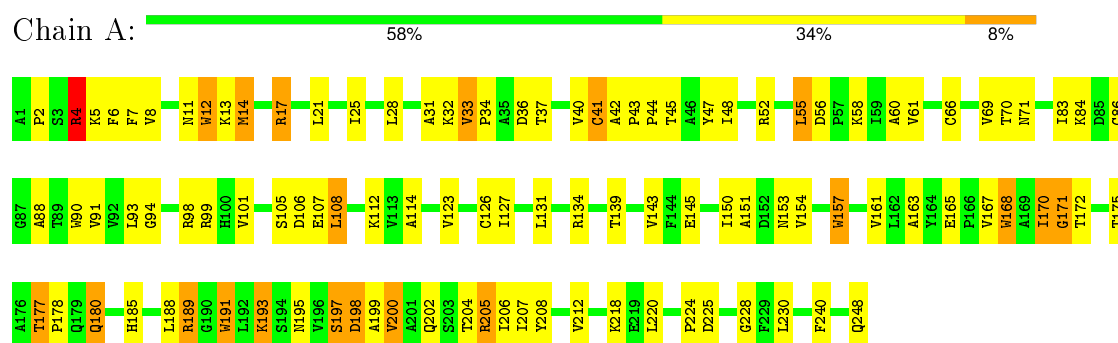
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

3 Residue-property plots

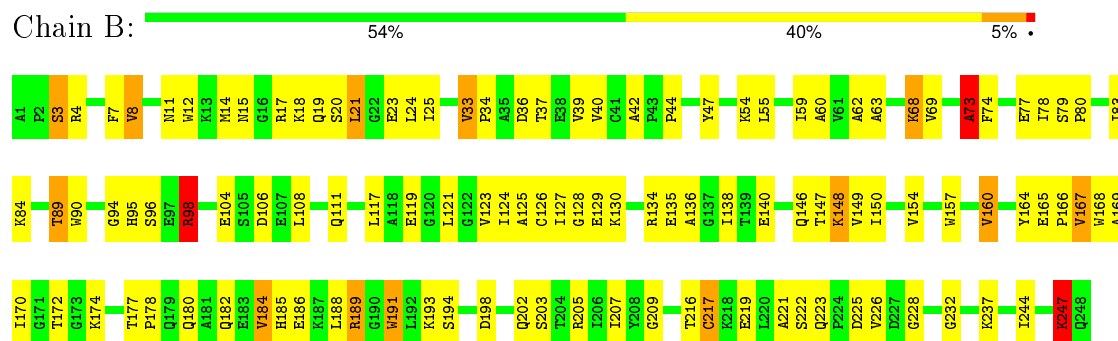
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 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 ⓘ

