



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:18 am GMT

PDB ID : 4OKN  
Title : Crystal structure of human muscle L-lactate dehydrogenase, ternary complex with NADH and oxalate  
Authors : Kolappan, S.; Craig, L.  
Deposited on : 2014-01-22  
Resolution : 2.10 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

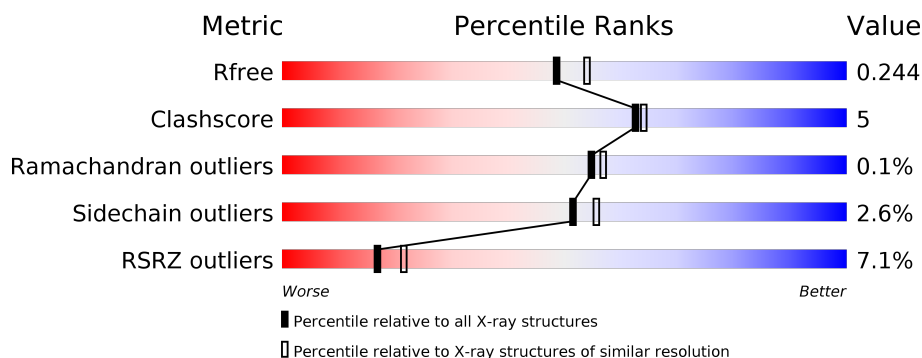
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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.

Mol	Chain	Length	Quality of chain
1	A	337	<div> <div>6%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	B	337	<div> <div>9%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	337	<div> <div>4%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	D	337	<div> <div>4%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	E	337	<div> <div>7%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	F	337	<div> <div>7%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	337	
1	H	337	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	G	402	-	-	X	-
4	SO4	E	404	-	-	-	X
4	SO4	F	403	-	-	-	X
5	KAN	B	403	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21753 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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2567	1639	439	476	13			
1	B	331	Total	C	N	O	S	0	0	0
			2567	1639	439	476	13			
1	C	331	Total	C	N	O	S	0	0	0
			2567	1639	439	476	13			
1	D	331	Total	C	N	O	S	0	0	0
			2567	1639	439	476	13			
1	E	331	Total	C	N	O	S	0	1	0
			2575	1643	440	479	13			
1	F	331	Total	C	N	O	S	0	0	0
			2567	1639	439	476	13			
1	G	331	Total	C	N	O	S	0	0	0
			2567	1639	439	476	13			
1	H	331	Total	C	N	O	S	0	0	0
			2567	1639	439	476	13			

There are 48 discrepancies between the modelled and reference sequences:

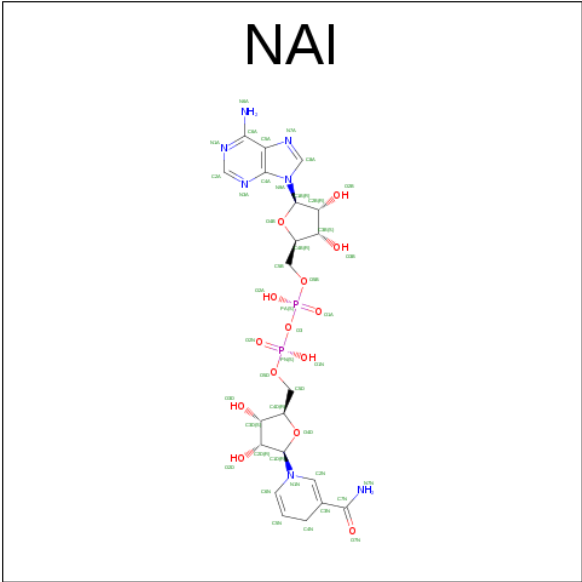
Chain	Residue	Modelled	Actual	Comment	Reference
A	333	HIS	-	EXPRESSION TAG	UNP P00338
A	334	HIS	-	EXPRESSION TAG	UNP P00338
A	335	HIS	-	EXPRESSION TAG	UNP P00338
A	336	HIS	-	EXPRESSION TAG	UNP P00338
A	337	HIS	-	EXPRESSION TAG	UNP P00338
A	338	HIS	-	EXPRESSION TAG	UNP P00338
B	333	HIS	-	EXPRESSION TAG	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
B	338	HIS	-	EXPRESSION TAG	UNP P00338
C	333	HIS	-	EXPRESSION TAG	UNP P00338

*Continued on next page...*

*Continued from previous page...*

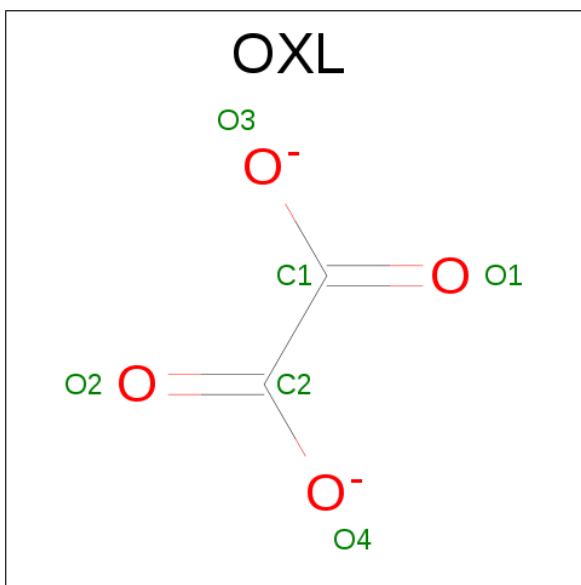
Chain	Residue	Modelled	Actual	Comment	Reference
C	334	HIS	-	EXPRESSION TAG	UNP P00338
C	335	HIS	-	EXPRESSION TAG	UNP P00338
C	336	HIS	-	EXPRESSION TAG	UNP P00338
C	337	HIS	-	EXPRESSION TAG	UNP P00338
C	338	HIS	-	EXPRESSION TAG	UNP P00338
D	333	HIS	-	EXPRESSION TAG	UNP P00338
D	334	HIS	-	EXPRESSION TAG	UNP P00338
D	335	HIS	-	EXPRESSION TAG	UNP P00338
D	336	HIS	-	EXPRESSION TAG	UNP P00338
D	337	HIS	-	EXPRESSION TAG	UNP P00338
D	338	HIS	-	EXPRESSION TAG	UNP P00338
E	333	HIS	-	EXPRESSION TAG	UNP P00338
E	334	HIS	-	EXPRESSION TAG	UNP P00338
E	335	HIS	-	EXPRESSION TAG	UNP P00338
E	336	HIS	-	EXPRESSION TAG	UNP P00338
E	337	HIS	-	EXPRESSION TAG	UNP P00338
E	338	HIS	-	EXPRESSION TAG	UNP P00338
F	333	HIS	-	EXPRESSION TAG	UNP P00338
F	334	HIS	-	EXPRESSION TAG	UNP P00338
F	335	HIS	-	EXPRESSION TAG	UNP P00338
F	336	HIS	-	EXPRESSION TAG	UNP P00338
F	337	HIS	-	EXPRESSION TAG	UNP P00338
F	338	HIS	-	EXPRESSION TAG	UNP P00338
G	333	HIS	-	EXPRESSION TAG	UNP P00338
G	334	HIS	-	EXPRESSION TAG	UNP P00338
G	335	HIS	-	EXPRESSION TAG	UNP P00338
G	336	HIS	-	EXPRESSION TAG	UNP P00338
G	337	HIS	-	EXPRESSION TAG	UNP P00338
G	338	HIS	-	EXPRESSION TAG	UNP P00338
H	333	HIS	-	EXPRESSION TAG	UNP P00338
H	334	HIS	-	EXPRESSION TAG	UNP P00338
H	335	HIS	-	EXPRESSION TAG	UNP P00338
H	336	HIS	-	EXPRESSION TAG	UNP P00338
H	337	HIS	-	EXPRESSION TAG	UNP P00338
H	338	HIS	-	EXPRESSION TAG	UNP P00338

