



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2014 – 12:47 AM EDT

PDB ID : 4AJP
Title : Human LDHA in complex with 2-((4-((3-((2-methyl-1,3-benzothiazol-6yl)amino)-3-oxo-propyl)amino)-4-oxo-butyl)phenyl)methyl)propanedioicacid
Authors : Tucker, J.A.; Brassington, C.; Caputo, A.; Ward, R.; Pearson, S.; Watson, M.; Tart, J.; Davies, G.
Deposited on : 2012-02-16
Resolution : 2.38 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

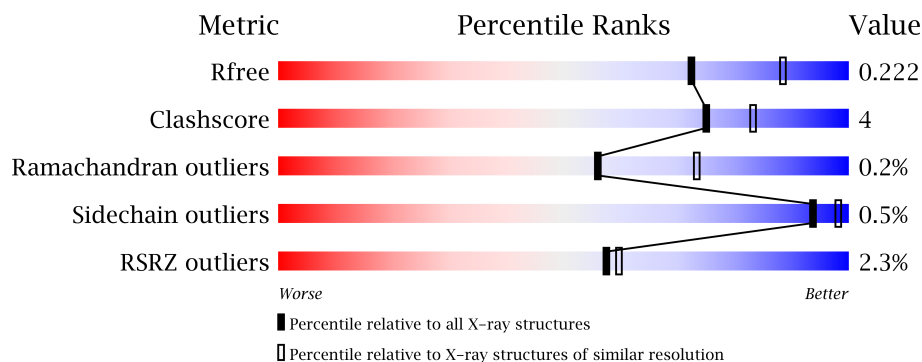
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.38 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))
R_{free}	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	1334	-	X
4	GOL	C	1332	-	X
4	GOL	C	1333	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10715 atoms, of which 0 are hydrogen and 0 are deuterium.

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 L-LACTATE DEHYDROGENASE A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	1	0
			2527	1614	428	472	13			
1	B	329	Total	C	N	O	S	0	2	0
			2520	1609	429	468	14			
1	C	329	Total	C	N	O	S	0	2	0
			2527	1611	430	473	13			
1	D	331	Total	C	N	O	S	0	1	0
			2534	1618	431	472	13			

There are 24 discrepancies between the modelled and reference sequences:

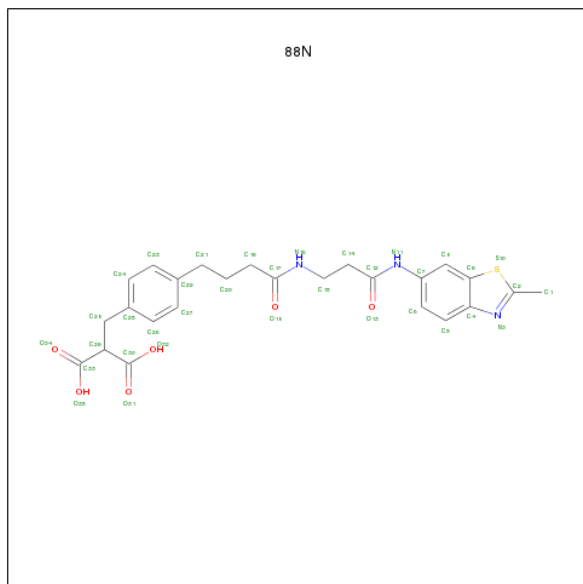
Chain	Residue	Modelled	Actual	Comment	Reference
A	332	HIS	-	EXPRESSION TAG	UNP P00338
A	333	HIS	-	EXPRESSION TAG	UNP P00338
A	334	HIS	-	EXPRESSION TAG	UNP P00338
A	335	HIS	-	EXPRESSION TAG	UNP P00338
A	336	HIS	-	EXPRESSION TAG	UNP P00338
A	337	HIS	-	EXPRESSION TAG	UNP P00338
B	332	HIS	-	EXPRESSION TAG	UNP P00338
B	333	HIS	-	EXPRESSION TAG	UNP P00338
B	334	HIS	-	EXPRESSION TAG	UNP P00338
B	335	HIS	-	EXPRESSION TAG	UNP P00338
B	336	HIS	-	EXPRESSION TAG	UNP P00338
B	337	HIS	-	EXPRESSION TAG	UNP P00338
C	332	HIS	-	EXPRESSION TAG	UNP P00338
C	333	HIS	-	EXPRESSION TAG	UNP P00338
C	334	HIS	-	EXPRESSION TAG	UNP P00338
C	335	HIS	-	EXPRESSION TAG	UNP P00338
C	336	HIS	-	EXPRESSION TAG	UNP P00338
C	337	HIS	-	EXPRESSION TAG	UNP P00338
D	332	HIS	-	EXPRESSION TAG	UNP P00338
D	333	HIS	-	EXPRESSION TAG	UNP P00338
D	334	HIS	-	EXPRESSION TAG	UNP P00338

