Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 04:44 PM JST

PDB ID	:	6JML
Title	:	Re-refined structure of R-state L-lactate dehydrogenase fromLactobacillus casei
Authors	:	Arai, K.; Miyanaga, A.; Uchikoba, H.; Fushinobu, S.; Taguchi, H.
Deposited on	:	2019-03-12
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

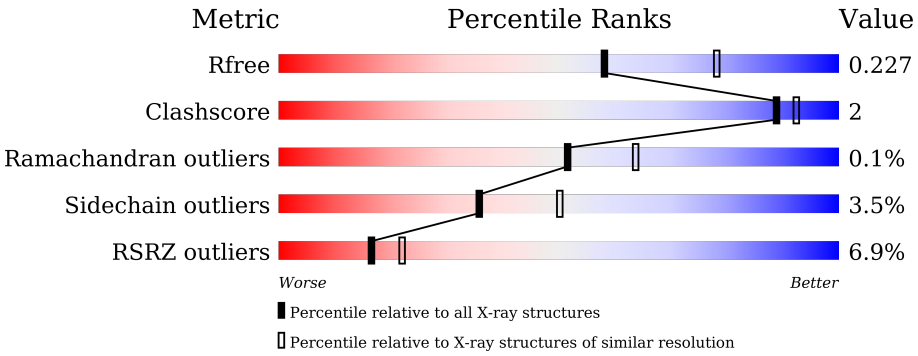
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	326	11% 87% 7% 5%
1	B	326	5% 88% 9% .
1	C	326	3% 83% 8% 9%
1	D	326	9% 85% 7% . 7%
1	E	326	6% 88% 8% .
1	F	326	6% 88% 8% .

2 Entry composition (i)

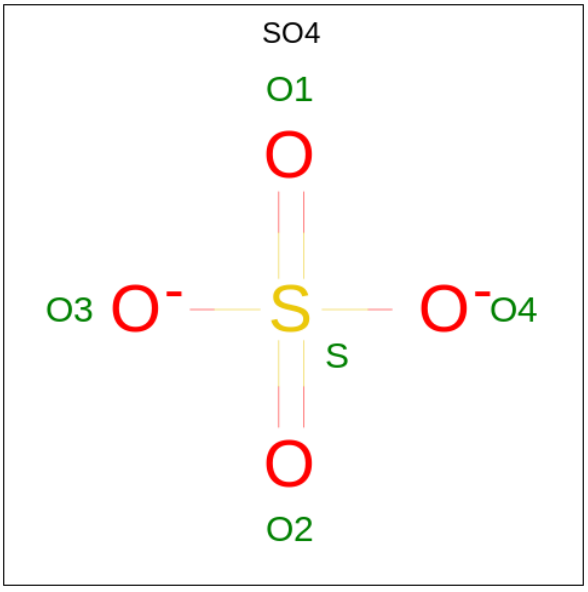
There are 3 unique types of molecules in this entry. The entry contains 14535 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2371	1515	393	457	6			
1	B	315	Total	C	N	O	S	0	0	0
			2414	1541	401	466	6			
1	C	296	Total	C	N	O	S	0	0	0
			2277	1456	377	438	6			
1	D	304	Total	C	N	O	S	0	0	0
			2327	1484	387	450	6			
1	E	314	Total	C	N	O	S	0	0	0
			2409	1538	400	465	6			
1	F	315	Total	C	N	O	S	0	0	0
			2414	1541	401	466	6			

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



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

- Molecule 3 is water.

