



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:22 PM UTC

PDB ID : 1IPD / pdb_00001ipd
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 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

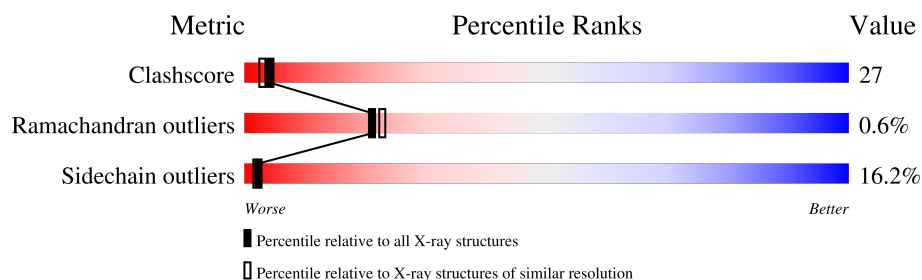
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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	345	

2 Entry composition [i](#)

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 (CCD ID: SO4) (formula: O₄S).



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.

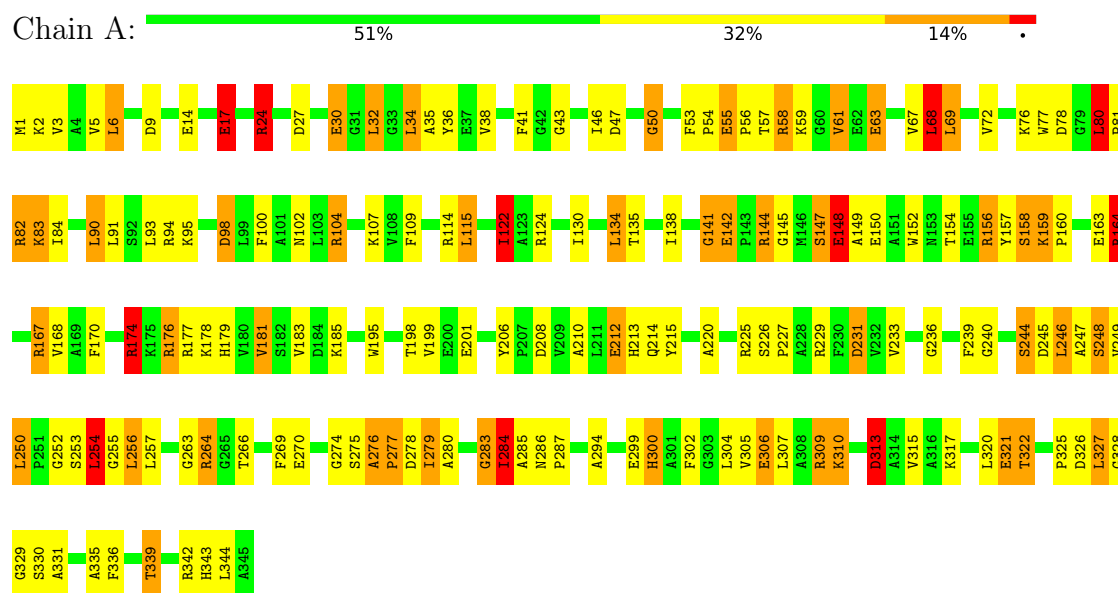
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		

3 Residue-property plots

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: 3-ISOPROPYLMALATE DEHYDROGENASE



4 Data and refinement statistics

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	78.60 Å 78.60 Å 158.10 Å 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	1.23	3/2645 (0.1%)	2.16	100/3590 (2.8%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	GLY	N-CA	6.72	1.55	1.45
1	A	305	VAL	C-N	-5.63	1.26	1.33
1	A	135	THR	CA-CB	5.48	1.62	1.53

