Full wwPDB X-ray Structure Validation Report (i)

Feb 8, 2022 – 03:24 am GMT

PDB ID	:	7NRZ
Title	:	Crystal structure of malate dehydrogenase from Trypanosoma cruzi
Authors	:	Sonani, R.R.; Kurpiewska, K.; Lewinski, K.; Dubin, G.
Deposited on	:	2021-03-04
Resolution	:	2.60 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 following versions of software and data (see references (1)) were used in the production of this report:

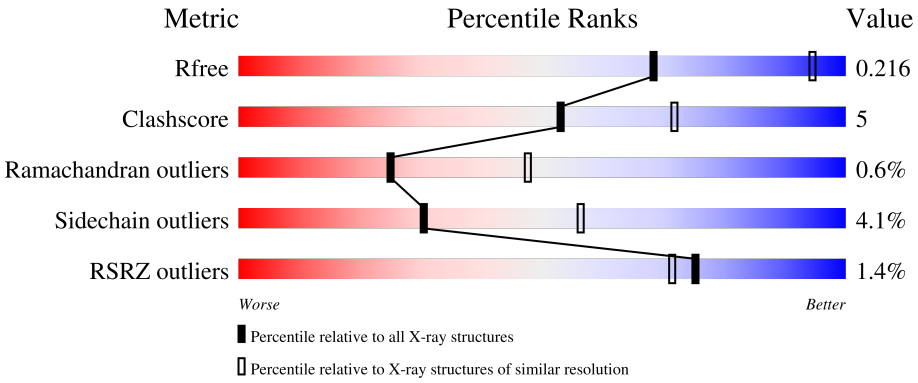
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	323	86% 14%
1	B	323	84% 15%
1	C	323	85% 15%
1	D	323	86% 12%
1	E	323	89% 11%

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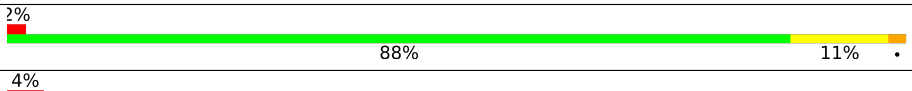
Mol	Chain	Length	Quality of chain
1	F	323	
1	G	323	
1	H	323	

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	A	414	-	-	-	X
2	EDO	C	407	-	-	-	X
2	EDO	D	411	-	-	-	X
2	EDO	G	1008	-	-	-	X
3	PEG	B	1806	-	-	X	-
5	PG4	D	404	-	-	-	X
6	CL	G	1011	-	-	X	-

2 Entry composition (i)

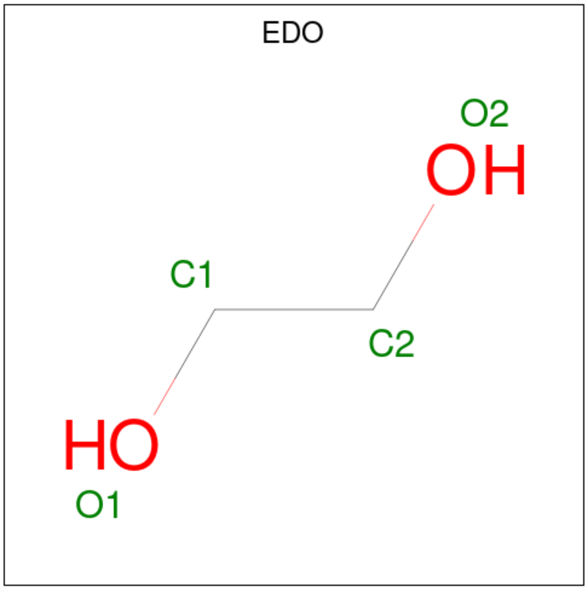
There are 7 unique types of molecules in this entry. The entry contains 19867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	1	0
			2394	1524	418	439	13			
1	B	323	Total	C	N	O	S	0	1	0
			2388	1521	415	439	13			
1	C	323	Total	C	N	O	S	0	0	0
			2384	1519	413	439	13			
1	D	323	Total	C	N	O	S	0	1	0
			2388	1520	416	440	12			
1	E	323	Total	C	N	O	S	0	0	0
			2365	1508	406	439	12			
1	F	323	Total	C	N	O	S	0	0	0
			2384	1519	413	439	13			
1	G	323	Total	C	N	O	S	0	0	0
			2377	1514	412	439	12			
1	H	323	Total	C	N	O	S	0	0	0
			2390	1522	416	439	13			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

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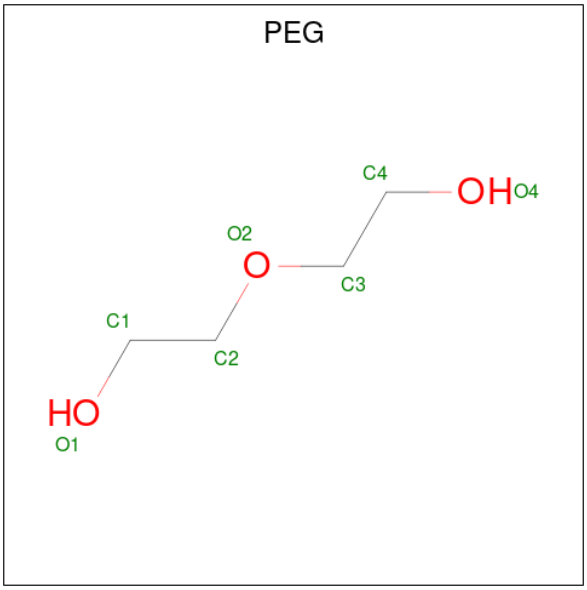
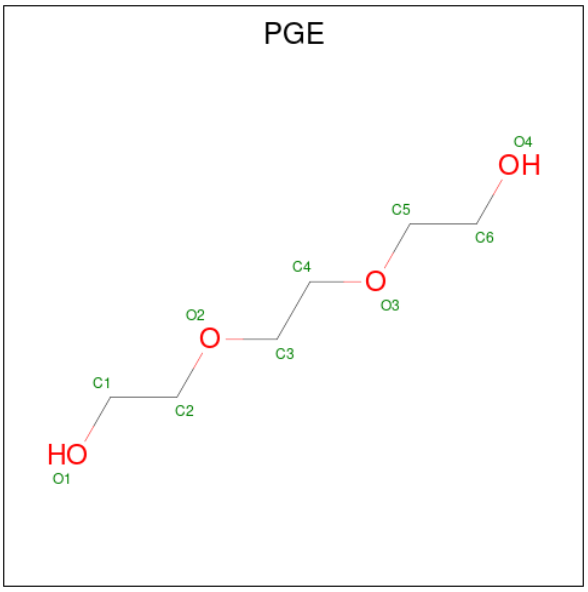
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

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



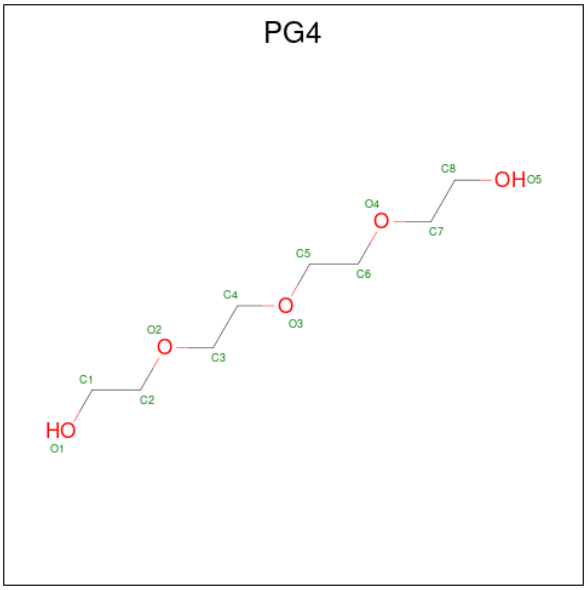
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 13 8 5	0	0
5	E	1	Total C O 13 8 5	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Cl 1 1	0	0

- Molecule 7 is water.

