Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 07:08 pm GMT

PDB ID	:	6ZZR
Title	:	The Crystal Structure of human LDHA from Biortus
Authors	:	Wang, F.; Lin, D.; Cheng, W.; Bao, X.; Zhu, B.; Shang, H.
Deposited on	:	2020-08-05
Resolution	:	2.65 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 (i) 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 (1)) were used in the production of this report:

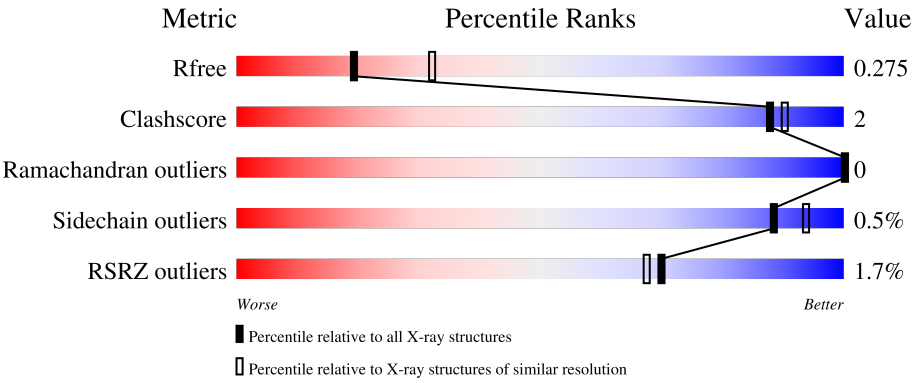
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	AAA	348	89% 6% 5%
1	BBB	348	90% 5% 5%
1	CCC	348	88% 7% 5%
1	DDD	348	91% 5%
1	EEE	348	90% 5% 5%

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Mol	Chain	Length	Quality of chain
1	FFF	348	2% 91% 5%
1	GGG	348	4% 90% 6%
1	HHH	348	2% 90% 5% 5%

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
2	EDO	AAA	406	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20943 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	AAA	331	Total	C	N	O	S	0	1	0
			2571	1641	439	478	13			
1	BBB	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	CCC	331	Total	C	N	O	S	0	2	0
			2580	1646	440	481	13			
1	DDD	331	Total	C	N	O	S	0	1	0
			2571	1641	439	478	13			
1	EEE	331	Total	C	N	O	S	0	2	0
			2573	1643	439	478	13			
1	FFF	331	Total	C	N	O	S	0	2	0
			2574	1643	439	479	13			
1	GGG	326	Total	C	N	O	S	0	2	0
			2534	1621	432	468	13			
1	HHH	331	Total	C	N	O	S	0	2	0
			2574	1643	439	479	13			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-15	MET	-	initiating methionine	UNP P00338
AAA	-14	GLY	-	expression tag	UNP P00338
AAA	-13	GLY	-	expression tag	UNP P00338
AAA	-12	SER	-	expression tag	UNP P00338
AAA	-11	HIS	-	expression tag	UNP P00338
AAA	-10	HIS	-	expression tag	UNP P00338
AAA	-9	HIS	-	expression tag	UNP P00338
AAA	-8	HIS	-	expression tag	UNP P00338
AAA	-7	HIS	-	expression tag	UNP P00338
AAA	-6	HIS	-	expression tag	UNP P00338
AAA	-5	GLU	-	expression tag	UNP P00338
AAA	-4	ASN	-	expression tag	UNP P00338
AAA	-3	LEU	-	expression tag	UNP P00338

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	TYR	-	expression tag	UNP P00338
AAA	-1	PHE	-	expression tag	UNP P00338
AAA	0	GLN	-	expression tag	UNP P00338
AAA	1	GLY	-	expression tag	UNP P00338
BBB	-15	MET	-	initiating methionine	UNP P00338
BBB	-14	GLY	-	expression tag	UNP P00338
BBB	-13	GLY	-	expression tag	UNP P00338
BBB	-12	SER	-	expression tag	UNP P00338
BBB	-11	HIS	-	expression tag	UNP P00338
BBB	-10	HIS	-	expression tag	UNP P00338
BBB	-9	HIS	-	expression tag	UNP P00338
BBB	-8	HIS	-	expression tag	UNP P00338
BBB	-7	HIS	-	expression tag	UNP P00338
BBB	-6	HIS	-	expression tag	UNP P00338
BBB	-5	GLU	-	expression tag	UNP P00338
BBB	-4	ASN	-	expression tag	UNP P00338
BBB	-3	LEU	-	expression tag	UNP P00338
BBB	-2	TYR	-	expression tag	UNP P00338
BBB	-1	PHE	-	expression tag	UNP P00338
BBB	0	GLN	-	expression tag	UNP P00338
BBB	1	GLY	-	expression tag	UNP P00338
CCC	-15	MET	-	initiating methionine	UNP P00338
CCC	-14	GLY	-	expression tag	UNP P00338
CCC	-13	GLY	-	expression tag	UNP P00338
CCC	-12	SER	-	expression tag	UNP P00338
CCC	-11	HIS	-	expression tag	UNP P00338
CCC	-10	HIS	-	expression tag	UNP P00338
CCC	-9	HIS	-	expression tag	UNP P00338
CCC	-8	HIS	-	expression tag	UNP P00338
CCC	-7	HIS	-	expression tag	UNP P00338
CCC	-6	HIS	-	expression tag	UNP P00338
CCC	-5	GLU	-	expression tag	UNP P00338
CCC	-4	ASN	-	expression tag	UNP P00338
CCC	-3	LEU	-	expression tag	UNP P00338
CCC	-2	TYR	-	expression tag	UNP P00338
CCC	-1	PHE	-	expression tag	UNP P00338
CCC	0	GLN	-	expression tag	UNP P00338
CCC	1	GLY	-	expression tag	UNP P00338
DDD	-15	MET	-	initiating methionine	UNP P00338
DDD	-14	GLY	-	expression tag	UNP P00338
DDD	-13	GLY	-	expression tag	UNP P00338
DDD	-12	SER	-	expression tag	UNP P00338