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	CD-NE-CZ	15.17	145.64	124.40
1	A	276	ALA	O-C-N	13.28	127.64	121.53
1	A	313	ASP	CA-CB-CG	-12.76	99.84	112.60
1	A	124	ARG	CD-NE-CZ	10.34	138.88	124.40
1	A	142	GLU	CB-CG-CD	10.27	130.05	112.60
1	A	47	ASP	CA-CB-CG	9.88	122.48	112.60
1	A	78	ASP	CA-CB-CG	-9.35	103.25	112.60
1	A	164	ARG	CD-NE-CZ	-9.12	111.63	124.40
1	A	158	SER	CB-CA-C	-8.90	94.29	109.51
1	A	167	ARG	NE-CZ-NH1	8.83	130.33	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	LEU	N-CA-C	8.77	121.43	109.24
1	A	148	GLU	N-CA-C	-8.74	102.63	113.38
1	A	167	ARG	CD-NE-CZ	8.33	136.07	124.40
1	A	114	ARG	CD-NE-CZ	-8.27	112.82	124.40
1	A	264	ARG	CD-NE-CZ	-8.14	113.01	124.40
1	A	164	ARG	NE-CZ-NH1	-8.02	113.48	121.50
1	A	305	VAL	CA-C-N	7.96	131.28	120.54
1	A	305	VAL	C-N-CA	7.96	131.28	120.54
1	A	141	GLY	N-CA-C	7.80	120.49	111.36
1	A	164	ARG	NE-CZ-NH2	7.65	126.08	119.20
1	A	156	ARG	CD-NE-CZ	-7.64	113.70	124.40
1	A	124	ARG	NE-CZ-NH1	7.51	129.01	121.50
1	A	157	TYR	CA-C-N	7.48	134.86	122.07
1	A	157	TYR	C-N-CA	7.48	134.86	122.07
1	A	61	VAL	CB-CA-C	7.45	122.50	112.22
1	A	134	LEU	N-CA-C	7.35	122.42	113.38
1	A	274	GLY	CA-C-N	7.32	130.68	120.29
1	A	274	GLY	C-N-CA	7.32	130.68	120.29
1	A	9	ASP	O-C-N	7.12	131.40	122.43
1	A	55	GLU	CB-CG-CD	7.10	124.66	112.60
1	A	32	LEU	N-CA-C	7.03	121.11	112.54
1	A	147	SER	O-C-N	6.89	133.43	122.61
1	A	68	LEU	CA-C-O	-6.88	113.39	120.54
1	A	147	SER	N-CA-C	-6.81	99.42	108.34
1	A	6	LEU	O-C-N	6.75	127.46	121.32
1	A	269	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	284	ILE	N-CA-C	6.70	123.27	109.34
1	A	24	ARG	CB-CG-CD	6.65	126.60	111.30
1	A	215	TYR	CA-C-O	-6.64	113.48	121.05
1	A	233	VAL	CA-C-O	-6.56	113.41	120.36
1	A	174	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	A	53	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	41	PHE	CA-C-N	6.49	130.65	120.65
1	A	41	PHE	C-N-CA	6.49	130.65	120.65
1	A	284	ILE	CA-C-O	-6.43	112.74	120.78
1	A	142	GLU	CA-CB-CG	6.39	126.88	114.10
1	A	300	HIS	CA-CB-CG	-6.38	107.42	113.80
1	A	210	ALA	CA-C-O	-6.34	113.83	121.05
1	A	283	GLY	N-CA-C	-6.32	98.20	113.18
1	A	122	ILE	CB-CA-C	6.25	119.82	111.94
1	A	275	SER	O-C-N	6.22	129.24	122.15