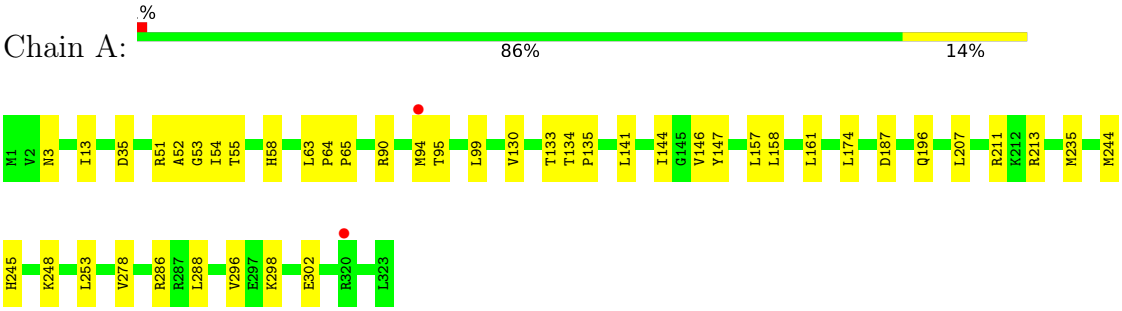
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	62	Total O 62 62	0	0
7	B	56	Total O 56 56	0	0
7	C	59	Total O 59 59	0	0
7	D	57	Total O 57 57	0	0
7	E	44	Total O 44 44	0	0
7	F	45	Total O 45 45	0	0
7	G	42	Total O 42 42	0	0
7	H	34	Total O 34 34	0	0

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.

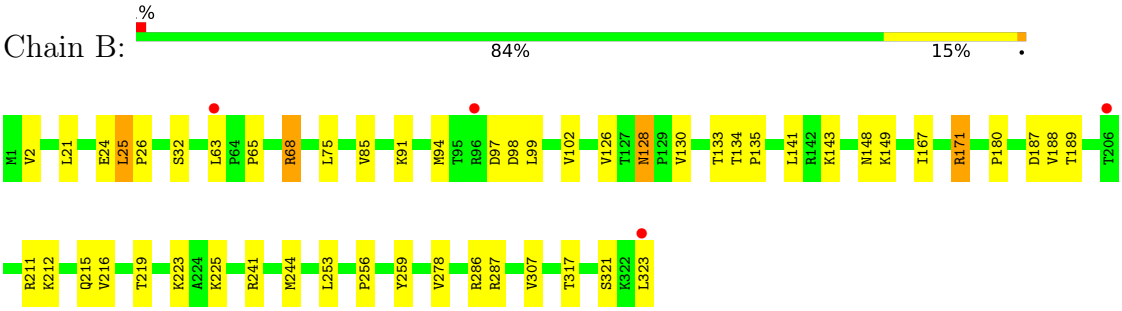
• Molecule 1: Malate dehydrogenase

Chain A:



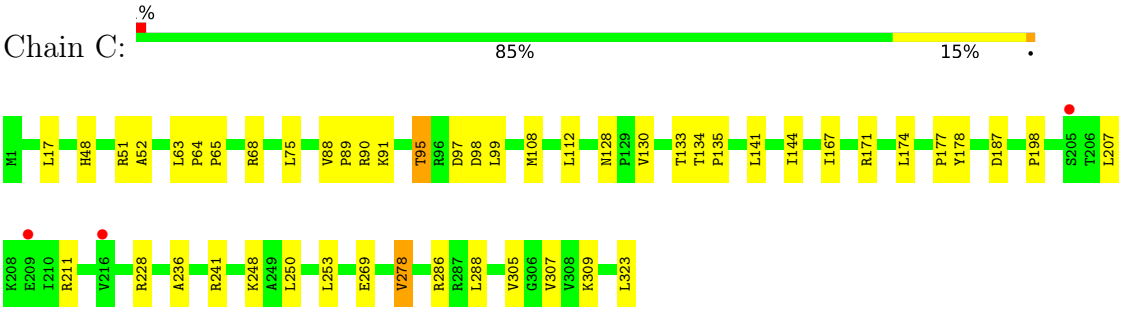
• Molecule 1: Malate dehydrogenase

Chain B:



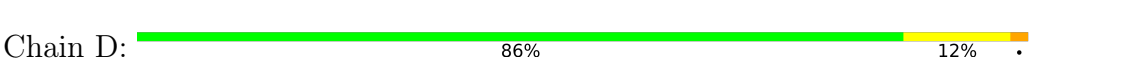
• Molecule 1: Malate dehydrogenase

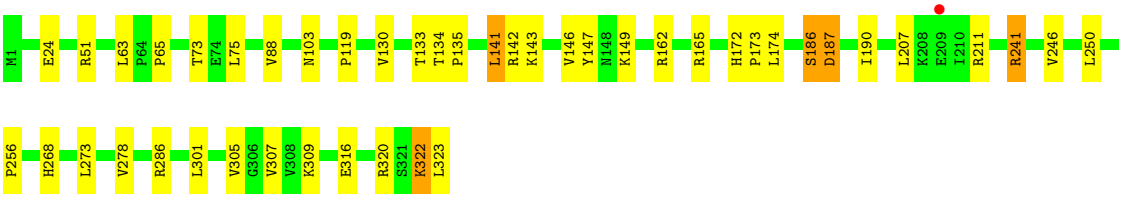
Chain C:



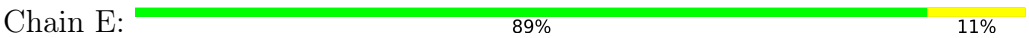
• Molecule 1: Malate dehydrogenase

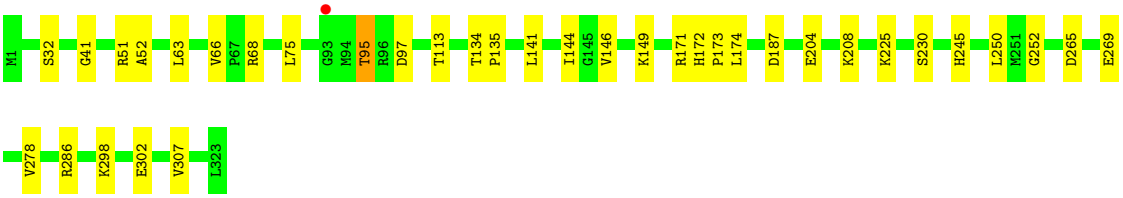
Chain D:



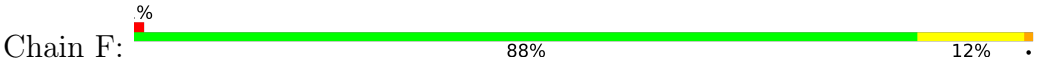


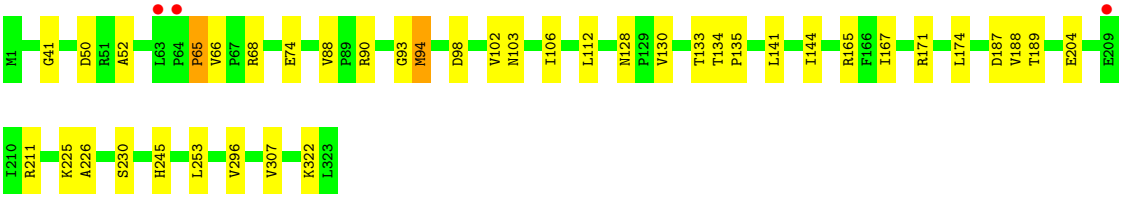
• Molecule 1: Malate dehydrogenase



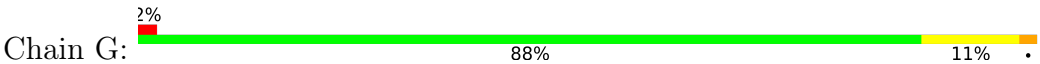


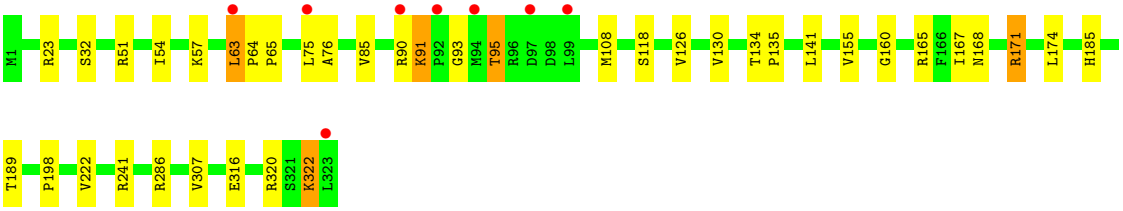
• Molecule 1: Malate dehydrogenase



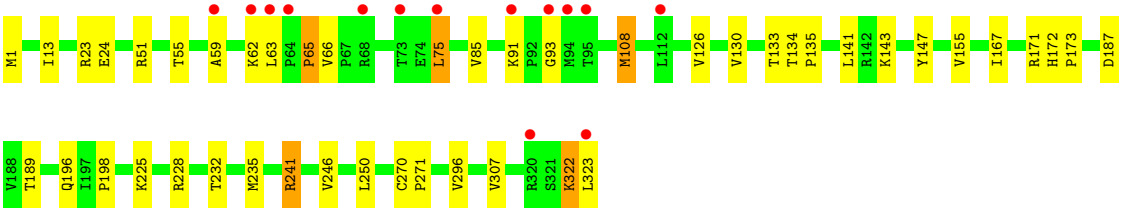


• Molecule 1: Malate dehydrogenase





• Molecule 1: Malate dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.04Å 148.33Å 251.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.32 – 2.60 48.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (23.32-2.60) 99.0 (48.52-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.203 , 0.216 0.206 , 0.216	Depositor DCC
R_{free} test set	4657 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19867	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: CL, EDO, PGE, PEG, PG4

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	0.30	0/2439	0.52	0/3320
1	B	0.35	0/2433	0.58	0/3313
1	C	0.34	0/2426	0.56	0/3303
1	D	0.34	0/2430	0.54	0/3310
1	E	0.36	0/2407	0.58	0/3282
1	F	0.34	0/2426	0.56	0/3303
1	G	0.32	0/2419	0.54	0/3296
1	H	0.30	0/2432	0.52	0/3310
All	All	0.33	0/19412	0.55	0/26437