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-11	HIS	-	expression tag	UNP P00338
DDD	-10	HIS	-	expression tag	UNP P00338
DDD	-9	HIS	-	expression tag	UNP P00338
DDD	-8	HIS	-	expression tag	UNP P00338
DDD	-7	HIS	-	expression tag	UNP P00338
DDD	-6	HIS	-	expression tag	UNP P00338
DDD	-5	GLU	-	expression tag	UNP P00338
DDD	-4	ASN	-	expression tag	UNP P00338
DDD	-3	LEU	-	expression tag	UNP P00338
DDD	-2	TYR	-	expression tag	UNP P00338
DDD	-1	PHE	-	expression tag	UNP P00338
DDD	0	GLN	-	expression tag	UNP P00338
DDD	1	GLY	-	expression tag	UNP P00338
EEE	-15	MET	-	initiating methionine	UNP P00338
EEE	-14	GLY	-	expression tag	UNP P00338
EEE	-13	GLY	-	expression tag	UNP P00338
EEE	-12	SER	-	expression tag	UNP P00338
EEE	-11	HIS	-	expression tag	UNP P00338
EEE	-10	HIS	-	expression tag	UNP P00338
EEE	-9	HIS	-	expression tag	UNP P00338
EEE	-8	HIS	-	expression tag	UNP P00338
EEE	-7	HIS	-	expression tag	UNP P00338
EEE	-6	HIS	-	expression tag	UNP P00338
EEE	-5	GLU	-	expression tag	UNP P00338
EEE	-4	ASN	-	expression tag	UNP P00338
EEE	-3	LEU	-	expression tag	UNP P00338
EEE	-2	TYR	-	expression tag	UNP P00338
EEE	-1	PHE	-	expression tag	UNP P00338
EEE	0	GLN	-	expression tag	UNP P00338
EEE	1	GLY	-	expression tag	UNP P00338
FFF	-15	MET	-	initiating methionine	UNP P00338
FFF	-14	GLY	-	expression tag	UNP P00338
FFF	-13	GLY	-	expression tag	UNP P00338
FFF	-12	SER	-	expression tag	UNP P00338
FFF	-11	HIS	-	expression tag	UNP P00338
FFF	-10	HIS	-	expression tag	UNP P00338
FFF	-9	HIS	-	expression tag	UNP P00338
FFF	-8	HIS	-	expression tag	UNP P00338
FFF	-7	HIS	-	expression tag	UNP P00338
FFF	-6	HIS	-	expression tag	UNP P00338
FFF	-5	GLU	-	expression tag	UNP P00338
FFF	-4	ASN	-	expression tag	UNP P00338

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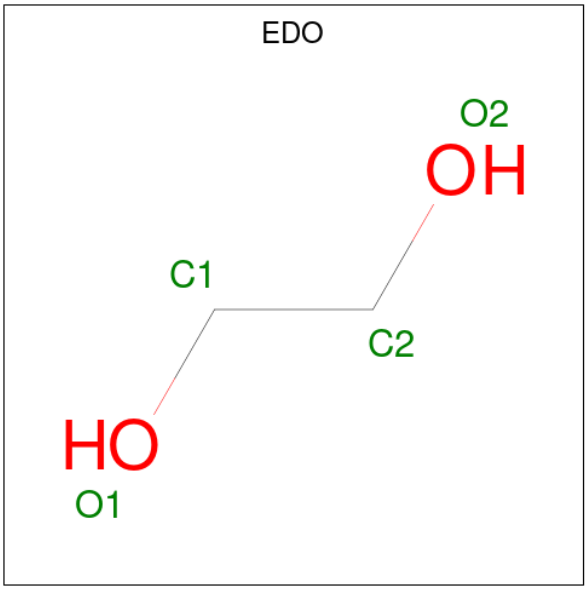
Chain	Residue	Modelled	Actual	Comment	Reference
FFF	-3	LEU	-	expression tag	UNP P00338
FFF	-2	TYR	-	expression tag	UNP P00338
FFF	-1	PHE	-	expression tag	UNP P00338
FFF	0	GLN	-	expression tag	UNP P00338
FFF	1	GLY	-	expression tag	UNP P00338
GGG	-15	MET	-	initiating methionine	UNP P00338
GGG	-14	GLY	-	expression tag	UNP P00338
GGG	-13	GLY	-	expression tag	UNP P00338
GGG	-12	SER	-	expression tag	UNP P00338
GGG	-11	HIS	-	expression tag	UNP P00338
GGG	-10	HIS	-	expression tag	UNP P00338
GGG	-9	HIS	-	expression tag	UNP P00338
GGG	-8	HIS	-	expression tag	UNP P00338
GGG	-7	HIS	-	expression tag	UNP P00338
GGG	-6	HIS	-	expression tag	UNP P00338
GGG	-5	GLU	-	expression tag	UNP P00338
GGG	-4	ASN	-	expression tag	UNP P00338
GGG	-3	LEU	-	expression tag	UNP P00338
GGG	-2	TYR	-	expression tag	UNP P00338
GGG	-1	PHE	-	expression tag	UNP P00338
GGG	0	GLN	-	expression tag	UNP P00338
GGG	1	GLY	-	expression tag	UNP P00338
HHH	-15	MET	-	initiating methionine	UNP P00338
HHH	-14	GLY	-	expression tag	UNP P00338
HHH	-13	GLY	-	expression tag	UNP P00338
HHH	-12	SER	-	expression tag	UNP P00338
HHH	-11	HIS	-	expression tag	UNP P00338
HHH	-10	HIS	-	expression tag	UNP P00338
HHH	-9	HIS	-	expression tag	UNP P00338
HHH	-8	HIS	-	expression tag	UNP P00338
HHH	-7	HIS	-	expression tag	UNP P00338
HHH	-6	HIS	-	expression tag	UNP P00338
HHH	-5	GLU	-	expression tag	UNP P00338
HHH	-4	ASN	-	expression tag	UNP P00338
HHH	-3	LEU	-	expression tag	UNP P00338
HHH	-2	TYR	-	expression tag	UNP P00338
HHH	-1	PHE	-	expression tag	UNP P00338
HHH	0	GLN	-	expression tag	UNP P00338
HHH	1	GLY	-	expression tag	UNP P00338

