Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:33 am BST

PDB ID	:	5MZ8
Title	:	Crystal structure of aldehyde dehydrogenase 21 (ALDH21) from Physcomitrella patens in complex with the reaction product succinate
Authors	:	Kopecny, D.; Vigouroux, A.; Briozzo, P.; Morera, S.
Deposited on	:	2017-01-31
Resolution	:	2.20 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 following versions of software and data (see references ①) were used in the production of this report:

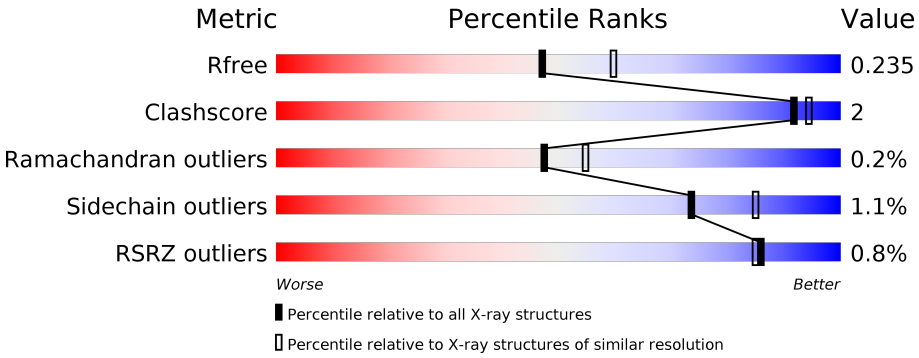
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	515	% 89% 5% 7%
1	B	515	88% 5% 7%
1	C	515	% 89% • 7%
1	D	515	% 88% 5% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15790 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 aldehyde dehydrogenase 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3720	2379	627	696	18			
1	B	480	Total	C	N	O	S	0	0	0
			3713	2374	626	695	18			
1	C	481	Total	C	N	O	S	0	0	0
			3720	2379	627	696	18			
1	D	481	Total	C	N	O	S	0	0	0
			3720	2379	627	696	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A9SS48
A	-16	GLY	-	expression tag	UNP A9SS48
A	-15	SER	-	expression tag	UNP A9SS48
A	-14	SER	-	expression tag	UNP A9SS48
A	-13	HIS	-	expression tag	UNP A9SS48
A	-12	HIS	-	expression tag	UNP A9SS48
A	-11	HIS	-	expression tag	UNP A9SS48
A	-10	HIS	-	expression tag	UNP A9SS48
A	-9	HIS	-	expression tag	UNP A9SS48
A	-8	HIS	-	expression tag	UNP A9SS48
A	-7	SER	-	expression tag	UNP A9SS48
A	-6	GLN	-	expression tag	UNP A9SS48
A	-5	ASP	-	expression tag	UNP A9SS48
A	-4	PRO	-	expression tag	UNP A9SS48
A	-3	ASN	-	expression tag	UNP A9SS48
A	-2	SER	-	expression tag	UNP A9SS48
A	-1	SER	-	expression tag	UNP A9SS48
A	0	SER	-	expression tag	UNP A9SS48
B	-17	MET	-	initiating methionine	UNP A9SS48
B	-16	GLY	-	expression tag	UNP A9SS48
B	-15	SER	-	expression tag	UNP A9SS48