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	A	2394	0	2506	31	0
1	B	2388	0	2495	33	0
1	C	2384	0	2493	24	0
1	D	2388	0	2487	33	0
1	E	2365	0	2453	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2384	0	2493	22	0
1	G	2377	0	2475	26	0
1	H	2390	0	2504	31	0
2	A	60	0	90	9	0
2	B	48	0	72	3	0
2	C	36	0	54	3	0
2	D	44	0	66	3	0
2	E	16	0	24	1	0
2	F	56	0	84	2	0
2	G	40	0	60	2	0
2	H	16	0	24	3	0
3	A	14	0	20	0	0
3	B	7	0	10	5	0
3	C	7	0	10	0	0
3	F	7	0	10	1	0
4	A	20	0	28	5	0
5	D	13	0	18	2	0
5	E	13	0	18	2	0
6	G	1	0	0	2	0
7	A	62	0	0	2	0
7	B	56	0	0	0	0
7	C	59	0	0	0	0
7	D	57	0	0	0	0
7	E	44	0	0	1	0
7	F	45	0	0	1	0
7	G	42	0	0	0	0
7	H	34	0	0	0	0
All	All	19867	0	20494	214	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 (214) 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:ILE:HD13	1:H:232:THR:HA	1.54	0.88
1:H:143:LYS:HE2	1:H:323:LEU:HD21	1.54	0.87
1:H:13:ILE:CD1	1:H:232:THR:HA	2.07	0.85
1:E:51:ARG:HE	5:E:403:PG4:H51	1.42	0.82
1:C:52:ALA:H	2:C:409:EDO:H11	1.43	0.82
1:H:246:VAL:O	1:H:250:LEU:HD13	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ARG:NH2	1:G:222:VAL:HG21	1.96	0.81
1:H:13:ILE:HD12	1:H:235:MET:HB3	1.64	0.79
1:D:143:LYS:NZ	1:D:323:LEU:HB3	2.00	0.76
1:D:51:ARG:HD2	5:D:404:PG4:H61	1.68	0.75
1:G:171:ARG:NH1	1:G:198:PRO:O	2.20	0.75
1:A:244:MET:HB3	2:A:412:EDO:H21	1.70	0.74
1:H:143:LYS:CE	1:H:323:LEU:HD21	2.16	0.74
1:G:171:ARG:NH2	6:G:1011:CL:CL	2.59	0.73
1:F:90:ARG:HD2	1:F:230:SER:HB3	1.70	0.73
1:D:143:LYS:HZ2	1:D:323:LEU:HB3	1.54	0.72
1:A:63:LEU:HD12	1:A:64:PRO:HA	1.73	0.71
1:F:204:GLU:OE2	1:F:211:ARG:NH2	2.24	0.71
1:D:88:VAL:H	1:D:103:ASN:HD21	1.41	0.69
1:D:256:PRO:HA	2:D:411:EDO:H22	1.73	0.69
1:B:278:VAL:CG1	1:B:286[A]:ARG:HB2	2.23	0.68
1:A:13:ILE:HD13	1:A:235:MET:HG2	1.75	0.68
1:F:52:ALA:H	3:F:807:PEG:H42	1.59	0.68
1:B:278:VAL:HG12	1:B:286[A]:ARG:HB2	1.76	0.67
1:H:108:MET:HE1	1:H:322:LYS:HB2	1.77	0.67
1:C:108:MET:SD	1:C:323:LEU:CD1	2.82	0.67
1:A:90:ARG:HB2	1:A:99:LEU:HD13	1.77	0.65
1:H:59:ALA:HB3	1:H:75:LEU:HD12	1.77	0.65
1:B:278:VAL:CG1	1:B:286[B]:ARG:HB2	2.27	0.64
1:D:278:VAL:CG1	1:D:286[B]:ARG:HB3	2.28	0.64
1:A:52:ALA:H	4:A:407:PGE:H52	1.63	0.63
1:E:298:LYS:O	1:E:302:GLU:HG3	1.98	0.63
1:A:286[B]:ARG:HA	2:A:404:EDO:H12	1.81	0.62
1:C:108:MET:SD	1:C:323:LEU:HD13	2.40	0.61
1:A:248:LYS:NZ	2:A:412:EDO:H22	2.16	0.61
1:F:112:LEU:HD22	1:F:144:ILE:HD11	1.83	0.61
1:A:55:THR:HA	2:A:409:EDO:H21	1.83	0.61
1:G:91:LYS:HG3	1:G:93:GLY:H	1.65	0.60
1:B:143:LYS:HE2	1:B:323:LEU:HG	1.82	0.60
1:D:246:VAL:O	1:D:250:LEU:HD13	2.01	0.60
1:B:286[B]:ARG:HA	3:B:1806:PEG:H22	1.83	0.60
1:F:189:THR:HG22	1:F:307:VAL:HG13	1.83	0.60
1:B:25:LEU:HD12	1:B:26:PRO:HD2	1.84	0.59
1:B:128:ASN:H	2:B:1810:EDO:H11	1.67	0.59
1:D:88:VAL:HG22	1:D:103:ASN:HD21	1.67	0.58
1:C:112:LEU:HD22	1:C:144:ILE:HD11	1.84	0.58
1:H:189:THR:HG22	1:H:307:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286[A]:ARG:HA	2:A:404:EDO:H12	1.83	0.58
1:G:189:THR:HG22	1:G:307:VAL:HG13	1.86	0.58
1:B:286[A]:ARG:HA	3:B:1806:PEG:H22	1.85	0.58
1:H:143:LYS:HE2	1:H:323:LEU:CD2	2.30	0.58
1:B:219:THR:HG22	1:B:223:LYS:HD2	1.84	0.57
1:H:13:ILE:HD13	1:H:232:THR:CA	2.31	0.57
1:C:278:VAL:HG12	1:C:288:LEU:HD11	1.87	0.57
1:A:207:LEU:HD23	1:A:211:ARG:NH2	2.20	0.56
1:E:252:GLY:HA3	1:H:1:MET:HE1	1.87	0.56
1:B:63:LEU:HD12	1:B:65:PRO:HD3	1.87	0.56
1:A:63:LEU:HD12	1:A:65:PRO:HD3	1.88	0.55
1:G:51:ARG:HB3	1:G:54:ILE:HD13	1.88	0.55
1:E:32:SER:HB3	1:E:75:LEU:HD11	1.88	0.55
1:H:59:ALA:HB2	1:H:75:LEU:HG	1.89	0.54
1:D:143:LYS:NZ	1:D:323:LEU:HD13	2.22	0.54
1:G:90:ARG:NH2	1:G:222:VAL:CG2	2.69	0.54
1:D:278:VAL:HG12	1:D:286[B]:ARG:HB3	1.87	0.54
1:A:90:ARG:NH2	1:A:94:MET:O	2.39	0.54
1:B:287:ARG:NH1	3:B:1806:PEG:H42	2.23	0.53
1:C:167:ILE:HG13	1:C:171:ARG:HH21	1.72	0.53
1:B:167:ILE:HG13	1:B:171:ARG:HD3	1.89	0.53
1:A:196:GLN:HG2	4:A:418:PGE:H5	1.91	0.52
1:B:99:LEU:HD23	1:B:128:ASN:HD21	1.74	0.52
1:B:148:ASN:HB3	2:B:1807:EDO:H21	1.92	0.52
1:D:134:THR:HB	1:D:135:PRO:HD3	1.91	0.52
1:A:144:ILE:HG13	1:A:146:VAL:HG22	1.92	0.52
1:B:211:ARG:O	1:B:215:GLN:HG3	2.09	0.52
1:G:90:ARG:HH22	1:G:222:VAL:HG21	1.69	0.52
1:G:76:ALA:O	1:G:118:SER:OG	2.27	0.52
1:C:48:HIS:HB3	1:D:162:ARG:HG2	1.91	0.51
1:E:149:LYS:NZ	1:E:265:ASP:OD1	2.40	0.51
1:G:90:ARG:HH22	1:G:222:VAL:CG2	2.23	0.51
1:C:51:ARG:HE	2:C:409:EDO:H12	1.77	0.50
1:D:63:LEU:HD12	1:D:65:PRO:HD3	1.93	0.50
1:G:108:MET:HE1	1:G:322:LYS:HB2	1.93	0.50
1:B:32:SER:HB3	1:B:75:LEU:HD11	1.92	0.50
1:C:95:THR:C	1:C:97:ASP:H	2.15	0.50
1:F:98:ASP:O	1:F:102:VAL:HG22	2.11	0.50
2:F:814:EDO:H22	1:H:198:PRO:HG3	1.94	0.50
1:A:53:GLY:O	1:A:54:ILE:HD12	2.12	0.49
1:E:52:ALA:H	5:E:403:PG4:H52	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:ASN:HB2	2:F:811:EDO:H12	1.95	0.49
1:B:287:ARG:H	3:B:1806:PEG:H22	1.77	0.49
1:B:287:ARG:HH11	3:B:1806:PEG:H42	1.78	0.49
1:B:134:THR:HB	1:B:135:PRO:HD3	1.93	0.49
1:D:301:LEU:O	1:D:305:VAL:HG23	2.13	0.49
1:F:88:VAL:HG12	1:F:103:ASN:OD1	2.13	0.49
1:D:143:LYS:HZ1	1:D:323:LEU:HD13	1.77	0.49
1:B:25:LEU:HD13	1:B:244:MET:CE	2.43	0.48
1:E:134:THR:HB	1:E:135:PRO:HD3	1.95	0.48
1:E:245:HIS:ND1	7:E:501:HOH:O	2.35	0.48
1:A:278:VAL:HG23	1:A:288:LEU:HD11	1.95	0.48
1:D:88:VAL:HG22	1:D:103:ASN:ND2	2.29	0.48
1:D:316:GLU:O	1:D:320:ARG:HG3	2.13	0.48
1:A:158:LEU:HA	1:A:161:LEU:HG	1.95	0.48
1:E:225:LYS:HG2	1:F:41:GLY:HA3	1.96	0.48
1:C:177:PRO:HA	5:D:404:PG4:H22	1.96	0.47