5.1 Standard geometry ⓘ

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	1.01	0/1903	1.91	50/2577 (1.9%)
1	B	1.00	1/1903 (0.1%)	1.84	41/2577 (1.6%)
All	All	1.01	1/3806 (0.0%)	1.88	91/5154 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	SER	CA-CB	5.15	1.60	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	B	134	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	17	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	A	61	VAL	CA-CB-CG2	-9.40	96.80	110.90
1	B	189	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	B	189	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	A	191	TRP	CD1-CG-CD2	9.12	113.59	106.30
1	B	90	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	A	40	VAL	CG1-CB-CG2	-8.76	96.88	110.90
1	A	41	CYS	CA-CB-SG	-8.33	99.00	114.00
1	A	191	TRP	CE2-CD2-CG	-8.28	100.67	107.30
1	B	98	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	90	TRP	CD1-CG-CD2	8.12	112.79	106.30
1	A	12	TRP	CG-CD2-CE3	8.09	141.18	133.90
1	A	86	CYS	CA-CB-SG	-8.07	99.47	114.00
1	B	217	CYS	CA-CB-SG	8.07	128.52	114.00
1	B	168	TRP	CE2-CD2-CG	-8.04	100.87	107.30
1	B	168	TRP	CD1-CG-CD2	7.90	112.62	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	B	191	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	17	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	90	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	A	98	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	89	THR	CA-CB-CG2	-7.37	102.09	112.40
1	B	98	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	191	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	A	12	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	B	157	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	A	157	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	B	12	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	A	157	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	A	168	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	B	12	TRP	CE2-CD2-CG	-6.97	101.73	107.30
1	A	139	THR	CA-CB-CG2	6.95	122.13	112.40
1	B	55	LEU	CB-CG-CD2	-6.77	99.49	111.00
1	A	4	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	90	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	123	VAL	CG1-CB-CG2	-6.50	100.50	110.90
1	B	157	TRP	CD1-CG-CD2	6.49	111.49	106.30
1	A	230	LEU	N-CA-C	-6.27	94.07	111.00
1	A	212	VAL	CA-CB-CG1	-6.20	101.61	110.90
1	A	61	VAL	CA-CB-CG1	6.13	120.09	110.90
1	A	12	TRP	CD1-CG-CD2	6.05	111.14	106.30
1	A	191	TRP	CB-CG-CD1	-6.02	119.18	127.00
1	A	197	SER	N-CA-CB	-6.00	101.50	110.50
1	B	68	LYS	CB-CA-C	-5.96	98.47	110.40
1	A	200	VAL	CA-CB-CG1	-5.96	101.97	110.90
1	B	124	ILE	N-CA-C	-5.92	95.01	111.00
1	A	69	VAL	CA-CB-CG2	-5.88	102.08	110.90
1	B	33	VAL	CA-CB-CG2	-5.88	102.08	110.90
1	A	177	THR	CA-CB-CG2	-5.85	104.21	112.40
1	A	198	ASP	CB-CA-C	-5.82	98.77	110.40
1	B	98	ARG	CD-NE-CZ	5.76	131.66	123.60
1	A	60	ALA	CB-CA-C	-5.74	101.49	110.10
1	B	188	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	101	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	A	99	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	73	ALA	O-C-N	-5.67	113.63	122.70
1	A	191	TRP	CG-CD2-CE3	5.64	138.97	133.90
1	B	24	LEU	CA-CB-CG	5.59	128.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	B	73	ALA	CA-C-N	5.56	129.43	117.20
1	A	52	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	91	VAL	CA-CB-CG1	-5.53	102.60	110.90
1	A	189	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	59	ILE	CG1-CB-CG2	-5.50	99.30	111.40
1	B	184	VAL	CG1-CB-CG2	-5.45	102.17	110.90
1	B	167	VAL	CG1-CB-CG2	-5.43	102.20	110.90
1	A	91	VAL	CA-CB-CG2	5.42	119.03	110.90
1	B	237	LYS	CB-CG-CD	-5.42	97.52	111.60
1	A	139	THR	CA-CB-OG1	-5.40	97.66	109.00
1	A	180	GLN	CA-CB-CG	5.37	125.22	113.40
1	B	90	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	B	168	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	A	14	MET	N-CA-C	-5.34	96.58	111.00
1	A	208	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	A	206	ILE	N-CA-C	-5.23	96.88	111.00
1	A	12	TRP	CB-CG-CD1	-5.20	120.23	127.00
1	A	205	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	198	ASP	N-CA-CB	5.17	119.90	110.60
1	B	191	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	B	14	MET	CA-CB-CG	5.13	122.03	113.30
1	B	154	VAL	CA-C-N	-5.12	105.94	117.20
1	A	55	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	168	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	108	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	B	117	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	B	37	THR	N-CA-CB	-5.06	100.68	110.30
1	B	191	TRP	CG-CD2-CE3	5.03	138.43	133.90
1	A	157	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	B	247	LYS	O-C-N	5.01	130.72	122.70

