



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 PM GMT

PDB ID : 6LDH  
Title : REFINED CRYSTAL STRUCTURE OF DOGFISH M4 APO-LACTATE DE-HYDROGENASE  
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Deposited on : 1987-11-25  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

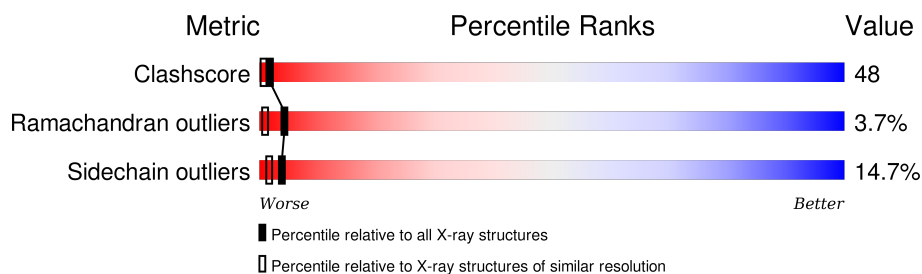
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	330	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2841 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 M4 APO-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2545	1620	439	468	18	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ASN	TRP	CONFLICT	UNP P00341
A	206	VAL	ASN	CONFLICT	UNP P00341
A	208	SER	LEU	CONFLICT	UNP P00341
A	209	ILE	LYS	CONFLICT	UNP P00341
A	210	LYS	GLU	CONFLICT	UNP P00341
A	214	LEU	GLU	CONFLICT	UNP P00341
A	215	ASP	LEU	CONFLICT	UNP P00341
A	308	ASN	ASP	CONFLICT	UNP P00341

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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.

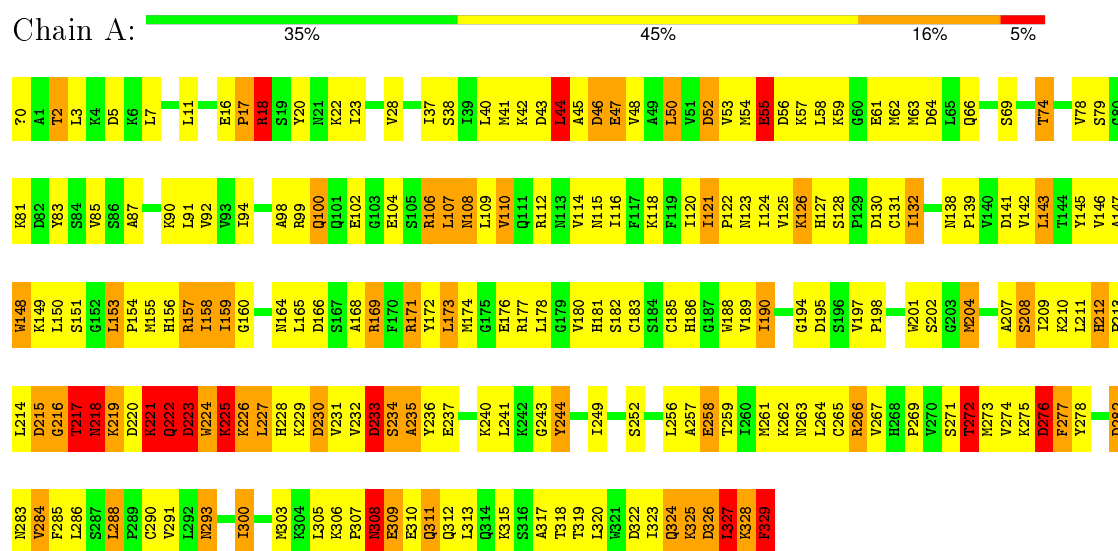
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	286	Total	O	0	0
			286	286		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: M4 APO-LACTATE DEHYDROGENASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	F 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.80 Å   146.80 Å   155.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2841	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	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, ACE

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	1.29	5/2590 (0.2%)	2.17	92/3502 (2.6%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	LYS	N-CA	-6.33	1.33	1.46
1	A	18	ARG	CA-CB	6.02	1.67	1.53
1	A	309	GLU	CD-OE1	-5.97	1.19	1.25
1	A	55	GLU	CD-OE1	-5.68	1.19	1.25
1	A	310	GLU	CB-CG	-5.15	1.42	1.52