1:G:32:SER:HB3	1:G:75:LEU:HD11	1.96	0.47
1:G:167:ILE:HG13	1:G:171:ARG:HD3	1.96	0.47
1:G:316:GLU:O	1:G:320:ARG:HG2	2.13	0.47
1:H:225:LYS:O	1:H:228:ARG:HG2	2.13	0.47
1:A:245:HIS:HD2	7:A:506:HOH:O	1.98	0.47
1:B:189:THR:HG22	1:B:307:VAL:HG13	1.96	0.47
1:C:134:THR:HB	1:C:135:PRO:HD3	1.96	0.47
1:H:167:ILE:O	1:H:171:ARG:HG3	2.14	0.47
1:F:245:HIS:HD2	7:F:920:HOH:O	1.98	0.47
1:A:35:ASP:OD1	2:A:405:EDO:H11	2.15	0.47
1:E:204:GLU:O	1:E:208:LYS:HG3	2.14	0.47
1:F:167:ILE:HG13	1:F:171:ARG:HD3	1.97	0.47
1:A:248:LYS:HZ1	2:A:412:EDO:H22	1.79	0.47
1:G:134:THR:HB	1:G:135:PRO:HD3	1.97	0.47
1:A:130:VAL:HA	1:A:133:THR:OG1	2.14	0.47
1:F:102:VAL:O	1:F:106:ILE:HG12	2.15	0.47
1:F:130:VAL:HA	1:F:133:THR:OG1	2.15	0.47
1:F:134:THR:HB	1:F:135:PRO:HD3	1.96	0.47
1:D:143:LYS:HZ3	1:D:323:LEU:HB3	1.79	0.47
1:H:85:VAL:HB	1:H:126:VAL:CG2	2.45	0.47
1:H:241:ARG:HB2	2:H:1103:EDO:H12	1.97	0.47
1:B:94:MET:HG2	1:B:98:ASP:HB3	1.95	0.46
1:B:94:MET:HB3	1:B:99:LEU:HD13	1.98	0.46
1:D:141:LEU:HB3	1:D:147:TYR:HB2	1.97	0.46
1:H:126:VAL:HG12	1:H:155:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:VAL:HA	1:D:133:THR:OG1	2.16	0.46
1:C:63:LEU:HD12	1:C:65:PRO:HD3	1.97	0.46
1:C:130:VAL:HA	1:C:133:THR:OG1	2.16	0.46
1:D:207:LEU:HD23	1:D:211:ARG:NH2	2.30	0.46
1:F:90:ARG:HD2	1:F:230:SER:CB	2.42	0.46
1:F:90:ARG:H	1:F:90:ARG:HG2	1.58	0.45
1:D:119:PRO:HB3	1:D:146:VAL:HG21	1.98	0.45
1:D:322:LYS:O	1:D:323:LEU:HB2	2.17	0.45
1:H:134:THR:HB	1:H:135:PRO:HD3	1.98	0.45
1:H:143:LYS:NZ	1:H:323:LEU:HD21	2.32	0.45
1:B:317:THR:O	1:B:321:SER:OG	2.32	0.45
4:A:418:PGE:H22	4:A:418:PGE:H42	1.58	0.45
1:F:204:GLU:OE2	1:F:211:ARG:NH1	2.50	0.45
1:H:13:ILE:HD11	1:H:232:THR:HA	1.94	0.45
1:A:134:THR:HB	1:A:135:PRO:HD3	1.98	0.45
1:C:207:LEU:HD23	1:C:211:ARG:NH2	2.32	0.45
1:B:130:VAL:HA	1:B:133:THR:OG1	2.16	0.45
1:C:108:MET:SD	1:C:323:LEU:HD11	2.57	0.45
1:D:241:ARG:HH11	2:D:405:EDO:H21	1.81	0.45
1:G:130:VAL:CG2	1:G:185:HIS:HB3	2.47	0.45
1:A:3:ASN:HB2	2:A:413:EDO:H12	1.99	0.44
1:C:88:VAL:HG22	1:C:89:PRO:HD2	2.00	0.44
1:E:32:SER:HB3	1:E:75:LEU:HD21	1.99	0.44
1:D:305:VAL:HG12	1:D:309:LYS:HD2	1.98	0.44
1:A:58:HIS:HD2	7:A:524:HOH:O	2.01	0.44
1:H:91:LYS:O	1:H:93:GLY:N	2.50	0.44
1:B:225:LYS:NZ	2:B:1809:EDO:H11	2.33	0.44
1:A:90:ARG:HH21	1:A:95:THR:HA	1.83	0.44
1:A:298:LYS:HE2	1:A:302:GLU:OE2	2.18	0.44
1:A:147:TYR:HB3	2:E:401:EDO:H22	2.00	0.44
1:H:23:ARG:HE	1:H:23:ARG:HB3	1.39	0.44
1:G:286:ARG:HA	2:G:1007:EDO:H12	2.00	0.43
1:F:225:LYS:O	1:F:226:ALA:C	2.57	0.43
1:C:305:VAL:HG12	1:C:309:LYS:HE2	2.00	0.43
1:D:88:VAL:H	1:D:103:ASN:ND2	2.10	0.43
1:C:178:TYR:HB2	2:C:406:EDO:H22	2.00	0.43
1:B:68:ARG:HH11	1:B:68:ARG:HB3	1.84	0.43
1:G:63:LEU:HA	1:G:64:PRO:C	2.39	0.43
1:B:180:PRO:HB3	1:B:259:TYR:CZ	2.54	0.43
1:D:278:VAL:HG12	1:D:286[A]:ARG:HB3	2.00	0.43
1:F:188:VAL:HG13	1:F:307:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:HD12	1:C:236:ALA:HA	2.00	0.42
1:D:142:ARG:HE	2:D:409:EDO:H22	1.85	0.42
1:A:51:ARG:HE	4:A:407:PGE:H5	1.84	0.42
1:C:64:PRO:HA	1:C:65:PRO:HD3	1.98	0.42
1:E:63:LEU:HD12	1:E:63:LEU:HA	1.92	0.42
1:A:213:ARG:HH22	2:A:411:EDO:H11	1.83	0.42
1:H:130:VAL:HA	1:H:133:THR:OG1	2.19	0.42
1:D:273:LEU:HD23	1:D:273:LEU:HA	1.94	0.42
1:E:41:GLY:HA3	1:F:225:LYS:HG3	2.01	0.42
1:G:168:ASN:OD1	6:G:1011:CL:CL	2.75	0.42
1:H:141:LEU:HD23	1:H:147:TYR:HD1	1.83	0.42
1:H:196:GLN:O	2:H:1101:EDO:H12	2.20	0.42
4:A:418:PGE:H2	1:C:198:PRO:HA	2.02	0.42
1:B:21:LEU:O	1:B:25:LEU:HB2	2.19	0.42
1:C:91:LYS:HE2	1:C:228:ARG:HH11	1.85	0.42
1:G:64:PRO:HA	1:G:65:PRO:HD3	1.93	0.42
1:C:278:VAL:HG13	1:C:286:ARG:HB2	2.02	0.41
1:E:144:ILE:HG13	1:E:146:VAL:HG22	2.01	0.41
1:F:204:GLU:O	1:F:204:GLU:HG3	2.19	0.41
1:G:160:GLY:HA3	2:G:1002:EDO:H21	2.02	0.41
1:B:212:LYS:O	1:B:216:VAL:HG22	2.20	0.41
1:G:126:VAL:HG12	1:G:155:VAL:HB	2.02	0.41
1:B:25:LEU:HD13	1:B:244:MET:HE1	2.02	0.41
1:D:172:HIS:CG	1:D:173:PRO:HA	2.56	0.41
1:G:90:ARG:HH21	1:G:222:VAL:HG21	1.80	0.41
1:A:63:LEU:HA	1:A:64:PRO:C	2.41	0.41
1:F:93:GLY:O	1:F:94:MET:HG2	2.21	0.41
1:H:51:ARG:HA	1:H:51:ARG:HD2	1.81	0.41
1:D:63:LEU:HD12	1:D:63:LEU:HA	1.89	0.41
1:D:186:SER:O	1:D:190:ILE:HG13	2.20	0.41
1:E:172:HIS:CG	1:E:173:PRO:HA	2.55	0.41
1:B:85:VAL:HA	1:B:126:VAL:HG22	2.03	0.41
1:E:68:ARG:HA	1:E:113:THR:OG1	2.21	0.41
1:E:278:VAL:CG1	1:E:286:ARG:HB2	2.52	0.40
1:G:85:VAL:HB	1:G:126:VAL:CG2	2.52	0.40
1:H:108:MET:HE3	1:H:108:MET:HB3	1.96	0.40
1:A:157:LEU:HG	1:A:161:LEU:HD21	2.01	0.40
1:D:141:LEU:HD12	1:D:141:LEU:HA	1.76	0.40
1:G:23:ARG:HH21	2:H:1103:EDO:H11	1.86	0.40
1:G:57:LYS:HB3	1:G:57:LYS:HE2	1.87	0.40
1:H:172:HIS:CG	1:H:173:PRO:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PRO:O	1:B:278:VAL:HA	2.22	0.40
1:C:95:THR:C	1:C:97:ASP:N	2.75	0.40
1:H:270:CYS:HA	1:H:271:PRO:HD3	1.94	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	322/323 (100%)	314 (98%)	7 (2%)	1 (0%)	41	64
1	B	322/323 (100%)	312 (97%)	9 (3%)	1 (0%)	41	64
1	C	321/323 (99%)	314 (98%)	6 (2%)	1 (0%)	41	64
1	D	322/323 (100%)	312 (97%)	8 (2%)	2 (1%)	25	47
1	E	321/323 (99%)	311 (97%)	9 (3%)	1 (0%)	41	64
1	F	321/323 (99%)	308 (96%)	8 (2%)	5 (2%)	9	19
1	G	321/323 (99%)	309 (96%)	11 (3%)	1 (0%)	41	64
1	H	321/323 (99%)	313 (98%)	5 (2%)	3 (1%)	17	35
All	All	2571/2584 (100%)	2493 (97%)	63 (2%)	15 (1%)	25	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ASP
1	B	97	ASP
1	C	187	ASP
1	D	268	HIS
1	F	65	PRO
1	F	94	MET
1	F	187	ASP

