Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:14 pm BST

PDB ID	:	1IPD
Title	:	THREE-DIMENSIONAL STRUCTURE OF A HIGHLY THERMOSTABLE ENZYME, 3-ISOPROPYLMALATE DEHYDROGENASE OF THERMUS THERMOPHILUS AT 2.2 ANGSTROMS RESOLUTION
Authors	:	Imada, K.; Sato, M.; Tanaka, N.; Katsube, Y.; Matsuura, Y.; Oshima, T.
Deposited on	:	1992-01-29
Resolution	:	2.20 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:

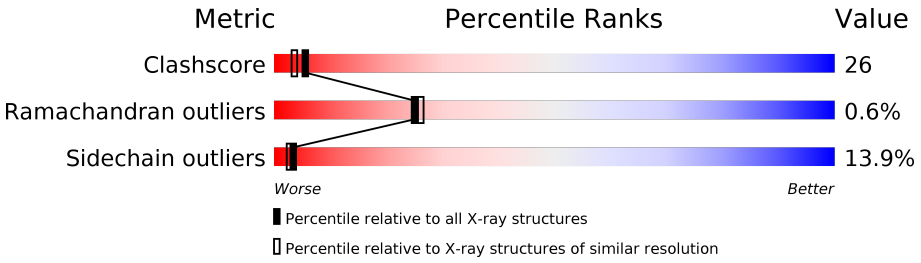
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	57% 30% 12% .

2 Entry composition

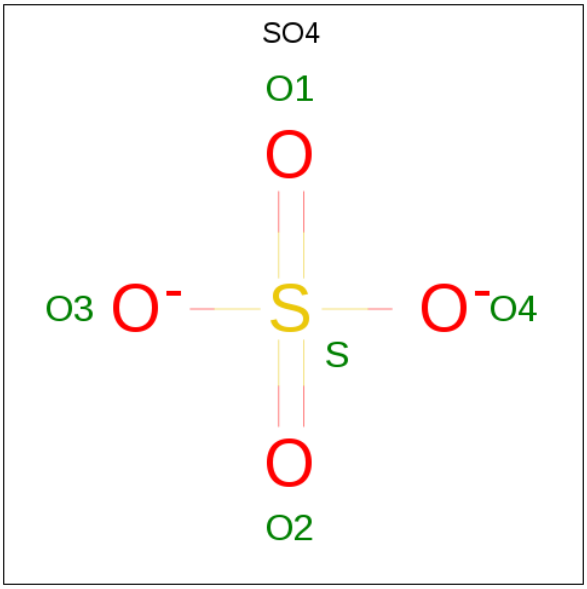
There are 3 unique types of molecules in this entry. The entry contains 2661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-ISOPROPYLMALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2590	1651	449	484	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		

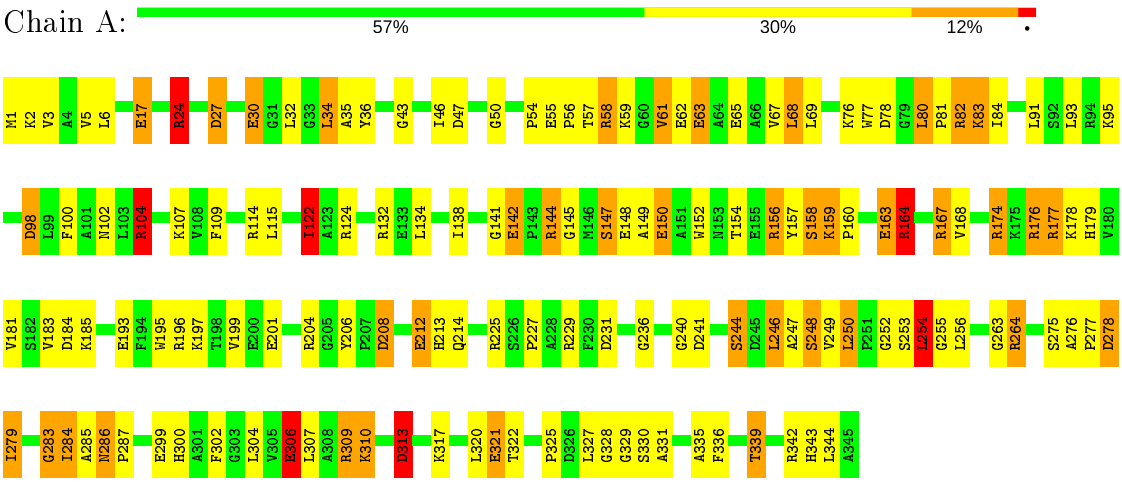
3 Residue-property plots (i)

