



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 AM UTC

PDB ID : 2V5L / pdb_00002v5l
Title : Structures of the Open and Closed State of Trypanosomal Triosephosphate Isomerase: as Observed in a New Crystal Form: Implications for the Reaction Mechanism
Authors : Noble, M.E.M.; Zeelen, J.P.; Wierenga, R.K.
Deposited on : 2007-07-06
Resolution : 2.40 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

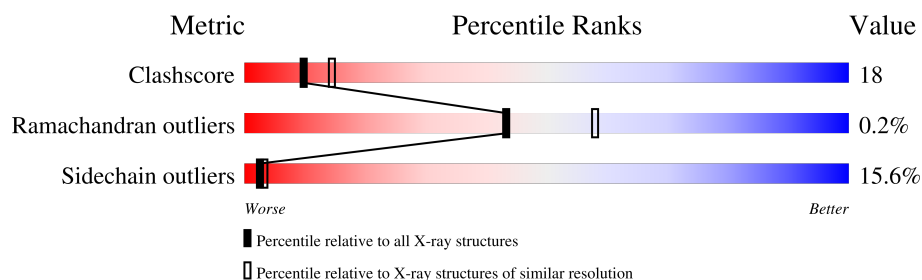
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	250	
1	B	250	

2 Entry composition [i](#)

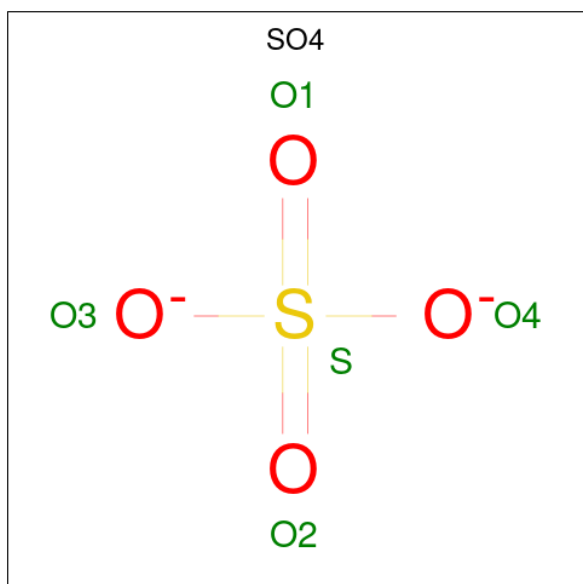
There are 3 unique types of molecules in this entry. The entry contains 3857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 water.

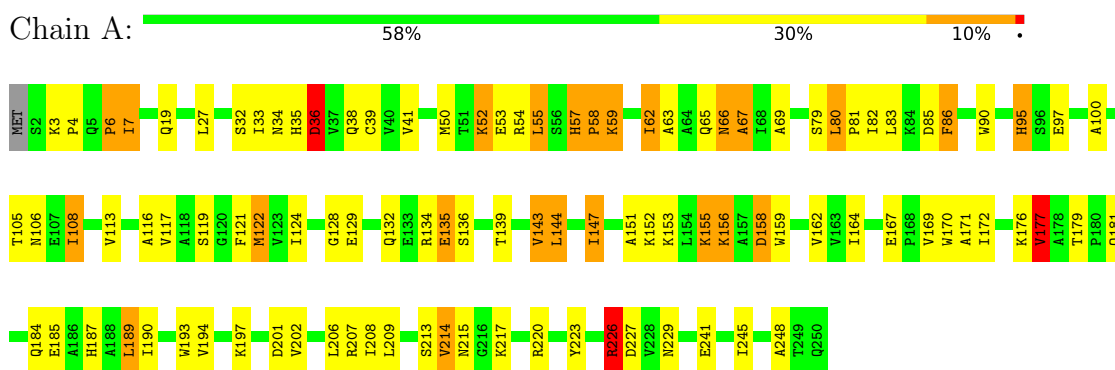
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	36	Total 36	O 36	0	0

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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.60Å 48.20Å 130.70Å 90.00° 100.60° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT NULL	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3857	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: SO4