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Mol	Chain	Res	Type
1	G	95	THR
1	H	187	ASP
1	D	187	ASP
1	E	95	THR
1	H	65	PRO
1	F	66	VAL
1	F	50	ASP
1	H	66	VAL

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	261/261 (100%)	257 (98%)	4 (2%)	65	83
1	B	260/261 (100%)	246 (95%)	14 (5%)	22	44
1	C	260/261 (100%)	244 (94%)	16 (6%)	18	37
1	D	259/261 (99%)	247 (95%)	12 (5%)	27	51
1	E	256/261 (98%)	245 (96%)	11 (4%)	29	54
1	F	260/261 (100%)	251 (96%)	9 (4%)	36	62
1	G	258/261 (99%)	249 (96%)	9 (4%)	36	62
1	H	261/261 (100%)	251 (96%)	10 (4%)	33	59
All	All	2075/2088 (99%)	1990 (96%)	85 (4%)	30	56

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	174	LEU
1	A	253	LEU
1	A	296	VAL
1	B	2	VAL
1	B	24	GLU
1	B	25	LEU

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Mol	Chain	Res	Type
1	B	68	ARG
1	B	91	LYS
1	B	102	VAL
1	B	128	ASN
1	B	141	LEU
1	B	149	LYS
1	B	171	ARG
1	B	187	ASP
1	B	188	VAL
1	B	241	ARG
1	B	253	LEU
1	C	68	ARG
1	C	75	LEU
1	C	90	ARG
1	C	95	THR
1	C	98	ASP
1	C	99	LEU
1	C	128	ASN
1	C	141	LEU
1	C	174	LEU
1	C	241	ARG
1	C	248	LYS
1	C	250	LEU
1	C	253	LEU
1	C	269	GLU
1	C	278	VAL
1	C	307	VAL
1	D	24	GLU
1	D	73	THR
1	D	75	LEU
1	D	141	LEU
1	D	149	LYS
1	D	165	ARG
1	D	174	LEU
1	D	186	SER
1	D	187	ASP
1	D	241	ARG
1	D	307	VAL
1	D	322	LYS
1	E	66	VAL
1	E	95	THR
1	E	97	ASP

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Mol	Chain	Res	Type
1	E	141	LEU
1	E	171	ARG
1	E	174	LEU
1	E	187	ASP
1	E	230	SER
1	E	250	LEU
1	E	269	GLU
1	E	307	VAL
1	F	65	PRO
1	F	68	ARG
1	F	74	GLU
1	F	141	LEU
1	F	165	ARG
1	F	174	LEU
1	F	253	LEU
1	F	296	VAL
1	F	322	LYS
1	G	63	LEU
1	G	91	LYS
1	G	95	THR
1	G	141	LEU
1	G	165	ARG
1	G	171	ARG
1	G	174	LEU
1	G	241	ARG
1	G	322	LYS
1	H	24	GLU
1	H	55	THR
1	H	62	LYS
1	H	63	LEU
1	H	65	PRO
1	H	75	LEU
1	H	108	MET
1	H	241	ARG
1	H	296	VAL
1	H	322	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	ASN
1	D	103	ASN

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Mol	Chain	Res	Type
1	G	101	ASN

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

Of 89 ligands modelled in this entry, 1 is monoatomic - leaving 88 for Mogul analysis.