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: 3-ISOPROPYLMALATE DEHYDROGENASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	78.60Å 78.60Å 158.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2661	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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	1.00	1/2645 (0.0%)	1.88	65/3590 (1.8%)

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	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	GLY	N-CA	6.04	1.55	1.46

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ARG	NE-CZ-NH1	20.07	130.33	120.30
1	A	124	ARG	NE-CZ-NH1	17.41	129.01	120.30
1	A	225	ARG	CD-NE-CZ	15.74	145.64	123.60
1	A	225	ARG	NE-CZ-NH1	14.47	127.54	120.30
1	A	174	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	A	164	ARG	NE-CZ-NH1	-13.65	113.48	120.30
1	A	174	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	A	164	ARG	NE-CZ-NH2	11.57	126.08	120.30
1	A	114	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	A	124	ARG	CD-NE-CZ	10.91	138.88	123.60
1	A	98	ASP	CB-CG-OD1	-9.83	109.45	118.30
1	A	313	ASP	CB-CG-OD1	-9.59	109.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	ASP	CB-CG-OD2	9.46	126.82	118.30
1	A	167	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	167	ARG	CD-NE-CZ	8.90	136.07	123.60
1	A	193	GLU	OE1-CD-OE2	8.83	133.90	123.30
1	A	98	ASP	CB-CG-OD2	8.70	126.13	118.30
1	A	164	ARG	CD-NE-CZ	-8.55	111.63	123.60
1	A	104	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	124	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	208	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	A	204	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	A	158	SER	CB-CA-C	-8.32	94.29	110.10
1	A	82	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	176	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	A	78	ASP	CB-CG-OD1	-8.04	111.07	118.30
1	A	114	ARG	CD-NE-CZ	-7.70	112.82	123.60
1	A	104	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	A	278	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	264	ARG	CD-NE-CZ	-7.57	113.01	123.60
1	A	176	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	A	156	ARG	CD-NE-CZ	-7.07	113.70	123.60
1	A	204	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	A	241	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	A	147	SER	O-C-N	6.71	133.43	122.70
1	A	184	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	147	SER	N-CA-CB	6.60	120.40	110.50
1	A	196	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	A	313	ASP	OD1-CG-OD2	6.21	135.10	123.30
1	A	47	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	313	ASP	CA-CB-CG	-6.16	99.84	113.40
1	A	142	GLU	CA-CB-CG	6.13	126.88	113.40
1	A	58	ARG	CD-NE-CZ	5.99	131.98	123.60
1	A	283	GLY	N-CA-C	-5.96	98.20	113.10
1	A	24	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	306	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	142	GLU	CB-CG-CD	5.87	130.05	114.20
1	A	212	GLU	CA-CB-CG	5.86	126.28	113.40
1	A	321	GLU	CA-CB-CG	5.84	126.26	113.40
1	A	61	VAL	CB-CA-C	5.84	122.50	111.40
1	A	24	ARG	CB-CG-CD	5.77	126.60	111.60
1	A	264	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	132	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	256	LEU	CA-CB-CG	5.49	127.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	GLU	OE1-CD-OE2	5.46	129.85	123.30
1	A	177	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	150	GLU	CG-CD-OE1	5.39	129.08	118.30
1	A	65	GLU	CG-CD-OE1	5.38	129.07	118.30
1	A	27	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	A	65	GLU	CG-CD-OE2	-5.36	107.59	118.30
1	A	157	TYR	C-N-CA	5.26	134.86	121.70
1	A	167	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	A	122	ILE	CA-CB-CG2	5.07	121.04	110.90
1	A	163	GLU	CG-CD-OE1	5.06	128.42	118.30
1	A	196	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	ARG	Sidechain

5.2 Too-close contacts (i)

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	2590	0	2625	135	1
2	A	10	0	0	1	1
3	A	61	0	0	14	0
All	All	2661	0	2625	135	1

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 26.