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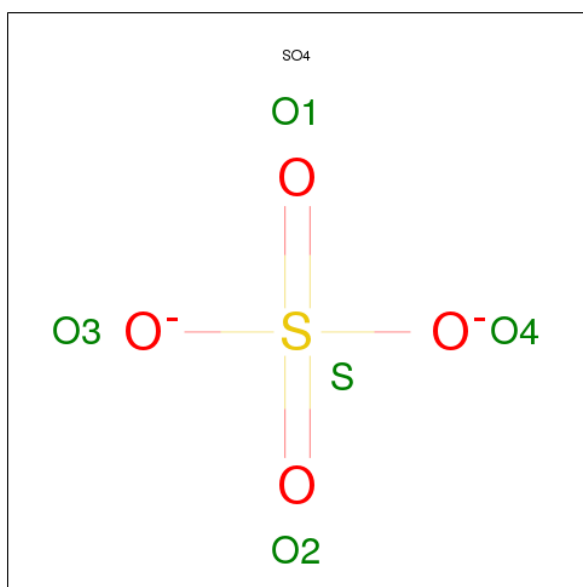
Chain	Residue	Modelled	Actual	Comment	Reference
D	335	HIS	-	EXPRESSION TAG	UNP P00338
D	336	HIS	-	EXPRESSION TAG	UNP P00338
D	337	HIS	-	EXPRESSION TAG	UNP P00338

- Molecule 2 is {4-[4-({3-[(2-METHYL-1,3-BENZOTHAZOL-6-YL)AMINO]-3-OXOPROPYL}AMINO)-4-OXOBUTYL]BENZYL}PROPANEDIOICACID (three-letter code: 88N) (formula: C₂₅H₂₇N₃O₆S).



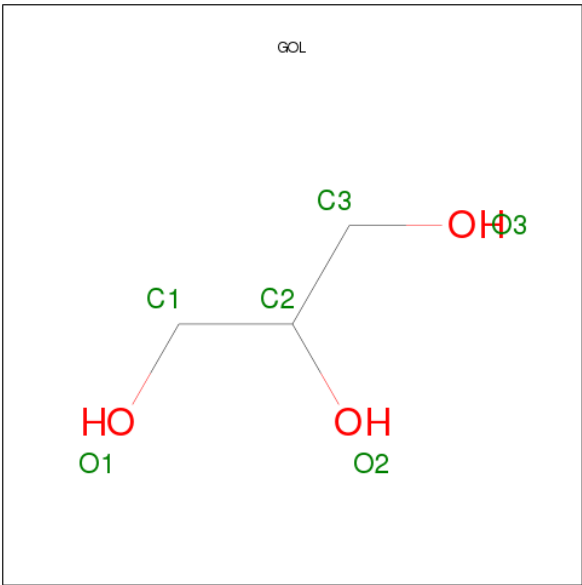
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	25	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			35	25	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			35	25	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			35	25	3	6	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	109	Total	O	0	0
			109	109		
5	C	88	Total	O	0	0
			88	88		
5	D	76	Total	O	0	0
			76	76		

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.

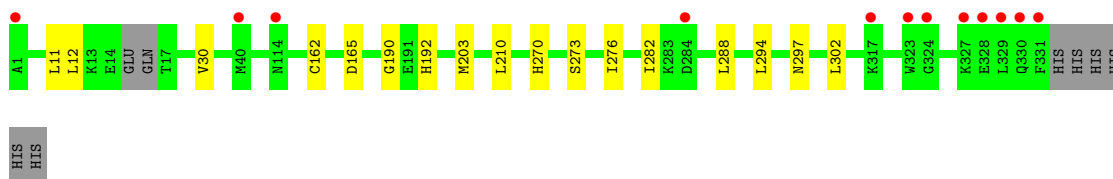
• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN

Chain A: 