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	SER	-	expression tag	UNP A9SS48
B	-13	HIS	-	expression tag	UNP A9SS48
B	-12	HIS	-	expression tag	UNP A9SS48
B	-11	HIS	-	expression tag	UNP A9SS48
B	-10	HIS	-	expression tag	UNP A9SS48
B	-9	HIS	-	expression tag	UNP A9SS48
B	-8	HIS	-	expression tag	UNP A9SS48
B	-7	SER	-	expression tag	UNP A9SS48
B	-6	GLN	-	expression tag	UNP A9SS48
B	-5	ASP	-	expression tag	UNP A9SS48
B	-4	PRO	-	expression tag	UNP A9SS48
B	-3	ASN	-	expression tag	UNP A9SS48
B	-2	SER	-	expression tag	UNP A9SS48
B	-1	SER	-	expression tag	UNP A9SS48
B	0	SER	-	expression tag	UNP A9SS48
C	-17	MET	-	initiating methionine	UNP A9SS48
C	-16	GLY	-	expression tag	UNP A9SS48
C	-15	SER	-	expression tag	UNP A9SS48
C	-14	SER	-	expression tag	UNP A9SS48
C	-13	HIS	-	expression tag	UNP A9SS48
C	-12	HIS	-	expression tag	UNP A9SS48
C	-11	HIS	-	expression tag	UNP A9SS48
C	-10	HIS	-	expression tag	UNP A9SS48
C	-9	HIS	-	expression tag	UNP A9SS48
C	-8	HIS	-	expression tag	UNP A9SS48
C	-7	SER	-	expression tag	UNP A9SS48
C	-6	GLN	-	expression tag	UNP A9SS48
C	-5	ASP	-	expression tag	UNP A9SS48
C	-4	PRO	-	expression tag	UNP A9SS48
C	-3	ASN	-	expression tag	UNP A9SS48
C	-2	SER	-	expression tag	UNP A9SS48
C	-1	SER	-	expression tag	UNP A9SS48
C	0	SER	-	expression tag	UNP A9SS48
D	-17	MET	-	initiating methionine	UNP A9SS48
D	-16	GLY	-	expression tag	UNP A9SS48
D	-15	SER	-	expression tag	UNP A9SS48
D	-14	SER	-	expression tag	UNP A9SS48
D	-13	HIS	-	expression tag	UNP A9SS48
D	-12	HIS	-	expression tag	UNP A9SS48
D	-11	HIS	-	expression tag	UNP A9SS48
D	-10	HIS	-	expression tag	UNP A9SS48
D	-9	HIS	-	expression tag	UNP A9SS48

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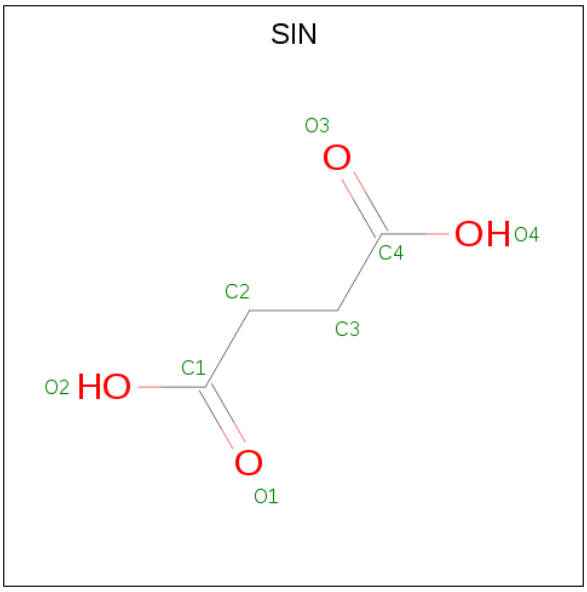
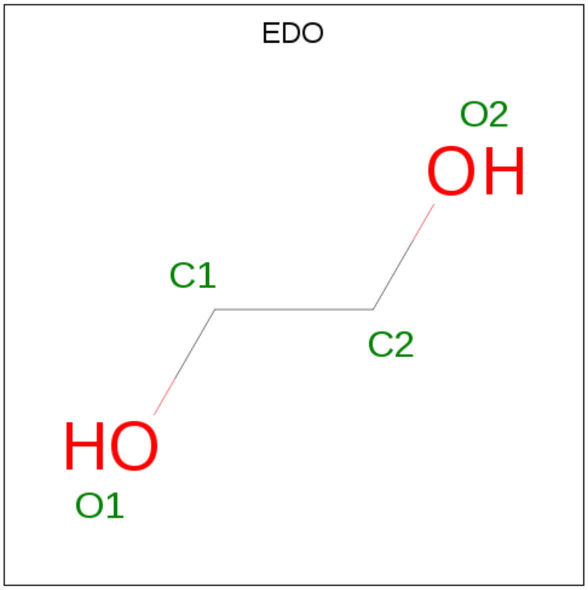
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP A9SS48
D	-7	SER	-	expression tag	UNP A9SS48
D	-6	GLN	-	expression tag	UNP A9SS48
D	-5	ASP	-	expression tag	UNP A9SS48
D	-4	PRO	-	expression tag	UNP A9SS48
D	-3	ASN	-	expression tag	UNP A9SS48
D	-2	SER	-	expression tag	UNP A9SS48
D	-1	SER	-	expression tag	UNP A9SS48
D	0	SER	-	expression tag	UNP A9SS48