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



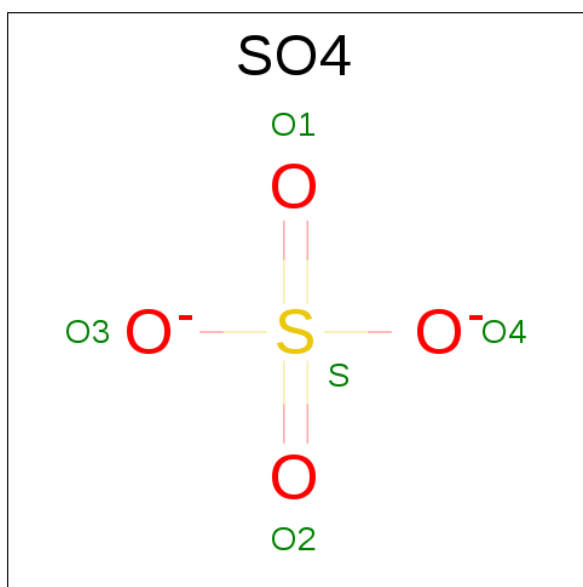
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

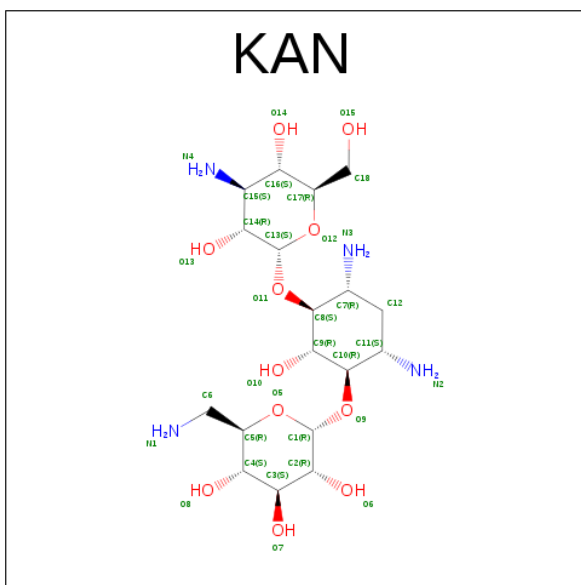
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is KANAMYCIN A (three-letter code: KAN) (formula: C<sub>18</sub>H<sub>36</sub>N<sub>4</sub>O<sub>11</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			33	18	4	11		

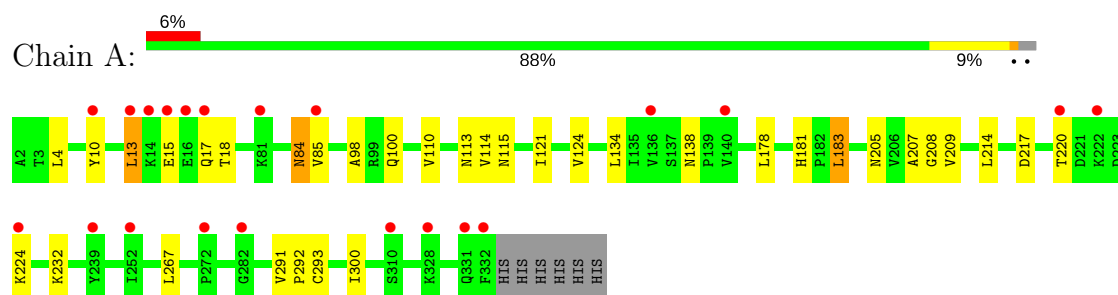
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	85	Total O 85 85	0	0
6	B	98	Total O 98 98	0	0
6	C	106	Total O 106 106	0	0
6	D	131	Total O 131 131	0	0
6	E	121	Total O 121 121	0	0
6	F	96	Total O 96 96	0	0
6	G	79	Total O 79 79	0	0
6	H	59	Total O 59 59	0	0

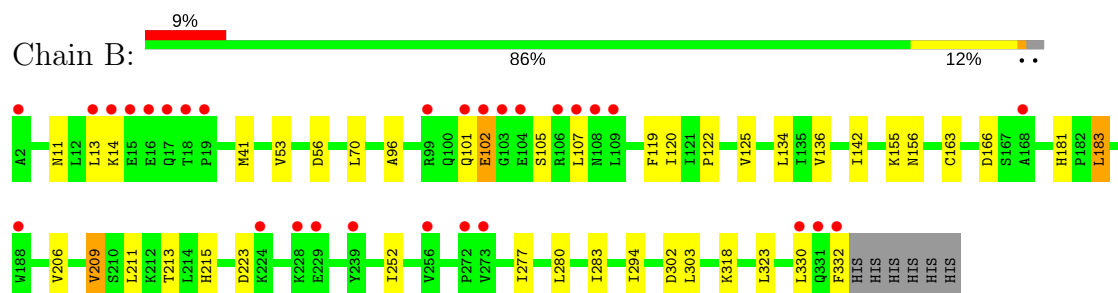
### 3 Residue-property plots

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

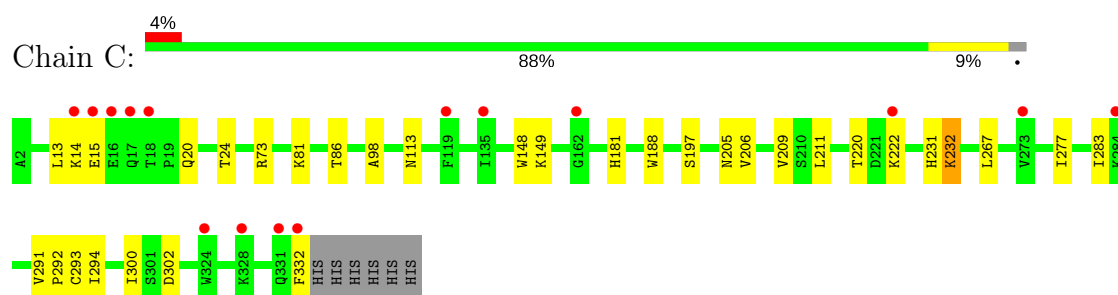
#### • Molecule 1: L-lactate dehydrogenase A chain



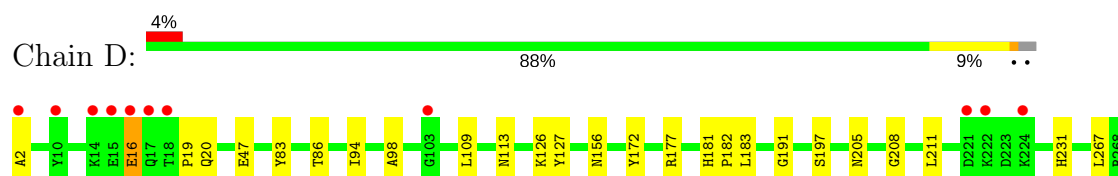
#### • Molecule 1: L-lactate dehydrogenase A chain



#### • Molecule 1: L-lactate dehydrogenase A chain

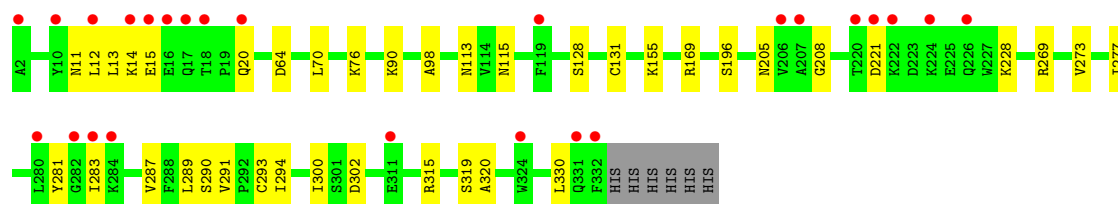
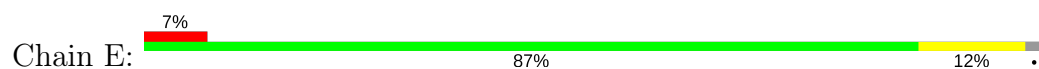