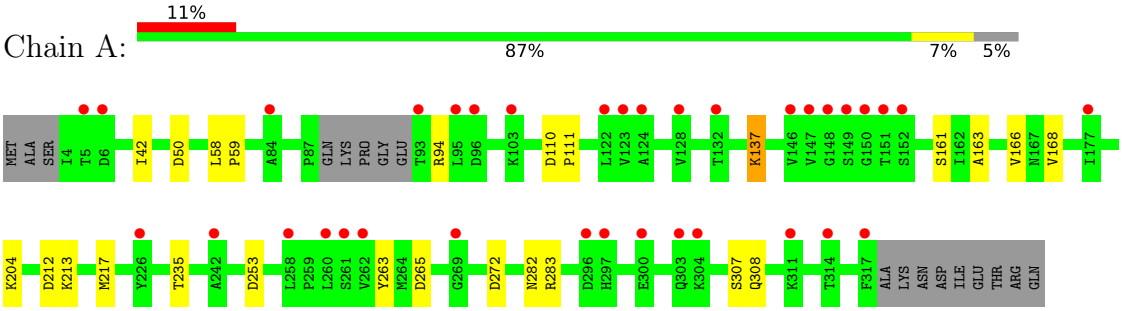
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	44	Total O 44 44	0	0
3	B	54	Total O 54 54	0	0
3	C	39	Total O 39 39	0	0
3	D	36	Total O 36 36	0	0
3	E	47	Total O 47 47	0	0
3	F	43	Total O 43 43	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

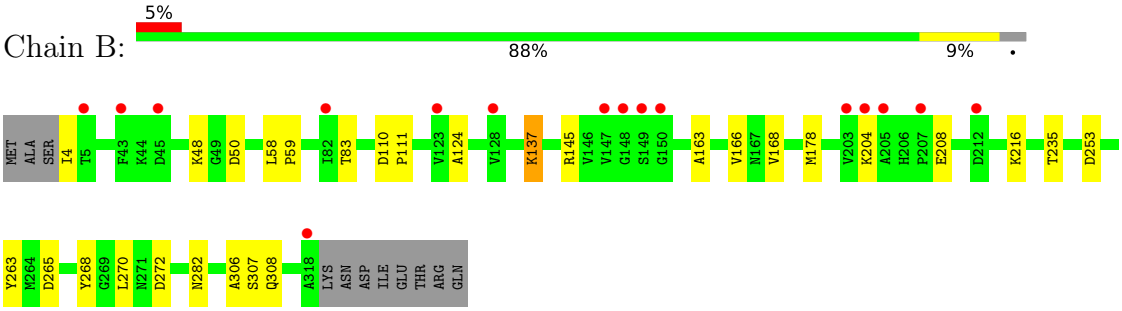
• Molecule 1: L-lactate dehydrogenase

Chain A:



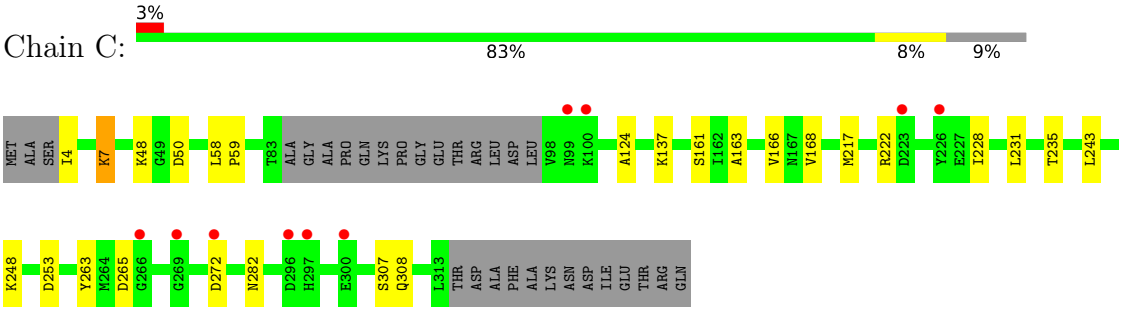
• Molecule 1: L-lactate dehydrogenase

Chain B:



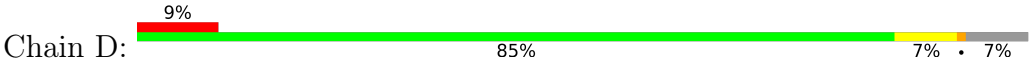
• Molecule 1: L-lactate dehydrogenase

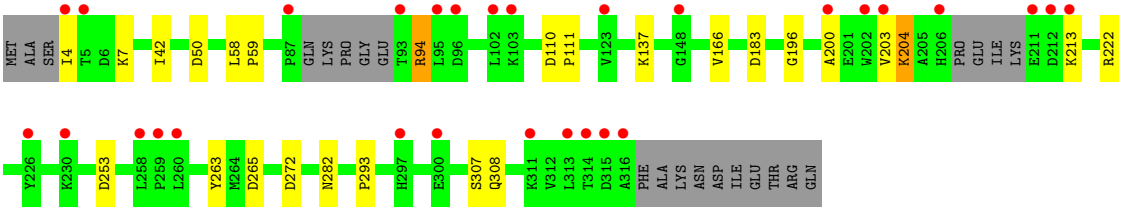
Chain C:



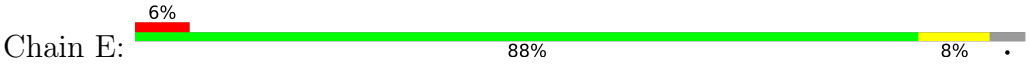
• Molecule 1: L-lactate dehydrogenase

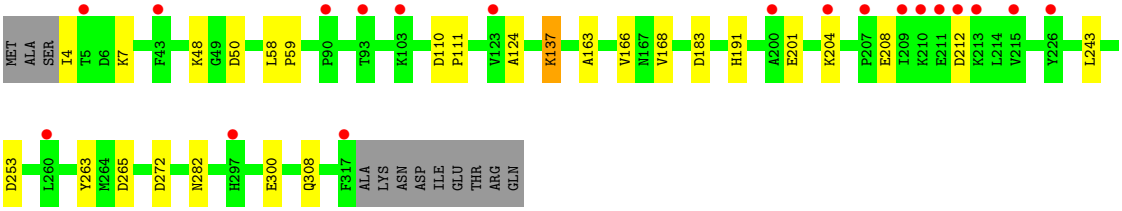
Chain D:



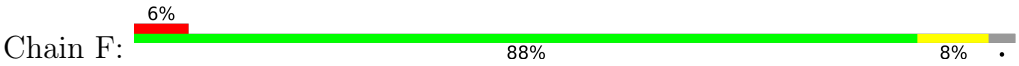


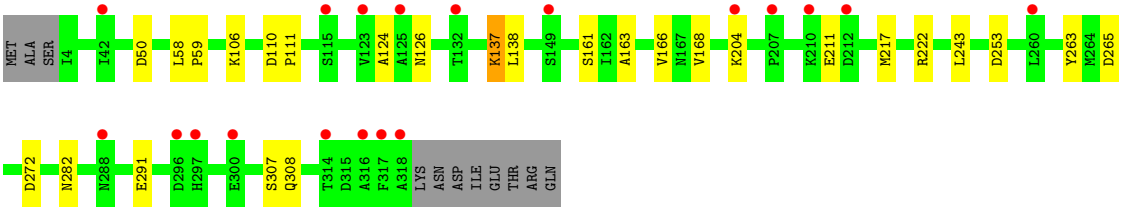
• Molecule 1: L-lactate dehydrogenase





• Molecule 1: L-lactate dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.38Å 82.89Å 179.77Å 90.00° 91.21° 90.00°	Depositor
Resolution (Å)	34.10 – 2.30 34.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.10-2.30) 99.9 (34.10-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.194 , 0.222 0.201 , 0.227	Depositor DCC
R_{free} test set	5411 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14535	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.80	0/2413	0.92	2/3273 (0.1%)
1	B	0.85	1/2458 (0.0%)	0.93	4/3335 (0.1%)
1	C	0.82	0/2317	0.95	2/3141 (0.1%)
1	D	0.81	0/2366	0.91	2/3208 (0.1%)
1	E	0.83	1/2453 (0.0%)	0.93	1/3328 (0.0%)
1	F	0.84	1/2458 (0.0%)	0.92	2/3335 (0.1%)
All	All	0.83	3/14465 (0.0%)	0.93	13/19620 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	291	GLU	CD-OE2	-6.15	1.18	1.25
1	E	300	GLU	CD-OE2	-5.91	1.19	1.25
1	B	124	ALA	C-O	-5.06	1.13	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	222	ARG	NE-CZ-NH1	-8.25	116.17	120.30
1	B	83	THR	C-N-CA	-6.49	105.48	121.70
1	B	145	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	D	183	ASP	CB-CA-C	-6.03	98.34	110.40
1	A	212	ASP	CB-CA-C	5.95	122.30	110.40
1	D	222	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	E	183	ASP	CB-CA-C	-5.46	99.49	110.40
1	A	283	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	F	137	LYS	CA-CB-CG	5.28	125.02	113.40
1	B	83	THR	CA-C-N	5.24	128.72	117.20
1	B	145	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	F	222	ARG	NE-CZ-NH1	-5.14	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	248	LYS	CD-CE-NZ	5.11	123.45	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2371	0	2392	9	0
1	B	2414	0	2435	8	0
1	C	2277	0	2301	9	0
1	D	2327	0	2345	11	0
1	E	2409	0	2430	11	0
1	F	2414	0	2435	10	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	44	0	0	2	0
3	B	54	0	0	0	0
3	C	39	0	0	0	0
3	D	36	0	0	1	0
3	E	47	0	0	0	0
3	F	43	0	0	2	0
All	All	14535	0	14338	55	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 2.

All (55) 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:D:94:ARG:CG	1:D:94:ARG:HH21	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:HG23	3:A:502:HOH:O	1.88	0.71