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0

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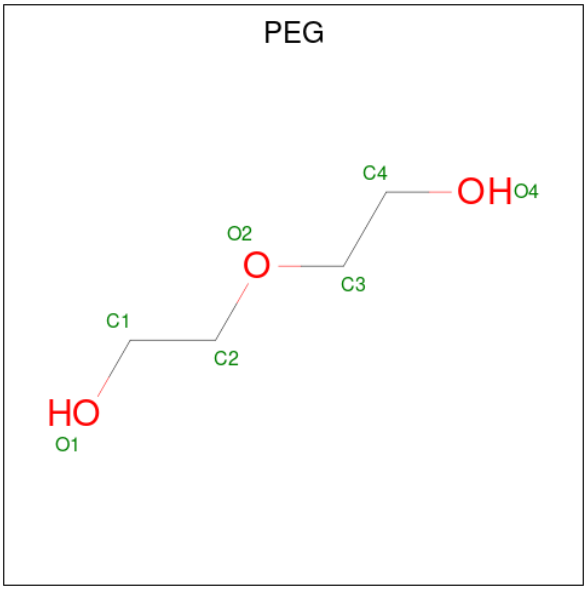
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	EEE	1	Total C O 4 2 2	0	0
2	EEE	1	Total C O 4 2 2	0	0
2	FFF	1	Total C O 4 2 2	0	0
2	FFF	1	Total C O 4 2 2	0	0
2	FFF	1	Total C O 4 2 2	0	0
2	GGG	1	Total C O 4 2 2	0	0
2	GGG	1	Total C O 4 2 2	0	0
2	HHH	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

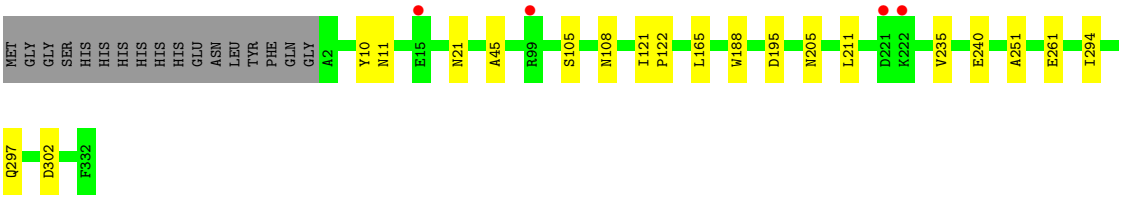
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	63	Total O 63 63	0	0
4	BBB	56	Total O 56 56	0	0
4	CCC	38	Total O 38 38	0	0
4	DDD	52	Total O 52 52	0	0
4	EEE	29	Total O 29 29	0	0
4	FFF	25	Total O 25 25	0	0
4	GGG	16	Total O 16 16	0	0
4	HHH	9	Total O 9 9	0	0

3 Residue-property plots (i)

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.

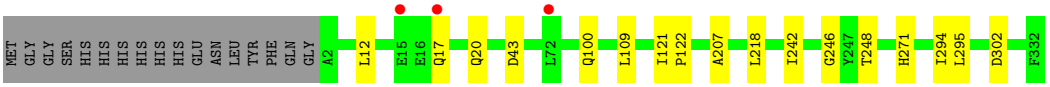
• Molecule 1: L-lactate dehydrogenase A chain

Chain AAA:



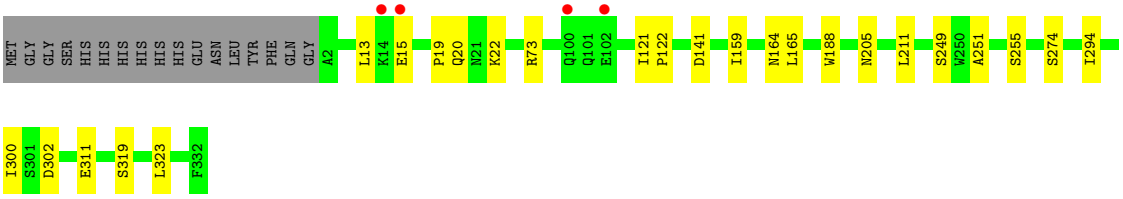
• Molecule 1: L-lactate dehydrogenase A chain