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	NE-CZ-NH1	29.32	134.96	120.30
1	A	18	ARG	NE-CZ-NH2	-23.73	108.43	120.30
1	A	327	LEU	C-N-CA	21.91	176.49	121.70
1	A	43	ASP	CB-CG-OD1	13.97	130.88	118.30
1	A	266	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	233	ASP	CB-CG-OD1	10.24	127.52	118.30
1	A	169	ARG	NE-CZ-NH2	10.01	125.31	120.30
1	A	50	LEU	CA-CB-CG	9.82	137.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	A	220	ASP	C-N-CA	9.25	144.82	121.70
1	A	46	ASP	CB-CG-OD1	9.23	126.60	118.30
1	A	99	ARG	CD-NE-CZ	9.15	136.41	123.60
1	A	18	ARG	CB-CA-C	-9.14	92.11	110.40
1	A	195	ASP	CB-CG-OD1	8.97	126.38	118.30
1	A	171	ARG	CD-NE-CZ	8.87	136.02	123.60
1	A	276	ASP	C-N-CA	8.80	143.69	121.70
1	A	18	ARG	N-CA-CB	-8.63	95.06	110.60
1	A	326	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	171	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	A	208	SER	CA-CB-OG	8.28	133.55	111.20
1	A	310	GLU	CB-CG-CD	8.04	135.92	114.20
1	A	48	VAL	CA-CB-CG1	7.67	122.40	110.90
1	A	143	LEU	CB-CA-C	7.57	124.58	110.20
1	A	221	LYS	N-CA-C	7.54	131.35	111.00
1	A	47	GLU	CG-CD-OE1	7.50	133.30	118.30
1	A	166	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	310	GLU	CG-CD-OE1	7.44	133.18	118.30
1	A	110	VAL	CB-CA-C	7.31	125.28	111.40
1	A	64	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	324	GLN	CB-CA-C	7.29	124.98	110.40
1	A	115	ASN	CA-CB-CG	7.20	129.24	113.40
1	A	141	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	46	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	A	18	ARG	NH1-CZ-NH2	-7.10	111.59	119.40
1	A	310	GLU	CA-CB-CG	7.07	128.96	113.40
1	A	195	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	208	SER	N-CA-CB	7.02	121.03	110.50
1	A	64	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	324	GLN	CA-C-O	6.96	134.71	120.10
1	A	215	ASP	CB-CG-OD1	6.72	124.34	118.30
1	A	110	VAL	CA-CB-CG1	6.70	120.96	110.90
1	A	11	LEU	CB-CA-C	6.65	122.84	110.20
1	A	18	ARG	N-CA-C	6.54	128.67	111.00
1	A	55	GLU	CG-CD-OE2	-6.40	105.49	118.30
1	A	44	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	224	TRP	N-CA-CB	6.33	122.00	110.60
1	A	127	HIS	CA-CB-CG	-6.33	102.85	113.60
1	A	157	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	41	MET	C-N-CA	6.31	137.47	121.70
1	A	55	GLU	OE1-CD-OE2	6.30	130.86	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ARG	CD-NE-CZ	-6.18	114.95	123.60
1	A	16	GLU	CG-CD-OE1	6.13	130.56	118.30
1	A	157	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	223	ASP	C-N-CA	6.10	136.96	121.70
1	A	327	LEU	O-C-N	-6.08	112.96	122.70
1	A	195	ASP	CA-CB-CG	6.07	126.75	113.40
1	A	227	LEU	CB-CA-C	6.03	121.66	110.20
1	A	173	LEU	CB-CA-C	5.92	121.46	110.20
1	A	328	LYS	N-CA-CB	5.91	121.24	110.60
1	A	244	TYR	CB-CG-CD1	5.89	124.53	121.00
1	A	48	VAL	CB-CA-C	5.88	122.58	111.40
1	A	218	ASN	CA-CB-CG	-5.83	100.56	113.40
1	A	310	GLU	CG-CD-OE2	-5.76	106.78	118.30
1	A	244	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	157	ARG	CD-NE-CZ	-5.71	115.61	123.60
1	A	148	TRP	CA-CB-CG	-5.69	102.88	113.70
1	A	225	LYS	CB-CG-CD	5.62	126.21	111.60
1	A	326	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	A	230	ASP	CB-CA-C	5.55	121.50	110.40
1	A	282	ASP	C-N-CA	5.54	135.54	121.70
1	A	277	PHE	CB-CA-C	-5.47	99.45	110.40
1	A	59	LYS	CA-CB-CG	-5.46	101.40	113.40
1	A	272	THR	OG1-CB-CG2	5.45	122.54	110.00
1	A	222	GLN	N-CA-CB	5.43	120.37	110.60
1	A	235	ALA	CB-CA-C	-5.40	102.00	110.10
1	A	102	GLU	CA-CB-CG	5.40	125.28	113.40
1	A	217	THR	CA-CB-CG2	5.39	119.94	112.40
1	A	153	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	177	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	217	THR	CB-CA-C	-5.22	97.50	111.60
1	A	325	LYS	CA-CB-CG	5.19	124.81	113.40
1	A	216	GLY	N-CA-C	-5.16	100.20	113.10
1	A	284	VAL	C-N-CA	5.14	134.56	121.70
1	A	329	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	A	52	ASP	CB-CG-OD1	5.12	122.90	118.30
1	A	147	ALA	CB-CA-C	5.11	117.77	110.10
1	A	204	MET	CA-CB-CG	-5.09	104.64	113.30
1	A	308	ASN	C-N-CA	5.08	134.41	121.70
1	A	47	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	A	157	ARG	CG-CD-NE	5.07	122.44	111.80
1	A	18	ARG	CA-CB-CG	-5.04	102.31	113.40
1	A	258	GLU	OE1-CD-OE2	5.01	129.31	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	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	2545	0	2610	248	13
2	A	10	0	0	1	0
3	A	286	0	0	34	5
All	All	2841	0	2610	248	16

