



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:00 PM UTC

PDB ID : 5TIM / pdb_00005tim
Title : REFINED 1.83 ANGSTROMS STRUCTURE OF TRYPANOSOMAL TRIOSEPHOSPHATE ISOMERASE, CRYSTALLIZED IN THE PRESENCE OF 2.4 M-AMMONIUM SULPHATE. A COMPARISON WITH THE STRUCTURE OF THE TRYPANOSOMAL TRIOSEPHOSPHATE ISOMERASE-GLYCEROL-3-PHOSPHATE COMPLEX
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Deposited on : 1991-04-23
Resolution : 1.83 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

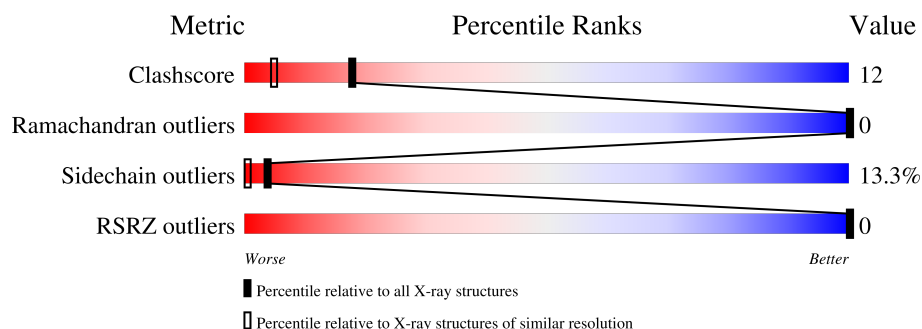
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4063 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.

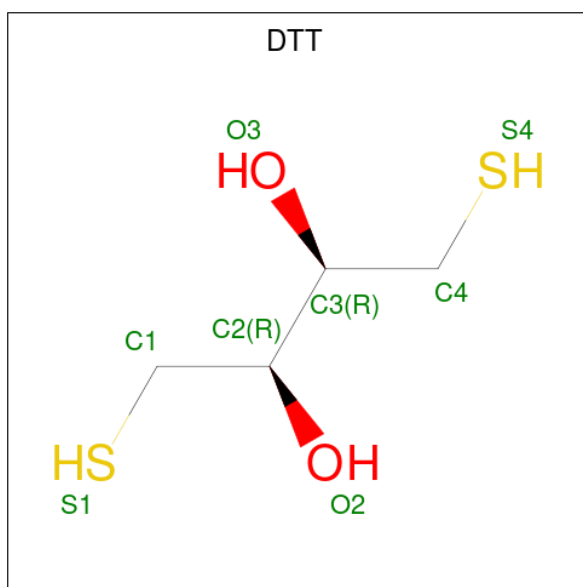
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			
1	B	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is water.

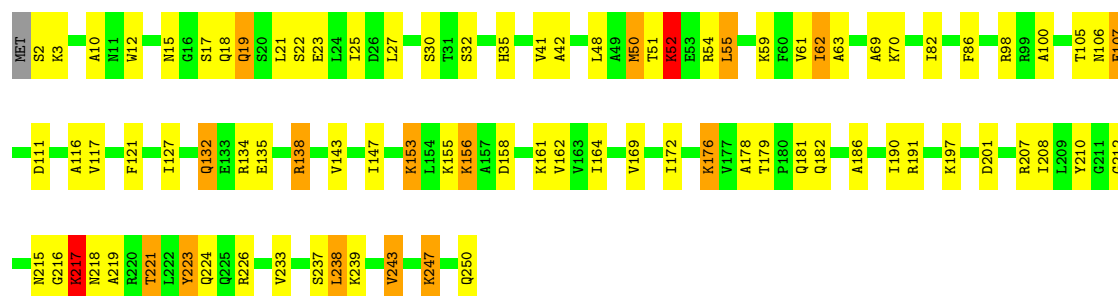
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	122	Total	O	0	0
			122	122		

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 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.