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	1.61	15/1917 (0.8%)	1.83	25/2599 (1.0%)
1	B	1.49	6/1917 (0.3%)	1.75	22/2599 (0.8%)
All	All	1.55	21/3834 (0.5%)	1.79	47/5198 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
All	All	1	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	VAL	N-CA	-8.67	1.36	1.46
1	A	124	ILE	CA-CB	-6.79	1.45	1.53
1	A	95	HIS	CG-ND1	6.18	1.45	1.38
1	A	6	PRO	CA-C	-6.16	1.46	1.52
1	B	347	HIS	CE1-NE2	6.07	1.38	1.32
1	B	494	VAL	C-O	5.69	1.30	1.24
1	A	113	VAL	CA-CB	-5.59	1.47	1.54
1	A	19	GLN	N-CA	-5.57	1.39	1.46
1	A	181	GLN	N-CA	-5.57	1.39	1.46
1	B	507	ARG	NE-CZ	5.53	1.39	1.33
1	A	65	GLN	C-O	-5.45	1.16	1.24
1	A	214	VAL	C-O	-5.43	1.18	1.24
1	A	67	ALA	C-N	-5.29	1.27	1.33
1	A	177	VAL	CA-CB	-5.20	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	ARG	N-CA	-5.20	1.40	1.46
1	B	424	ILE	CA-CB	-5.17	1.47	1.53
1	A	7	ILE	CA-C	-5.12	1.46	1.52
1	B	305	GLN	CA-C	-5.11	1.48	1.53
1	A	135	GLU	C-O	-5.09	1.18	1.24
1	B	344	THR	C-O	-5.03	1.16	1.23
1	A	179	THR	CB-OG1	-5.02	1.35	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLU	N-CA-C	8.19	120.12	111.03
1	B	365	GLN	OE1-CD-NE2	7.70	130.30	122.60
1	A	57	HIS	CA-C-N	7.60	127.27	119.82
1	A	57	HIS	C-N-CA	7.60	127.27	119.82
1	B	527	ASP	CA-CB-CG	-6.93	105.67	112.60
1	A	132	GLN	O-C-N	6.86	129.14	122.07
1	B	546	ILE	CB-CA-C	-6.63	103.07	112.22
1	B	404	GLU	O-C-N	-6.59	114.91	123.02
1	B	413	VAL	O-C-N	6.50	128.52	121.83
1	A	177	VAL	N-CA-C	6.27	116.94	108.17
1	A	69	ALA	N-CA-C	6.18	117.81	111.14
1	B	391	ILE	CA-C-O	-6.16	115.78	120.96
1	B	518	ASN	CA-CB-CG	6.13	118.73	112.60
1	B	497	LYS	CA-C-N	-6.12	116.72	122.66
1	B	497	LYS	C-N-CA	-6.12	116.72	122.66
1	B	507	ARG	NH1-CZ-NH2	-6.12	111.34	119.30
1	A	85	ASP	CA-C-O	5.88	126.78	120.55
1	B	392	VAL	CB-CA-C	-5.83	102.76	110.98
1	A	116	ALA	O-C-N	5.70	128.02	122.09
1	A	58	PRO	CB-CA-C	-5.70	103.30	111.62
1	B	372	GLY	CA-C-O	5.68	124.83	120.91
1	B	420	GLY	O-C-N	-5.65	115.35	122.41
1	B	528	VAL	CB-CA-C	-5.63	104.49	111.08
1	A	52	LYS	O-C-N	5.59	127.90	122.09
1	A	121	PHE	CA-C-O	-5.58	114.81	121.56
1	B	357	HIS	CA-C-N	5.52	125.23	119.82
1	B	357	HIS	C-N-CA	5.52	125.23	119.82
1	B	404	GLU	CA-C-O	5.51	126.88	120.49
1	A	213	SER	CA-C-N	-5.50	115.34	122.99
1	A	213	SER	C-N-CA	-5.50	115.34	122.99
1	B	533	VAL	N-CA-C	5.41	117.01	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ASN	CA-CB-CG	-5.40	107.20	112.60
1	B	519	ALA	N-CA-C	5.39	117.23	111.36
1	B	313	LYS	CB-CA-C	-5.32	109.46	115.79
1	A	158	ASP	N-CA-C	5.25	117.75	111.71
1	A	100	ALA	O-C-N	-5.25	116.42	122.09
1	A	85	ASP	O-C-N	-5.23	116.57	122.12
1	A	36	ASP	N-CA-CB	5.22	119.31	110.49
1	A	66	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	86	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	80	LEU	CA-C-O	5.11	123.30	118.34
1	A	229	ASN	CA-C-N	-5.11	112.55	122.82
1	A	229	ASN	C-N-CA	-5.11	112.55	122.82
1	B	329	ASN	CA-CB-CG	5.11	117.70	112.60
1	A	116	ALA	CA-C-O	-5.10	115.44	120.90
1	B	333	ILE	CA-CB-CG1	5.10	119.06	110.40
1	A	227	ASP	N-CA-C	5.01	119.08	112.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	36	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	466	TYR	Sidechain

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	62	0
1	B	1883	0	1917	72	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	45	0	0	0	0
3	B	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3857	0	3834	134	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 18.