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 48.

All (248) 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:219:LYS:HE2	3:A:400:HOH:O	1.31	1.27
1:A:273:MET:CE	1:A:275:LYS:HB2	1.70	1.20
1:A:107:LEU:HD11	1:A:325:LYS:HE3	1.20	1.15
1:A:273:MET:HE1	1:A:283:ASN:HA	1.35	1.08
1:A:62:MET:HE2	1:A:78:VAL:HA	1.35	1.07
1:A:62:MET:HE3	1:A:79:SER:N	1.69	1.06
1:A:210:LYS:HG2	1:A:213:PRO:CD	1.87	1.05
1:A:62:MET:HE3	1:A:79:SER:H	1.13	1.03
1:A:197:VAL:HG23	1:A:228:HIS:HE1	1.20	1.03
1:A:100:GLN:HB2	1:A:109:LEU:HD22	1.36	1.02
1:A:57:LYS:HE3	3:A:570:HOH:O	1.59	1.02
1:A:81:LYS:O	3:A:430:HOH:O	1.77	1.01
1:A:273:MET:HE3	1:A:275:LYS:CB	1.92	0.98
1:A:312:GLN:HG2	3:A:525:HOH:O	1.62	0.98
1:A:273:MET:HE3	1:A:275:LYS:HB2	0.98	0.98
1:A:197:VAL:HG23	1:A:228:HIS:CE1	1.99	0.98
1:A:210:LYS:HG2	1:A:213:PRO:HD3	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:HB3	1:A:213:PRO:HG2	1.50	0.93
1:A:230:ASP:HA	1:A:233:ASP:HB2	1.51	0.92
1:A:0:ACE:H2	1:A:5:ASP:HB3	1.50	0.92
1:A:288:LEU:HD23	1:A:300:ILE:CD1	2.01	0.91
1:A:17:PRO:HA	1:A:18:ARG:HD3	1.52	0.91
1:A:210:LYS:HZ1	1:A:212:HIS:HB3	1.35	0.90
1:A:54:MET:CE	3:A:398:HOH:O	2.20	0.90
1:A:62:MET:CE	1:A:78:VAL:HA	2.03	0.88
1:A:284:VAL:HG11	1:A:317:ALA:HA	1.57	0.86
1:A:212:HIS:O	1:A:217:THR:HA	1.74	0.86
1:A:0:ACE:CH3	1:A:5:ASP:HB3	2.06	0.86
1:A:58:LEU:HD23	3:A:438:HOH:O	1.74	0.85
1:A:327:LEU:HD22	3:A:549:HOH:O	1.77	0.85
1:A:210:LYS:HG2	1:A:213:PRO:HD2	1.58	0.85
1:A:57:LYS:HG3	3:A:570:HOH:O	1.76	0.84
1:A:229:LYS:HG2	3:A:536:HOH:O	1.77	0.84
1:A:226:LYS:HD3	3:A:535:HOH:O	1.78	0.83
1:A:107:LEU:CD1	1:A:325:LYS:HE3	2.08	0.83
1:A:142:VAL:O	1:A:146:VAL:HG23	1.80	0.81
1:A:54:MET:HE1	3:A:398:HOH:O	1.77	0.81
1:A:98:ALA:HB1	1:A:112:ARG:NH1	1.96	0.81
1:A:194:GLY:H	1:A:197:VAL:CG1	1.94	0.79
1:A:83:TYR:HE2	1:A:124:ILE:HD11	1.48	0.79
1:A:107:LEU:HD11	1:A:325:LYS:CE	2.09	0.77
1:A:83:TYR:OH	1:A:120:ILE:HG23	1.84	0.77
1:A:274:VAL:HG21	1:A:286:LEU:HD12	1.64	0.77
1:A:263:ASN:OD1	1:A:293:ASN:HB2	1.85	0.77
1:A:210:LYS:HB3	1:A:213:PRO:CG	2.15	0.76
1:A:236:TYR:C	1:A:240:LYS:HE2	2.05	0.76
1:A:236:TYR:O	1:A:240:LYS:HE2	1.86	0.75
1:A:218:ASN:OD1	1:A:219:LYS:N	2.19	0.75
1:A:190:ILE:HD13	1:A:190:ILE:C	2.06	0.74
1:A:100:GLN:CB	1:A:109:LEU:HD22	2.18	0.74
1:A:210:LYS:CG	1:A:213:PRO:CD	2.66	0.74
1:A:181:HIS:HD2	1:A:183:CYS:SG	2.11	0.74
1:A:210:LYS:NZ	1:A:212:HIS:HB3	2.03	0.73
1:A:210:LYS:O	1:A:213:PRO:HD2	1.89	0.73
1:A:181:HIS:CD2	1:A:183:CYS:SG	2.82	0.73
1:A:216:GLY:O	1:A:217:THR:HG23	1.89	0.72
1:A:230:ASP:O	1:A:234:SER:HB2	1.89	0.71
1:A:215:ASP:HB3	1:A:217:THR:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLN:CG	3:A:525:HOH:O	2.31	0.69
1:A:83:TYR:CE2	1:A:124:ILE:HD11	2.27	0.69