- Molecule 2 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 4 4	0	0
2	B	1	Total C O 8 4 4	0	0
2	C	1	Total C O 8 4 4	0	0
2	D	1	Total C O 8 4 4	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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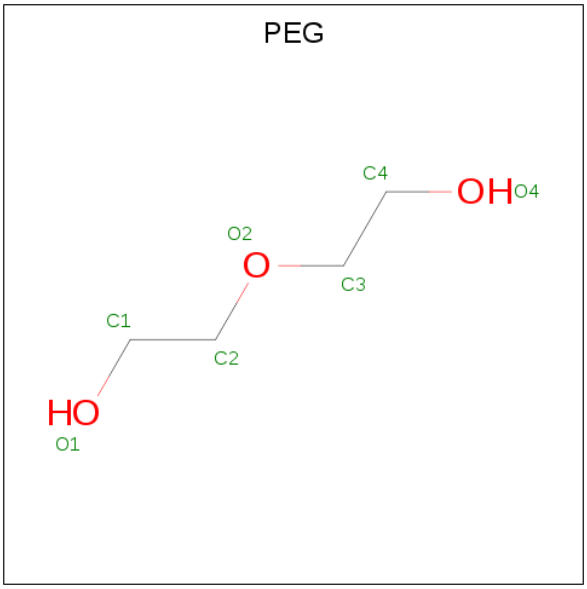
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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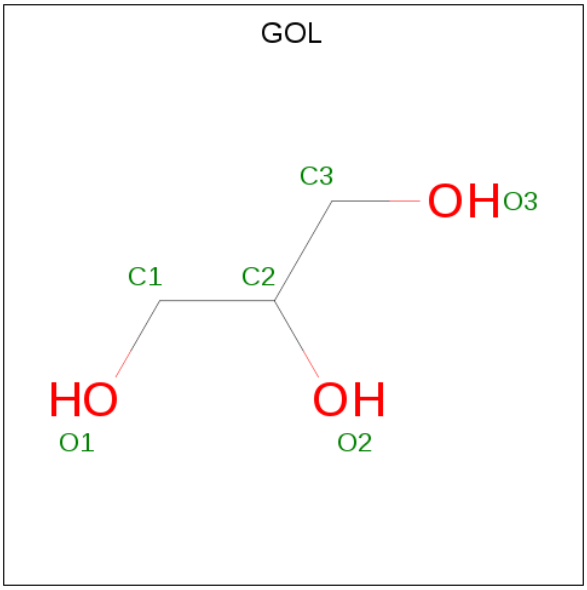
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	160	Total O 160 160	0	0
6	B	178	Total O 178 178	0	0
6	C	175	Total O 175 175	0	0

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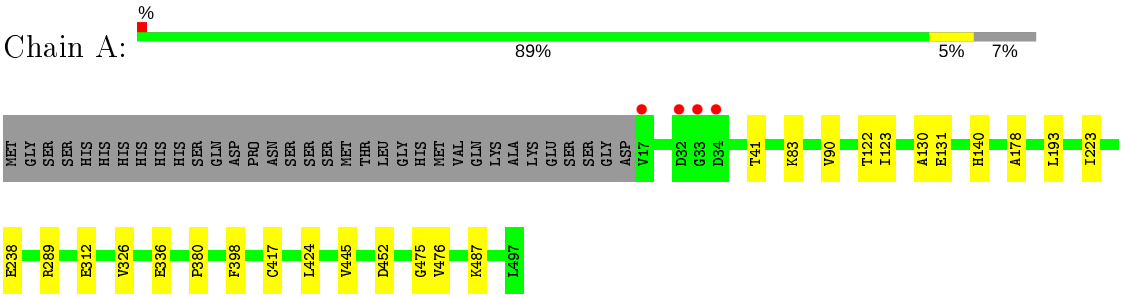
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	135	Total 135	O 135	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