#### • Molecule 1: L-lactate dehydrogenase A chain

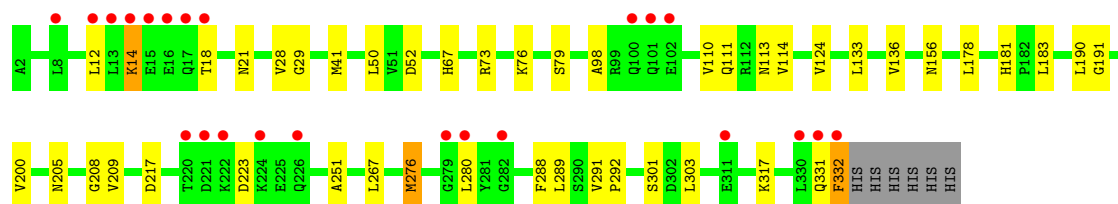
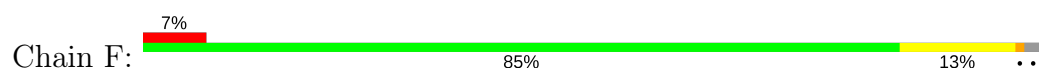




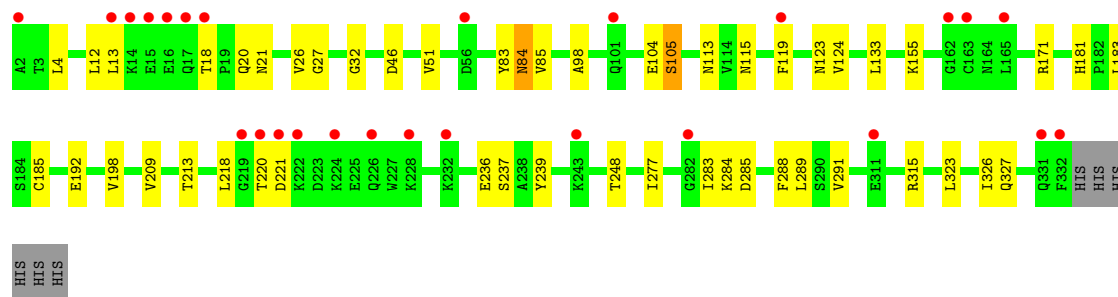
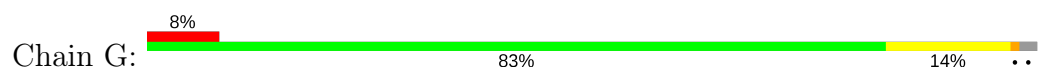
- Molecule 1: L-lactate dehydrogenase A chain



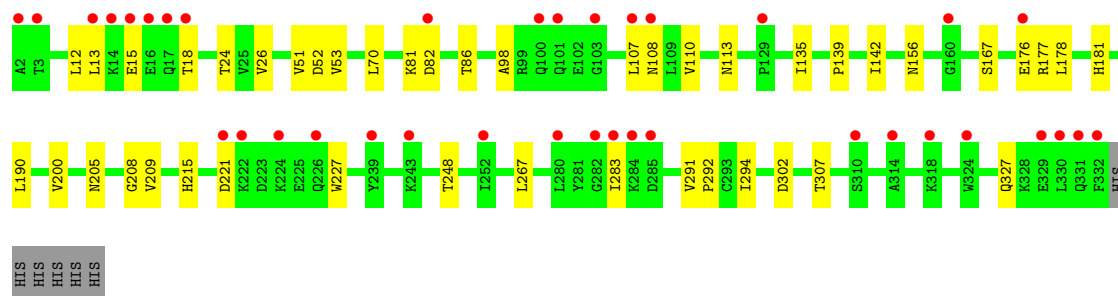
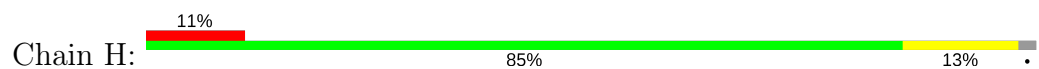
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.55Å 159.62Å 266.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 – 2.10 34.22 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.00-2.10) 99.9 (34.22-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.89	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.206 , 0.245 0.209 , 0.244	Depositor DCC
$R_{free}$ test set	8172 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, NAI, SO4, KAN