1:A:210:LYS:C	1:A:213:PRO:HD2	2.14	0.68
1:A:100:GLN:HB2	1:A:109:LEU:CD2	2.20	0.68
1:A:20:TYR:O	1:A:90:LYS:HD3	1.93	0.68
1:A:194:GLY:N	1:A:197:VAL:HG13	2.08	0.68
1:A:165:LEU:CD2	1:A:249:ILE:HG12	2.23	0.68
1:A:46:ASP:OD2	3:A:593:HOH:O	2.12	0.67
1:A:186:HIS:ND1	2:A:330:SO4:O1	2.23	0.67
1:A:53:VAL:HA	1:A:81:LYS:HD2	1.75	0.67
1:A:308:ASN:ND2	3:A:404:HOH:O	2.27	0.66
1:A:194:GLY:H	1:A:197:VAL:HG11	1.58	0.66
1:A:278:TYR:HE2	1:A:288:LEU:HD21	1.61	0.66
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.61	0.66
1:A:18:ARG:CG	1:A:18:ARG:O	2.41	0.66
1:A:54:MET:HE3	3:A:398:HOH:O	1.87	0.65
1:A:194:GLY:N	1:A:197:VAL:CG1	2.58	0.65
1:A:264:LEU:HB3	1:A:266:ARG:HG3	1.79	0.65
1:A:225:LYS:HG3	3:A:560:HOH:O	1.97	0.64
1:A:210:LYS:CG	1:A:213:PRO:HD2	2.29	0.63
1:A:303:MET:CE	1:A:305:LEU:HD21	2.30	0.62
1:A:94:ILE:HD13	1:A:121:ILE:HD11	1.80	0.62
1:A:232:VAL:HG23	3:A:594:HOH:O	2.00	0.62
1:A:2:THR:HG22	1:A:5:ASP:H	1.65	0.62
1:A:259:THR:HG23	1:A:264:LEU:HB2	1.82	0.62
1:A:215:ASP:C	1:A:217:THR:H	2.01	0.62
1:A:318:THR:HG23	1:A:319:THR:N	2.15	0.62
1:A:329:PHE:CD2	1:A:329:PHE:O	2.53	0.62
1:A:57:LYS:CG	3:A:570:HOH:O	2.41	0.61
1:A:155:MET:O	3:A:584:HOH:O	2.16	0.61
1:A:273:MET:CE	1:A:275:LYS:CB	2.62	0.61
1:A:230:ASP:O	1:A:234:SER:CB	2.48	0.61
1:A:0:ACE:CH3	1:A:5:ASP:CB	2.78	0.60
1:A:138:ASN:ND2	3:A:452:HOH:O	2.35	0.59
1:A:212:HIS:CD2	1:A:218:ASN:H	2.21	0.59
1:A:315:LYS:O	1:A:318:THR:HG22	2.01	0.59
1:A:323:ILE:O	1:A:325:LYS:N	2.34	0.59
1:A:173:LEU:HD12	1:A:231:VAL:HG23	1.84	0.59
1:A:106:ARG:O	1:A:110:VAL:HG23	2.03	0.59
1:A:190:ILE:O	1:A:198:PRO:HD2	2.03	0.59
1:A:258:GLU:HG3	1:A:262:LYS:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:HIS:CD2	1:A:183:CYS:H	2.21	0.58
1:A:309:GLU:OE2	3:A:528:HOH:O	2.17	0.58
1:A:217:THR:O	1:A:218:ASN:HB2	2.03	0.57
1:A:312:GLN:NE2	3:A:408:HOH:O	2.37	0.57
1:A:40:LEU:HD23	1:A:74:THR:HG21	1.85	0.57
1:A:307:PRO:O	1:A:311:GLN:HB2	2.03	0.57
1:A:109:LEU:HD12	1:A:109:LEU:O	2.04	0.57
1:A:233:ASP:O	1:A:236:TYR:N	2.29	0.57
1:A:98:ALA:HB1	1:A:112:ARG:HH12	1.68	0.57
1:A:125:VAL:HG21	1:A:151:SER:HB2	1.85	0.57
1:A:318:THR:CG2	1:A:319:THR:H	2.17	0.57
1:A:121:ILE:HB	1:A:122:PRO:HD3	1.86	0.57
1:A:132:ILE:CD1	1:A:159:ILE:HG13	2.35	0.56
1:A:18:ARG:HG2	1:A:18:ARG:O	2.05	0.56
1:A:197:VAL:O	1:A:228:HIS:NE2	2.39	0.56
1:A:288:LEU:HB3	1:A:300:ILE:HD11	1.87	0.56
1:A:194:GLY:O	1:A:197:VAL:HG22	2.06	0.56
1:A:257:ALA:O	1:A:261:MET:HG2	2.06	0.56
1:A:38:SER:O	1:A:42:LYS:HB2	2.06	0.55
1:A:229:LYS:HD2	3:A:535:HOH:O	2.06	0.55
1:A:212:HIS:HB3	1:A:213:PRO:HD3	1.88	0.55
1:A:22:LYS:HE3	1:A:47:GLU:OE2	2.06	0.55
1:A:303:MET:HE3	1:A:305:LEU:HD21	1.87	0.55
1:A:210:LYS:NZ	1:A:212:HIS:CB	2.68	0.55