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	G	1005	-	3,3,3	0.10	0	2,2,2	0.27	0
2	EDO	B	1804	-	3,3,3	0.50	0	2,2,2	0.17	0
2	EDO	D	407	-	3,3,3	0.15	0	2,2,2	0.12	0
2	EDO	D	408	-	3,3,3	0.48	0	2,2,2	0.27	0
2	EDO	A	405	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	B	1811	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	C	409	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	G	1003	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	F	813	-	3,3,3	0.16	0	2,2,2	0.17	0
2	EDO	G	1006	-	3,3,3	0.50	0	2,2,2	0.22	0
2	EDO	G	1008	-	3,3,3	0.45	0	2,2,2	0.41	0
2	EDO	A	402	-	3,3,3	0.49	0	2,2,2	0.17	0
2	EDO	A	415	-	3,3,3	0.15	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	H	1104	-	3,3,3	0.46	0	2,2,2	0.25	0
2	EDO	A	410	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	A	416	-	3,3,3	0.06	0	2,2,2	0.38	0
2	EDO	C	408	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	F	808	-	3,3,3	0.45	0	2,2,2	0.25	0
2	EDO	F	814	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	F	804	-	3,3,3	0.48	0	2,2,2	0.30	0
2	EDO	F	806	-	3,3,3	0.45	0	2,2,2	0.38	0
3	PEG	F	807	-	6,6,6	0.49	0	5,5,5	0.21	0
2	EDO	A	404	-	3,3,3	0.49	0	2,2,2	0.31	0
2	EDO	G	1002	-	3,3,3	0.47	0	2,2,2	0.23	0
2	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.35	0
5	PG4	E	403	-	12,12,12	0.51	0	11,11,11	0.22	0
2	EDO	F	812	-	3,3,3	0.39	0	2,2,2	0.78	0
2	EDO	A	413	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	F	801	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	H	1102	-	3,3,3	0.21	0	2,2,2	0.21	0
2	EDO	F	815	-	3,3,3	0.44	0	2,2,2	0.34	0
2	EDO	H	1101	-	3,3,3	0.48	0	2,2,2	0.28	0
2	EDO	C	404	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	D	410	-	3,3,3	0.48	0	2,2,2	0.29	0
2	EDO	B	1812	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	C	402	-	3,3,3	0.45	0	2,2,2	0.38	0
5	PG4	D	404	-	12,12,12	0.53	0	11,11,11	0.25	0
3	PEG	A	406	-	6,6,6	0.48	0	5,5,5	0.28	0
2	EDO	A	408	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	F	805	-	3,3,3	0.49	0	2,2,2	0.19	0
2	EDO	F	811	-	3,3,3	0.41	0	2,2,2	0.38	0
2	EDO	H	1103	-	3,3,3	0.46	0	2,2,2	0.35	0
2	EDO	D	409	-	3,3,3	0.44	0	2,2,2	0.40	0
2	EDO	D	402	-	3,3,3	0.49	0	2,2,2	0.19	0
2	EDO	A	411	-	3,3,3	0.50	0	2,2,2	0.24	0
3	PEG	A	419	-	6,6,6	0.49	0	5,5,5	0.27	0
2	EDO	F	809	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	C	410	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	F	803	-	3,3,3	0.48	0	2,2,2	0.30	0
2	EDO	B	1805	-	3,3,3	0.46	0	2,2,2	0.40	0
2	EDO	D	405	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	F	810	-	3,3,3	0.42	0	2,2,2	0.51	0
2	EDO	G	1001	-	3,3,3	0.44	0	2,2,2	0.39	0
2	EDO	B	1813	-	3,3,3	0.47	0	2,2,2	0.35	0
3	PEG	B	1806	-	6,6,6	0.48	0	5,5,5	0.30	0
2	EDO	C	403	-	3,3,3	0.18	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	C	407	-	3,3,3	0.49	0	2,2,2	0.20	0
2	EDO	G	1010	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	B	1802	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	B	1801	-	3,3,3	0.49	0	2,2,2	0.32	0
2	EDO	G	1009	-	3,3,3	0.16	0	2,2,2	0.09	0
4	PGE	A	407	-	9,9,9	0.32	0	8,8,8	0.25	0
2	EDO	D	406	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	A	409	-	3,3,3	0.46	0	2,2,2	0.42	0
3	PEG	C	401	-	6,6,6	0.48	0	5,5,5	0.31	0
2	EDO	C	405	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	B	1808	-	3,3,3	0.48	0	2,2,2	0.19	0
2	EDO	E	404	-	3,3,3	0.49	0	2,2,2	0.23	0
2	EDO	A	412	-	3,3,3	0.49	0	2,2,2	0.29	0
2	EDO	E	402	-	3,3,3	0.52	0	2,2,2	0.08	0
2	EDO	A	401	-	3,3,3	0.49	0	2,2,2	0.15	0
2	EDO	A	414	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	G	1007	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	B	1809	-	3,3,3	0.49	0	2,2,2	0.19	0
2	EDO	C	406	-	3,3,3	0.48	0	2,2,2	0.16	0
4	PGE	A	418	-	9,9,9	0.32	0	8,8,8	0.24	0
2	EDO	B	1803	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	B	1810	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	F	802	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	B	1807	-	3,3,3	0.44	0	2,2,2	0.29	0
2	EDO	A	417	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	D	403	-	3,3,3	0.09	0	2,2,2	0.40	0
2	EDO	E	405	-	3,3,3	0.46	0	2,2,2	0.35	0
2	EDO	D	412	-	3,3,3	0.47	0	2,2,2	0.29	0
2	EDO	D	411	-	3,3,3	0.49	0	2,2,2	0.17	0
2	EDO	D	401	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	E	401	-	3,3,3	0.45	0	2,2,2	0.39	0
2	EDO	G	1004	-	3,3,3	0.46	0	2,2,2	0.36	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	G	1005	-	-	1/1/1/1	-
2	EDO	B	1804	-	-	0/1/1/1	-
2	EDO	D	407	-	-	1/1/1/1	-
2	EDO	D	408	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	405	-	-	1/1/1/1	-
2	EDO	B	1811	-	-	1/1/1/1	-
2	EDO	C	409	-	-	0/1/1/1	-
2	EDO	G	1003	-	-	1/1/1/1	-
2	EDO	F	813	-	-	0/1/1/1	-
2	EDO	G	1006	-	-	1/1/1/1	-
2	EDO	G	1008	-	-	1/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
2	EDO	A	415	-	-	1/1/1/1	-
2	EDO	H	1104	-	-	1/1/1/1	-
2	EDO	A	410	-	-	1/1/1/1	-
2	EDO	A	416	-	-	0/1/1/1	-
2	EDO	C	408	-	-	1/1/1/1	-
2	EDO	F	808	-	-	1/1/1/1	-
2	EDO	F	814	-	-	0/1/1/1	-
2	EDO	F	804	-	-	1/1/1/1	-
2	EDO	F	806	-	-	0/1/1/1	-
3	PEG	F	807	-	-	2/4/4/4	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	G	1002	-	-	1/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
5	PG4	E	403	-	-	4/10/10/10	-
2	EDO	F	812	-	-	0/1/1/1	-
2	EDO	A	413	-	-	0/1/1/1	-
2	EDO	F	801	-	-	1/1/1/1	-
2	EDO	H	1102	-	-	1/1/1/1	-
2	EDO	F	815	-	-	0/1/1/1	-
2	EDO	H	1101	-	-	0/1/1/1	-
2	EDO	C	404	-	-	1/1/1/1	-
2	EDO	D	410	-	-	0/1/1/1	-
2	EDO	B	1812	-	-	1/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
5	PG4	D	404	-	-	8/10/10/10	-
3	PEG	A	406	-	-	2/4/4/4	-
2	EDO	A	408	-	-	0/1/1/1	-
2	EDO	F	805	-	-	1/1/1/1	-
2	EDO	F	811	-	-	1/1/1/1	-
2	EDO	H	1103	-	-	1/1/1/1	-
2	EDO	D	409	-	-	1/1/1/1	-
2	EDO	D	402	-	-	0/1/1/1	-
2	EDO	A	411	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	419	-	-	1/4/4/4	-
2	EDO	F	809	-	-	0/1/1/1	-
2	EDO	C	410	-	-	0/1/1/1	-
2	EDO	F	803	-	-	1/1/1/1	-
2	EDO	B	1805	-	-	1/1/1/1	-
2	EDO	D	405	-	-	1/1/1/1	-
2	EDO	F	810	-	-	0/1/1/1	-
2	EDO	G	1001	-	-	0/1/1/1	-
2	EDO	B	1813	-	-	1/1/1/1	-
3	PEG	B	1806	-	-	0/4/4/4	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	C	407	-	-	0/1/1/1	-
2	EDO	G	1010	-	-	0/1/1/1	-
2	EDO	B	1802	-	-	0/1/1/1	-
2	EDO	B	1801	-	-	0/1/1/1	-
2	EDO	G	1009	-	-	0/1/1/1	-
4	PGE	A	407	-	-	5/7/7/7	-
2	EDO	D	406	-	-	0/1/1/1	-
2	EDO	A	409	-	-	0/1/1/1	-
3	PEG	C	401	-	-	2/4/4/4	-
2	EDO	C	405	-	-	1/1/1/1	-
2	EDO	B	1808	-	-	0/1/1/1	-
2	EDO	E	404	-	-	0/1/1/1	-
2	EDO	A	412	-	-	1/1/1/1	-
2	EDO	E	402	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	A	414	-	-	1/1/1/1	-
2	EDO	G	1007	-	-	0/1/1/1	-
2	EDO	B	1809	-	-	1/1/1/1	-
2	EDO	C	406	-	-	1/1/1/1	-
4	PGE	A	418	-	-	4/7/7/7	-
2	EDO	B	1803	-	-	1/1/1/1	-
2	EDO	B	1810	-	-	0/1/1/1	-
2	EDO	F	802	-	-	0/1/1/1	-
2	EDO	B	1807	-	-	0/1/1/1	-
2	EDO	A	417	-	-	1/1/1/1	-
2	EDO	D	403	-	-	1/1/1/1	-
2	EDO	E	405	-	-	0/1/1/1	-
2	EDO	D	412	-	-	0/1/1/1	-
2	EDO	D	411	-	-	0/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	G	1004	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	418	PGE	C4-C3-O2-C2
5	D	404	PG4	O3-C5-C6-O4
5	D	404	PG4	O2-C3-C4-O3
5	E	403	PG4	C6-C5-O3-C4
4	A	407	PGE	O2-C3-C4-O3
5	D	404	PG4	C1-C2-O2-C3
4	A	418	PGE	O2-C3-C4-O3
5	E	403	PG4	O1-C1-C2-O2
2	A	414	EDO	O1-C1-C2-O2
2	D	403	EDO	O1-C1-C2-O2
4	A	418	PGE	O1-C1-C2-O2
3	A	419	PEG	O2-C3-C4-O4
2	A	411	EDO	O1-C1-C2-O2
2	A	415	EDO	O1-C1-C2-O2
2	B	1805	EDO	O1-C1-C2-O2
2	B	1812	EDO	O1-C1-C2-O2
2	C	403	EDO	O1-C1-C2-O2
2	C	405	EDO	O1-C1-C2-O2
2	D	407	EDO	O1-C1-C2-O2
2	D	408	EDO	O1-C1-C2-O2
2	F	801	EDO	O1-C1-C2-O2
2	G	1003	EDO	O1-C1-C2-O2
2	H	1103	EDO	O1-C1-C2-O2
3	A	406	PEG	O1-C1-C2-O2
3	C	401	PEG	O1-C1-C2-O2
3	F	807	PEG	O2-C3-C4-O4
5	D	404	PG4	O1-C1-C2-O2
2	A	410	EDO	O1-C1-C2-O2
2	G	1006	EDO	O1-C1-C2-O2
5	E	403	PG4	O2-C3-C4-O3
2	A	405	EDO	O1-C1-C2-O2
2	B	1803	EDO	O1-C1-C2-O2
3	C	401	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	D	404	PG4	C4-C3-O2-C2
5	D	404	PG4	C3-C4-O3-C5
4	A	418	PGE	C3-C4-O3-C5
5	D	404	PG4	C5-C6-O4-C7
2	F	804	EDO	O1-C1-C2-O2
4	A	407	PGE	C3-C4-O3-C5
5	D	404	PG4	C8-C7-O4-C6
4	A	407	PGE	C4-C3-O2-C2
2	B	1811	EDO	O1-C1-C2-O2
2	B	1813	EDO	O1-C1-C2-O2
2	F	805	EDO	O1-C1-C2-O2
2	G	1002	EDO	O1-C1-C2-O2
2	H	1102	EDO	O1-C1-C2-O2
2	C	404	EDO	O1-C1-C2-O2
5	E	403	PG4	O3-C5-C6-O4
2	A	412	EDO	O1-C1-C2-O2
2	F	803	EDO	O1-C1-C2-O2
2	F	808	EDO	O1-C1-C2-O2
2	G	1008	EDO	O1-C1-C2-O2
3	A	406	PEG	C1-C2-O2-C3
2	B	1809	EDO	O1-C1-C2-O2
2	C	406	EDO	O1-C1-C2-O2
2	D	401	EDO	O1-C1-C2-O2
2	D	405	EDO	O1-C1-C2-O2
2	G	1005	EDO	O1-C1-C2-O2
2	H	1104	EDO	O1-C1-C2-O2
4	A	407	PGE	C1-C2-O2-C3
2	A	417	EDO	O1-C1-C2-O2
2	C	408	EDO	O1-C1-C2-O2
2	D	409	EDO	O1-C1-C2-O2
2	F	811	EDO	O1-C1-C2-O2
4	A	407	PGE	C6-C5-O3-C4
3	F	807	PEG	O1-C1-C2-O2