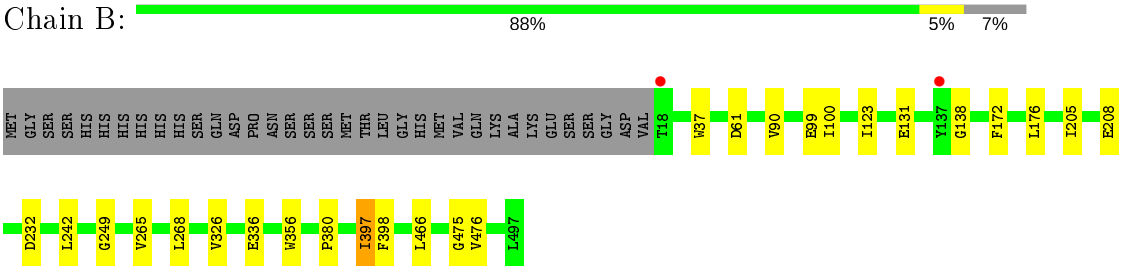
- Molecule 1: aldehyde dehydrogenase 21

Chain A:



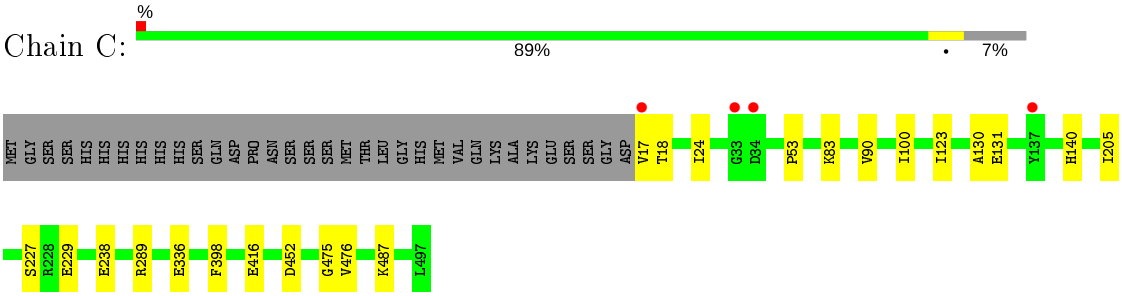
- Molecule 1: aldehyde dehydrogenase 21

Chain B:



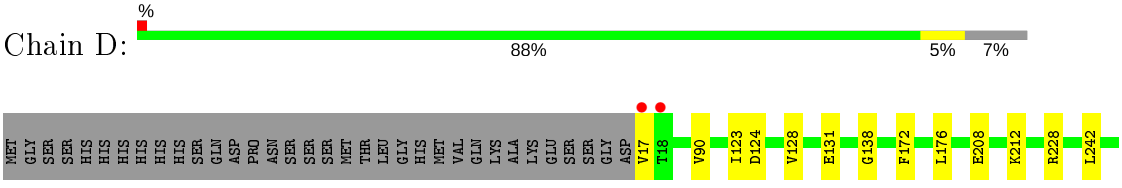
- Molecule 1: aldehyde dehydrogenase 21

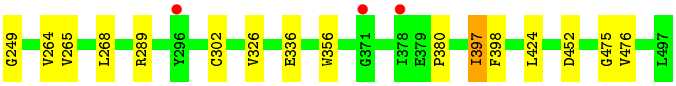
Chain C:



- Molecule 1: aldehyde dehydrogenase 21

Chain D:




G249
V264
V265
L268
R289
Y296
C302
V326
E336
W356
G371
I378
E379
P380
I397
F398
L424
D452
G475
V476
L497

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.58Å 151.81Å 159.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.07 – 2.20 50.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.07-2.20) 100.0 (50.07-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.188 , 0.220 0.204 , 0.235	Depositor DCC
R_{free} test set	5648 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15790	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8344e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, PEG, SIN, EDO

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	0.46	0/3796	0.67	1/5133 (0.0%)
1	B	0.47	0/3789	0.67	1/5123 (0.0%)
1	C	0.45	0/3796	0.66	1/5133 (0.0%)
1	D	0.46	0/3796	0.67	1/5133 (0.0%)
All	All	0.46	0/15177	0.67	4/20522 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	475	GLY	N-CA-C	-6.38	97.16	113.10
1	A	475	GLY	N-CA-C	-6.37	97.18	113.10
1	B	475	GLY	N-CA-C	-6.22	97.54	113.10
1	C	475	GLY	N-CA-C	-6.13	97.77	113.10