1:D:200:ALA:O	1:D:203:VAL:HG12	1.93	0.68
1:F:137:LYS:HD2	3:F:525:HOH:O	1.91	0.68
1:C:161:SER:OG	1:C:217:MET:HG3	1.95	0.67
1:D:42:ILE:HG13	3:D:523:HOH:O	1.97	0.65
1:D:94:ARG:HH21	1:D:94:ARG:HG2	1.63	0.63
1:C:4:ILE:O	1:C:7:LYS:HG3	2.01	0.61
1:C:231:LEU:HD13	1:E:48:LYS:HG3	1.89	0.54
1:D:4:ILE:HG12	1:D:7:LYS:HD3	1.89	0.53
1:A:161:SER:OG	1:A:217:MET:HG3	2.09	0.52
1:B:263:TYR:CZ	1:B:272:ASP:HA	2.47	0.50
1:E:263:TYR:CZ	1:E:272:ASP:HA	2.47	0.50
1:F:161:SER:OG	1:F:217:MET:HG3	2.10	0.49
1:C:124:ALA:HB2	1:C:243:LEU:HD21	1.95	0.49
1:D:263:TYR:CZ	1:D:272:ASP:HA	2.48	0.49
1:F:263:TYR:CZ	1:F:272:ASP:HA	2.48	0.49
1:A:263:TYR:CZ	1:A:272:ASP:HA	2.48	0.49
1:C:263:TYR:CZ	1:C:272:ASP:HA	2.49	0.47
1:B:137:LYS:HD2	1:B:137:LYS:HA	1.71	0.46
1:F:58:LEU:N	1:F:59:PRO:CD	2.79	0.46
1:E:58:LEU:N	1:E:59:PRO:CD	2.79	0.46
1:D:293:PRO:HG2	1:E:201:GLU:CG	2.47	0.45
1:E:4:ILE:HG12	1:E:7:LYS:HD3	1.97	0.45
1:A:58:LEU:N	1:A:59:PRO:CD	2.80	0.45
1:C:58:LEU:N	1:C:59:PRO:CD	2.80	0.44
1:D:58:LEU:N	1:D:59:PRO:CD	2.80	0.44
1:B:163:ALA:HB1	1:B:168:VAL:O	2.17	0.44
1:E:163:ALA:HB1	1:E:168:VAL:O	2.17	0.44
1:D:253:ASP:OD1	1:D:282:ASN:HB2	2.18	0.44
1:D:110:ASP:HB2	1:D:111:PRO:HD3	2.00	0.43
1:F:110:ASP:HB2	1:F:111:PRO:HD3	2.00	0.43
1:C:163:ALA:HB1	1:C:168:VAL:O	2.19	0.43
1:E:137:LYS:HD2	1:E:137:LYS:HA	1.88	0.43
1:B:58:LEU:N	1:B:59:PRO:CD	2.80	0.43
1:C:253:ASP:OD1	1:C:282:ASN:HB2	2.19	0.43
1:B:253:ASP:OD1	1:B:282:ASN:HB2	2.19	0.42
1:A:163:ALA:HB1	1:A:168:VAL:O	2.19	0.42
1:B:110:ASP:HB2	1:B:111:PRO:HD3	2.02	0.42
1:F:137:LYS:CD	3:F:525:HOH:O	2.62	0.42
1:A:110:ASP:HB2	1:A:111:PRO:HD3	2.02	0.42
1:E:110:ASP:HB2	1:E:111:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:ALA:HB1	1:F:168:VAL:O	2.19	0.42
1:B:270:LEU:HD22	1:B:306:ALA:CB	2.50	0.41
1:C:228:ILE:HB	1:C:235:THR:HG22	2.01	0.41
1:B:178:MET:HE1	1:B:268:TYR:CZ	2.55	0.41
1:F:106:LYS:HD2	1:F:138:LEU:HD22	2.02	0.41
1:E:124:ALA:HB2	1:E:243:LEU:HD21	2.02	0.41
1:E:253:ASP:OD1	1:E:282:ASN:HB2	2.21	0.41
1:A:253:ASP:OD1	1:A:282:ASN:HB2	2.21	0.41
1:A:137:LYS:HD2	1:A:137:LYS:HA	1.90	0.40
1:D:196:GLY:O	1:E:191:HIS:HD2	2.05	0.40
1:F:253:ASP:OD1	1:F:282:ASN:HB2	2.20	0.40
1:F:124:ALA:HB2	1:F:243:LEU:HD21	2.03	0.40
1:A:42:ILE:HG13	3:A:538:HOH:O	2.20	0.40