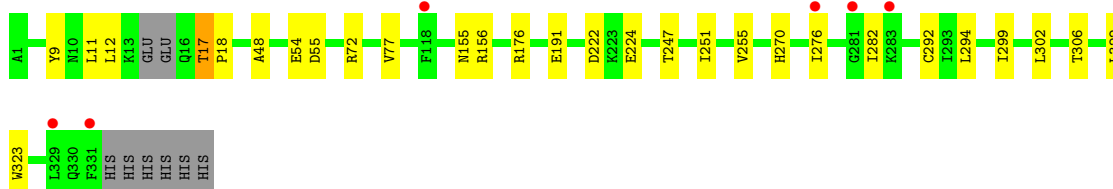
• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN

Chain B: 



• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.98Å 136.78Å 83.79Å 90.00° 102.31° 90.00°	Depositor
Resolution (Å)	56.85 – 2.38 56.85 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (56.85-2.38) 98.8 (56.85-2.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.166 , 0.215 0.174 , 0.222	Depositor DCC
R_{free} test set	2804 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 55746 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10715	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 88N, 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	0.63	2/2570 (0.1%)	0.68	0/3483
1	B	0.61	0/2562	0.71	0/3474
1	C	0.61	1/2570 (0.0%)	0.67	1/3484 (0.0%)
1	D	0.60	1/2577 (0.0%)	0.69	0/3494
All	All	0.61	4/10279 (0.0%)	0.69	1/13935 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	TRP	CD2-CE2	5.55	1.48	1.41
1	A	147	TRP	CD2-CE2	5.40	1.47	1.41
1	D	249	TRP	CD2-CE2	5.33	1.47	1.41
1	C	323	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2527	0	2564	18	0
1	B	2520	0	2557	27	0
1	C	2527	0	2556	33	0
1	D	2534	0	2572	24	0
2	A	35	0	25	0	0
2	B	35	0	25	1	0
2	C	35	0	25	0	0
2	D	35	0	25	0	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	B	6	0	8	1	0
4	C	12	0	16	3	0
5	A	121	0	0	2	0
5	B	109	0	0	1	0
5	C	88	0	0	0	0
5	D	76	0	0	0	0
All	All	10715	0	10373	82	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:11:LEU:HD11	1:C:302:LEU:CD1	1.72	1.16
1:B:302:LEU:HD11	1:C:11:LEU:HD11	1.37	1.05
1:B:302:LEU:CD1	1:C:11:LEU:HD11	1.88	1.02
1:B:11:LEU:HD11	1:C:302:LEU:HD12	1.46	0.97
1:D:276:ILE:CD1	1:D:282:ILE:HD13	2.01	0.91
1:C:17:THR:HG22	1:C:18:PRO:HD2	1.58	0.85
1:B:302:LEU:CD1	1:C:11:LEU:CD1	2.59	0.81
1:C:276:ILE:CD1	1:C:282:ILE:HD13	2.11	0.80
1:A:11:LEU:HD11	1:D:302:LEU:HD13	1.62	0.79
1:A:12:LEU:HA	1:A:13:LYS:CB	2.13	0.79
1:B:276:ILE:HD13	1:B:282:ILE:CD1	2.14	0.77
1:B:276:ILE:HD13	1:B:282:ILE:HD13	1.66	0.76
1:D:276:ILE:HD13	1:D:282:ILE:HD13	1.67	0.75
1:C:276:ILE:HD11	1:C:282:ILE:HD13	1.68	0.74
1:A:276:ILE:HD13	1:A:282:ILE:HD13	1.68	0.74
1:A:11:LEU:CD1	1:D:302:LEU:HD13	2.17	0.74
1:B:11:LEU:CD1	1:C:302:LEU:HD12	2.18	0.74
1:C:17:THR:HG22	1:C:18:PRO:CD	2.19	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:302:LEU:HD12	1:C:11:LEU:CD1	2.20	0.72
1:B:276:ILE:CD1	1:B:282:ILE:HD13	2.21	0.71
1:B:270:HIS:CD2	1:B:294:LEU:HD22	2.27	0.69
1:B:11:LEU:CD1	1:C:302:LEU:CD1	2.64	0.69
1:B:302:LEU:HD12	1:C:11:LEU:HD11	1.75	0.66
1:B:302:LEU:HD13	1:C:9:TYR:HD2	1.63	0.63
1:D:276:ILE:HD11	1:D:282:ILE:HD13	1.79	0.63
1:B:11:LEU:HD11	1:C:302:LEU:HD13	1.74	0.62
1:A:12:LEU:CA	1:A:13:LYS:CB	2.78	0.61
4:B:1332:GOL:O3	5:B:2108:HOH:O	2.16	0.59
1:C:156:ARG:NE	4:C:1333:GOL:O2	2.36	0.58
1:A:276:ILE:HG12	1:A:288:LEU:HD11	1.87	0.56
1:C:54[B]:GLU:HG2	1:C:55[B]:ASP:H	1.70	0.56
1:A:11:LEU:HD11	1:D:302:LEU:CD1	2.35	0.55
1:B:12:LEU:HD11	1:C:155:ASN:ND2	2.20	0.55