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	0.37	0/2611	0.59	0/3532
1	B	0.39	0/2611	0.59	0/3532
1	C	0.40	0/2611	0.60	0/3532
1	D	0.42	0/2611	0.62	0/3532
1	E	0.43	0/2619	0.62	0/3543
1	F	0.41	0/2611	0.60	1/3532 (0.0%)
1	G	0.38	0/2611	0.60	0/3532
1	H	0.35	0/2611	0.56	0/3532
All	All	0.40	0/20896	0.60	1/28267 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	41	MET	CA-CB-CG	-5.09	104.65	113.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2567	0	2653	23	0
1	B	2567	0	2653	28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2567	0	2653	22	0
1	D	2567	0	2653	31	0
1	E	2575	0	2656	32	0
1	F	2567	0	2653	31	0
1	G	2567	0	2653	37	0
1	H	2567	0	2653	30	0
2	A	44	0	27	1	0
2	C	44	0	27	1	0
2	D	44	0	27	1	0
2	E	44	0	27	0	0
2	F	44	0	27	3	0
2	G	44	0	27	2	0
2	H	44	0	27	1	0
3	A	6	0	0	1	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	1	0
3	E	6	0	0	0	0
3	F	6	0	0	1	0
3	G	6	0	0	2	0
3	H	6	0	0	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	1	0
5	B	33	0	36	5	0
6	A	85	0	0	4	0
6	B	98	0	0	4	0
6	C	106	0	0	4	0
6	D	131	0	0	6	0
6	E	121	0	0	4	0
6	F	96	0	0	1	0
6	G	79	0	0	4	0
6	H	59	0	0	6	0
All	All	21753	0	21452	213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (213) 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:H:13:LEU:O	1:H:13:LEU:HD12	1.63	0.99
1:B:41:MET:SD	6:B:559:HOH:O	2.24	0.96
1:B:56:ASP:HB3	6:B:573:HOH:O	1.66	0.95
1:D:277:ILE:HB	6:D:616:HOH:O	1.66	0.93
1:F:303:LEU:HD13	1:G:12:LEU:HD21	1.50	0.93
1:D:98:ALA:H	1:D:113:ASN:HD21	1.25	0.85
1:G:183:LEU:HD12	1:H:70:LEU:HD12	1.63	0.81
1:E:277:ILE:HD12	1:E:283:ILE:HG21	1.64	0.79
1:A:291:VAL:HB	6:A:573:HOH:O	1.84	0.77
1:F:181:HIS:CE1	1:F:183:LEU:HD13	2.20	0.77
1:E:277:ILE:HD11	1:E:283:ILE:HD13	1.70	0.73
1:C:232:LYS:HD2	6:C:601:HOH:O	1.88	0.73
1:C:206:VAL:O	1:C:209:VAL:HG12	1.90	0.72
1:C:86:THR:HG22	6:C:506:HOH:O	1.91	0.69
1:H:13:LEU:CD1	1:H:13:LEU:O	2.41	0.68
1:A:98:ALA:H	1:A:113:ASN:HD21	1.41	0.67
1:D:86:THR:HG22	6:D:517:HOH:O	1.95	0.67
1:B:183:LEU:HD23	1:D:269:ARG:HD3	1.77	0.66
1:D:181:HIS:CE1	1:D:183:LEU:HD13	2.30	0.65
1:G:171:ARG:HD3	1:G:185:CYS:O	1.97	0.65
1:H:26:VAL:HG22	1:H:51:VAL:CG2	2.26	0.65
1:C:98:ALA:H	1:C:113:ASN:HD21	1.43	0.64
1:C:291:VAL:HG22	1:C:292:PRO:HD2	1.79	0.64
1:H:98:ALA:H	1:H:113:ASN:HD21	1.46	0.64
1:F:291:VAL:HG22	1:F:292:PRO:HD2	1.78	0.64
1:D:277:ILE:HD11	1:D:289:LEU:HD12	1.80	0.63
1:E:15:GLU:OE2	1:E:15:GLU:N	2.31	0.62
1:E:281:TYR:H	1:E:283:ILE:HG22	1.65	0.61
1:E:98:ALA:H	1:E:113:ASN:HD21	1.48	0.61
1:E:169:ARG:HD3	1:F:67:HIS:CG	2.36	0.61
1:B:13:LEU:N	1:B:13:LEU:HD23	2.16	0.61
1:B:120:ILE:HD11	5:B:403:KAN:H11	1.83	0.60
1:E:277:ILE:CD1	1:E:283:ILE:HD13	2.31	0.60
1:A:84:ASN:HD22	1:A:85:VAL:N	1.99	0.59
1:G:20:GLN:CD	1:G:46:ASP:OD2	2.41	0.59
1:G:171:ARG:CD	1:G:185:CYS:O	2.51	0.59
1:D:19:PRO:HG3	1:D:47:GLU:OE1	2.03	0.59
1:G:98:ALA:H	1:G:113:ASN:HD21	1.51	0.58
1:F:98:ALA:H	1:F:113:ASN:HD21	1.49	0.57
1:G:104:GLU:O	1:G:105:SER:HB3	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ASN:HA	1:D:211:LEU:HD13	1.87	0.57
1:A:291:VAL:CB	6:A:573:HOH:O	2.47	0.56
1:B:156:ASN:ND2	1:C:13:LEU:HD11	2.21	0.56
1:C:291:VAL:HG22	1:C:292:PRO:CD	2.36	0.56
2:A:401:NAI:H42N	3:A:402:OXL:C1	2.35	0.56
1:H:167:SER:HB2	4:H:403:SO4:O3	2.06	0.55
1:F:301:SER:HA	1:G:13:LEU:HD23	1.87	0.55
1:G:181:HIS:CE1	1:G:183:LEU:HD13	2.42	0.55
1:A:217:ASP:O	1:A:220:THR:HG22	2.06	0.55
1:F:156:ASN:HB3	1:G:13:LEU:HD21	1.88	0.55
1:B:163:CYS:HA	1:B:166:ASP:OD2	2.07	0.54
1:E:277:ILE:CD1	1:E:283:ILE:HG21	2.35	0.54
1:C:277:ILE:HD13	1:C:283:ILE:HD13	1.89	0.54
1:H:26:VAL:HG22	1:H:51:VAL:HG21	1.88	0.54
1:A:291:VAL:HG13	1:A:292:PRO:HD2	1.88	0.54
1:G:288:PHE:H	1:G:327:GLN:HE22	1.54	0.54
1:C:294:ILE:HD12	1:C:302:ASP:HB2	1.90	0.54
1:G:26:VAL:HG22	1:G:51:VAL:CG1	2.38	0.54
1:D:307:THR:CB	6:D:518:HOH:O	2.55	0.53
1:C:220:THR:HB	6:C:550:HOH:O	2.08	0.53
1:D:277:ILE:HD12	1:D:283:ILE:HD13	1.90	0.53
5:B:403:KAN:H13	5:B:403:KAN:O10	2.08	0.53
1:G:4:LEU:HD13	1:H:215:HIS:HB2	1.90	0.53
1:E:169:ARG:NH1	6:E:503:HOH:O	2.41	0.53
1:F:291:VAL:HG22	1:F:292:PRO:CD	2.38	0.53
1:E:115:ASN:ND2	6:E:550:HOH:O	2.42	0.53
1:G:119:PHE:HB2	6:G:563:HOH:O	2.08	0.53
1:E:12:LEU:HD23	6:H:549:HOH:O	2.08	0.53
1:B:206:VAL:O	1:B:209:VAL:HG12	2.09	0.52
1:E:293:CYS:HB3	1:E:300:ILE:HG23	1.91	0.52
1:B:294:ILE:HD12	1:B:302:ASP:HB2	1.91	0.52
1:F:217:ASP:HB3	1:F:223:ASP:HB3	1.92	0.52
1:H:190:LEU:HD22	1:H:200:VAL:HG21	1.92	0.52
1:B:206:VAL:O	1:B:209:VAL:CG1	2.58	0.52
1:D:277:ILE:CD1	1:D:289:LEU:HD12	2.40	0.52
1:F:191:GLY:HA2	1:F:289:LEU:HD13	1.91	0.52
1:B:181:HIS:HB2	1:D:267:LEU:O	2.10	0.51
1:E:20:GLN:O	1:E:90:LYS:NZ	2.43	0.51
1:F:21:ASN:HD21	1:G:21:ASN:HD21	1.57	0.51
1:E:283:ILE:HD12	1:E:320:ALA:HB1	1.93	0.51
1:F:111:GLN:HE21	1:F:111:GLN:HA	1.76	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:VAL:O	1:F:114:VAL:HG23	2.11	0.51
1:E:315:ARG:NE	6:E:553:HOH:O	2.43	0.50
1:C:148:TRP:CZ3	1:C:149:LYS:HE2	2.47	0.50
1:F:276:MET:HG2	1:F:288:PHE:CE2	2.46	0.50
1:F:98:ALA:N	1:F:113:ASN:HD21	2.09	0.50
1:D:86:THR:CG2	6:D:517:HOH:O	2.55	0.50
1:H:81:LYS:HE3	6:H:545:HOH:O	2.11	0.50
1:G:124:VAL:HG11	1:G:133:LEU:HD21	1.93	0.49
1:D:94:ILE:HD12	1:D:94:ILE:N	2.26	0.49
1:H:24:THR:OG1	1:H:86:THR:HG23	2.11	0.49
1:H:81:LYS:CE	6:H:545:HOH:O	2.59	0.49
1:D:86:THR:HG22	1:D:86:THR:O	2.13	0.49
2:F:401:NAI:H42N	3:F:402:OXL:C2	2.43	0.49
2:H:401:NAI:H42N	3:H:402:OXL:C2	2.43	0.49
1:A:10:TYR:HB2	1:D:305:LYS:HD2	1.95	0.49
1:G:104:GLU:O	1:G:105:SER:CB	2.61	0.48
1:G:84:ASN:HD22	1:G:85:VAL:N	2.11	0.48