Chain BBB:



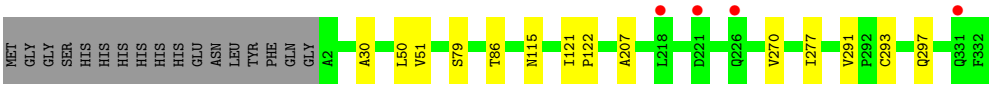
• Molecule 1: L-lactate dehydrogenase A chain

Chain CCC:



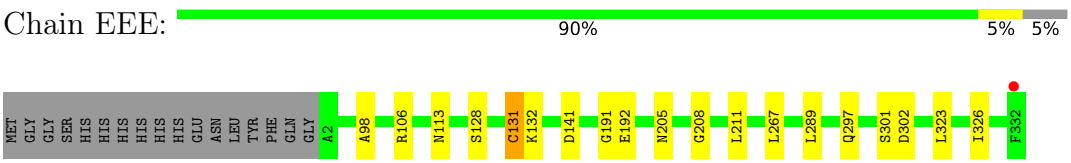
• Molecule 1: L-lactate dehydrogenase A chain

Chain DDD:



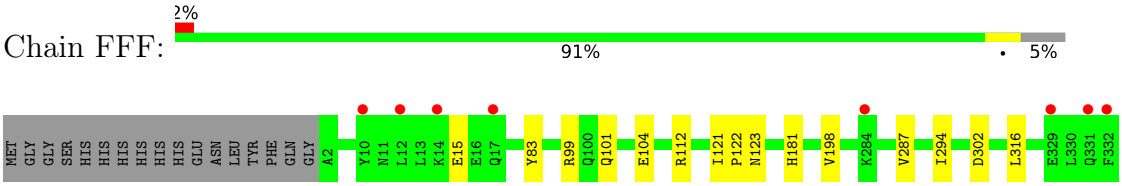
• Molecule 1: L-lactate dehydrogenase A chain

Chain EEE:



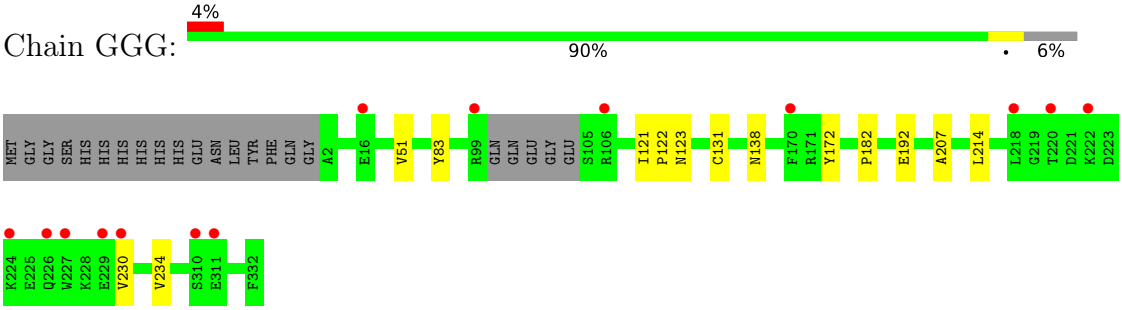
• Molecule 1: L-lactate dehydrogenase A chain

Chain FFF:



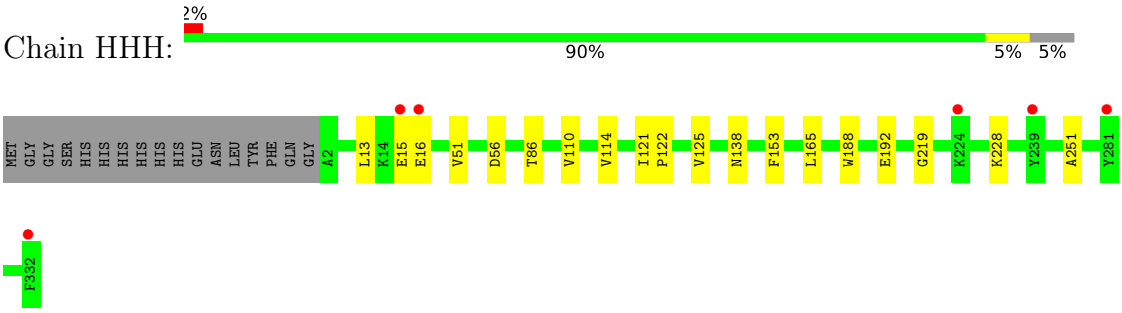
• Molecule 1: L-lactate dehydrogenase A chain

Chain GGG:



• Molecule 1: L-lactate dehydrogenase A chain

Chain HHH:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.96Å 66.48Å 250.84Å 90.00° 100.10° 90.00°	Depositor
Resolution (Å)	46.73 – 2.65 46.73 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.73-2.65) 97.5 (46.73-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.212 , 0.277 0.210 , 0.275	Depositor DCC
R_{free} test set	4012 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20943	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: EDO, PEG