1:C:156:ARG:NH2	4:C:1333:GOL:O2	2.38	0.55
1:B:276:ILE:HD13	1:B:282:ILE:HD12	1.88	0.54
1:A:12:LEU:HD11	1:D:155:ASN:ND2	2.23	0.54
1:B:11:LEU:HD11	1:C:302:LEU:HD11	1.82	0.54
1:B:203[B]:MET:HG2	1:B:210:LEU:HD12	1.92	0.52
1:B:302:LEU:HD12	1:B:302:LEU:N	2.25	0.52
1:A:53:ILE:HD12	5:A:2024:HOH:O	2.11	0.51
1:C:251:ILE:O	1:C:255:VAL:HG23	2.11	0.50
1:B:203[B]:MET:SD	1:B:210:LEU:HD12	2.52	0.50
1:D:251:ILE:O	1:D:255:VAL:HG23	2.11	0.49
1:D:106:LEU:O	1:D:109:VAL:HG23	2.13	0.49
1:D:272:VAL:O	1:D:289:SER:HA	2.13	0.49
1:B:190:GLY:HA2	1:B:288:LEU:HD13	1.95	0.48
1:D:180:HIS:CE1	1:D:182:LEU:HD12	2.49	0.48
1:C:276:ILE:CD1	1:C:282:ILE:CD1	2.89	0.48
1:B:297:ASN:HB3	1:C:12:LEU:HD21	1.95	0.47
1:D:113:VAL:HG21	1:D:329:LEU:CD2	2.45	0.47
1:A:125:LYS:HE2	1:A:126:TYR:CZ	2.49	0.47
1:C:276:ILE:HD13	1:C:282:ILE:HD13	1.96	0.46
1:C:270:HIS:CD2	1:C:294:LEU:HD22	2.51	0.46
1:A:203:MET:HB3	1:A:210:LEU:HD12	1.97	0.45
1:B:165:ASP:OD2	1:B:192:HIS:ND1	2.49	0.45
1:C:306:THR:HG23	1:C:306:THR:O	2.17	0.45
1:D:293:ILE:HD12	1:D:301:ASP:HB2	1.98	0.45
1:A:251:ILE:HG22	5:A:2104:HOH:O	2.15	0.45
1:A:276:ILE:HG12	1:A:288:LEU:CD1	2.46	0.45
1:D:191:GLU:HG3	1:D:322:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:278:GLY:C	1:D:279:LEU:HD12	2.37	0.45
1:D:274:THR:HG21	1:D:292:CYS:SG	2.57	0.44
1:C:176:ARG:NH2	1:C:224:GLU:O	2.47	0.44
1:D:141:ILE:HD13	1:D:325:ILE:CG2	2.48	0.44
1:D:141:ILE:HD13	1:D:325:ILE:HG21	2.00	0.43
1:A:276:ILE:HD13	1:A:282:ILE:CD1	2.43	0.43
1:C:54[B]:GLU:CD	1:C:54[B]:GLU:H	2.23	0.42
1:B:30:VAL:HG21	2:B:1333:88N:C27	2.50	0.42
1:A:302:LEU:HD13	1:D:11:LEU:HD11	2.02	0.41
1:C:292:CYS:HB3	1:C:299:ILE:HG23	2.01	0.41
1:C:156:ARG:NH2	4:C:1333:GOL:HO2	2.17	0.41
1:A:300:SER:HA	1:D:12:LEU:HD23	2.03	0.41
1:B:276:ILE:HG12	1:B:288:LEU:HG	2.02	0.41
1:A:155:ASN:CG	1:D:12:LEU:HD21	2.40	0.41
1:C:48:ALA:HA	1:C:77:VAL:O	2.21	0.41
1:A:269:VAL:HA	1:A:292:CYS:O	2.21	0.41
1:D:240:VAL:CG1	1:D:247:THR:HG22	2.50	0.41
1:D:276:ILE:HG12	1:D:288:LEU:HD11	2.03	0.40
1:D:165:ASP:OD1	1:D:192:HIS:ND1	2.46	0.40
1:C:54[B]:GLU:HG2	1:C:55[B]:ASP:N	2.34	0.40
1:B:162:CYS:HA	1:B:165:ASP:OD2	2.22	0.40
1:C:191:GLU:HG3	1:C:322:LEU:HD21	2.03	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	326/337 (97%)	318 (98%)	7 (2%)	1 (0%)	50	66
1	B	327/337 (97%)	321 (98%)	6 (2%)	0	100	100
1	C	327/337 (97%)	320 (98%)	6 (2%)	1 (0%)	50	66
1	D	330/337 (98%)	322 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1310/1348 (97%)	1281 (98%)	27 (2%)	2 (0%)	56 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	ASP
1	A	222	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	276/293 (94%)	274 (99%)	2 (1%)	91 97
1	B	274/293 (94%)	273 (100%)	1 (0%)	95 98
1	C	276/293 (94%)	274 (99%)	2 (1%)	91 97
1	D	275/293 (94%)	275 (100%)	0	100 100
All	All	1101/1172 (94%)	1096 (100%)	5 (0%)	94 98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	A	288	LEU
1	B	273	SER
1	C	17	THR
1	C	247	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