1:A:106:ARG:HG3	3:A:508:HOH:O	2.06	0.54
1:A:225:LYS:HZ3	1:A:226:LYS:NZ	2.06	0.54
1:A:210:LYS:HZ1	1:A:212:HIS:CB	2.12	0.54
1:A:272:THR:O	1:A:285:PHE:HA	2.07	0.54
1:A:23:ILE:HD12	1:A:45:ALA:HB2	1.88	0.54
1:A:110:VAL:O	1:A:114:VAL:HG23	2.08	0.54
1:A:100:GLN:HA	1:A:104:GLU:OE1	2.08	0.54
1:A:326:ASP:O	1:A:327:LEU:HB2	2.07	0.54
1:A:174:MET:O	1:A:178:LEU:N	2.34	0.54
1:A:249:ILE:O	1:A:252:SER:HB3	2.08	0.53
1:A:94:ILE:CD1	1:A:121:ILE:HD11	2.38	0.53
1:A:306:LYS:O	1:A:309:GLU:HB2	2.08	0.53
1:A:66:GLN:O	1:A:69:SER:OG	2.14	0.53
1:A:202:SER:O	1:A:210:LYS:HD2	2.08	0.53
1:A:267:VAL:HA	1:A:290:CYS:O	2.09	0.53
1:A:210:LYS:HE3	1:A:213:PRO:HD3	1.89	0.53
1:A:318:THR:HG23	1:A:319:THR:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HB2	1:A:156:HIS:CD2	2.44	0.53
1:A:121:ILE:O	1:A:125:VAL:HG23	2.09	0.53
1:A:325:LYS:HG2	1:A:325:LYS:O	2.09	0.52
1:A:132:ILE:HD11	1:A:159:ILE:HG13	1.91	0.52
1:A:0:ACE:H2	1:A:5:ASP:CB	2.33	0.52
1:A:142:VAL:HG22	1:A:320:LEU:CD2	2.39	0.52
1:A:188:TRP:CZ3	1:A:269:PRO:HD3	2.45	0.52
1:A:112:ARG:O	1:A:116:ILE:HG13	2.08	0.52
1:A:126:LYS:HG3	1:A:126:LYS:O	2.09	0.52
1:A:229:LYS:HE2	3:A:462:HOH:O	2.09	0.51
1:A:210:LYS:CB	1:A:213:PRO:HD2	2.40	0.51
1:A:318:THR:CG2	1:A:319:THR:N	2.71	0.51
1:A:186:HIS:O	1:A:204:MET:HA	2.11	0.51
1:A:110:VAL:HG22	1:A:139:PRO:HG3	1.91	0.50
1:A:243:GLY:O	1:A:244:TYR:HB3	2.11	0.50
1:A:106:ARG:O	1:A:110:VAL:CG2	2.59	0.50
1:A:57:LYS:O	1:A:61:GLU:HG2	2.11	0.50
1:A:62:MET:CE	1:A:79:SER:H	2.04	0.50
1:A:219:LYS:HB3	1:A:219:LYS:NZ	2.26	0.50
1:A:219:LYS:NZ	1:A:219:LYS:CB	2.75	0.50
1:A:110:VAL:HG11	1:A:142:VAL:HG11	1.93	0.50
1:A:83:TYR:CE2	1:A:124:ILE:CD1	2.93	0.49
1:A:288:LEU:HD23	1:A:300:ILE:HD11	1.92	0.49
1:A:288:LEU:HD23	1:A:300:ILE:HD12	1.90	0.49
1:A:22:LYS:HG3	1:A:47:GLU:HB3	1.95	0.49
1:A:233:ASP:C	1:A:235:ALA:N	2.66	0.49
1:A:318:THR:CB	3:A:608:HOH:O	2.60	0.49
1:A:62:MET:HE1	3:A:479:HOH:O	2.13	0.48
1:A:190:ILE:HD13	1:A:190:ILE:O	2.13	0.48
1:A:165:LEU:O	1:A:168:ALA:HB3	2.13	0.48
1:A:219:LYS:HB3	1:A:219:LYS:HZ3	1.78	0.48
1:A:110:VAL:CG1	1:A:142:VAL:HG11	2.43	0.48
1:A:63:MET:CE	3:A:381:HOH:O	2.62	0.48
1:A:214:LEU:C	1:A:216:GLY:H	2.17	0.48
1:A:320:LEU:O	1:A:324:GLN:HG3	2.14	0.48
1:A:164:ASN:O	3:A:484:HOH:O	2.20	0.47
1:A:18:ARG:HG2	1:A:18:ARG:NH1	2.26	0.47
1:A:145:TYR:O	1:A:148:TRP:HB3	2.14	0.47
1:A:0:ACE:H1	1:A:5:ASP:CB	2.45	0.47
1:A:217:THR:OG1	1:A:218:ASN:N	2.40	0.47
1:A:110:VAL:HG11	1:A:323:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:CE	1:A:213:PRO:HD3	2.45	0.46
1:A:278:TYR:CE2	1:A:288:LEU:HD21	2.47	0.46
1:A:210:LYS:CB	1:A:213:PRO:CD	2.93	0.46
1:A:58:LEU:HG	1:A:79:SER:HB2	1.97	0.46
1:A:229:LYS:HB2	1:A:229:LYS:HE3	1.32	0.46
1:A:318:THR:HA	3:A:608:HOH:O	2.15	0.46