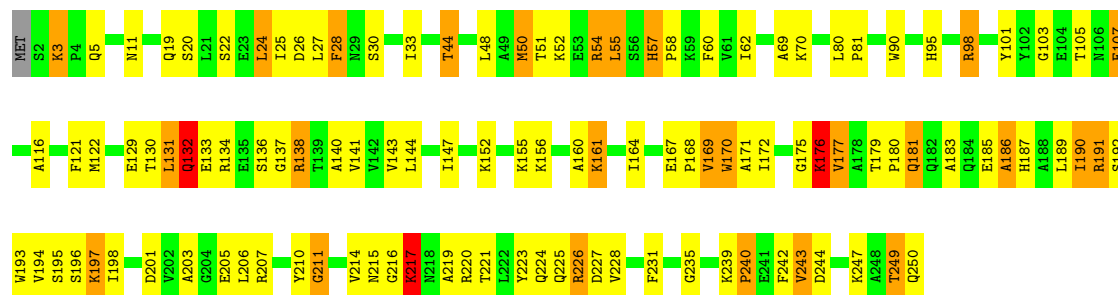
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.14Å 97.69Å 46.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.83 6.00 – 1.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.83) 81.0 (6.00-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 1.83Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.183 , (Not available) 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 106.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4063	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: SO4, DTT

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	1.53	7/1917 (0.4%)	1.99	36/2599 (1.4%)
1	B	1.45	4/1917 (0.2%)	2.07	60/2599 (2.3%)
All	All	1.49	11/3834 (0.3%)	2.03	96/5198 (1.8%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	HIS	CE1-NE2	6.32	1.38	1.32
1	A	107	GLU	CD-OE2	6.30	1.37	1.25
1	A	117	VAL	CA-C	6.22	1.60	1.52
1	A	186	ALA	CA-C	6.13	1.60	1.52
1	A	219	ALA	CA-C	6.12	1.60	1.52
1	B	187	HIS	CD2-NE2	5.83	1.44	1.37
1	A	51	THR	C-N	-5.49	1.26	1.33
1	B	186	ALA	N-CA	5.30	1.52	1.46
1	B	134	ARG	CA-C	5.23	1.59	1.52
1	A	106	ASN	N-CA	-5.14	1.40	1.46
1	A	135	GLU	CD-OE2	5.04	1.34	1.25