All (134) 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:325:ILE:HG23	1:B:355:LEU:HD23	1.45	0.96
1:A:147:ILE:HD12	1:A:193:TRP:CZ3	2.11	0.86
1:B:444:LEU:HD13	1:B:493:TRP:CD1	2.11	0.85
1:B:327:LEU:HD21	1:B:543:VAL:HG21	1.63	0.81
1:B:354:ARG:HH11	1:B:354:ARG:HB2	1.43	0.80
1:B:452:LYS:HE2	1:B:452:LYS:O	1.85	0.76
1:A:105:THR:OG1	1:A:108:ILE:HD12	1.84	0.76
1:A:144:LEU:HD13	1:A:193:TRP:CD1	2.22	0.74
1:B:357:HIS:ND1	1:B:358:PRO:HD2	2.06	0.70
1:B:546:ILE:HD13	1:B:546:ILE:N	2.07	0.69
1:A:4:PRO:HB2	1:A:207:ARG:HD2	1.73	0.69
1:B:318:GLN:O	1:B:350:MET:HE1	1.92	0.69
1:B:362:ILE:CD1	1:B:388:VAL:HG22	2.23	0.68
1:A:62:ILE:O	1:A:62:ILE:HD13	1.94	0.68
1:B:413:VAL:HG22	1:B:423:VAL:HG11	1.76	0.67
1:B:380:LEU:HB2	1:B:381:PRO:HD3	1.75	0.67
1:A:35:HIS:O	1:A:59:LYS:NZ	2.28	0.66
1:A:38:GLN:HE21	1:A:39:CYS:N	1.93	0.66
1:A:6:PRO:HD2	1:A:36:ASP:O	1.97	0.64
1:B:312:TRP:CD1	1:B:538:LEU:HD13	2.33	0.64
1:B:497:LYS:HB2	1:B:497:LYS:NZ	2.12	0.64
1:B:547:LYS:O	1:B:550:GLN:HG3	1.96	0.64
1:A:147:ILE:HD11	1:A:159:TRP:HH2	1.63	0.63
1:A:80:LEU:HB2	1:A:81:PRO:HD3	1.79	0.62
1:B:479:THR:HB	1:B:480:PRO:HD2	1.81	0.62
1:B:501:ASP:N	1:B:501:ASP:OD1	2.26	0.62
1:A:129:GLU:OE2	1:A:139:THR:HG23	1.99	0.62
1:B:317:SER:HB3	1:B:320:SER:OG	1.99	0.62
1:B:479:THR:N	1:B:482:GLN:OE1	2.31	0.61
1:A:144:LEU:HA	1:A:147:ILE:HG22	1.82	0.60
1:B:487:HIS:CE1	1:B:508:ILE:HG22	2.36	0.60
1:B:497:LYS:HB2	1:B:497:LYS:HZ3	1.65	0.59
1:A:117:VAL:HG11	1:A:158:ASP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:O	1:A:147:ILE:HD13	2.03	0.58
1:B:417:VAL:HG11	1:B:458:ASP:HB3	1.85	0.58
1:B:327:LEU:C	1:B:327:LEU:HD23	2.27	0.58
1:A:62:ILE:HD13	1:A:62:ILE:C	2.29	0.58
1:A:143:VAL:HG23	1:A:144:LEU:HD23	1.85	0.58
1:B:354:ARG:HH11	1:B:354:ARG:CB	2.15	0.58
1:B:444:LEU:HD13	1:B:493:TRP:HD1	1.66	0.57
1:B:367:ALA:O	1:B:412:LYS:HE2	2.04	0.57
1:A:57:HIS:ND1	1:A:58:PRO:HD2	2.19	0.56
1:B:331:THR:HG22	1:B:333:ILE:HD13	1.86	0.56
1:A:177:VAL:O	1:A:177:VAL:HG12	2.06	0.56
1:A:4:PRO:HB2	1:A:207:ARG:CD	2.36	0.55
1:B:362:ILE:HD11	1:B:388:VAL:HG22	1.88	0.55
1:A:147:ILE:HD11	1:A:159:TRP:CH2	2.43	0.54
1:A:147:ILE:HD13	1:A:147:ILE:C	2.32	0.54
1:B:478:ALA:HA	1:B:482:GLN:OE1	2.07	0.54
1:A:147:ILE:HD12	1:A:193:TRP:HZ3	1.69	0.54
1:A:143:VAL:CG2	1:A:144:LEU:HD23	2.38	0.54
1:A:129:GLU:OE1	1:A:129:GLU:N	2.36	0.54
1:B:354:ARG:O	1:B:354:ARG:HG2	2.07	0.53
1:A:156:LYS:HZ2	1:A:201:ASP:CG	2.17	0.53
1:B:305:GLN:O	1:B:507:ARG:HD2	2.08	0.53
1:A:52:LYS:NZ	1:A:86:PHE:O	2.41	0.53
1:B:517:LYS:N	1:B:517:LYS:HD3	2.25	0.52
1:A:3:LYS:NZ	1:A:223:TYR:O	2.43	0.52
1:A:66:ASN:O	1:A:67:ALA:HB2	2.10	0.52
1:B:487:HIS:ND1	1:B:508:ILE:HG22	2.25	0.51
1:A:144:LEU:HD23	1:A:144:LEU:N	2.26	0.51
1:B:469:VAL:HA	1:B:472:ILE:HD12	1.93	0.51
1:A:184:GLN:HE22	1:A:226:ARG:HG2	1.76	0.51
1:B:431:LEU:HD11	1:B:476:LYS:HE2	1.93	0.50
1:A:194:VAL:CG1	1:A:202:VAL:HG12	2.42	0.50
1:B:506:LEU:HG	1:B:507:ARG:N	2.27	0.49
1:B:444:LEU:HD21	1:B:489:LEU:HD12	1.93	0.49
1:A:6:PRO:HG3	1:A:223:TYR:OH	2.12	0.49
1:A:79:SER:HB2	1:A:81:PRO:HD2	1.95	0.49
1:B:321:LEU:O	1:B:325:ILE:HG13	2.13	0.49