There are no symmetry-related clashes.

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	305/326 (94%)	296 (97%)	9 (3%)	0	100	100
1	B	313/326 (96%)	301 (96%)	12 (4%)	0	100	100
1	C	292/326 (90%)	282 (97%)	10 (3%)	0	100	100
1	D	298/326 (91%)	288 (97%)	9 (3%)	1 (0%)	41	50
1	E	312/326 (96%)	303 (97%)	9 (3%)	0	100	100
1	F	313/326 (96%)	303 (97%)	10 (3%)	0	100	100
All	All	1833/1956 (94%)	1773 (97%)	59 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	204	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/269 (95%)	246 (96%)	9 (4%)	36	50
1	B	259/269 (96%)	247 (95%)	12 (5%)	27	38
1	C	246/269 (91%)	238 (97%)	8 (3%)	38	53
1	D	250/269 (93%)	241 (96%)	9 (4%)	35	49
1	E	259/269 (96%)	251 (97%)	8 (3%)	40	55
1	F	259/269 (96%)	251 (97%)	8 (3%)	40	55
All	All	1528/1614 (95%)	1474 (96%)	54 (4%)	36	50

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	94	ARG
1	A	137	LYS
1	A	166	VAL
1	A	204	LYS
1	A	213	LYS
1	A	265	ASP
1	A	307	SER
1	A	308	GLN
1	B	4	ILE
1	B	48	LYS
1	B	50	ASP
1	B	137	LYS
1	B	166	VAL
1	B	204	LYS
1	B	208	GLU
1	B	216	LYS
1	B	235	THR