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ASN	CA-CB-CG	-10.18	102.42	112.60
1	B	69	ALA	N-CA-C	8.18	119.97	111.14
1	B	177	VAL	CB-CA-C	-8.17	100.00	111.28
1	B	210	TYR	CA-C-N	8.13	127.18	121.65
1	B	210	TYR	C-N-CA	8.13	127.18	121.65
1	A	132	GLN	N-CA-C	7.93	119.93	111.28
1	A	143	VAL	N-CA-CB	7.91	118.93	110.62
1	B	226	ARG	N-CA-C	7.89	119.88	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	LYS	N-CA-C	7.71	119.58	111.03
1	A	191	ARG	CD-NE-CZ	7.67	135.13	124.40
1	B	103	GLY	CA-C-N	-7.48	112.20	122.30
1	B	103	GLY	C-N-CA	-7.48	112.20	122.30
1	B	194	VAL	N-CA-CB	7.31	118.62	110.51
1	A	217	LYS	N-CA-C	7.21	119.14	111.28
1	B	11	ASN	CA-CB-CG	7.13	119.73	112.60
1	B	134	ARG	NE-CZ-NH2	-6.90	112.99	119.20
1	A	233	VAL	N-CA-C	6.89	118.21	108.36
1	A	216	GLY	O-C-N	6.81	128.78	122.17
1	B	172	ILE	N-CA-C	6.77	117.88	107.99
1	A	41	VAL	N-CA-CB	6.76	120.42	111.90
1	B	48	LEU	N-CA-C	6.72	118.60	111.28
1	A	117	VAL	CA-C-N	6.67	129.22	120.28
1	A	117	VAL	C-N-CA	6.67	129.22	120.28
1	B	195	SER	N-CA-CB	6.57	119.89	110.16
1	B	141	VAL	O-C-N	6.57	128.34	121.91
1	B	219	ALA	N-CA-C	6.47	119.33	111.82
1	B	121	PHE	CA-CB-CG	6.45	120.25	113.80
1	B	190	ILE	N-CA-C	6.42	117.10	110.36
1	A	61	VAL	CG1-CB-CG2	-6.38	96.76	110.80
1	B	176	LYS	N-CA-C	6.35	119.56	108.52
1	A	17	SER	N-CA-C	-6.31	99.88	109.85
1	B	211	GLY	O-C-N	-6.29	118.45	123.49
1	B	216	GLY	CA-C-N	6.28	129.18	120.63
1	B	216	GLY	C-N-CA	6.28	129.18	120.63
1	A	17	SER	CA-C-O	-6.26	114.14	121.46
1	A	98	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	A	191	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	B	192	SER	N-CA-CB	6.11	119.20	110.16
1	B	206	LEU	N-CA-C	6.10	118.55	109.59
1	A	134	ARG	CG-CD-NE	-6.07	98.65	112.00
1	B	28	PHE	CA-CB-CG	6.05	119.85	113.80
1	B	240	PRO	N-CA-CB	5.97	109.83	103.39
1	B	138	ARG	N-CA-CB	5.94	119.94	110.73
1	B	107	GLU	CB-CG-CD	5.92	122.67	112.60
1	A	208	ILE	N-CA-CB	5.92	119.13	111.67
1	B	207	ARG	N-CA-CB	5.88	120.06	110.17
1	A	186	ALA	CA-C-N	5.78	128.02	120.28
1	A	186	ALA	C-N-CA	5.78	128.02	120.28
1	B	90	TRP	N-CA-CB	5.75	120.83	110.83
1	A	52	LYS	CB-CA-C	5.74	119.97	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	GLY	N-CA-C	5.70	120.85	113.27
1	A	100	ALA	CA-C-N	-5.70	113.20	122.26
1	A	100	ALA	C-N-CA	-5.70	113.20	122.26
1	B	101	TYR	N-CA-C	5.68	120.87	113.88
1	B	28	PHE	CA-C-O	5.63	126.39	120.42
1	B	26	ASP	CA-CB-CG	-5.61	106.99	112.60
1	B	132	GLN	N-CA-CB	-5.59	101.04	110.49
1	B	81	PRO	CB-CA-C	-5.58	103.41	112.62
1	A	41	VAL	CA-C-O	-5.57	114.35	120.48
1	B	244	ASP	N-CA-CB	5.57	118.31	110.12
1	B	57	HIS	CA-C-O	5.53	124.36	119.71
1	B	54	ARG	N-CA-C	5.51	119.17	112.23
1	B	138	ARG	N-CA-C	5.43	119.89	112.88
1	B	175	GLY	N-CA-C	-5.43	108.62	115.08
1	B	143	VAL	N-CA-CB	5.39	116.86	110.55
1	B	243	VAL	O-C-N	5.36	127.07	121.87
1	A	164	ILE	N-CA-CB	5.35	116.56	110.72
1	B	249	THR	O-C-N	5.34	128.75	122.34
1	A	106	ASN	CA-CB-CG	-5.33	107.27	112.60
1	A	121	PHE	CA-C-O	-5.33	115.75	121.56
1	A	207	ARG	N-CA-CB	5.32	118.94	110.16
1	B	164	ILE	N-CA-CB	5.32	116.52	110.72
1	A	221	THR	O-C-N	5.32	127.75	122.12
1	A	69	ALA	N-CA-C	5.31	116.75	111.07
1	B	242	PHE	CA-C-N	5.31	127.73	120.46
1	B	242	PHE	C-N-CA	5.31	127.73	120.46
1	B	191	ARG	O-C-N	5.30	127.74	122.12
1	B	131	LEU	N-CA-CB	-5.25	102.12	109.94
1	A	223	TYR	N-CA-C	5.24	117.74	111.71
1	A	117	VAL	CB-CA-C	5.24	118.59	111.88
1	B	98	ARG	CA-C-N	5.24	127.25	120.44
1	B	98	ARG	C-N-CA	5.24	127.25	120.44
1	B	203	ALA	CA-C-O	5.23	126.05	120.20
1	B	19	GLN	N-CA-CB	-5.22	102.49	110.07
1	B	239	LYS	CA-C-O	5.21	126.03	120.66
1	A	52	LYS	CA-CB-CG	5.20	124.50	114.10
1	B	44	THR	CA-CB-OG1	5.19	117.39	109.60
1	A	147	ILE	CA-CB-CG2	5.18	119.31	110.50
1	B	169	VAL	N-CA-CB	5.18	116.95	110.47
1	A	116	ALA	CA-C-O	5.17	126.25	120.82
1	A	22	SER	N-CA-C	-5.16	104.92	111.11
1	B	183	ALA	CA-C-O	5.16	126.01	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	VAL	CA-CB-CG2	-5.09	101.74	110.40
1	A	162	VAL	N-CA-C	5.08	115.90	108.53
1	B	175	GLY	CA-C-O	5.03	124.50	119.27
1	B	20	SER	CA-C-O	5.02	125.87	120.55