1:F:14:LYS:HE3	1:F:14:LYS:HA	1.94	0.48
1:D:191:GLY:C	1:D:289:LEU:HD22	2.33	0.48
1:H:283:ILE:HD11	6:H:511:HOH:O	2.14	0.48
1:A:4:LEU:HD21	1:B:211:LEU:HG	1.96	0.47
1:C:222:LYS:C	6:C:550:HOH:O	2.51	0.47
1:H:205:ASN:HD22	1:H:208:GLY:H	1.62	0.47
1:B:330:LEU:HD23	6:B:580:HOH:O	2.13	0.47
1:E:155:LYS:HE2	1:H:12:LEU:HD11	1.97	0.47
1:A:293:CYS:HB3	1:A:300:ILE:HG23	1.96	0.47
1:B:53:VAL:HG13	5:B:403:KAN:HN21	1.79	0.47
1:E:269:ARG:HD3	1:G:183:LEU:HD23	1.95	0.47
1:G:27:GLY:O	1:G:32:GLY:HA3	2.14	0.47
1:G:192:GLU:HG3	1:G:323:LEU:HD21	1.96	0.47
1:H:135:ILE:N	1:H:135:ILE:HD12	2.29	0.47
1:C:197:SER:OG	1:C:231:HIS:HE1	1.98	0.47
1:D:83:TYR:O	1:D:86:THR:HB	2.15	0.47
1:F:29:GLY:HA3	2:F:401:NAI:O5B	2.15	0.47
1:F:156:ASN:CB	1:G:13:LEU:HD21	2.43	0.47
1:A:100:GLN:NE2	1:A:138:ASN:HD22	2.11	0.47
1:E:289:LEU:C	1:E:289:LEU:HD12	2.36	0.47
1:H:86:THR:HG22	1:H:86:THR:O	2.14	0.47
1:H:177:ARG:HD2	1:H:227:TRP:CH2	2.50	0.47
2:G:401:NAI:H42N	3:G:402:OXL:C2	2.44	0.46
1:E:221:ASP:OD2	1:E:228:LYS:HE3	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LYS:HD3	1:D:127:TYR:CE1	2.50	0.46
1:E:283:ILE:HD11	1:E:287:VAL:HB	1.97	0.46
1:B:277:ILE:HD13	1:B:283:ILE:HD13	1.97	0.46
1:F:205:ASN:HD22	1:F:208:GLY:H	1.64	0.46
1:G:213:THR:HG22	6:G:531:HOH:O	2.15	0.46
1:D:98:ALA:N	1:D:113:ASN:HD21	2.04	0.46
1:G:284:LYS:O	1:G:285:ASP:HB2	2.16	0.46
1:H:291:VAL:HG13	1:H:292:PRO:HD2	1.97	0.45
1:H:327:GLN:NE2	6:H:506:HOH:O	2.43	0.45
1:A:291:VAL:CG1	6:A:573:HOH:O	2.65	0.45
1:A:291:VAL:HG12	6:A:573:HOH:O	2.16	0.45
1:B:136:VAL:HG13	1:B:252:ILE:HD11	1.98	0.45
1:E:76:LYS:NZ	6:E:536:HOH:O	2.50	0.45
1:D:191:GLY:HA2	1:D:289:LEU:HD22	1.97	0.45
2:D:401:NAI:H42N	3:D:402:OXL:C2	2.46	0.45
1:D:98:ALA:H	1:D:113:ASN:ND2	2.04	0.45
1:H:294:ILE:HD12	1:H:302:ASP:HB2	1.98	0.45
1:B:213:THR:HB	6:D:614:HOH:O	2.17	0.45
1:D:277:ILE:CD1	1:D:283:ILE:HD13	2.47	0.45
2:G:401:NAI:H42N	3:G:402:OXL:C1	2.47	0.45
1:C:293:CYS:HB3	1:C:300:ILE:HG23	1.99	0.44
1:E:98:ALA:N	1:E:113:ASN:HD21	2.13	0.44
1:F:124:VAL:HG21	1:F:133:LEU:HD21	1.99	0.44
1:A:181:HIS:HB2	1:C:267:LEU:O	2.17	0.44
1:G:183:LEU:HD11	1:H:70:LEU:O	2.17	0.44
1:E:12:LEU:CD2	6:H:549:HOH:O	2.66	0.44
1:F:190:LEU:HD22	1:F:200:VAL:HG21	2.00	0.44
1:E:205:ASN:HD22	1:E:208:GLY:H	1.65	0.44
1:B:13:LEU:N	1:B:13:LEU:CD2	2.80	0.44
1:D:191:GLY:CA	1:D:289:LEU:HD22	2.48	0.44
1:C:98:ALA:N	1:C:113:ASN:HD21	2.14	0.43
1:G:84:ASN:HD22	1:G:85:VAL:H	1.66	0.43
1:E:64:ASP:O	1:F:251:ALA:HB2	2.18	0.43
1:G:220:THR:HG22	1:G:221:ASP:O	2.18	0.43
1:B:215:HIS:CE1	1:B:223:ASP:HB2	2.54	0.43
1:H:52:ASP:OD1	1:H:53:VAL:N	2.51	0.43
1:B:107:LEU:HD21	6:B:580:HOH:O	2.18	0.43
1:F:28:VAL:HG22	1:F:52:ASP:HB2	2.01	0.43
1:G:198:VAL:HG22	1:G:315:ARG:HB3	2.00	0.43
1:A:183:LEU:HD12	1:B:70:LEU:HD12	2.01	0.43
1:B:119:PHE:CD2	5:B:403:KAN:H5	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ALA:HB1	5:B:403:KAN:H7	2.01	0.43
1:C:24:THR:OG1	1:C:86:THR:HG23	2.19	0.43
1:D:172:TYR:HA	1:D:182:PRO:HG3	2.00	0.43
1:B:142:ILE:HG13	1:B:323:LEU:HD22	2.01	0.43
1:C:14:LYS:HG3	1:C:15:GLU:N	2.34	0.43
1:G:83:TYR:CG	1:G:123:ASN:HB3	2.53	0.43
1:F:181:HIS:HB2	1:H:267:LEU:O	2.19	0.43
1:F:12:LEU:HG	6:F:583:HOH:O	2.18	0.42
1:F:289:LEU:HD12	1:F:289:LEU:C	2.40	0.42
1:G:115:ASN:HB3	6:G:568:HOH:O	2.19	0.42
1:B:101:GLN:O	1:B:102:GLU:C	2.58	0.42
1:H:13:LEU:HD13	1:H:15:GLU:HB2	2.01	0.42
1:C:205:ASN:HA	1:C:211:LEU:HD13	2.01	0.42
1:A:13:LEU:HD21	1:D:156:ASN:CG	2.40	0.42
1:G:289:LEU:C	1:G:289:LEU:HD12	2.40	0.42
1:G:277:ILE:CD1	1:G:283:ILE:HG21	2.50	0.42
1:B:280:LEU:HD11	1:B:303:LEU:HD11	2.01	0.42
1:A:84:ASN:HD22	1:A:85:VAL:H	1.64	0.41
1:F:267:LEU:O	1:H:181:HIS:HB2	2.21	0.41
1:E:273:VAL:O	1:E:290:SER:HA	2.20	0.41
1:A:110:VAL:O	1:A:114:VAL:HG23	2.20	0.41
1:A:121:ILE:O	1:A:124:VAL:HG22	2.21	0.41
1:D:277:ILE:HD12	1:D:283:ILE:CD1	2.50	0.41
1:E:70:LEU:HD12	1:F:183:LEU:HD12	2.01	0.41
1:H:139:PRO:HG2	1:H:142:ILE:HB	2.02	0.41
1:D:197:SER:OG	1:D:231:HIS:HE1	2.03	0.41
1:E:11:ASN:C	1:E:12:LEU:HD12	2.41	0.41
1:H:107:LEU:O	1:H:110:VAL:HG23	2.20	0.41
1:A:205:ASN:HD22	1:A:208:GLY:H	1.67	0.41
1:A:267:LEU:O	1:C:181:HIS:HB2	2.20	0.41
1:G:155:LYS:NZ	6:G:509:HOH:O	2.53	0.41
1:E:196:SER:OG	1:E:319:SER:HA	2.21	0.41
1:G:236:GLU:HA	1:G:239:TYR:HD1	1.85	0.41
1:A:115:ASN:HD21	1:G:326:ILE:HD11	1.86	0.41
1:E:294:ILE:HD12	1:E:302:ASP:HB2	2.01	0.41
1:B:122:PRO:HA	1:B:125:VAL:HG22	2.02	0.41
1:F:136:VAL:O	2:F:401:NAI:H2N	2.21	0.41
1:G:98:ALA:N	1:G:113:ASN:HD21	2.18	0.41
1:E:13:LEU:HD11	1:H:156:ASN:ND2	2.36	0.41
1:B:11:ASN:HA	1:C:302:ASP:OD2	2.20	0.40
1:D:205:ASN:HD22	1:D:208:GLY:H	1.69	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:ND2	1:G:326:ILE:HD11	2.37	0.40
1:D:289:LEU:HD21	1:D:323:LEU:CD2	2.51	0.40
1:D:2:ALA:HA	6:D:620:HOH:O	2.19	0.40
1:F:331:GLN:O	1:F:332:PHE:C	2.60	0.40
1:A:207:ALA:HA	1:C:188:TRP:CZ2	2.56	0.40
2:C:401:NAI:H42N	3:C:402:OXL:C1	2.52	0.40
1:E:128:SER:HB3	1:E:131:CYS:HB3	2.04	0.40
1:F:50:LEU:O	1:F:79:SER:HA	2.21	0.40
1:H:82:ASP:N	1:H:82:ASP:OD1	2.55	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	329/337 (98%)	320 (97%)	9 (3%)	0	100	100
1	B	329/337 (98%)	318 (97%)	10 (3%)	1 (0%)	44	44
1	C	329/337 (98%)	319 (97%)	10 (3%)	0	100	100
1	D	329/337 (98%)	318 (97%)	10 (3%)	1 (0%)	44	44
1	E	330/337 (98%)	315 (96%)	15 (4%)	0	100	100
1	F	329/337 (98%)	319 (97%)	10 (3%)	0	100	100
1	G	329/337 (98%)	312 (95%)	16 (5%)	1 (0%)	44	44
1	H	329/337 (98%)	313 (95%)	16 (5%)	0	100	100
All	All	2633/2696 (98%)	2534 (96%)	96 (4%)	3 (0%)	55	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	SER