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	AAA	0.66	0/2618	0.71	0/3540
1	BBB	0.66	0/2612	0.71	0/3532
1	CCC	0.66	0/2627	0.71	0/3552
1	DDD	0.66	0/2618	0.71	0/3540
1	EEE	0.67	0/2623	0.71	0/3548
1	FFF	0.67	0/2624	0.71	0/3548
1	GGG	0.67	0/2583	0.72	0/3492
1	HHH	0.68	0/2624	0.72	0/3548
All	All	0.67	0/20929	0.71	0/28300

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	2571	0	2658	14	0
1	BBB	2568	0	2653	11	0
1	CCC	2580	0	2663	14	0
1	DDD	2571	0	2658	9	0
1	EEE	2573	0	2663	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FFF	2574	0	2663	8	0
1	GGG	2534	0	2631	9	0
1	HHH	2574	0	2663	10	0
2	AAA	36	0	54	3	0
2	BBB	4	0	6	0	0
2	CCC	8	0	12	0	0
2	DDD	16	0	24	1	0
2	EEE	8	0	12	1	0
2	FFF	12	0	18	0	0
2	GGG	8	0	12	2	0
2	HHH	4	0	6	1	0
3	BBB	14	0	20	2	0
4	AAA	63	0	0	1	0
4	BBB	56	0	0	2	0
4	CCC	38	0	0	0	0
4	DDD	52	0	0	0	0
4	EEE	29	0	0	0	0
4	FFF	25	0	0	0	0
4	GGG	16	0	0	1	0
4	HHH	9	0	0	0	0
All	All	20943	0	21416	84	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 (84) 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:EEE:98:ALA:H	1:EEE:113:ASN:HD21	1.37	0.73
1:AAA:11:ASN:H	2:AAA:409:EDO:H22	1.59	0.67
1:BBB:43:ASP:OD1	3:BBB:402:PEG:H32	1.95	0.66
1:GGG:138:ASN:HD21	2:GGG:402:EDO:C2	2.11	0.63
1:EEE:301:SER:HA	1:HHH:13:LEU:HD21	1.80	0.62
1:GGG:138:ASN:HD21	2:GGG:402:EDO:H22	1.65	0.60
1:CCC:294:ILE:HD12	1:CCC:302:ASP:HB2	1.88	0.56
1:GGG:192:GLU:HG2	4:GGG:504:HOH:O	2.05	0.56
1:EEE:98:ALA:N	1:EEE:113:ASN:HD21	2.02	0.55
1:FFF:294:ILE:HD12	1:FFF:302:ASP:HB2	1.88	0.55
1:EEE:191:GLY:C	1:EEE:289:LEU:HD22	2.27	0.54
1:BBB:294:ILE:HD12	1:BBB:302:ASP:HB2	1.90	0.54
1:AAA:105:SER:H	1:AAA:108:ASN:HD22	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:13:LEU:HD12	1:CCC:15:GLU:HB3	1.90	0.52
1:EEE:205:ASN:HA	1:EEE:211:LEU:HD13	1.92	0.52
1:EEE:205:ASN:HD22	1:EEE:208:GLY:H	1.57	0.51
1:EEE:191:GLY:HA2	1:EEE:289:LEU:HD22	1.93	0.50
1:DDD:51:VAL:HG21	1:DDD:86:THR:CG2	2.42	0.50
1:BBB:248:THR:CG2	4:BBB:508:HOH:O	2.60	0.49
1:FFF:83:TYR:CG	1:FFF:123:ASN:HB3	2.47	0.49
1:AAA:121:ILE:HB	1:AAA:122:PRO:HD3	1.95	0.49
1:DDD:121:ILE:HB	1:DDD:122:PRO:HD3	1.94	0.49
1:AAA:294:ILE:HD12	1:AAA:302:ASP:HB2	1.94	0.49
1:BBB:248:THR:HG23	4:BBB:508:HOH:O	2.12	0.49
1:BBB:100:GLN:HB2	1:BBB:109:LEU:HD22	1.96	0.48
4:AAA:515:HOH:O	3:BBB:402:PEG:H22	2.13	0.48
1:CCC:19:PRO:HB2	1:CCC:22:LYS:HB2	1.96	0.48
1:CCC:141:ASP:OD1	1:CCC:274:SER:OG	2.32	0.47
1:FFF:101:GLN:HB3	1:FFF:104:GLU:HB2	1.95	0.47
1:AAA:261:GLU:OE2	1:CCC:73:ARG:HD2	2.15	0.47
1:GGG:121:ILE:HB	1:GGG:122:PRO:HD3	1.96	0.47
1:HHH:110:VAL:O	1:HHH:114:VAL:HG23	2.15	0.47
1:AAA:297:GLN:HE22	1:CCC:20:GLN:HG2	1.80	0.46
1:GGG:51:VAL:HG11	1:GGG:83:TYR:CZ	2.51	0.46
1:GGG:172:TYR:HA	1:GGG:182:PRO:HG3	1.98	0.46
1:BBB:20:GLN:HG2	1:DDD:297:GLN:HE22	1.81	0.45
1:EEE:132:LYS:HE3	1:EEE:297:GLN:O	2.16	0.45
1:FFF:198:VAL:HG21	1:FFF:316:LEU:CD1	2.46	0.45
1:EEE:132:LYS:CE	1:EEE:297:GLN:O	2.64	0.45
1:HHH:138:ASN:HD21	2:HHH:401:EDO:H11	1.82	0.45
1:DDD:270:VAL:HA	1:DDD:293:CYS:O	2.17	0.45
1:FFF:99:ARG:O	1:FFF:112:ARG:NH1	2.50	0.44
1:AAA:195:ASP:HA	1:AAA:235:VAL:CG2	2.47	0.44