1:A:130:ASP:HA	1:A:157:ARG:HH12	1.80	0.46
1:A:153:LEU:HB2	1:A:158:ILE:HD11	1.96	0.46
1:A:288:LEU:HB3	1:A:300:ILE:CD1	2.45	0.46
1:A:288:LEU:HD23	1:A:300:ILE:HD13	1.92	0.46
1:A:329:PHE:CG	1:A:329:PHE:O	2.68	0.46
1:A:44:LEU:HD11	1:A:258:GLU:HB2	1.98	0.46
1:A:210:LYS:CG	1:A:213:PRO:HD3	2.31	0.45
1:A:165:LEU:HB3	3:A:519:HOH:O	2.16	0.45
1:A:171:ARG:HD3	1:A:186:HIS:HA	1.99	0.45
1:A:325:LYS:HB3	1:A:325:LYS:HE2	1.54	0.45
1:A:50:LEU:O	1:A:79:SER:HA	2.17	0.45
1:A:157:ARG:C	1:A:158:ILE:HG12	2.37	0.45
1:A:171:ARG:CD	1:A:185:CYS:O	2.65	0.45
1:A:171:ARG:HD2	1:A:185:CYS:O	2.17	0.45
1:A:264:LEU:HD13	1:A:266:ARG:HD3	1.97	0.45
1:A:145:TYR:OH	1:A:149:LYS:NZ	2.49	0.45
1:A:172:TYR:HA	1:A:182:SER:HB3	1.99	0.45
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.73	0.45
1:A:100:GLN:HG3	1:A:104:GLU:HB3	1.98	0.44
1:A:83:TYR:HD2	1:A:124:ILE:HD13	1.82	0.44
1:A:210:LYS:HB3	1:A:213:PRO:CD	2.47	0.44
1:A:142:VAL:HG22	1:A:320:LEU:HD22	1.98	0.44
1:A:165:LEU:HD22	1:A:249:ILE:HG12	1.95	0.44
1:A:178:LEU:HD11	1:A:211:LEU:HD21	2.00	0.44
1:A:210:LYS:HE3	1:A:213:PRO:HG3	2.00	0.44
1:A:237:GLU:HA	1:A:240:LYS:HE3	1.98	0.44
1:A:237:GLU:O	1:A:241:LEU:HB2	2.17	0.44
1:A:229:LYS:O	1:A:232:VAL:HG12	2.18	0.44
1:A:92:VAL:HG21	1:A:124:ILE:CG2	2.48	0.43
1:A:62:MET:CE	1:A:78:VAL:CA	2.86	0.43
1:A:288:LEU:CB	1:A:300:ILE:HD11	2.49	0.43
1:A:312:GLN:HG2	3:A:557:HOH:O	2.18	0.43
1:A:114:VAL:O	1:A:118:LYS:HG3	2.18	0.43
1:A:225:LYS:NZ	1:A:226:LYS:CE	2.81	0.43
1:A:277:PHE:O	1:A:278:TYR:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:C	1:A:235:ALA:H	2.22	0.42
1:A:265:CYS:HA	1:A:291:VAL:HG13	2.00	0.42
1:A:28:VAL:HG22	1:A:52:ASP:HB2	2.02	0.42
1:A:313:LEU:HA	1:A:313:LEU:HD12	1.72	0.42
1:A:83:TYR:CD2	1:A:124:ILE:HD13	2.55	0.42
1:A:303:MET:HE3	1:A:303:MET:HB2	1.92	0.42
1:A:303:MET:HE1	1:A:305:LEU:HD21	2.02	0.41
1:A:128:SER:HB3	1:A:131:CYS:HB3	2.01	0.41
1:A:28:VAL:HG11	1:A:50:LEU:HD13	2.02	0.41
1:A:223:ASP:HB3	3:A:349:HOH:O	2.19	0.41
1:A:212:HIS:CD2	1:A:218:ASN:N	2.86	0.41
1:A:62:MET:CE	3:A:479:HOH:O	2.67	0.41
1:A:276:ASP:OD1	1:A:276:ASP:O	2.38	0.41
1:A:160:GLY:HA3	1:A:271:SER:HB3	2.01	0.41
1:A:52:ASP:OD1	1:A:54:MET:CE	2.69	0.41
1:A:61:GLU:HA	1:A:61:GLU:OE2	2.19	0.41
1:A:94:ILE:HG21	1:A:94:ILE:HD13	1.88	0.41
1:A:7:LEU:O	1:A:7:LEU:HG	2.21	0.41
1:A:189:VAL:HG13	1:A:197:VAL:HB	2.03	0.40
1:A:83:TYR:CD2	1:A:124:ILE:CD1	3.04	0.40
1:A:173:LEU:HD12	1:A:231:VAL:CG2	2.48	0.40
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.82	0.40
1:A:305:LEU:HD12	1:A:313:LEU:HD22	2.04	0.40
1:A:201:TRP:CD1	1:A:219:LYS:HG2	2.57	0.40
1:A:55:GLU:HB2	1:A:56:ASP:H	1.71	0.40
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.76	0.40