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	16	GLU
1	G	105	SER

### 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	287/293 (98%)	275 (96%)	12 (4%)	34	33
1	B	287/293 (98%)	279 (97%)	8 (3%)	49	52
1	C	287/293 (98%)	282 (98%)	5 (2%)	66	72
1	D	287/293 (98%)	281 (98%)	6 (2%)	59	64
1	E	288/293 (98%)	285 (99%)	3 (1%)	80	85
1	F	287/293 (98%)	277 (96%)	10 (4%)	41	42
1	G	287/293 (98%)	280 (98%)	7 (2%)	54	59
1	H	287/293 (98%)	279 (97%)	8 (3%)	49	52
All	All	2297/2344 (98%)	2238 (97%)	59 (3%)	51	55

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	15	GLU
1	A	17	GLN
1	A	18	THR
1	A	84	ASN
1	A	134	LEU
1	A	178	LEU
1	A	183	LEU
1	A	209	VAL
1	A	214	LEU
1	A	224	LYS
1	A	232	LYS
1	B	14	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	102	GLU
1	B	134	LEU
1	B	155	LYS
1	B	183	LEU
1	B	209	VAL
1	B	318	LYS
1	B	332	PHE
1	C	20	GLN
1	C	73	ARG
1	C	81	LYS
1	C	232	LYS
1	C	332	PHE
1	D	16	GLU
1	D	20	GLN
1	D	109	LEU
1	D	177	ARG
1	D	307	THR
1	D	323	LEU
1	E	14	LYS
1	E	291	VAL
1	E	330	LEU
1	F	14	LYS
1	F	18	THR
1	F	73	ARG
1	F	76	LYS
1	F	178	LEU
1	F	209	VAL
1	F	276	MET
1	F	280	LEU
1	F	317	LYS
1	F	332	PHE
1	G	18	THR
1	G	84	ASN
1	G	209	VAL
1	G	218	LEU
1	G	237	SER
1	G	248	THR
1	G	291	VAL
1	H	18	THR
1	H	108	ASN
1	H	176	GLU
1	H	178	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	209	VAL
1	H	221	ASP
1	H	248	THR
1	H	307	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	17	GLN
1	A	84	ASN
1	A	100	GLN
1	A	108	ASN
1	A	113	ASN
1	A	115	ASN
1	A	205	ASN
1	A	231	HIS
1	A	331	GLN
1	B	17	GLN
1	B	21	ASN
1	B	205	ASN
1	B	231	HIS
1	B	327	GLN
1	C	20	GLN
1	C	21	ASN
1	C	113	ASN
1	C	226	GLN
1	C	231	HIS
1	C	298	ASN
1	D	113	ASN
1	D	130	ASN
1	D	205	ASN
1	D	231	HIS
1	D	331	GLN
1	E	113	ASN
1	E	115	ASN
1	E	205	ASN
1	E	331	GLN
1	F	20	GLN
1	F	21	ASN
1	F	100	GLN
1	F	108	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	111	GLN
1	F	113	ASN
1	F	123	ASN
1	F	130	ASN
1	F	205	ASN
1	F	231	HIS
1	F	298	ASN
1	G	7	GLN
1	G	84	ASN
1	G	113	ASN
1	G	123	ASN
1	G	205	ASN
1	G	327	GLN
1	H	100	GLN
1	H	108	ASN
1	H	113	ASN
1	H	115	ASN
1	H	205	ASN
1	H	231	HIS
1	H	297	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