1:EEE:289:LEU:HD23	1:EEE:289:LEU:HA	1.83	0.44
1:AAA:240:GLU:HB3	2:AAA:405:EDO:H22	2.00	0.44
1:EEE:106:ARG:HH12	2:EEE:402:EDO:H11	1.83	0.44
1:CCC:205:ASN:HA	1:CCC:211:LEU:HD13	1.99	0.44
1:AAA:195:ASP:HA	1:AAA:235:VAL:HG21	1.99	0.44
1:CCC:319:SER:O	1:CCC:323:LEU:HG	2.18	0.44
1:HHH:125:VAL:HG22	1:HHH:153:PHE:CZ	2.53	0.44
1:DDD:277:ILE:HD11	1:DDD:291:VAL:HG11	2.00	0.43
1:EEE:141:ASP:OD2	1:EEE:192:GLU:HA	2.18	0.43
1:BBB:242:ILE:O	1:BBB:246:GLY:N	2.51	0.43
1:CCC:164:ASN:ND2	1:CCC:255[B]:SER:OG	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:191:GLY:CA	1:EEE:289:LEU:HD22	2.48	0.43
1:BBB:121:ILE:HB	1:BBB:122:PRO:HD3	1.99	0.43
1:EEE:289:LEU:HD21	1:EEE:323:LEU:HD12	2.01	0.42
1:AAA:10:TYR:CD1	2:AAA:409:EDO:H12	2.54	0.42
1:CCC:159:ILE:HG23	1:CCC:300:ILE:HD11	2.01	0.42
1:AAA:21:ASN:O	1:AAA:45:ALA:HA	2.20	0.42
1:BBB:207:ALA:HA	1:CCC:188:TRP:CE2	2.53	0.42
1:HHH:219:GLY:HA2	1:HHH:228:LYS:HG2	2.02	0.42
1:GGG:83:TYR:CG	1:GGG:123:ASN:HB3	2.54	0.42
1:HHH:15:GLU:HG2	1:HHH:16:GLU:N	2.35	0.42
1:HHH:51:VAL:HG21	1:HHH:86:THR:CG2	2.48	0.42
1:CCC:165:LEU:HD11	1:CCC:251:ALA:HB1	2.00	0.42
1:DDD:30:ALA:HA	2:DDD:402:EDO:H22	2.01	0.42
1:AAA:165:LEU:HD11	1:AAA:251:ALA:HB1	2.02	0.42
1:AAA:205:ASN:HA	1:AAA:211:LEU:HD13	2.01	0.41
1:DDD:50:LEU:O	1:DDD:79:SER:HA	2.20	0.41
1:DDD:115:ASN:HD21	1:EEE:326:ILE:HD11	1.86	0.41
1:BBB:271:HIS:CD2	1:BBB:295:LEU:HD12	2.55	0.41
1:GGG:230:VAL:O	1:GGG:234:VAL:HG23	2.20	0.41
1:CCC:311[B]:GLU:H	1:CCC:311[B]:GLU:CD	2.23	0.41
1:CCC:121:ILE:HB	1:CCC:122:PRO:HD3	2.02	0.41
1:EEE:267:LEU:O	1:FFF:181:HIS:HB2	2.20	0.41
1:GGG:207:ALA:HA	1:HHH:188:TRP:CE2	2.56	0.41
1:EEE:128:SER:HB3	1:EEE:131:CYS:HB3	2.02	0.41
1:BBB:12:LEU:HD12	1:BBB:12:LEU:N	2.36	0.40
1:FFF:121:ILE:HB	1:FFF:122:PRO:HD3	2.02	0.40
1:AAA:188:TRP:CE2	1:DDD:207:ALA:HA	2.55	0.40
1:FFF:198:VAL:HG21	1:FFF:316:LEU:HD12	2.02	0.40
1:HHH:121:ILE:HB	1:HHH:122:PRO:HD3	2.03	0.40
1:HHH:165:LEU:HD11	1:HHH:251:ALA:HB1	2.02	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	AAA	330/348 (95%)	317 (96%)	13 (4%)	0	100	100
1	BBB	329/348 (94%)	318 (97%)	11 (3%)	0	100	100
1	CCC	331/348 (95%)	319 (96%)	12 (4%)	0	100	100
1	DDD	330/348 (95%)	320 (97%)	10 (3%)	0	100	100
1	EEE	331/348 (95%)	321 (97%)	10 (3%)	0	100	100
1	FFF	331/348 (95%)	318 (96%)	13 (4%)	0	100	100
1	GGG	324/348 (93%)	313 (97%)	11 (3%)	0	100	100
1	HHH	331/348 (95%)	320 (97%)	11 (3%)	0	100	100
All	All	2637/2784 (95%)	2546 (96%)	91 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	288/301 (96%)	288 (100%)	0	100	100
1	BBB	287/301 (95%)	285 (99%)	2 (1%)	84	91
1	CCC	289/301 (96%)	288 (100%)	1 (0%)	92	96
1	DDD	288/301 (96%)	288 (100%)	0	100	100
1	EEE	289/301 (96%)	287 (99%)	2 (1%)	84	91
1	FFF	289/301 (96%)	287 (99%)	2 (1%)	84	91
1	GGG	285/301 (95%)	283 (99%)	2 (1%)	84	91
1	HHH	289/301 (96%)	287 (99%)	2 (1%)	84	91
All	All	2304/2408 (96%)	2293 (100%)	11 (0%)	88	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	17	GLN
1	BBB	218	LEU
1	CCC	249	SER
1	EEE	131	CYS
1	EEE	302	ASP
1	FFF	15	GLU
1	FFF	287	VAL
1	GGG	131	CYS
1	GGG	214	LEU
1	HHH	56	ASP
1	HHH	192	GLU