1	A	122	ILE	CA-CB-CG2	6.20	121.04	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	GLU	CA-CB-CG	6.09	126.28	114.10
1	A	321	GLU	CA-CB-CG	6.08	126.26	114.10
1	A	225	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	A	14	GLU	CA-C-O	-6.01	114.05	120.42
1	A	198	THR	CA-CB-OG1	-5.91	100.73	109.60
1	A	322	THR	O-C-N	5.83	125.95	121.23
1	A	17	GLU	CB-CG-CD	5.79	122.45	112.60
1	A	90	LEU	CA-C-N	5.75	128.31	120.54
1	A	90	LEU	C-N-CA	5.75	128.31	120.54
1	A	256	LEU	CA-C-N	5.72	129.56	121.61
1	A	256	LEU	C-N-CA	5.72	129.56	121.61
1	A	82	ARG	N-CA-C	-5.71	106.16	113.01
1	A	98	ASP	CA-CB-CG	-5.71	106.89	112.60
1	A	266	THR	O-C-N	5.69	126.97	121.28
1	A	313	ASP	N-CA-CB	-5.68	101.77	110.12
1	A	294	ALA	N-CA-C	-5.64	105.04	111.07
1	A	277	PRO	CA-C-N	5.63	128.09	120.38
1	A	277	PRO	C-N-CA	5.63	128.09	120.38
1	A	141	GLY	CA-C-O	5.61	126.35	121.41
1	A	130	ILE	N-CA-CB	5.50	116.72	110.72
1	A	245	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	170	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	58	ARG	CD-NE-CZ	5.42	131.98	124.40
1	A	176	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	239	PHE	O-C-N	5.36	128.26	122.15
1	A	212	GLU	CA-C-O	-5.35	115.36	121.40
1	A	147	SER	N-CA-CB	5.29	120.40	110.87
1	A	176	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	69	LEU	CA-C-O	-5.25	115.14	120.71
1	A	231	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	134	LEU	N-CA-CB	-5.25	102.71	110.53
1	A	53	PHE	CA-C-N	5.23	125.17	119.78
1	A	53	PHE	C-N-CA	5.23	125.17	119.78
1	A	226	SER	O-C-N	5.22	127.32	121.32
1	A	50	GLY	N-CA-C	-5.21	108.14	114.92
1	A	275	SER	CB-CA-C	-5.20	102.01	110.85
1	A	270	GLU	O-C-N	5.14	125.85	121.84
1	A	147	SER	CB-CA-C	-5.12	101.04	113.19
1	A	80	LEU	O-C-N	5.08	124.96	121.71
1	A	313	ASP	OD1-CG-OD2	5.08	135.10	122.90
1	A	72	VAL	N-CA-C	5.08	116.02	108.46
1	A	174	ARG	NE-CZ-NH1	5.07	126.57	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	VAL	N-CA-CB	5.06	118.22	111.64
1	A	114	ARG	NE-CZ-NH2	-5.06	114.65	119.20
1	A	130	ILE	O-C-N	5.05	128.71	122.95
1	A	220	ALA	CA-C-N	5.02	127.01	120.28
1	A	220	ALA	C-N-CA	5.02	127.01	120.28
1	A	300	HIS	N-CA-C	5.01	116.82	111.36