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Mol	Chain	Res	Type
1	B	265	ASP
1	B	307	SER
1	B	308	GLN
1	C	7	LYS
1	C	48	LYS
1	C	50	ASP
1	C	137	LYS
1	C	166	VAL
1	C	265	ASP
1	C	307	SER
1	C	308	GLN
1	D	50	ASP
1	D	94	ARG
1	D	137	LYS
1	D	166	VAL
1	D	204	LYS
1	D	213	LYS
1	D	265	ASP
1	D	307	SER
1	D	308	GLN
1	E	50	ASP
1	E	137	LYS
1	E	166	VAL
1	E	204	LYS
1	E	208	GLU
1	E	212	ASP
1	E	265	ASP
1	E	308	GLN
1	F	50	ASP
1	F	126	ASN
1	F	166	VAL
1	F	204	LYS
1	F	211	GLU
1	F	265	ASP
1	F	307	SER
1	F	308	GLN

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

Mol	Chain	Res	Type
1	E	191	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

12 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	D	401	-	4,4,4	0.40	0	6,6,6	0.49	0
2	SO4	D	402	-	4,4,4	0.85	0	6,6,6	0.43	0
2	SO4	A	402	-	4,4,4	0.31	0	6,6,6	0.20	0
2	SO4	E	402	-	4,4,4	0.48	0	6,6,6	0.32	0
2	SO4	B	402	-	4,4,4	0.27	0	6,6,6	0.47	0
2	SO4	F	402	-	4,4,4	0.37	0	6,6,6	0.46	0
2	SO4	C	401	-	4,4,4	0.32	0	6,6,6	0.44	0
2	SO4	B	401	-	4,4,4	0.30	0	6,6,6	0.70	0
2	SO4	F	401	-	4,4,4	0.23	0	6,6,6	0.63	0
2	SO4	A	401	-	4,4,4	0.45	0	6,6,6	0.31	0
2	SO4	E	401	-	4,4,4	0.37	0	6,6,6	0.74	0
2	SO4	C	402	-	4,4,4	0.45	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	309/326 (94%)	0.43	35 (11%) 5 7	28, 47, 76, 92	0
1	B	315/326 (96%)	0.18	16 (5%) 28 35	29, 45, 69, 87	0
1	C	296/326 (90%)	0.06	10 (3%) 45 52	30, 44, 70, 95	0
1	D	304/326 (93%)	0.53	29 (9%) 8 11	30, 48, 93, 117	0
1	E	314/326 (96%)	0.16	19 (6%) 21 27	29, 42, 69, 94	0
1	F	315/326 (96%)	0.26	19 (6%) 21 28	31, 46, 68, 87	0
All	All	1853/1956 (94%)	0.27	128 (6%) 16 22	28, 45, 73, 117	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	THR	6.6
1	F	318	ALA	6.3
1	D	5	THR	6.1
1	D	93	THR	5.9
1	D	95	LEU	5.8
1	D	203	VAL	5.3
1	D	96	ASP	4.7
1	A	226	TYR	4.7
1	F	212	ASP	4.7
1	D	226	TYR	4.6
1	E	207	PRO	4.4
1	D	87	PRO	4.4
1	E	212	ASP	4.3
1	A	123	VAL	4.3
1	A	260	LEU	4.1
1	A	128	VAL	3.9
1	E	209	ILE	3.8
1	B	212	ASP	3.7
1	E	210	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	211	GLU	3.5
1	A	317	PHE	3.4
1	D	315	ASP	3.4
1	C	266	GLY	3.4
1	A	93	THR	3.4
1	A	147	VAL	3.3
1	D	297	HIS	3.3
1	C	226	TYR	3.3
1	A	5	THR	3.3
1	D	260	LEU	3.3
1	E	215	VAL	3.3
1	C	272	ASP	3.3
1	D	103	LYS	3.3
1	D	300	GLU	3.3
1	A	124	ALA	3.2
1	E	5	THR	3.1
1	A	303	GLN	3.1
1	B	204	LYS	3.1
1	A	261	SER	3.1
1	A	148	GLY	3.1
1	F	317	PHE	3.0
1	A	296	ASP	3.0
1	E	204	LYS	3.0
1	D	206	HIS	3.0
1	A	95	LEU	2.9
1	D	200	ALA	2.9
1	C	269	GLY	2.9
1	A	96	ASP	2.9
1	B	203	VAL	2.8
1	A	311	LYS	2.8
1	A	122	LEU	2.8
1	C	297	HIS	2.8
1	B	43	PHE	2.8
1	D	313	LEU	2.8
1	A	149	SER	2.8
1	A	314	THR	2.8
1	E	43	PHE	2.8
1	E	200	ALA	2.8
1	D	102	LEU	2.7
1	B	82	ILE	2.7
1	D	311	LYS	2.7
1	A	262	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	THR	2.7
1	C	296	ASP	2.6
1	F	204	LYS	2.6
1	F	149	SER	2.6
1	A	151	THR	2.6
1	D	148	GLY	2.6
1	E	93	THR	2.6
1	A	150	GLY	2.6
1	D	123	VAL	2.6
1	A	103	LYS	2.6
1	A	84	ALA	2.5
1	C	100	LYS	2.5
1	C	99	ASN	2.5
1	F	314	THR	2.5
1	B	45	ASP	2.5
1	F	300	GLU	2.4
1	A	297	HIS	2.4
1	B	207	PRO	2.4
1	F	297	HIS	2.4
1	F	260	LEU	2.4
1	D	211	GLU	2.4
1	D	316	ALA	2.4
1	B	147	VAL	2.4
1	B	5	THR	2.4
1	B	123	VAL	2.4
1	E	317	PHE	2.4
1	F	115	SER	2.4
1	E	226	TYR	2.3
1	B	318	ALA	2.3
1	D	230	LYS	2.3
1	F	210	LYS	2.2
1	F	296	ASP	2.2
1	D	259	PRO	2.2
1	E	260	LEU	2.2
1	B	128	VAL	2.2
1	A	304	LYS	2.2
1	E	297	HIS	2.2
1	F	207	PRO	2.2
1	F	288	ASN	2.2
1	A	242	ALA	2.2
1	B	205	ALA	2.2
1	F	316	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	300	GLU	2.2
1	F	123	VAL	2.1
1	D	4	ILE	2.1
1	F	42	ILE	2.1
1	D	202	TRP	2.1
1	E	213	LYS	2.1
1	A	146	VAL	2.1
1	B	149	SER	2.1
1	A	152	SER	2.1
1	A	258	LEU	2.1
1	A	269	GLY	2.1
1	B	148	GLY	2.1
1	B	150	GLY	2.1
1	E	90	PRO	2.1
1	C	223	ASP	2.1
1	F	125	ALA	2.1
1	D	212	ASP	2.1
1	F	132	THR	2.1
1	C	300	GLU	2.0
1	A	6	ASP	2.0
1	A	177	ILE	2.0
1	D	258	LEU	2.0
1	E	103	LYS	2.0
1	E	123	VAL	2.0
1	D	213	LYS	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	SO4	F	401	5/5	0.96	0.12	55,56,64,65	0
2	SO4	E	402	5/5	0.97	0.16	48,49,51,52	0
2	SO4	B	401	5/5	0.97	0.13	49,56,56,65	0
2	SO4	E	401	5/5	0.98	0.08	47,48,52,54	0
2	SO4	A	401	5/5	0.98	0.09	49,52,56,59	0
2	SO4	D	401	5/5	0.98	0.07	46,52,56,57	0
2	SO4	D	402	5/5	0.99	0.12	39,43,45,46	0
2	SO4	C	401	5/5	0.99	0.07	50,50,52,53	0
2	SO4	C	402	5/5	0.99	0.12	39,40,42,46	0
2	SO4	B	402	5/5	0.99	0.11	41,41,43,44	0
2	SO4	F	402	5/5	0.99	0.13	39,40,42,42	0
2	SO4	A	402	5/5	1.00	0.09	39,39,42,44	0

6.5 Other polymers (i)

There are no such residues in this entry.