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

26 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	EDO	FFF	401	-	3,3,3	0.11	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PEG	BBB	402	-	6,6,6	0.15	0	5,5,5	0.10	0
2	EDO	DDD	402	-	3,3,3	0.15	0	2,2,2	0.33	0
2	EDO	DDD	401	-	3,3,3	0.08	0	2,2,2	0.24	0
2	EDO	AAA	406	-	3,3,3	0.13	0	2,2,2	0.35	0
3	PEG	BBB	403	-	6,6,6	0.21	0	5,5,5	0.15	0
2	EDO	DDD	403	-	3,3,3	0.18	0	2,2,2	0.39	0
2	EDO	CCC	402	-	3,3,3	0.14	0	2,2,2	0.33	0
2	EDO	EEE	402	-	3,3,3	0.16	0	2,2,2	0.36	0
2	EDO	AAA	403	-	3,3,3	0.11	0	2,2,2	0.27	0
2	EDO	GGG	402	-	3,3,3	0.07	0	2,2,2	0.26	0
2	EDO	AAA	404	-	3,3,3	0.13	0	2,2,2	0.38	0
2	EDO	CCC	401	-	3,3,3	0.10	0	2,2,2	0.27	0
2	EDO	AAA	402	-	3,3,3	0.07	0	2,2,2	0.30	0
2	EDO	AAA	408	-	3,3,3	0.09	0	2,2,2	0.21	0
2	EDO	GGG	401	-	3,3,3	0.07	0	2,2,2	0.22	0
2	EDO	HHH	401	-	3,3,3	0.13	0	2,2,2	0.36	0
2	EDO	FFF	403	-	3,3,3	0.11	0	2,2,2	0.40	0
2	EDO	BBB	401	-	3,3,3	0.12	0	2,2,2	0.32	0
2	EDO	AAA	409	-	3,3,3	0.09	0	2,2,2	0.38	0
2	EDO	AAA	405	-	3,3,3	0.08	0	2,2,2	0.36	0
2	EDO	EEE	401	-	3,3,3	0.07	0	2,2,2	0.22	0
2	EDO	DDD	404	-	3,3,3	0.17	0	2,2,2	0.41	0
2	EDO	AAA	407	-	3,3,3	0.08	0	2,2,2	0.25	0
2	EDO	AAA	401	-	3,3,3	0.07	0	2,2,2	0.23	0
2	EDO	FFF	402	-	3,3,3	0.07	0	2,2,2	0.20	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	EDO	FFF	401	-	-	1/1/1/1	-
3	PEG	BBB	402	-	-	2/4/4/4	-
2	EDO	DDD	402	-	-	0/1/1/1	-
2	EDO	DDD	401	-	-	0/1/1/1	-
2	EDO	AAA	406	-	-	1/1/1/1	-
3	PEG	BBB	403	-	-	2/4/4/4	-
2	EDO	DDD	403	-	-	1/1/1/1	-
2	EDO	CCC	402	-	-	1/1/1/1	-
2	EDO	EEE	402	-	-	1/1/1/1	-
2	EDO	AAA	403	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	GGG	402	-	-	0/1/1/1	-
2	EDO	AAA	404	-	-	0/1/1/1	-
2	EDO	CCC	401	-	-	0/1/1/1	-
2	EDO	AAA	402	-	-	0/1/1/1	-
2	EDO	AAA	408	-	-	0/1/1/1	-
2	EDO	GGG	401	-	-	0/1/1/1	-
2	EDO	HHH	401	-	-	1/1/1/1	-
2	EDO	FFF	403	-	-	1/1/1/1	-
2	EDO	BBB	401	-	-	1/1/1/1	-
2	EDO	AAA	409	-	-	0/1/1/1	-
2	EDO	AAA	405	-	-	0/1/1/1	-
2	EDO	EEE	401	-	-	0/1/1/1	-
2	EDO	DDD	404	-	-	1/1/1/1	-
2	EDO	AAA	407	-	-	0/1/1/1	-
2	EDO	AAA	401	-	-	1/1/1/1	-
2	EDO	FFF	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	402	PEG	O1-C1-C2-O2
2	AAA	403	EDO	O1-C1-C2-O2
2	BBB	401	EDO	O1-C1-C2-O2
2	CCC	402	EDO	O1-C1-C2-O2
2	EEE	402	EDO	O1-C1-C2-O2
2	FFF	401	EDO	O1-C1-C2-O2
2	AAA	406	EDO	O1-C1-C2-O2
2	DDD	403	EDO	O1-C1-C2-O2
2	FFF	403	EDO	O1-C1-C2-O2
2	HHH	401	EDO	O1-C1-C2-O2
3	BBB	402	PEG	C1-C2-O2-C3
3	BBB	403	PEG	O2-C3-C4-O4
2	DDD	404	EDO	O1-C1-C2-O2
3	BBB	403	PEG	C4-C3-O2-C2
2	AAA	401	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	402	PEG	2	0
2	DDD	402	EDO	1	0
2	EEE	402	EDO	1	0
2	GGG	402	EDO	2	0
2	HHH	401	EDO	1	0
2	AAA	409	EDO	2	0
2	AAA	405	EDO	1	0