All (135) 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:83:LYS:HG2	1:A:84:ILE:HG23	1.19	1.16
1:A:176:ARG:NH1	1:A:231:ASP:OD1	1.93	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:O	1:A:61:VAL:HG22	1.65	0.97
1:A:310:LYS:HG3	3:A:403:HOH:O	1.63	0.96
1:A:321:GLU:OE2	1:A:342:ARG:NH2	1.99	0.95
1:A:158:SER:HB3	1:A:160:PRO:HD2	1.49	0.95
1:A:83:LYS:CG	1:A:84:ILE:HG23	1.99	0.91
1:A:164:ARG:NH1	3:A:366:HOH:O	2.01	0.90
1:A:300:HIS:HE1	3:A:378:HOH:O	1.53	0.88
1:A:122:ILE:CD1	1:A:227:PRO:HD2	2.04	0.86
1:A:55:GLU:CD	1:A:58:ARG:HD3	1.99	0.84
1:A:30:GLU:HB3	1:A:32:LEU:CD1	2.08	0.82
1:A:148:GLU:HA	1:A:148:GLU:OE1	1.79	0.81
1:A:201:GLU:OE1	3:A:393:HOH:O	1.99	0.80
1:A:102:ASN:HB2	1:A:134:LEU:HD11	1.67	0.77
1:A:122:ILE:HD12	1:A:227:PRO:HD2	1.68	0.75
1:A:276:ALA:O	1:A:279:ILE:HG13	1.86	0.74
1:A:55:GLU:OE1	1:A:58:ARG:HD3	1.88	0.73
1:A:283:GLY:O	3:A:352:HOH:O	2.09	0.71
1:A:30:GLU:HB3	1:A:32:LEU:HD13	1.71	0.70
1:A:102:ASN:HB2	1:A:134:LEU:CD1	2.22	0.70
1:A:164:ARG:HD2	3:A:366:HOH:O	1.91	0.70
1:A:80:LEU:HB3	1:A:81:PRO:HD2	1.75	0.68
1:A:246:LEU:O	1:A:249:VAL:HG22	1.95	0.67
1:A:174:ARG:HD3	1:A:208:ASP:OD2	1.95	0.67
1:A:236:GLY:HA3	3:A:396:HOH:O	1.95	0.67
1:A:247:ALA:HA	1:A:250:LEU:HD22	1.77	0.66
1:A:55:GLU:OE2	1:A:58:ARG:HD2	1.96	0.66
1:A:1:MET:HE2	1:A:34:LEU:HG	1.77	0.66
1:A:177:ARG:HH11	1:A:177:ARG:HG3	1.59	0.66
1:A:240:GLY:O	1:A:244:SER:OG	2.13	0.66
1:A:174:ARG:HA	1:A:178:LYS:HD3	1.79	0.65
1:A:279:ILE:HG23	1:A:284:ILE:HD11	1.79	0.65
1:A:27:ASP:C	1:A:27:ASP:OD1	2.33	0.65
1:A:2:LYS:HA	1:A:35:ALA:O	1.97	0.64
1:A:177:ARG:NH1	1:A:177:ARG:HG3	2.11	0.64
1:A:145:GLY:HA3	1:A:152:TRP:CZ2	2.32	0.63
1:A:2:LYS:CE	1:A:63:GLU:HG3	2.30	0.61
1:A:55:GLU:OE2	1:A:58:ARG:CD	2.48	0.61
1:A:1:MET:HB3	1:A:34:LEU:HA	1.82	0.60
1:A:55:GLU:CD	1:A:58:ARG:CD	2.67	0.60
1:A:147:SER:HB2	1:A:150:GLU:H	1.67	0.60
1:A:5:VAL:C	1:A:6:LEU:HD12	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:HB3	1:A:32:LEU:HD11	1.82	0.60
1:A:83:LYS:HG2	1:A:84:ILE:CG2	2.13	0.58
1:A:310:LYS:CD	3:A:403:HOH:O	2.50	0.58
1:A:54:PRO:O	1:A:58:ARG:HG3	2.03	0.57
1:A:55:GLU:HA	1:A:58:ARG:HG3	1.86	0.57
1:A:159:LYS:O	1:A:163:GLU:HG3	2.04	0.57
1:A:122:ILE:CD1	1:A:227:PRO:CD	2.80	0.57
1:A:279:ILE:CG2	1:A:284:ILE:HD11	2.34	0.56
1:A:310:LYS:CG	3:A:403:HOH:O	2.35	0.56
1:A:17:GLU:OE2	1:A:24:ARG:NH2	2.38	0.56
1:A:174:ARG:CD	1:A:208:ASP:OD2	2.55	0.54
1:A:322:THR:OG1	1:A:339:THR:HG21	2.07	0.54
1:A:98:ASP:OD2	1:A:264:ARG:CZ	2.55	0.54
1:A:80:LEU:CB	1:A:81:PRO:HD2	2.37	0.54
1:A:322:THR:HG21	1:A:339:THR:HG21	1.89	0.53
1:A:61:VAL:HG12	1:A:67:VAL:HG22	1.91	0.53
1:A:115:LEU:O	1:A:252:GLY:HA3	2.10	0.51
1:A:310:LYS:HD3	3:A:403:HOH:O	2.10	0.51
1:A:81:PRO:HG2	1:A:84:ILE:HG12	1.93	0.51
1:A:322:THR:CG2	1:A:339:THR:HG21	2.41	0.51
1:A:325:PRO:HD3	1:A:331:ALA:O	2.11	0.50
1:A:254:LEU:CD1	1:A:254:LEU:N	2.73	0.50
1:A:167:ARG:HG2	1:A:206:TYR:OH	2.12	0.49
1:A:253:SER:C	1:A:255:GLY:H	2.16	0.48
1:A:279:ILE:HG22	1:A:284:ILE:CG1	2.43	0.48