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	59	0
2	B	9	0	2	3	0
All	All	3745	0	3760	106	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 (106) 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:NZ	1:A:193:LYS:HB3	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:14:MET:HE2	1:B:74:PHE:HD2	1.66	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:B:125:ALA:HB1	1:B:150:ILE:HG12	1.87	0.56
1:A:177:THR:H	1:A:180:GLN:HG2	1.70	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:B:80:PRO:HB2	1:B:119:GLU:HG3	1.89	0.53
1:A:185:HIS:HB3	1:A:225:ASP:HB2	1.90	0.53
1:B:34:PRO:HB2	1:B:36:ASP:HB3	1.91	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:B:223:GLN:HA	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:31:ALA:O	1:A:58:LYS:NZ	2.44	0.47
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: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:B:98:ARG:HG3	1:B:98:ARG:HH11	1.82	0.45
1:A:143:VAL:CG1	1:A:188:LEU:HD11	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:TRP:O	1:A:172:THR:HG21	2.18	0.43
1:A:83:ILE:HG22	1:A:88:ALA:HB3	2.01	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:B:185:HIS:HD1	1:B:226:VAL:HA	1.83	0.43
1:A:12:TRP:CD1	1:A:12:TRP:N	2.84	0.43
1:B:170:ILE:HA	2:B:549:PGA:O2P	2.20	0.42
1:B:68:LYS:HG2	1:B:111:GLN:HB3	2.00	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:193:LYS:HZ2	1:A:193:LYS:HB3	1.86	0.41
1:A:151:ALA:HA	1:A:157:TRP:CZ2	2.56	0.41
1:A:41:CYS:O	1:A:43:PRO:HD3	2.21	0.41
1:B:18:LYS:HG3	1:B:47:TYR:CE1	2.56	0.41
1:B:207:ILE:HD13	1:B:207:ILE:HG21	1.81	0.41
1:B:189:ARG:HH21	1:B:225:ASP:HA	1.86	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:B:232:GLY:HA3	2:B:549:PGA:O1P	2.21	0.40
1:B:80:PRO:HA	1:B:121:LEU:HD11	2.03	0.40
1:A:4:ARG:HH21	1:A:189:ARG:CZ	2.34	0.40
1:B:80:PRO:O	1:B:83:ILE:N	2.55	0.40
1:B:94:GLY:C	1:B:126:CYS:HB2	2.41	0.40
1:A:84:LYS:HB3	1:A:84:LYS:HE2	1.83	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%)	24	58
1	B	246/248 (99%)	221 (90%)	21 (8%)	4 (2%)	12	38
All	All	492/496 (99%)	445 (90%)	41 (8%)	6 (1%)	16	47

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%)	175 (90%)	20 (10%)	9	26
1	B	195/195 (100%)	170 (87%)	25 (13%)	5	16
All	All	390/390 (100%)	345 (88%)	45 (12%)	7	21

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	8	VAL
1	A	33	VAL
1	A	56	ASP
1	A	70	THR
1	A	105	SER
1	A	106	ASP
1	A	107	GLU
1	A	108	LEU
1	A	127	ILE
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	202	GLN
1	A	205	ARG
1	A	218	LYS
1	A	224	PRO
1	B	3	SER
1	B	8	VAL
1	B	19	GLN
1	B	20	SER
1	B	21	LEU
1	B	23	GLU
1	B	84	LYS
1	B	89	THR
1	B	98	ARG
1	B	108	LEU
1	B	129	GLU
1	B	135	GLU
1	B	140	GLU
1	B	147	THR
1	B	148	LYS
1	B	160	VAL
1	B	178	PRO
1	B	202	GLN
1	B	203	SER
1	B	205	ARG
1	B	216	THR
1	B	217	CYS
1	B	219	GLU

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Mol	Chain	Res	Type
1	B	222	SER
1	B	247	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	248	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	5,8,8	0.86	0	6,11,11	1.85	3 (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	-	-	0/4/6/6	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	549	PGA	O1P-P-O2P	-2.13	101.72	107.14
2	B	549	PGA	O3P-P-O1P	-2.07	100.59	106.56
2	B	549	PGA	O4P-P-O2P	2.66	119.15	110.58

There are no chirality outliers.

There are no torsion outliers.

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 will therefore be empty.

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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