There are no ring outliers.

27 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	EDO	1	0
2	C	409	EDO	2	0
2	F	814	EDO	1	0
3	F	807	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	EDO	2	0
2	G	1002	EDO	1	0
5	E	403	PG4	2	0
2	A	413	EDO	1	0
2	H	1101	EDO	1	0
5	D	404	PG4	2	0
2	F	811	EDO	1	0
2	H	1103	EDO	2	0
2	D	409	EDO	1	0
2	A	411	EDO	1	0
2	D	405	EDO	1	0
3	B	1806	PEG	5	0
4	A	407	PGE	2	0
2	A	409	EDO	1	0
2	A	412	EDO	3	0
2	G	1007	EDO	1	0
2	B	1809	EDO	1	0
2	C	406	EDO	1	0
4	A	418	PGE	3	0
2	B	1810	EDO	1	0
2	B	1807	EDO	1	0
2	D	411	EDO	1	0
2	E	401	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	A	323/323 (100%)	-0.04	2 (0%)	89	88	30, 48, 74, 99	0
1	B	323/323 (100%)	-0.09	4 (1%)	79	76	33, 48, 75, 116	0
1	C	323/323 (100%)	-0.09	3 (0%)	84	82	32, 50, 78, 121	0
1	D	323/323 (100%)	-0.07	1 (0%)	94	93	34, 54, 79, 113	0
1	E	323/323 (100%)	-0.11	1 (0%)	94	93	40, 54, 85, 130	0
1	F	323/323 (100%)	-0.06	3 (0%)	84	82	36, 54, 83, 125	0
1	G	323/323 (100%)	0.06	8 (2%)	57	51	37, 57, 90, 145	0
1	H	323/323 (100%)	0.13	14 (4%)	35	28	42, 62, 93, 141	0
All	All	2584/2584 (100%)	-0.03	36 (1%)	75	71	30, 54, 85, 145	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	90	ARG	4.3
1	H	63	LEU	4.1
1	F	63	LEU	3.6
1	H	62	LYS	3.6
1	H	93	GLY	3.1
1	H	64	PRO	3.1
1	G	94	MET	3.1
1	H	320	ARG	3.1
1	G	63	LEU	3.1
1	H	73	THR	3.1
1	D	209	GLU	2.9
1	H	68	ARG	2.8
1	G	97	ASP	2.7
1	F	64	PRO	2.6
1	G	99	LEU	2.6
1	B	63	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	96	ARG	2.4
1	C	205	SER	2.4
1	A	94	MET	2.4
1	H	94	MET	2.4
1	F	209	GLU	2.4
1	E	93	GLY	2.4
1	B	323	LEU	2.3
1	G	92	PRO	2.2
1	H	75	LEU	2.2
1	H	112	LEU	2.2
1	B	206	THR	2.1
1	A	320	ARG	2.1
1	G	75	LEU	2.1
1	H	323	LEU	2.1
1	H	95	THR	2.1
1	H	59	ALA	2.1
1	C	209	GLU	2.1
1	G	323	LEU	2.0
1	H	91	LYS	2.0
1	C	216	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 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	F	804	4/4	0.56	0.28	85,92,93,93	0
2	EDO	D	411	4/4	0.61	0.42	73,76,79,79	0
2	EDO	D	403	4/4	0.61	0.34	76,80,82,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	404	4/4	0.65	0.25	65,72,72,75	0
2	EDO	G	1007	4/4	0.69	0.26	71,72,72,74	0
2	EDO	C	407	4/4	0.71	0.63	80,81,83,84	0
2	EDO	B	1813	4/4	0.73	0.17	86,88,89,89	0
2	EDO	G	1008	4/4	0.75	0.48	61,62,62,66	0
3	PEG	A	419	7/7	0.75	0.39	83,86,89,91	0
5	PG4	D	404	13/13	0.75	0.40	72,83,88,89	0
2	EDO	B	1809	4/4	0.77	0.27	67,68,69,69	0
2	EDO	A	416	4/4	0.77	0.36	20,20,20,20	0
4	PGE	A	418	10/10	0.77	0.34	71,79,86,87	0
2	EDO	D	405	4/4	0.77	0.39	68,69,72,72	0
2	EDO	A	414	4/4	0.79	0.53	62,65,65,65	0
2	EDO	F	801	4/4	0.79	0.28	69,72,73,73	0
2	EDO	C	405	4/4	0.80	0.19	66,70,72,77	0
6	CL	G	1011	1/1	0.80	0.19	85,85,85,85	0
2	EDO	D	412	4/4	0.81	0.45	81,85,86,88	0
2	EDO	F	814	4/4	0.81	0.27	59,63,64,66	0
3	PEG	A	406	7/7	0.82	0.28	58,62,73,74	0
2	EDO	D	410	4/4	0.82	0.32	75,76,78,81	0
3	PEG	C	401	7/7	0.82	0.39	74,83,87,91	0
2	EDO	C	408	4/4	0.82	0.42	67,68,69,70	0
2	EDO	A	412	4/4	0.82	0.59	78,79,83,83	0
5	PG4	E	403	13/13	0.82	0.23	60,80,92,93	0
2	EDO	A	413	4/4	0.82	0.20	62,63,66,66	0
2	EDO	A	410	4/4	0.83	0.17	73,76,77,78	0
2	EDO	B	1810	4/4	0.83	0.25	66,68,68,72	0
2	EDO	G	1006	4/4	0.83	0.24	62,66,67,68	0
2	EDO	H	1103	4/4	0.84	0.43	70,70,70,72	0
2	EDO	A	411	4/4	0.84	0.35	50,53,53,55	0
2	EDO	G	1005	4/4	0.85	0.25	70,70,71,71	0
2	EDO	A	403	4/4	0.85	0.21	56,58,59,61	0
2	EDO	B	1811	4/4	0.86	0.30	67,68,69,70	0
4	PGE	A	407	10/10	0.86	0.27	66,74,81,81	0
2	EDO	C	410	4/4	0.86	0.24	58,62,64,65	0
2	EDO	A	401	4/4	0.86	0.24	51,54,55,57	0
2	EDO	F	810	4/4	0.86	0.21	64,68,71,76	0
3	PEG	B	1806	7/7	0.86	0.25	64,71,77,79	0
2	EDO	B	1808	4/4	0.87	0.23	41,43,45,47	0
2	EDO	H	1101	4/4	0.87	0.18	73,73,76,76	0
2	EDO	E	402	4/4	0.88	0.18	49,52,52,54	0
2	EDO	G	1004	4/4	0.88	0.18	68,70,73,74	0
2	EDO	H	1104	4/4	0.88	0.21	54,57,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	D	407	4/4	0.89	0.46	53,55,59,59	0
2	EDO	A	405	4/4	0.89	0.20	66,68,70,71	0
2	EDO	F	803	4/4	0.90	0.31	78,80,83,84	0
2	EDO	C	404	4/4	0.90	0.25	59,64,65,66	0
3	PEG	F	807	7/7	0.90	0.28	71,83,88,90	0
2	EDO	B	1801	4/4	0.90	0.24	60,62,66,71	0
2	EDO	B	1812	4/4	0.90	0.29	67,73,74,74	0
2	EDO	A	408	4/4	0.90	0.21	49,49,50,50	0
2	EDO	E	404	4/4	0.90	0.19	54,59,59,62	0
2	EDO	D	409	4/4	0.90	0.21	69,70,70,72	0
2	EDO	E	401	4/4	0.91	0.20	60,63,65,65	0
2	EDO	F	812	4/4	0.91	0.14	34,34,34,34	0
2	EDO	B	1804	4/4	0.91	0.17	48,50,51,55	0
2	EDO	F	806	4/4	0.92	0.25	63,67,68,72	0
2	EDO	F	813	4/4	0.92	0.33	20,20,20,20	0
2	EDO	C	406	4/4	0.92	0.22	50,51,56,57	0
2	EDO	F	811	4/4	0.93	0.33	87,88,88,89	0
2	EDO	D	406	4/4	0.93	0.30	58,60,60,61	0
2	EDO	C	403	4/4	0.93	0.29	57,58,58,59	0
2	EDO	H	1102	4/4	0.93	0.22	45,49,50,52	0
2	EDO	D	408	4/4	0.93	0.19	51,56,60,64	0
2	EDO	F	805	4/4	0.93	0.25	56,58,59,60	0
2	EDO	B	1807	4/4	0.93	0.22	58,61,61,64	0
2	EDO	C	402	4/4	0.93	0.22	45,46,47,49	0
2	EDO	G	1009	4/4	0.94	0.28	20,20,20,20	0
2	EDO	G	1010	4/4	0.94	0.28	56,56,57,58	0
2	EDO	A	402	4/4	0.94	0.22	42,43,44,45	0
2	EDO	F	802	4/4	0.94	0.30	51,53,55,57	0
2	EDO	D	401	4/4	0.95	0.17	48,50,53,56	0
2	EDO	F	815	4/4	0.95	0.20	64,65,66,67	0
2	EDO	G	1002	4/4	0.95	0.20	46,47,49,54	0
2	EDO	D	402	4/4	0.95	0.20	51,52,54,58	0
2	EDO	A	415	4/4	0.95	0.13	20,20,20,20	0
2	EDO	B	1803	4/4	0.95	0.17	49,49,50,51	0
2	EDO	C	409	4/4	0.95	0.19	60,68,69,70	0
2	EDO	A	409	4/4	0.95	0.21	63,64,65,68	0
2	EDO	G	1001	4/4	0.96	0.16	55,58,60,65	0
2	EDO	B	1805	4/4	0.96	0.18	47,48,49,49	0
2	EDO	G	1003	4/4	0.96	0.21	55,57,60,62	0
2	EDO	F	809	4/4	0.96	0.14	62,62,63,64	0
2	EDO	F	808	4/4	0.97	0.23	62,63,66,67	0
2	EDO	B	1802	4/4	0.97	0.20	37,41,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	417	4/4	0.97	0.13	35,36,38,39	0
2	EDO	E	405	4/4	0.97	0.13	46,46,46,48	0

6.5 Other polymers (i)

There are no such residues in this entry.