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	3720	0	3765	14	0
1	B	3713	0	3756	12	0
1	C	3720	0	3765	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3720	0	3765	13	0
2	A	8	0	4	0	0
2	B	8	0	4	0	0
2	C	8	0	4	0	0
2	D	8	0	4	0	0
3	A	36	0	54	4	0
3	B	60	0	90	2	0
3	C	40	0	60	3	0
3	D	28	0	42	0	0
4	A	21	0	30	3	0
4	B	7	0	10	0	0
4	C	14	0	20	0	0
4	D	7	0	10	0	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
5	D	12	0	16	1	0
6	A	160	0	0	0	0
6	B	178	0	0	0	0
6	C	175	0	0	0	0
6	D	135	0	0	0	0
All	All	15790	0	15415	48	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 (48) 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:A:445:VAL:HG13	4:A:512:PEG:H12	1.63	0.80
1:A:487:LYS:HE3	3:A:509:EDO:H21	1.75	0.67
1:A:487:LYS:CE	3:A:509:EDO:H21	2.26	0.65
1:D:264:VAL:H	5:D:504:GOL:H32	1.64	0.62
1:A:417:CYS:O	4:A:512:PEG:H21	2.00	0.61
3:A:509:EDO:H22	1:B:466:LEU:HD11	1.82	0.60
1:A:131:GLU:HG2	1:C:131:GLU:HG2	1.87	0.57
1:B:208:GLU:HG2	3:B:509:EDO:H22	1.86	0.57
1:B:99:GLU:HA	3:B:510:EDO:H22	1.89	0.54
1:C:24:ILE:HG23	1:C:53:PRO:HD2	1.89	0.53
1:A:193:LEU:HD23	1:A:223:ILE:HG12	1.90	0.53
1:D:90:VAL:HG13	1:D:123:ILE:HG23	1.92	0.52
1:C:487:LYS:CE	3:C:510:EDO:H22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ASP:O	1:D:128:VAL:HG23	2.11	0.51
1:D:249:GLY:HA2	1:D:268:LEU:HD13	1.94	0.50
1:D:289:ARG:HD3	1:D:452:ASP:OD1	2.11	0.49
1:A:289:ARG:HD3	1:A:452:ASP:OD1	2.14	0.48
1:A:326:VAL:HG13	1:A:380:PRO:HB2	1.95	0.48
1:C:289:ARG:HD3	1:C:452:ASP:OD1	2.13	0.48
1:D:326:VAL:HG13	1:D:380:PRO:HB2	1.97	0.47
1:B:356:TRP:HE3	1:B:397:ILE:HD12	1.80	0.47
1:B:242:LEU:HD11	1:B:265:VAL:HG23	1.96	0.47
1:D:208:GLU:O	1:D:212:LYS:HD3	2.16	0.46
1:D:302:CYS:O	1:D:424:LEU:HD23	2.16	0.46
1:C:416:GLU:HG2	5:C:502:GOL:H31	1.97	0.46
1:A:83:LYS:HG3	1:A:130:ALA:O	2.17	0.45
1:B:90:VAL:HG13	1:B:123:ILE:HG23	1.99	0.45
1:C:83:LYS:HG3	1:C:130:ALA:O	2.17	0.45
1:B:249:GLY:HA2	1:B:268:LEU:HD13	1.99	0.45
1:C:238:GLU:HB2	3:C:512:EDO:H21	1.99	0.44
1:C:227:SER:HB2	1:C:229:GLU:OE2	2.17	0.44
1:D:242:LEU:HD11	1:D:265:VAL:HG23	1.99	0.44
1:C:90:VAL:HG13	1:C:123:ILE:HG23	1.99	0.44
1:B:326:VAL:HG13	1:B:380:PRO:HB2	2.00	0.43
1:A:41:THR:HG21	3:A:506:EDO:H12	2.01	0.43
1:C:487:LYS:HE3	3:C:510:EDO:H22	2.01	0.43
1:B:131:GLU:HG2	1:D:131:GLU:HG2	2.00	0.42
1:B:138:GLY:HA3	1:C:140:HIS:HB3	2.01	0.42
1:A:140:HIS:HB3	1:D:138:GLY:HA3	2.01	0.42
1:A:445:VAL:CG1	4:A:512:PEG:H12	2.42	0.42
1:C:17:VAL:HG13	1:C:18:THR:H	1.85	0.41
1:B:100:ILE:HG12	1:B:205:ILE:HG21	2.02	0.41
1:C:100:ILE:HG12	1:C:205:ILE:HG21	2.01	0.41
1:D:356:TRP:HE3	1:D:397:ILE:HD12	1.85	0.41
1:B:172:PHE:HB2	1:B:176:LEU:HG	2.03	0.40
1:D:172:PHE:HB2	1:D:176:LEU:HG	2.03	0.40
1:A:90:VAL:HG13	1:A:123:ILE:HG23	2.03	0.40
1:A:122:THR:HG23	1:A:178:ALA:HB2	2.04	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	479/515 (93%)	461 (96%)	17 (4%)	1 (0%)	47	55
1	B	478/515 (93%)	462 (97%)	15 (3%)	1 (0%)	47	55
1	C	479/515 (93%)	466 (97%)	12 (2%)	1 (0%)	47	55
1	D	479/515 (93%)	465 (97%)	13 (3%)	1 (0%)	47	55
All	All	1915/2060 (93%)	1854 (97%)	57 (3%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	476	VAL
1	A	476	VAL
1	B	476	VAL
1	D	476	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	395/425 (93%)	390 (99%)	5 (1%)	69	81
1	B	394/425 (93%)	388 (98%)	6 (2%)	65	78
1	C	395/425 (93%)	393 (100%)	2 (0%)	88	94
1	D	395/425 (93%)	390 (99%)	5 (1%)	69	81
All	All	1579/1700 (93%)	1561 (99%)	18 (1%)	73	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	GLU
1	A	312	GLU
1	A	336	GLU
1	A	398	PHE
1	A	424	LEU
1	B	37	TRP
1	B	61	ASP
1	B	232	ASP
1	B	336	GLU
1	B	397	ILE
1	B	398	PHE
1	C	336	GLU
1	C	398	PHE
1	D	17	VAL
1	D	228	ARG
1	D	336	GLU
1	D	397	ILE
1	D	398	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	B	153	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