18 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	88N	A	1332	-	37,37,37	0.41	0	49,50,50	0.99	5 (10%)
3	SO4	A	1333	-	4,4,4	0.45	0	6,6,6	0.39	0
3	SO4	A	1334	-	4,4,4	0.28	0	6,6,6	0.17	0
3	SO4	A	1335	-	4,4,4	0.29	0	6,6,6	0.41	0
3	SO4	A	1336	-	4,4,4	0.23	0	6,6,6	0.31	0
4	GOL	B	1332	-	5,5,5	0.30	0	5,5,5	0.37	0
2	88N	B	1333	-	37,37,37	0.40	0	49,50,50	1.05	5 (10%)
3	SO4	B	1334	-	4,4,4	0.16	0	6,6,6	0.61	0
3	SO4	B	1335	-	4,4,4	0.37	0	6,6,6	0.25	0
3	SO4	B	1336	-	4,4,4	0.47	0	6,6,6	0.24	0
4	GOL	C	1332	-	5,5,5	0.23	0	5,5,5	0.38	0
4	GOL	C	1333	-	5,5,5	0.32	0	5,5,5	0.66	0
2	88N	C	1334	-	37,37,37	0.39	0	49,50,50	1.03	5 (10%)
3	SO4	C	1335	-	4,4,4	0.40	0	6,6,6	0.11	0
3	SO4	C	1336	-	4,4,4	0.40	0	6,6,6	0.29	0
2	88N	D	1332	-	37,37,37	0.41	0	49,50,50	0.95	5 (10%)
3	SO4	D	1333	-	4,4,4	0.29	0	6,6,6	0.33	0
3	SO4	D	1334	-	4,4,4	0.42	0	6,6,6	0.30	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	88N	A	1332	-	-	0/28/28/28	0/3/3/3
3	SO4	A	1333	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1334	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1335	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1336	-	-	0/0/0/0	0/0/0/0
4	GOL	B	1332	-	-	0/4/4/4	0/0/0/0
2	88N	B	1333	-	-	0/28/28/28	0/3/3/3
3	SO4	B	1334	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1335	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1336	-	-	0/0/0/0	0/0/0/0
4	GOL	C	1332	-	-	0/4/4/4	0/0/0/0
4	GOL	C	1333	-	-	0/4/4/4	0/0/0/0
2	88N	C	1334	-	-	0/28/28/28	0/3/3/3
3	SO4	C	1335	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1336	-	-	0/0/0/0	0/0/0/0
2	88N	D	1332	-	-	0/28/28/28	0/3/3/3
3	SO4	D	1333	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1334	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1333	88N	C9-C4-N3	2.97	114.94	108.08
2	C	1334	88N	C9-C4-N3	2.95	114.88	108.08
2	D	1332	88N	C9-C4-N3	2.93	114.85	108.08
2	A	1332	88N	C9-C4-N3	2.92	114.83	108.08
2	A	1332	88N	C2-N3-C4	2.80	110.73	106.57
2	D	1332	88N	C2-N3-C4	2.77	110.68	106.57
2	B	1333	88N	C2-N3-C4	2.77	110.68	106.57
2	C	1334	88N	C2-N3-C4	2.72	110.60	106.57
2	A	1332	88N	C7-C8-C9	-2.56	118.69	121.25
2	B	1333	88N	C7-C8-C9	-2.52	118.72	121.25
2	C	1334	88N	C7-C8-C9	-2.51	118.73	121.25