1:B:493:TRP:CD1	1:B:497:LYS:HZ1	2.29	0.49
1:A:172:ILE:O	1:A:172:ILE:HG22	2.12	0.49
1:B:468:PRO:O	1:B:472:ILE:HG13	2.12	0.49
1:A:79:SER:OG	1:A:82:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LYS:HB3	1:B:540:PRO:HD2	1.96	0.48
1:A:57:HIS:CE1	1:A:59:LYS:HB2	2.48	0.48
1:B:362:ILE:C	1:B:362:ILE:HD12	2.39	0.48
1:A:41:VAL:O	1:A:41:VAL:HG12	2.13	0.48
1:B:430:THR:OG1	1:B:433:GLU:HG3	2.14	0.48
1:B:493:TRP:O	1:B:497:LYS:HB2	2.14	0.47
1:A:129:GLU:CD	1:A:139:THR:HG23	2.41	0.46
1:A:245:ILE:O	1:A:248:ALA:HB3	2.16	0.46
1:A:215:ASN:HB2	1:A:241:GLU:OE2	2.15	0.46
1:A:128:GLY:HA3	1:A:167:GLU:O	2.15	0.46
1:B:444:LEU:O	1:B:447:ILE:HG22	2.16	0.46
1:A:63:ALA:HB2	1:A:90:TRP:CB	2.46	0.46
1:B:380:LEU:N	1:B:381:PRO:CD	2.79	0.46
1:B:431:LEU:HG	1:B:435:GLU:HG3	1.98	0.46
1:A:151:ALA:HB2	1:A:159:TRP:HZ2	1.81	0.46
1:B:351:THR:O	1:B:355:LEU:HB2	2.16	0.45
1:B:355:LEU:HD13	1:B:360:PHE:HB2	1.97	0.45
1:B:410:ALA:CB	1:B:453:LYS:NZ	2.78	0.45
1:A:80:LEU:N	1:A:81:PRO:CD	2.79	0.45
1:A:170:TRP:H	1:A:170:TRP:CD1	2.34	0.45
1:A:38:GLN:NE2	1:A:39:CYS:N	2.63	0.44
1:A:190:ILE:O	1:A:194:VAL:HG23	2.17	0.44
1:A:170:TRP:CE3	1:A:171:ALA:HB2	2.53	0.44
1:B:368:ILE:HD13	1:B:377:GLU:HB3	2.00	0.44
1:B:495:SER:HA	1:B:503:ALA:HB2	2.00	0.44
1:A:122:MET:HE3	1:A:122:MET:HB3	1.77	0.44
1:A:187:HIS:CE1	1:A:208:ILE:HG22	2.53	0.43
1:B:526:ARG:HA	1:B:526:ARG:HD2	1.74	0.43
1:A:169:VAL:HA	1:A:172:ILE:HD12	2.01	0.43
1:B:327:LEU:CD2	1:B:543:VAL:HG21	2.41	0.43
1:B:467:GLU:O	1:B:469:VAL:N	2.51	0.43
1:B:533:VAL:HG12	1:B:534:GLY:N	2.34	0.42
1:A:155:LYS:O	1:A:158:ASP:N	2.51	0.42
1:B:342:ALA:HA	1:B:363:ALA:O	2.19	0.42
1:A:38:GLN:HE21	1:A:38:GLN:C	2.27	0.42
1:B:313:LYS:HB3	1:B:314:CYS:H	1.57	0.42
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.49	0.42
1:B:410:ALA:HB1	1:B:453:LYS:CE	2.50	0.42
1:B:497:LYS:NZ	1:B:497:LYS:CB	2.77	0.42
1:A:38:GLN:NE2	1:A:38:GLN:HA	2.34	0.42
1:B:525:GLN:H	1:B:525:GLN:HG2	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:HIS:CE1	1:B:397:GLU:CD	2.97	0.42
1:B:442:VAL:O	1:B:445:THR:HB	2.20	0.41
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.90	0.41
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.87	0.41
1:A:194:VAL:HG21	1:A:206:LEU:CD2	2.51	0.41
1:B:429:GLU:CD	1:B:470:TRP:CD1	2.99	0.41
1:B:444:LEU:HD21	1:B:489:LEU:CD1	2.50	0.41
1:A:7:ILE:HB	1:A:209:LEU:HD21	2.02	0.41
1:A:33:ILE:HD12	1:A:57:HIS:CE1	2.56	0.41
1:A:144:LEU:CD1	1:A:193:TRP:CD1	2.99	0.41
1:B:370:LYS:HE3	1:B:370:LYS:HB2	1.60	0.41
1:A:95:HIS:CE1	1:A:97:GLU:HG3	2.56	0.41
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.84	0.41
1:B:383:LEU:HA	1:B:383:LEU:HD23	1.83	0.41
1:B:395:HIS:HE1	1:B:397:GLU:HG3	1.86	0.41
1:B:357:HIS:HA	1:B:358:PRO:HD3	1.78	0.40
1:B:447:ILE:HG21	1:B:447:ILE:HD13	1.86	0.40
1:B:395:HIS:CE1	1:B:397:GLU:HG3	2.57	0.40
1:B:493:TRP:CD1	1:B:497:LYS:NZ	2.90	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	247/250 (99%)	238 (96%)	8 (3%)	1 (0%)	30	43
1	B	247/250 (99%)	235 (95%)	12 (5%)	0	100	100
All	All	494/500 (99%)	473 (96%)	20 (4%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASP

