



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2018 – 10:47 AM EDT

PDB ID : 2V5L
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031021

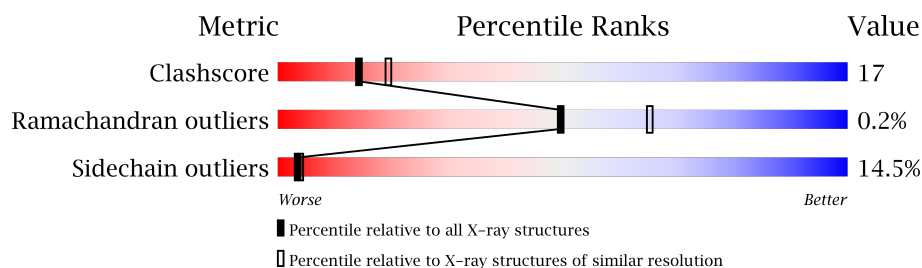
1 Overall quality at a glance

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	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (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 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 $\leq 5\%$.

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 (three-letter code: 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.

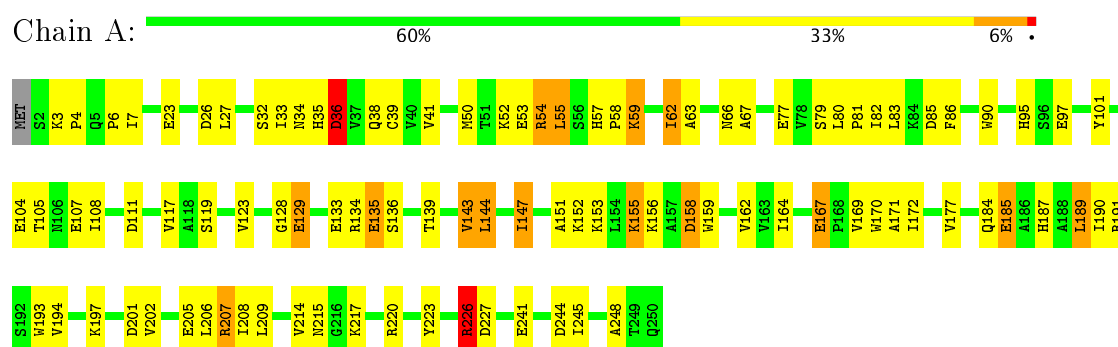
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	36	Total 36	O 36	0	0

3 Residue-property plots [i](#)

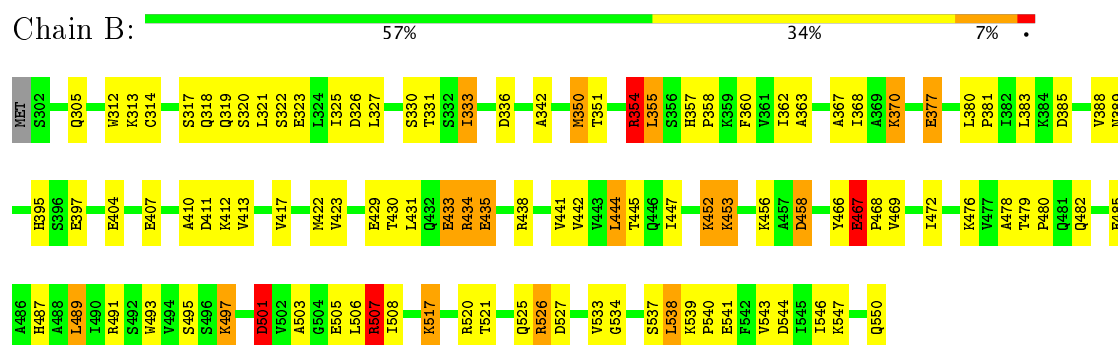
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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	94.60 Å 48.20 Å 130.70 Å 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	1.25	14/1917 (0.7%)	1.50	21/2599 (0.8%)
1	B	1.17	11/1917 (0.6%)	1.49	18/2599 (0.7%)
All	All	1.21	25/3834 (0.7%)	1.50	39/5198 (0.8%)

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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	467	GLU	CD-OE2	8.26	1.34	1.25
1	A	185	GLU	CD-OE2	7.55	1.33	1.25
1	A	53	GLU	CD-OE2	7.01	1.33	1.25
1	B	404	GLU	CD-OE2	6.90	1.33	1.25
1	A	133	GLU	CD-OE2	6.76	1.33	1.25
1	A	129	GLU	CD-OE2	6.72	1.33	1.25
1	A	167	GLU	CD-OE2	6.65	1.32	1.25
1	A	23	GLU	CD-OE2	6.57	1.32	1.25
1	B	433	GLU	CD-OE2	6.55	1.32	1.25
1	B	323	GLU	CD-OE2	6.45	1.32	1.25
1	B	407	GLU	CD-OE2	6.38	1.32	1.25
1	A	205	GLU	CD-OE2	6.35	1.32	1.25
1	A	77	GLU	CD-OE2	6.25	1.32	1.25
1	B	377	GLU	CD-OE1	-6.13	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	GLU	CD-OE2	6.12	1.32	1.25
1	B	429	GLU	CD-OE2	6.08	1.32	1.25
1	A	107	GLU	CD-OE2	5.78	1.32	1.25
1	A	129	GLU	CD-OE1	-5.76	1.19	1.25
1	A	135	GLU	CD-OE1	-5.39	1.19	1.25
1	B	541	GLU	CD-OE2	5.33	1.31	1.25
1	A	135	GLU	CD-OE2	5.24	1.31	1.25
1	A	104	GLU	CD-OE1	-5.20	1.20	1.25
1	B	435	GLU	CD-OE2	5.18	1.31	1.25
1	B	505	GLU	CD-OE2	5.11	1.31	1.25
1	A	162	VAL	N-CA	-5.10	1.36	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASP	CB-CG-OD1	11.53	128.67	118.30
1	B	385	ASP	CB-CG-OD2	-11.38	108.06	118.30
1	A	54	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	B	458	ASP	CB-CG-OD2	-10.81	108.57	118.30
1	B	507	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	B	544	ASP	CB-CG-OD2	-10.25	109.07	118.30
1	A	227	ASP	CB-CG-OD2	-9.97	109.33	118.30
1	A	158	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	B	491	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	A	201	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	227	ASP	CB-CG-OD1	8.61	126.05	118.30
1	B	354	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	A	244	ASP	CB-CG-OD1	8.38	125.85	118.30
1	B	501	ASP	CB-CG-OD2	-8.28	110.84	118.30
1	B	385	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	191	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	507	ARG	NH1-CZ-NH2	-7.33	111.34	119.40
1	B	411	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	B	544	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	336	ASP	CB-CG-OD1	6.91	124.51	118.30
1	A	201	ASP	CB-CG-OD1	6.83	124.44	118.30
1	B	354	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	26	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	111	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	B	527	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	B	434	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	85	ASP	CB-CG-OD1	6.26	123.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	123	VAL	CG1-CB-CG2	-6.18	101.01	110.90
1	A	111	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	85	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	54	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	326	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	162	VAL	CA-CB-CG2	-5.73	102.31	110.90
1	A	244	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	101	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	101	TYR	CB-CG-CD1	5.34	124.21	121.00
1	A	226	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	507	ARG	NE-CZ-NH2	5.02	122.81	120.30