All (16) 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:329:PHE:CE1	1:A:329:PHE:CE1[32_555]	0.72	1.48
1:A:329:PHE:CE1	1:A:329:PHE:CZ[32_555]	1.37	0.83
1:A:329:PHE:CB	3:A:419:HOH:O[32_555]	1.39	0.81
1:A:329:PHE:CD1	1:A:329:PHE:CZ[32_555]	1.42	0.78
3:A:364:HOH:O	3:A:364:HOH:O[32_555]	1.61	0.59
3:A:590:HOH:O	3:A:590:HOH:O[14_555]	1.66	0.54
1:A:329:PHE:O	1:A:329:PHE:CE2[32_555]	1.88	0.32
1:A:108:ASN:ND2	1:A:329:PHE:CD2[32_555]	1.88	0.32
1:A:329:PHE:CD1	1:A:329:PHE:CE1[32_555]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:OD1	1:A:329:PHE:O[32_555]	2.00	0.20
1:A:329:PHE:CZ	1:A:329:PHE:CZ[32_555]	2.04	0.16
3:A:576:HOH:O	3:A:596:HOH:O[27_555]	2.08	0.12
1:A:329:PHE:CG	1:A:329:PHE:CZ[32_555]	2.11	0.09
1:A:188:TRP:NE1	1:A:207:ALA:O[14_555]	2.16	0.04
1:A:329:PHE:C	1:A:329:PHE:CE2[32_555]	2.19	0.01
1:A:126:LYS:O	3:A:602:HOH:O[27_555]	2.19	0.01