25 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	NAI	A	401	-	40,48,48	0.92	2 (5%)	41,73,73	1.72	6 (14%)
3	OXL	A	402	-	0,5,5	0.00	-	0,6,6	0.00	-
4	SO4	A	403	-	4,4,4	0.42	0	6,6,6	0.33	0
3	OXL	B	401	-	0,5,5	0.00	-	0,6,6	0.00	-
4	SO4	B	402	-	4,4,4	0.51	0	6,6,6	0.27	0
5	KAN	B	403	-	35,35,35	0.56	0	46,52,52	1.11	4 (8%)
2	NAI	C	401	-	40,48,48	1.00	2 (5%)	41,73,73	1.90	7 (17%)
3	OXL	C	402	-	0,5,5	0.00	-	0,6,6	0.00	-
4	SO4	C	403	-	4,4,4	0.41	0	6,6,6	0.20	0
2	NAI	D	401	-	40,48,48	1.02	4 (10%)	41,73,73	1.64	6 (14%)
3	OXL	D	402	-	0,5,5	0.00	-	0,6,6	0.00	-
4	SO4	D	403	-	4,4,4	0.64	0	6,6,6	0.34	0
2	NAI	E	401	-	40,48,48	1.07	2 (5%)	41,73,73	1.71	8 (19%)
3	OXL	E	402	-	0,5,5	0.00	-	0,6,6	0.00	-
4	SO4	E	403	-	4,4,4	0.44	0	6,6,6	0.60	0
4	SO4	E	404	-	4,4,4	0.55	0	6,6,6	0.26	0
2	NAI	F	401	-	40,48,48	0.96	2 (5%)	41,73,73	1.78	5 (12%)
3	OXL	F	402	-	0,5,5	0.00	-	0,6,6	0.00	-
4	SO4	F	403	-	4,4,4	0.37	0	6,6,6	0.29	0
2	NAI	G	401	-	40,48,48	0.98	2 (5%)	41,73,73	1.62	6 (14%)
3	OXL	G	402	-	0,5,5	0.00	-	0,6,6	0.00	-
4	SO4	G	403	-	4,4,4	0.54	0	6,6,6	0.43	0
2	NAI	H	401	-	40,48,48	1.03	2 (5%)	41,73,73	1.72	6 (14%)
3	OXL	H	402	-	0,5,5	0.00	-	0,6,6	0.00	-
4	SO4	H	403	-	4,4,4	0.42	0	6,6,6	0.51	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	NAI	A	401	-	-	0/25/72/72	0/5/5/5
3	OXL	A	402	-	-	0/0/4/4	0/0/0/0
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	OXL	B	401	-	-	0/0/4/4	0/0/0/0
4	SO4	B	402	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	KAN	B	403	-	-	0/12/72/72	0/3/3/3
2	NAI	C	401	-	-	0/25/72/72	0/5/5/5
3	OXL	C	402	-	-	0/0/4/4	0/0/0/0
4	SO4	C	403	-	-	0/0/0/0	0/0/0/0
2	NAI	D	401	-	-	0/25/72/72	0/5/5/5
3	OXL	D	402	-	-	0/0/4/4	0/0/0/0
4	SO4	D	403	-	-	0/0/0/0	0/0/0/0
2	NAI	E	401	-	-	0/25/72/72	0/5/5/5
3	OXL	E	402	-	-	0/0/4/4	0/0/0/0
4	SO4	E	403	-	-	0/0/0/0	0/0/0/0
4	SO4	E	404	-	-	0/0/0/0	0/0/0/0
2	NAI	F	401	-	-	0/25/72/72	0/5/5/5
3	OXL	F	402	-	-	0/0/4/4	0/0/0/0
4	SO4	F	403	-	-	0/0/0/0	0/0/0/0
2	NAI	G	401	-	-	0/25/72/72	0/5/5/5
3	OXL	G	402	-	-	0/0/4/4	0/0/0/0
4	SO4	G	403	-	-	0/0/0/0	0/0/0/0
2	NAI	H	401	-	-	0/25/72/72	0/5/5/5
3	OXL	H	402	-	-	0/0/4/4	0/0/0/0
4	SO4	H	403	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAI	C4N-C5N	-2.33	1.44	1.49
2	D	401	NAI	C2A-N3A	2.14	1.35	1.32
2	A	401	NAI	C6N-C5N	2.23	1.37	1.33
2	D	401	NAI	C5A-C4A	2.43	1.46	1.40
2	A	401	NAI	C5A-C4A	2.75	1.46	1.40
2	C	401	NAI	C5A-C4A	2.77	1.46	1.40
2	F	401	NAI	C5A-C4A	2.82	1.46	1.40
2	G	401	NAI	C5A-C4A	2.97	1.47	1.40
2	D	401	NAI	C6N-C5N	2.97	1.38	1.33
2	H	401	NAI	C5A-C4A	2.98	1.47	1.40
2	E	401	NAI	C5A-C4A	3.03	1.47	1.40
2	F	401	NAI	C6N-C5N	3.05	1.38	1.33
2	E	401	NAI	C6N-C5N	3.08	1.39	1.33
2	H	401	NAI	C6N-C5N	3.21	1.39	1.33
2	G	401	NAI	C6N-C5N	3.23	1.39	1.33
2	C	401	NAI	C6N-C5N	3.52	1.39	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAI	N3A-C2A-N1A	-8.21	121.71	128.86
2	C	401	NAI	N3A-C2A-N1A	-8.16	121.75	128.86
2	G	401	NAI	N3A-C2A-N1A	-7.40	122.41	128.86
2	D	401	NAI	N3A-C2A-N1A	-7.32	122.48	128.86
2	H	401	NAI	N3A-C2A-N1A	-7.02	122.74	128.86
2	A	401	NAI	N3A-C2A-N1A	-6.96	122.79	128.86
2	E	401	NAI	N3A-C2A-N1A	-6.94	122.81	128.86
2	A	401	NAI	C4B-O4B-C1B	-4.93	104.52	109.77
2	H	401	NAI	C4B-O4B-C1B	-4.81	104.65	109.77
2	E	401	NAI	C4B-O4B-C1B	-4.40	105.09	109.77
2	C	401	NAI	C4B-O4B-C1B	-3.73	105.80	109.77
2	F	401	NAI	C4B-O4B-C1B	-3.21	106.35	109.77
2	H	401	NAI	C4A-C5A-N7A	-3.21	106.31	109.41
2	C	401	NAI	C1D-N1N-C2N	-3.12	115.79	121.09
2	F	401	NAI	C1B-N9A-C4A	-3.00	121.46	126.64
2	D	401	NAI	C4B-O4B-C1B	-2.96	106.62	109.77
2	A	401	NAI	C1B-N9A-C4A	-2.78	121.84	126.64
2	C	401	NAI	C1B-N9A-C4A	-2.75	121.88	126.64
2	E	401	NAI	C4A-C5A-N7A	-2.71	106.79	109.41
2	G	401	NAI	C4A-C5A-N7A	-2.69	106.81	109.41
2	D	401	NAI	C1B-N9A-C4A	-2.67	122.03	126.64
2	G	401	NAI	C1D-N1N-C2N	-2.56	116.74	121.09
2	G	401	NAI	C4B-O4B-C1B	-2.51	107.10	109.77
2	G	401	NAI	C1B-N9A-C4A	-2.45	122.40	126.64
2	E	401	NAI	O4D-C1D-C2D	-2.34	101.47	106.64
2	A	401	NAI	C4A-C5A-N7A	-2.31	107.18	109.41
2	H	401	NAI	C1B-N9A-C4A	-2.29	122.67	126.64
2	E	401	NAI	C1B-N9A-C4A	-2.26	122.73	126.64
5	B	403	KAN	C3-C4-C5	-2.25	106.25	110.22
2	A	401	NAI	C1D-N1N-C2N	-2.23	117.30	121.09
2	D	401	NAI	C1D-N1N-C2N	-2.18	117.38	121.09
2	F	401	NAI	C4A-C5A-N7A	-2.10	107.39	109.41
2	E	401	NAI	C1D-N1N-C2N	-2.09	117.55	121.09
2	H	401	NAI	C1D-N1N-C2N	-2.04	117.63	121.09
2	C	401	NAI	O1N-PN-O2N	2.01	122.68	112.28
2	C	401	NAI	C2D-C1D-N1N	2.08	118.68	113.32
2	E	401	NAI	O1N-PN-O2N	2.11	123.19	112.28
2	D	401	NAI	O1N-PN-O2N	2.19	123.59	112.28
5	B	403	KAN	C1-O5-C5	2.23	117.92	113.72
2	A	401	NAI	C2A-N1A-C6A	2.29	122.78	118.77
2	D	401	NAI	N6A-C6A-N1A	2.30	123.32	118.77
2	H	401	NAI	C2A-N1A-C6A	2.31	122.82	118.77
5	B	403	KAN	C1-C2-C3	2.33	114.31	109.98