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	196/197 (100%)	164 (84%)	32 (16%)	2	3
1	B	196/197 (100%)	167 (85%)	29 (15%)	3	4
All	All	392/394 (100%)	331 (84%)	61 (16%)	2	3

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	32	SER
1	A	34	ASN
1	A	36	ASP
1	A	50	MET
1	A	54	ARG
1	A	55	LEU
1	A	59	LYS
1	A	62	ILE
1	A	108	ILE
1	A	119	SER
1	A	122	MET
1	A	134	ARG
1	A	135	GLU
1	A	136	SER
1	A	143	VAL
1	A	144	LEU
1	A	147	ILE
1	A	152	LYS
1	A	153	LYS
1	A	155	LYS
1	A	156	LYS
1	A	164	ILE

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Mol	Chain	Res	Type
1	A	176	LYS
1	A	177	VAL
1	A	185	GLU
1	A	189	LEU
1	A	197	LYS
1	A	214	VAL
1	A	217	LYS
1	A	220	ARG
1	A	226	ARG
1	B	319	GLN
1	B	322	SER
1	B	330	SER
1	B	333	ILE
1	B	350	MET
1	B	353	GLU
1	B	354	ARG
1	B	355	LEU
1	B	370	LYS
1	B	389	ASN
1	B	404	GLU
1	B	422	MET
1	B	434	ARG
1	B	438	ARG
1	B	441	VAL
1	B	444	LEU
1	B	452	LYS
1	B	453	LYS
1	B	456	LYS
1	B	461	LYS
1	B	467	GLU
1	B	489	LEU
1	B	497	LYS
1	B	501	ASP
1	B	517	LYS
1	B	521	THR
1	B	526	ARG
1	B	538	LEU
1	B	546	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	B	338	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	1551	-	4,4,4	0.81	0	6,6,6	0.30	0
2	SO4	A	1251	-	4,4,4	1.09	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

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 [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.