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, 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	AAA	331/348 (95%)	-0.12	4 (1%)	79 77	27, 39, 67, 105	0
1	BBB	331/348 (95%)	-0.32	3 (0%)	84 83	29, 40, 67, 99	0
1	CCC	331/348 (95%)	-0.23	4 (1%)	79 77	33, 44, 69, 95	0
1	DDD	331/348 (95%)	-0.13	4 (1%)	79 77	32, 43, 74, 99	0
1	EEE	331/348 (95%)	-0.20	1 (0%)	94 95	32, 47, 74, 108	1 (0%)
1	FFF	331/348 (95%)	0.02	8 (2%)	59 54	39, 55, 88, 108	1 (0%)
1	GGG	326/348 (93%)	0.15	14 (4%)	35 31	36, 58, 96, 105	2 (0%)
1	HHH	331/348 (95%)	0.18	6 (1%)	68 65	41, 61, 90, 108	0
All	All	2643/2784 (94%)	-0.08	44 (1%)	70 67	27, 49, 83, 108	4 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	GGG	106	ARG	4.6
1	EEE	332	PHE	4.2
1	HHH	332	PHE	3.9
1	FFF	332	PHE	3.7
1	HHH	239	TYR	3.6
1	HHH	15	GLU	3.5
1	GGG	224	LYS	3.4
1	HHH	281	TYR	3.4
1	GGG	226	GLN	3.3
1	FFF	12	LEU	3.3
1	AAA	99	ARG	3.2
1	FFF	14	LYS	3.0
1	GGG	16	GLU	3.0
1	FFF	17	GLN	3.0
1	AAA	15	GLU	2.9
1	DDD	331	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	FFF	331	GLN	2.9
1	HHH	16	GLU	2.8
1	CCC	15	GLU	2.8
1	GGG	220	THR	2.8
1	BBB	15	GLU	2.7
1	FFF	329	GLU	2.7
1	GGG	222	LYS	2.7
1	GGG	99	ARG	2.7
1	GGG	227	TRP	2.6
1	CCC	100	GLN	2.6
1	AAA	221	ASP	2.5
1	GGG	229	GLU	2.4
1	GGG	218	LEU	2.4
1	GGG	311	GLU	2.4
1	BBB	72	LEU	2.3
1	DDD	221	ASP	2.3
1	GGG	170	PHE	2.2
1	GGG	230	VAL	2.2
1	CCC	102	GLU	2.1
1	AAA	222	LYS	2.1
1	DDD	218	LEU	2.1
1	FFF	10	TYR	2.1
1	GGG	310	SER	2.1
1	BBB	17	GLN	2.0
1	DDD	226	GLN	2.0
1	FFF	284	LYS	2.0
1	HHH	224	LYS	2.0
1	CCC	14	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	EDO	AAA	405	4/4	0.65	0.34	72,74,75,76	0
2	EDO	AAA	409	4/4	0.71	0.23	57,58,58,59	0
2	EDO	AAA	401	4/4	0.75	0.33	59,61,62,63	0
2	EDO	AAA	406	4/4	0.79	0.68	61,61,61,62	0
2	EDO	DDD	401	4/4	0.80	0.37	65,65,65,66	0
2	EDO	BBB	401	4/4	0.83	0.39	57,59,59,59	0
2	EDO	AAA	407	4/4	0.83	0.60	53,55,55,56	0
2	EDO	DDD	402	4/4	0.83	0.27	50,51,52,52	0
2	EDO	FFF	401	4/4	0.83	0.81	72,72,72,73	0
2	EDO	DDD	404	4/4	0.84	0.35	54,56,56,56	0
2	EDO	FFF	402	4/4	0.85	0.17	61,62,63,64	0
2	EDO	AAA	404	4/4	0.86	0.35	51,52,53,54	0
2	EDO	GGG	401	4/4	0.86	0.56	66,67,67,67	0
2	EDO	CCC	402	4/4	0.88	0.21	58,59,59,60	0
2	EDO	HHH	401	4/4	0.89	0.26	45,47,47,47	0
3	PEG	BBB	402	7/7	0.89	0.41	54,57,60,60	0
2	EDO	DDD	403	4/4	0.90	0.24	34,35,36,37	0
3	PEG	BBB	403	7/7	0.90	0.20	37,41,46,47	0
2	EDO	CCC	401	4/4	0.91	0.65	52,54,54,55	0
2	EDO	AAA	408	4/4	0.93	0.35	42,43,44,44	0
2	EDO	EEE	401	4/4	0.93	0.11	59,61,61,61	0
2	EDO	AAA	403	4/4	0.94	0.28	36,37,38,38	0
2	EDO	FFF	403	4/4	0.95	0.16	42,44,44,45	0
2	EDO	AAA	402	4/4	0.95	0.14	48,48,48,48	0
2	EDO	GGG	402	4/4	0.95	0.09	56,57,57,57	0
2	EDO	EEE	402	4/4	0.96	0.18	27,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.