1:A:55:GLU:O	1:A:59:LYS:HG3	2.13	0.48
1:A:181:VAL:HG23	3:A:374:HOH:O	2.13	0.48
1:A:2:LYS:CE	1:A:63:GLU:O	2.62	0.48
1:A:287:PRO:HG2	1:A:336:PHE:CD2	2.49	0.48
1:A:185:LYS:HD3	1:A:185:LYS:HA	1.65	0.48
1:A:32:LEU:HD21	1:A:307:LEU:CD1	2.44	0.48
1:A:3:VAL:O	1:A:36:TYR:HA	2.13	0.48
1:A:55:GLU:CD	1:A:58:ARG:HH11	2.17	0.48
1:A:286:ASN:C	1:A:286:ASN:HD22	2.18	0.47
1:A:178:LYS:HE3	2:A:347:SO4:O1	2.14	0.47
1:A:195:TRP:O	1:A:199:VAL:HG23	2.14	0.47
1:A:98:ASP:OD2	1:A:264:ARG:NH1	2.47	0.47
1:A:287:PRO:HG2	1:A:336:PHE:HD2	1.79	0.47
1:A:325:PRO:HA	1:A:329:GLY:O	2.14	0.47
1:A:138:ILE:HA	1:A:154:THR:O	2.15	0.47
1:A:300:HIS:NE2	3:A:373:HOH:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLY:O	1:A:285:ALA:N	2.47	0.47
1:A:276:ALA:N	1:A:277:PRO:HD3	2.30	0.46
1:A:156:ARG:HH11	1:A:156:ARG:HD3	1.47	0.46
1:A:159:LYS:N	1:A:160:PRO:CD	2.79	0.46
1:A:302:PHE:O	1:A:304:LEU:HD13	2.15	0.46
1:A:54:PRO:C	1:A:56:PRO:HD2	2.36	0.46
1:A:212:GLU:OE1	1:A:229:ARG:NH2	2.46	0.46
1:A:30:GLU:HG2	1:A:307:LEU:HD21	1.98	0.46
1:A:5:VAL:O	1:A:6:LEU:HD12	2.16	0.45
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.63	0.45
1:A:344:LEU:HA	1:A:344:LEU:HD12	1.77	0.45
1:A:306:GLU:CD	1:A:306:GLU:H	2.18	0.45
1:A:179:HIS:CD2	3:A:374:HOH:O	2.70	0.45
1:A:321:GLU:OE2	1:A:343:HIS:NE2	2.48	0.44
1:A:27:ASP:HA	1:A:32:LEU:HB2	1.99	0.44
1:A:2:LYS:NZ	1:A:63:GLU:HG3	2.33	0.44
1:A:164:ARG:HH11	1:A:164:ARG:HD2	1.18	0.44
1:A:244:SER:O	1:A:248:SER:HB3	2.17	0.44
1:A:104:ARG:NH1	3:A:395:HOH:O	2.50	0.44
1:A:17:GLU:CD	1:A:24:ARG:HH22	2.21	0.44
1:A:115:LEU:HD11	1:A:327:LEU:HG	1.99	0.44
1:A:183:VAL:HA	1:A:214:GLN:O	2.17	0.44
1:A:27:ASP:O	1:A:27:ASP:OD1	2.35	0.44
1:A:54:PRO:HB2	1:A:56:PRO:HD2	2.00	0.44
1:A:213:HIS:C	1:A:214:GLN:HG2	2.38	0.44
1:A:2:LYS:HE3	1:A:63:GLU:O	2.18	0.43
1:A:55:GLU:N	1:A:56:PRO:HD2	2.33	0.43
1:A:335:ALA:O	1:A:339:THR:HG22	2.18	0.43
1:A:1:MET:CE	1:A:34:LEU:HG	2.47	0.43
1:A:46:ILE:O	1:A:50:GLY:N	2.48	0.43
1:A:30:GLU:CB	1:A:32:LEU:HD13	2.45	0.43
1:A:147:SER:HB3	1:A:148:GLU:H	1.48	0.43
1:A:1:MET:HE2	1:A:34:LEU:CG	2.47	0.43
1:A:145:GLY:HA3	1:A:152:TRP:CE2	2.54	0.42
1:A:55:GLU:N	1:A:56:PRO:CD	2.83	0.42
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.86	0.42
1:A:100:PHE:CE2	1:A:263:GLY:HA2	2.54	0.42
1:A:309:ARG:O	1:A:313:ASP:HB2	2.18	0.42
1:A:43:GLY:HA3	1:A:77:TRP:CH2	2.55	0.42
1:A:55:GLU:OE1	1:A:58:ARG:NH1	2.52	0.42
1:A:310:LYS:HE2	1:A:310:LYS:HB2	1.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HD3	1:A:343:HIS:ND1	2.35	0.41
1:A:325:PRO:O	1:A:328:GLY:N	2.49	0.41
1:A:213:HIS:O	1:A:214:GLN:HG2	2.20	0.41
1:A:107:LYS:HD3	1:A:109:PHE:CE1	2.55	0.41
1:A:279:ILE:HG22	1:A:284:ILE:HG13	2.03	0.41
1:A:141:GLY:O	1:A:144:ARG:HG2	2.21	0.41
1:A:147:SER:CB	1:A:149:ALA:H	2.33	0.41
1:A:122:ILE:HD11	1:A:227:PRO:CD	2.49	0.41
1:A:299:GLU:CD	1:A:309:ARG:HH22	2.24	0.40
1:A:54:PRO:CB	1:A:56:PRO:HD2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:NH1	2:A:346:SO4:O2[4_545]	2.10	0.10