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	1883	0	1917	39	0
1	B	1883	0	1917	56	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	8	0	8	0	0
4	A	157	0	0	7	0
4	B	122	0	0	4	0
All	All	4063	0	3842	94	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 12.

All (94) 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:247:LYS:HD2	4:A:970:HOH:O	1.82	0.79
1:A:243:VAL:HG13	4:A:970:HOH:O	1.83	0.78
1:B:160:ALA:C	1:B:161:LYS:HE2	2.09	0.77
1:B:168:PRO:HD2	1:B:211:GLY:O	1.90	0.72
1:B:27:LEU:O	1:B:30:SER:HB2	1.92	0.70
1:B:161:LYS:HE2	1:B:161:LYS:N	2.06	0.69
1:B:122:MET:HE1	4:B:881:HOH:O	1.92	0.68
1:B:25:ILE:CD1	1:B:50:MET:HE1	2.25	0.66
1:A:111:ASP:OD1	1:A:153:LYS:NZ	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:NZ	1:A:201:ASP:OD2	2.30	0.65
1:A:107:GLU:HB3	4:A:767:HOH:O	1.97	0.65
1:B:144:LEU:HD11	1:B:189:LEU:HD11	1.79	0.64
1:A:62:ILE:O	1:A:62:ILE:HD13	1.97	0.64
1:B:180:PRO:CB	1:B:225:GLN:HE21	2.11	0.63
1:B:129:GLU:OE2	1:B:170:TRP:NE1	2.31	0.63
1:A:201:ASP:N	1:A:201:ASP:OD1	2.29	0.63
1:B:180:PRO:HB2	1:B:225:GLN:NE2	2.14	0.62
1:A:25:ILE:HD12	1:A:55:LEU:HG	1.82	0.61
1:B:193:TRP:CE2	1:B:197:LYS:HD3	2.35	0.61
1:B:186:ALA:O	1:B:190:ILE:HG13	2.01	0.61
1:A:181:GLN:H	1:A:181:GLN:CD	2.09	0.60
1:A:221:THR:O	1:A:224:GLN:HB2	2.02	0.60
1:A:217:LYS:HD2	1:A:217:LYS:H	1.67	0.59
1:B:5:GLN:HB2	4:B:830:HOH:O	2.01	0.59
1:A:105:THR:OG1	1:A:107:GLU:HG2	2.03	0.59
1:B:179:THR:OG1	1:B:181:GLN:HG2	2.02	0.59
1:B:193:TRP:CZ2	1:B:197:LYS:HD3	2.37	0.59
1:B:167:GLU:O	1:B:167:GLU:HG3	2.03	0.58
1:B:156:LYS:HZ1	1:B:201:ASP:CG	2.11	0.58
1:A:12:TRP:CD1	1:A:238:LEU:HD13	2.38	0.57
1:A:62:ILE:HD13	1:A:62:ILE:C	2.30	0.56
1:A:10:ALA:HB1	1:A:237:SER:HB2	1.86	0.56
1:A:48:LEU:O	1:A:52:LYS:HB3	2.06	0.56
1:B:130:THR:HA	1:B:169:VAL:HB	1.88	0.55
1:B:180:PRO:HB2	1:B:225:GLN:HE21	1.68	0.55
1:B:3:LYS:NZ	1:B:223:TYR:O	2.38	0.55
1:A:82:ILE:HD13	1:B:44:THR:HG21	1.87	0.55
1:A:155:LYS:O	1:A:158:ASP:HB2	2.07	0.54
1:B:156:LYS:NZ	1:B:201:ASP:OD1	2.32	0.54
1:A:35:HIS:O	1:A:59:LYS:NZ	2.38	0.54
1:B:105:THR:OG1	1:B:107:GLU:HG2	2.08	0.54
1:B:217:LYS:HG2	4:B:759:HOH:O	2.08	0.54
1:B:193:TRP:O	1:B:197:LYS:HB2	2.08	0.53
1:A:138:ARG:NE	4:A:810:HOH:O	2.33	0.53
1:B:22:SER:HB3	1:B:54:ARG:CZ	2.39	0.52
1:A:21:LEU:O	1:A:25:ILE:HG12	2.10	0.52
1:B:170:TRP:H	1:B:170:TRP:CD1	2.28	0.51
1:B:161:LYS:HE2	1:B:161:LYS:CA	2.41	0.51