2	D	1332	88N	C7-C8-C9	-2.46	118.78	121.25
2	B	1333	88N	C8-C9-S10	2.25	128.99	124.84
2	B	1333	88N	C4-C9-S10	-2.19	109.28	112.03
2	C	1334	88N	C8-C9-S10	2.17	128.84	124.84
2	D	1332	88N	C8-C9-S10	2.12	128.74	124.84
2	C	1334	88N	C4-C9-S10	-2.10	109.39	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1332	88N	C4-C9-S10	-2.09	109.40	112.03
2	A	1332	88N	C8-C9-S10	2.06	128.64	124.84
2	A	1332	88N	C4-C9-S10	-2.04	109.47	112.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/337 (97%)	-0.06	5 (1%) 70 72	24, 33, 50, 87	0
1	B	329/337 (97%)	0.00	12 (3%) 41 43	24, 34, 54, 95	0
1	C	329/337 (97%)	0.02	6 (1%) 65 67	25, 36, 57, 74	1 (0%)
1	D	331/337 (98%)	-0.04	7 (2%) 60 62	25, 35, 56, 75	0
All	All	1318/1348 (97%)	-0.02	30 (2%) 57 60	24, 35, 55, 95	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	PHE	5.7
1	B	331	PHE	5.2
1	D	331	PHE	4.6
1	C	281	GLY	3.8
1	B	330	GLN	3.8
1	C	331	PHE	3.8
1	B	324	GLY	3.4
1	A	330	GLN	3.3
1	B	323	TRP	3.0
1	B	328	GLU	3.0
1	D	281	GLY	2.9
1	D	329	LEU	2.9
1	B	329	LEU	2.9
1	B	284	ASP	2.9
1	A	2	THR	2.8
1	B	1	ALA	2.7
1	C	118	PHE	2.7
1	C	276	ILE	2.6
1	B	317	LYS	2.4
1	D	325	ILE	2.3
1	D	2	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	286	VAL	2.2
1	C	283	LYS	2.2
1	D	1	ALA	2.2
1	B	114	ASN	2.1
1	C	329	LEU	2.1
1	A	12	LEU	2.1
1	B	327	LYS	2.0
1	B	40	MET	2.0
1	A	118	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	C	1332	6/6	0.19	3.16	47,50,51,52	0
3	SO4	A	1334	5/5	0.19	2.11	52,55,56,57	0
4	GOL	C	1333	6/6	0.19	2.01	38,41,43,44	0
3	SO4	C	1336	5/5	0.23	1.87	59,61,61,63	0
3	SO4	B	1335	5/5	0.15	0.99	54,55,58,61	0
3	SO4	A	1335	5/5	0.14	0.65	51,56,58,58	0
3	SO4	A	1336	5/5	0.17	0.62	63,65,68,68	0
3	SO4	D	1334	5/5	0.17	0.18	59,61,63,64	0
2	88N	C	1334	35/35	0.12	0.03	25,31,34,36	0
4	GOL	B	1332	6/6	0.12	0.01	42,47,50,52	0
3	SO4	D	1333	5/5	0.12	-0.12	42,44,45,47	0
2	88N	A	1332	35/35	0.11	-0.14	27,30,35,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	88N	B	1333	35/35	0.11	-0.22	26,29,35,35	0
2	88N	D	1332	35/35	0.10	-0.34	30,33,37,41	0
3	SO4	A	1333	5/5	0.10	-1.03	41,42,47,48	0
3	SO4	C	1335	5/5	0.10	-1.15	43,44,47,49	0
3	SO4	B	1336	5/5	0.12	-1.17	62,65,66,69	0
3	SO4	B	1334	5/5	0.10	-1.69	43,44,48,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.