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	343/345 (99%)	326 (95%)	15 (4%)	2 (1%)	25 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ILE
1	A	254	LEU

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	266/266 (100%)	229 (86%)	37 (14%)	3 3

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	24	ARG
1	A	30	GLU
1	A	34	LEU
1	A	63	GLU
1	A	68	LEU
1	A	69	LEU
1	A	76	LYS
1	A	80	LEU
1	A	82	ARG
1	A	83	LYS
1	A	91	LEU
1	A	93	LEU
1	A	95	LYS
1	A	104	ARG
1	A	122	ILE
1	A	142	GLU
1	A	144	ARG
1	A	159	LYS
1	A	164	ARG
1	A	168	VAL
1	A	197	LYS
1	A	244	SER
1	A	246	LEU
1	A	248	SER
1	A	250	LEU
1	A	254	LEU
1	A	275	SER
1	A	278	ASP
1	A	279	ILE

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Mol	Chain	Res	Type
1	A	286	ASN
1	A	306	GLU
1	A	310	LYS
1	A	313	ASP
1	A	320	LEU
1	A	330	SER
1	A	339	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	347	-	4,4,4	0.96	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	346	-	4,4,4	0.92	0	6,6,6	0.62	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	347	SO4	1	0
2	A	346	SO4	0	1

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

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.