1:B:180:PRO:HB3	1:B:225:GLN:HE21	1.76	0.51
1:A:169:VAL:HA	1:A:172:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:HA	4:A:616:HOH:O	2.11	0.50
1:B:3:LYS:HE2	1:B:228:VAL:O	2.12	0.49
1:A:52:LYS:NZ	1:A:86:PHE:O	2.31	0.49
1:A:217:LYS:HD2	1:A:217:LYS:N	2.26	0.49
1:B:24:LEU:CD2	1:B:28:PHE:CZ	2.96	0.49
1:A:221:THR:HG23	4:A:616:HOH:O	2.13	0.49
1:A:250:GLN:NE2	4:A:776:HOH:O	2.44	0.49
1:A:210:TYR:CZ	1:A:212:GLY:HA3	2.49	0.47
1:B:191:ARG:NE	1:B:227:ASP:OD1	2.44	0.47
1:B:215:ASN:OD1	1:B:217:LYS:N	2.49	0.46
1:B:180:PRO:HG3	1:B:221:THR:HG22	1.97	0.46
1:A:42:ALA:HB2	1:A:63:ALA:HB3	1.99	0.45
1:B:24:LEU:CD2	1:B:28:PHE:CE1	3.00	0.45
1:B:57:HIS:HA	1:B:58:PRO:HD2	1.76	0.45
1:B:221:THR:HA	1:B:224:GLN:HE21	1.81	0.45
1:B:24:LEU:HD22	1:B:28:PHE:CZ	2.52	0.45
1:A:176:LYS:HA	1:A:176:LYS:HD3	1.59	0.45
1:B:25:ILE:HD11	1:B:50:MET:HE1	1.99	0.44
1:B:225:GLN:OE1	1:B:225:GLN:HA	2.18	0.44
1:B:133:GLU:HG2	1:B:138:ARG:CZ	2.46	0.44
1:A:12:TRP:O	1:A:15:ASN:HB2	2.18	0.44
1:A:18:GLN:HG2	1:A:50:MET:HE1	2.00	0.44
1:A:178:ALA:HA	1:A:182:GLN:OE1	2.17	0.43
1:B:193:TRP:CE2	1:B:197:LYS:CD	2.99	0.43
1:A:3:LYS:NZ	1:A:223:TYR:O	2.52	0.43
1:A:127:ILE:HD11	1:A:190:ILE:HG12	2.00	0.43
1:B:176:LYS:O	1:B:176:LYS:HD3	2.19	0.43
1:B:214:VAL:HG11	1:B:231:PHE:CD1	2.54	0.43
1:B:220:ARG:O	1:B:224:GLN:HG3	2.18	0.43
1:B:130:THR:OG1	1:B:132:GLN:HB3	2.19	0.43
1:B:240:PRO:O	1:B:243:VAL:HB	2.19	0.42
1:A:179:THR:HB	1:A:181:GLN:OE1	2.19	0.42
1:B:50:MET:HE2	1:B:51:THR:N	2.34	0.42
1:A:12:TRP:HH2	1:A:25:ILE:HD11	1.85	0.42
1:A:19:GLN:O	1:A:23:GLU:HG3	2.20	0.42
1:B:140:ALA:O	1:B:144:LEU:HG	2.19	0.41
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.75	0.41
1:B:247:LYS:C	1:B:249:THR:H	2.29	0.41
1:B:55:LEU:HD11	1:B:60:PHE:HB3	2.03	0.40
1:B:80:LEU:HD13	1:B:116:ALA:HA	2.03	0.40
1:A:18:GLN:HG2	1:A:50:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLY:HA2	4:B:800:HOH:O	2.21	0.40
1:B:161:LYS:HD3	1:B:161:LYS:HA	1.83	0.40
1:B:168:PRO:HG2	1:B:171:ALA:HB3	2.03	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	247/250 (99%)	242 (98%)	5 (2%)	0	100	100
1	B	247/250 (99%)	237 (96%)	10 (4%)	0	100	100
All	All	494/500 (99%)	479 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/197 (100%)	172 (88%)	24 (12%)	5	0
1	B	196/197 (100%)	168 (86%)	28 (14%)	3	0
All	All	392/394 (100%)	340 (87%)	52 (13%)	4	0