## 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	328/330 (99%)	289 (88%)	27 (8%)	12 (4%)	<b>4</b> <b>1</b>

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	A	217	THR
1	A	218	ASN
1	A	221	LYS
1	A	222	GLN
1	A	223	ASP
1	A	327	LEU
1	A	87	ALA
1	A	234	SER
1	A	100	GLN
1	A	219	LYS
1	A	224	TRP

### 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	286/286 (100%)	244 (85%)	42 (15%)	<b>4</b> <b>2</b>

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	LEU
1	A	17	PRO
1	A	18	ARG
1	A	37	ILE
1	A	44	LEU
1	A	55	GLU
1	A	74	THR
1	A	85	VAL
1	A	91	LEU
1	A	107	LEU
1	A	108	ASN
1	A	121	ILE
1	A	123	ASN
1	A	126	LYS
1	A	132	ILE
1	A	150	LEU
1	A	158	ILE
1	A	159	ILE
1	A	169	ARG
1	A	176	GLU
1	A	180	VAL
1	A	190	ILE
1	A	209	ILE
1	A	212	HIS
1	A	221	LYS
1	A	222	GLN
1	A	225	LYS
1	A	226	LYS
1	A	233	ASP

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Mol	Chain	Res	Type
1	A	256	LEU
1	A	272	THR
1	A	276	ASP
1	A	282	ASP
1	A	288	LEU
1	A	293	ASN
1	A	300	ILE
1	A	308	ASN
1	A	311	GLN
1	A	322	ASP
1	A	328	LYS
1	A	329	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	66	GLN
1	A	127	HIS
1	A	138	ASN
1	A	181	HIS
1	A	293	ASN
1	A	295	HIS
1	A	312	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 ⓘ

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	330	-	4,4,4	1.52	1 (25%)	6,6,6	0.64	0
2	SO4	A	331	-	4,4,4	1.20	0	6,6,6	0.40	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	330	-	-	0/0/0/0	0/0/0/0
2	SO4	A	331	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	330	SO4	O4-S	2.60	1.56	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	330	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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.