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	58	0
1	B	1883	0	1917	69	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
All	All	3857	0	3834	127	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 17.

All (127) 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:HB2	1:B:354:ARG:HH11	1.43	0.80
1:B:452:LYS:O	1:B:452:LYS:HE2	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:N	1:B:546:ILE:HD13	2.07	0.69
1:A:4:PRO:HB2	1:A:207:ARG:HD2	1.73	0.69
1:B:362:ILE:CD1	1:B:388:VAL:HG22	2.23	0.68
1:A:62:ILE:HD13	1:A:62:ILE:O	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:OD1	1:B:501:ASP:N	2.26	0.62
1:B:497:LYS:HB2	1:B:497:LYS:HZ2	1.64	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:A:117:VAL:HG11	1:A:158:ASP:HB3	1.84	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:327:LEU:C	1:B:327:LEU:HD23	2.27	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:B:305:GLN:O	1:B:507:ARG:HD2	2.08	0.53
1:A:62:ILE:C	1:A:62:ILE:HD13	2.29	0.52
1:B:517:LYS:HD3	1:B:517:LYS:N	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:N	1:A:144:LEU:HD23	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:A:147:ILE:C	1:A:147:ILE:HD13	2.32	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:A:172:ILE:HG22	1:A:172:ILE:O	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
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:A:41:VAL:HG12	1:A:41:VAL:O	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:52:LYS:NZ	1:A:86:PHE:O	2.41	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:362:ILE:HD12	1:B:362:ILE:C	2.39	0.43
1:A:169:VAL:HA	1:A:172:ILE:HD12	2.01	0.43
1:B:467:GLU:O	1:B:469:VAL:N	2.51	0.43
1:B:327:LEU:CD2	1:B:543:VAL:HG21	2.41	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: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:CB	1:B:497:LYS:NZ	2.77	0.42
1:A:38:GLN:HA	1:A:38:GLN:NE2	2.34	0.42
1:B:525:GLN:HG2	1:B:525:GLN:H	1.61	0.42
1:B:442:VAL:O	1:B:445:THR:HB	2.20	0.41
1:A:129:GLU:CD	1:A:139:THR:HG23	2.41	0.41
1:A:55:LEU:HA	1:A:55:LEU:HD23	1.90	0.41
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.87	0.41
1:B:318:GLN:O	1:B:350:MET:HE1	2.20	0.41
1:A:194:VAL:HG21	1:A:206:LEU:CD2	2.51	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:144:LEU:CD1	1:A:193:TRP:CD1	2.99	0.41
1:A:33:ILE:HD12	1:A:57:HIS:CE1	2.56	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:HD23	1:B:383:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:B:447:ILE:HG21	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 [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%)	238 (96%)	8 (3%)	1 (0%)	36	51
1	B	247/250 (99%)	235 (95%)	12 (5%)	0	100	100
All	All	494/500 (99%)	473 (96%)	20 (4%)	1 (0%)	49	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASP

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/197 (100%)	167 (85%)	29 (15%)	3	4
1	B	196/197 (100%)	168 (86%)	28 (14%)	3	4
All	All	392/394 (100%)	335 (86%)	57 (14%)	3	4

All (57) 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	119	SER
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
1	A	185	GLU
1	A	189	LEU
1	A	197	LYS
1	A	207	ARG
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

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Mol	Chain	Res	Type
1	B	333	ILE
1	B	350	MET
1	B	354	ARG
1	B	355	LEU
1	B	370	LYS
1	B	389	ASN
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	467	GLU
1	B	489	LEU
1	B	497	LYS
1	B	501	ASP
1	B	507	ARG
1	B	517	LYS
1	B	520	ARG
1	B	521	THR
1	B	526	ARG
1	B	537	SER
1	B	538	LEU

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	38	GLN
1	A	224	GLN
1	B	338	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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	A	1251	-	4,4,4	1.14	0	6,6,6	0.41	0
2	SO4	B	1551	-	4,4,4	0.84	0	6,6,6	0.28	0

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	SO4	A	1251	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1551	-	-	0/0/0/0	0/0/0/0

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 ⓘ

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.