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	19	GLN
1	A	27	LEU
1	A	30	SER
1	A	32	SER
1	A	50	MET
1	A	52	LYS
1	A	54	ARG
1	A	55	LEU
1	A	62	ILE
1	A	70	LYS
1	A	132	GLN
1	A	138	ARG
1	A	153	LYS
1	A	156	LYS
1	A	161	LYS
1	A	176	LYS
1	A	197	LYS
1	A	217	LYS
1	A	226	ARG
1	A	238	LEU
1	A	239	LYS
1	A	243	VAL
1	A	247	LYS
1	B	3	LYS
1	B	24	LEU
1	B	33	ILE
1	B	50	MET
1	B	52	LYS
1	B	55	LEU
1	B	62	ILE
1	B	70	LYS
1	B	98	ARG
1	B	131	LEU
1	B	132	GLN
1	B	136	SER
1	B	147	ILE
1	B	152	LYS
1	B	155	LYS
1	B	161	LYS
1	B	170	TRP
1	B	176	LYS
1	B	177	VAL

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Mol	Chain	Res	Type
1	B	181	GLN
1	B	185	GLU
1	B	196	SER
1	B	197	LYS
1	B	198	ILE
1	B	205	GLU
1	B	217	LYS
1	B	226	ARG
1	B	250	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	B	34	ASN
1	B	89	ASN
1	B	224	GLN
1	B	225	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](#)

3 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	SO4	A	256	-	4,4,4	0.76	0	6,6,6	0.42	0
2	SO4	B	255	-	4,4,4	0.77	0	6,6,6	0.39	0
3	DTT	A	257	-	7,7,7	1.89	3 (42%)	4,8,8	1.57	1 (25%)

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
3	DTT	A	257	-	-	0/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	257	DTT	C4-S4	3.09	1.87	1.81
3	A	257	DTT	C3-C2	3.01	1.60	1.53
3	A	257	DTT	C1-C2	2.23	1.57	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	257	DTT	O3-C3-C2	2.47	114.77	109.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/250 (99%)	-0.82	0 100 100	7, 18, 36, 49	0
1	B	249/250 (99%)	-0.64	0 100 100	8, 22, 45, 70	0
All	All	498/500 (99%)	-0.73	0 100 100	7, 19, 43, 70	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	256	5/5	0.90	0.10	58,67,71,73	0
3	DTT	A	257	8/8	0.92	0.08	30,35,38,44	0
2	SO4	B	255	5/5	0.95	0.06	40,45,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.