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	KAN	O9-C10-C9	2.47	113.13	107.19
2	C	401	NAI	C2A-N1A-C6A	2.48	123.11	118.77
2	E	401	NAI	C2D-C1D-N1N	2.49	119.73	113.32
2	G	401	NAI	C2A-N1A-C6A	2.55	123.23	118.77
2	F	401	NAI	C2A-N1A-C6A	2.91	123.87	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAI	1	0
3	A	402	OXL	1	0
5	B	403	KAN	5	0
2	C	401	NAI	1	0
3	C	402	OXL	1	0
2	D	401	NAI	1	0
3	D	402	OXL	1	0
2	F	401	NAI	3	0
3	F	402	OXL	1	0
2	G	401	NAI	2	0
3	G	402	OXL	2	0
2	H	401	NAI	1	0
3	H	402	OXL	1	0
4	H	403	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/337 (98%)	0.42	21 (6%)	21	26	25, 37, 57, 68	2 (0%)
1	B	331/337 (98%)	0.47	29 (8%)	11	14	25, 36, 59, 83	4 (1%)
1	C	331/337 (98%)	0.39	15 (4%)	34	40	20, 32, 52, 81	0
1	D	331/337 (98%)	0.29	13 (3%)	40	47	19, 28, 51, 84	1 (0%)
1	E	331/337 (98%)	0.37	25 (7%)	15	19	21, 32, 60, 84	1 (0%)
1	F	331/337 (98%)	0.47	23 (6%)	18	22	20, 35, 63, 82	2 (0%)
1	G	331/337 (98%)	0.49	26 (7%)	13	17	24, 38, 57, 72	2 (0%)
1	H	331/337 (98%)	0.70	37 (11%)	6	7	27, 44, 75, 104	2 (0%)
All	All	2648/2696 (98%)	0.45	189 (7%)	17	21	19, 35, 61, 104	14 (0%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	332	PHE	10.3
1	F	17	GLN	9.8
1	G	14	LYS	6.3
1	A	15	GLU	6.3
1	A	17	GLN	6.3
1	G	332	PHE	6.3
1	E	15	GLU	6.0
1	D	17	GLN	6.0
1	C	332	PHE	5.9
1	H	331	GLN	5.8
1	E	16	GLU	5.7
1	E	332	PHE	5.7
1	F	13	LEU	5.6
1	H	13	LEU	5.6
1	D	332	PHE	5.5
1	D	15	GLU	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	220	THR	5.3
1	C	15	GLU	5.2
1	G	119	PHE	5.2
1	C	14	LYS	5.2
1	H	17	GLN	5.2
1	G	222	LYS	5.2
1	C	16	GLU	5.2
1	E	17	GLN	5.1
1	H	103	GLY	5.1
1	D	14	LYS	5.0
1	C	17	GLN	5.0
1	F	280	LEU	4.7
1	B	102	GLU	4.7
1	D	16	GLU	4.7
1	E	222	LYS	4.6
1	B	13	LEU	4.6
1	D	18	THR	4.5
1	H	284	LYS	4.4
1	G	17	GLN	4.4
1	G	16	GLU	4.4
1	A	13	LEU	4.4
1	F	332	PHE	4.3
1	B	106	ARG	4.3
1	F	16	GLU	4.3
1	H	16	GLU	4.3
1	H	2	ALA	4.2
1	E	331	GLN	4.1
1	H	283	ILE	4.1
1	F	101	GLN	4.0
1	B	16	GLU	4.0
1	B	107	LEU	3.9
1	B	332	PHE	3.8
1	G	224	LYS	3.8
1	F	15	GLU	3.8
1	H	101	GLN	3.8
1	A	222	LYS	3.8
1	B	103	GLY	3.8
1	G	221	ASP	3.7
1	D	331	GLN	3.6
1	B	101	GLN	3.6
1	H	224	LYS	3.6
1	G	331	GLN	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	16	GLU	3.5
1	F	222	LYS	3.5
1	F	14	LYS	3.5
1	C	119	PHE	3.4
1	F	224	LYS	3.4
1	E	10	TYR	3.4
1	E	282	GLY	3.4
1	D	103	GLY	3.3
1	H	324	TRP	3.3
1	G	13	LEU	3.3
1	B	99	ARG	3.3
1	H	310	SER	3.2
1	H	15	GLU	3.2
1	B	14	LYS	3.2
1	E	18	THR	3.2
1	G	101	GLN	3.2
1	E	283	ILE	3.2
1	A	332	PHE	3.2
1	E	220	THR	3.2
1	G	15	GLU	3.1
1	C	331	GLN	3.1
1	G	311	GLU	3.1
1	E	324	TRP	3.1
1	E	14	LYS	3.1
1	H	14	LYS	3.1
1	B	109	LEU	3.1
1	H	239	TYR	3.1
1	E	2	ALA	3.1
1	B	330	LEU	3.1
1	D	2	ALA	3.0
1	H	330	LEU	3.0
1	B	239	TYR	3.0
1	H	18	THR	3.0
1	A	224	LYS	3.0
1	H	82	ASP	3.0
1	D	222	LYS	3.0
1	A	252	ILE	2.9
1	B	17	GLN	2.9
1	H	329	GLU	2.9
1	A	239	TYR	2.9
1	F	282	GLY	2.9
1	F	18	THR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	221	ASP	2.8
1	C	18	THR	2.8
1	E	224	LYS	2.8
1	B	331	GLN	2.7
1	B	2	ALA	2.7
1	F	221	ASP	2.7
1	F	330	LEU	2.7
1	A	136	VAL	2.7
1	A	331	GLN	2.7
1	F	12	LEU	2.7
1	F	220	THR	2.7
1	H	221	ASP	2.7
1	B	15	GLU	2.6
1	A	282	GLY	2.6
1	H	314	ALA	2.6
1	C	222	LYS	2.6
1	C	284	LYS	2.6
1	H	107	LEU	2.6
1	E	119	PHE	2.6
1	E	20	GLN	2.6
1	D	224	LYS	2.6
1	H	318	LYS	2.5
1	B	108	ASN	2.5
1	C	328	LYS	2.5
1	F	331	GLN	2.5
1	H	100	GLN	2.5
1	A	140	VAL	2.5
1	F	102	GLU	2.5
1	H	252	ILE	2.4
1	B	272	PRO	2.4
1	H	108	ASN	2.4
1	A	14	LYS	2.4
1	H	129	PRO	2.4
1	E	12	LEU	2.4
1	G	165	LEU	2.4
1	A	220	THR	2.4
1	H	282	GLY	2.4
1	B	228	LYS	2.4
1	B	18	THR	2.4
1	G	56	ASP	2.4
1	G	163	CYS	2.3
1	B	229	GLU	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	206	VAL	2.3
1	G	2	ALA	2.3
1	D	10	TYR	2.3
1	B	273	VAL	2.3
1	D	221	ASP	2.3
1	H	160	GLY	2.3
1	B	188	TRP	2.3
1	H	222	LYS	2.2
1	B	19	PRO	2.2
1	C	324	TRP	2.2
1	E	284	LYS	2.2
1	G	282	GLY	2.2
1	B	104	GLU	2.2
1	E	207	ALA	2.2
1	E	311	GLU	2.2
1	G	243	LYS	2.2
1	C	273	VAL	2.2
1	G	228	LYS	2.2
1	F	100	GLN	2.1
1	B	224	LYS	2.1
1	A	328	LYS	2.1
1	H	243	LYS	2.1
1	H	285	ASP	2.1
1	F	8	LEU	2.1
1	G	18	THR	2.1
1	F	226	GLN	2.1
1	F	311	GLU	2.1
1	H	226	GLN	2.1
1	C	162	GLY	2.1
1	E	280	LEU	2.1
1	G	162	GLY	2.1
1	A	81	LYS	2.1
1	A	310	SER	2.1
1	A	272	PRO	2.1
1	B	168	ALA	2.1
1	H	3	THR	2.1
1	A	10	TYR	2.1
1	C	135	ILE	2.1
1	G	226	GLN	2.1
1	G	219	GLY	2.1
1	A	85	VAL	2.0
1	F	279	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	176	GLU	2.0
1	E	226	GLN	2.0
1	G	232	LYS	2.0
1	H	280	LEU	2.0
1	B	256	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	E	404	5/5	0.93	0.22	5.88	45,48,50,51	0
4	SO4	F	403	5/5	0.92	0.23	2.22	39,42,46,47	0
5	KAN	B	403	33/33	0.65	0.30	2.14	48,65,70,73	0
4	SO4	G	403	5/5	0.91	0.19	0.93	41,43,45,47	0
4	SO4	E	403	5/5	0.94	0.18	0.54	33,34,35,39	0
4	SO4	D	403	5/5	0.93	0.16	0.48	32,32,34,39	0
4	SO4	H	403	5/5	0.91	0.17	0.24	43,45,47,51	0
2	NAI	D	401	44/44	0.97	0.13	-0.47	18,22,27,28	0
2	NAI	F	401	44/44	0.94	0.11	-0.59	26,30,38,41	0
2	NAI	G	401	44/44	0.95	0.11	-0.60	29,34,42,47	0
2	NAI	E	401	44/44	0.96	0.11	-0.67	19,27,35,39	0
3	OXL	F	402	6/6	0.96	0.13	-0.68	30,31,32,33	0
2	NAI	C	401	44/44	0.96	0.10	-0.77	22,27,37,38	0
3	OXL	C	402	6/6	0.97	0.10	-0.87	21,23,23,26	0
2	NAI	H	401	44/44	0.95	0.11	-0.95	32,37,42,43	0
4	SO4	C	403	5/5	0.95	0.16	-1.10	36,37,39,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OXL	H	402	6/6	0.96	0.10	-1.13	34,35,36,37	0
2	NAI	A	401	44/44	0.96	0.10	-1.15	26,30,35,37	0
3	OXL	G	402	6/6	0.95	0.11	-1.28	30,31,35,35	0
3	OXL	A	402	6/6	0.97	0.11	-1.41	26,28,28,30	0
3	OXL	E	402	6/6	0.97	0.09	-1.56	16,18,19,22	0
4	SO4	A	403	5/5	0.96	0.12	-1.69	39,41,42,43	0
3	OXL	D	402	6/6	0.98	0.11	-1.79	16,17,19,20	0
3	OXL	B	401	6/6	0.95	0.10	-1.85	36,36,37,37	0
4	SO4	B	402	5/5	0.95	0.12	-2.42	43,45,47,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.