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 ⓘ

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	141	1
2	A	10	0	0	1	1
3	A	61	0	0	14	0
All	All	2661	0	2625	141	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 27.

All (141) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:NH1	3:A:366:HOH:O	2.01	0.90
1:A:55:GLU:CD	1:A:58:ARG:HD3	1.99	0.88
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: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:55:GLU:CD	1:A:58:ARG:CD	2.67	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:27:ASP:C	1:A:27:ASP:OD1	2.33	0.66
1:A:55:GLU:OE2	1:A:58:ARG:HD2	1.96	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:5:VAL:C	1:A:6:LEU:HD12	2.22	0.65
1:A:279:ILE:HG23	1:A:284:ILE:HD11	1.79	0.65
1:A:2:LYS:HA	1:A:35:ALA:O	1.97	0.64
1:A:177:ARG:HG3	1:A:177:ARG:NH1	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:147:SER:HB2	1:A:150:GLU:H	1.67	0.60
1:A:1:MET:HE2	1:A:34:LEU:HG	1.83	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:CD1	1:A:227:PRO:CD	2.80	0.57
1:A:159:LYS:O	1:A:163:GLU:HG3	2.04	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:1:MET:HE2	1:A:34:LEU:CG	2.36	0.55
1:A:174:ARG:CD	1:A:208:ASP:OD2	2.55	0.54
1:A:98:ASP:OD2	1:A:264:ARG:CZ	2.55	0.54
1:A:322:THR:OG1	1:A:339:THR:HG21	2.07	0.54
1:A:1:MET:HE2	1:A:34:LEU:HD23	1.89	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:253:SER:C	1:A:255:GLY:H	2.16	0.53
1:A:61:VAL:HG12	1:A:67:VAL:HG22	1.91	0.53
1:A:55:GLU:CD	1:A:58:ARG:HH11	2.17	0.52
1:A:286:ASN:HD22	1:A:286:ASN:C	2.18	0.52
1:A:1:MET:HE2	1:A:34:LEU:CD2	2.40	0.51
1:A:115:LEU:O	1:A:252:GLY:HA3	2.10	0.51
1:A:81:PRO:HG2	1:A:84:ILE:HG12	1.93	0.51
1:A:310:LYS:HD3	3:A:403:HOH:O	2.10	0.51
1:A:322:THR:CG2	1:A:339:THR:HG21	2.41	0.51
1:A:54:PRO:C	1:A:56:PRO:HD2	2.36	0.50
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:17:GLU:CD	1:A:24:ARG:HH22	2.21	0.48
1:A:55:GLU:O	1:A:59:LYS:HG3	2.13	0.48
1:A:279:ILE:HG22	1:A:284:ILE:CG1	2.43	0.48
1:A:2:LYS:CE	1:A:63:GLU:O	2.62	0.48
1:A:181:VAL:HG23	3:A:374:HOH:O	2.13	0.48
1:A:213:HIS:C	1:A:214:GLN:HG2	2.38	0.48
1:A:287:PRO:HG2	1:A:336:PHE:CD2	2.49	0.48
1:A:306:GLU:H	1:A:306:GLU:CD	2.18	0.48
1:A:32:LEU:HD21	1:A:307:LEU:CD1	2.44	0.48
1:A:185:LYS:HD3	1:A:185:LYS:HA	1.65	0.48
1:A:3:VAL:O	1:A:36:TYR:HA	2.13	0.48
1:A:178:LYS:HE3	2:A:347:SO4:O1	2.14	0.47
1:A:98:ASP:OD2	1:A:264:ARG:NH1	2.47	0.47
1:A:195:TRP:O	1:A:199:VAL:HG23	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:299:GLU:CD	1:A:309:ARG:HH22	2.24	0.45
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.63	0.45
1:A:344:LEU:HD12	1:A:344:LEU:HA	1.77	0.45
1:A:179:HIS:CD2	3:A:374:HOH:O	2.70	0.45
1:A:27:ASP:HA	1:A:32:LEU:HB2	1.99	0.44
1:A:321:GLU:OE2	1:A:343:HIS:NE2	2.48	0.44
1:A:2:LYS:NZ	1:A:63:GLU:HG3	2.33	0.44
1:A:36:TYR:C	1:A:36:TYR:CD1	2.95	0.44
1:A:325:PRO:O	1:A:326:ASP:C	2.61	0.44
1:A:164:ARG:HD2	1:A:164:ARG:HH11	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:27:ASP:OD1	1:A:27:ASP:O	2.35	0.44
1:A:54:PRO:HB2	1:A:56:PRO:HD2	2.00	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: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:1:MET:CE	1:A:34:LEU:HG	2.47	0.43
1:A:335:ALA:O	1:A:339:THR:HG22	2.18	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:212:GLU:CD	1:A:229:ARG:HH22	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:O	1:A:280:ALA:C	2.61	0.42
1:A:310:LYS:HE2	1:A:310:LYS:HB2	1.26	0.41
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:122:ILE:HD11	1:A:227:PRO:CD	2.49	0.41
1:A:147:SER:CB	1:A:149:ALA:H	2.33	0.41
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%)	21 23

All (2) Ramachandran outliers are listed below:

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

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	266/266 (100%)	223 (84%)	43 (16%)	2 2

All (43) 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	38	VAL
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	90	LEU
1	A	91	LEU
1	A	93	LEU
1	A	94	ARG
1	A	95	LYS
1	A	104	ARG
1	A	115	LEU
1	A	122	ILE
1	A	142	GLU
1	A	144	ARG
1	A	148	GLU
1	A	159	LYS
1	A	164	ARG
1	A	168	VAL
1	A	174	ARG
1	A	244	SER
1	A	246	LEU
1	A	248	SER

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Mol	Chain	Res	Type
1	A	250	LEU
1	A	254	LEU
1	A	256	LEU
1	A	278	ASP
1	A	279	ILE
1	A	306	GLU
1	A	310	LYS
1	A	313	ASP
1	A	315	VAL
1	A	320	LEU
1	A	327	LEU
1	A	330	SER
1	A	339	THR

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

Mol	Chain	Res	Type
1	A	102	ASN
1	A	153	ASN
1	A	286	ASN

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	A	346	-	4,4,4	0.97	0	6,6,6	0.59	0
2	SO4	A	347	-	4,4,4	1.00	0	6,6,6	0.24	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	346	SO4	0	1
2	A	347	SO4	1	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

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.