56 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	$\#\|Z\| > 2$
3	EDO	C	505	-	3,3,3	0.60	0	2,2,2	0.35	0
3	EDO	D	505	-	3,3,3	0.46	0	2,2,2	0.46	0
3	EDO	D	508	-	3,3,3	0.57	0	2,2,2	0.35	0
3	EDO	C	509	-	3,3,3	0.73	0	2,2,2	0.08	0
4	PEG	C	513	-	6,6,6	0.22	0	5,5,5	0.24	0
3	EDO	A	509	-	3,3,3	0.55	0	2,2,2	0.26	0
3	EDO	B	513	-	3,3,3	0.64	0	2,2,2	0.20	0
3	EDO	A	508	-	3,3,3	0.66	0	2,2,2	0.29	0
4	PEG	B	517	-	6,6,6	0.25	0	5,5,5	0.17	0
3	EDO	C	504	-	3,3,3	0.54	0	2,2,2	0.45	0
3	EDO	A	503	-	3,3,3	0.67	0	2,2,2	0.28	0
4	PEG	A	512	-	6,6,6	0.37	0	5,5,5	0.36	0
3	EDO	C	508	-	3,3,3	0.68	0	2,2,2	0.25	0
5	GOL	B	502	-	5,5,5	0.06	0	5,5,5	0.33	0
3	EDO	D	506	-	3,3,3	0.69	0	2,2,2	0.17	0
3	EDO	B	514	-	3,3,3	0.62	0	2,2,2	0.32	0
3	EDO	B	511	-	3,3,3	0.61	0	2,2,2	0.33	0
3	EDO	B	507	-	3,3,3	0.65	0	2,2,2	0.23	0
3	EDO	D	510	-	3,3,3	0.63	0	2,2,2	0.45	0
5	GOL	D	504	-	5,5,5	0.05	0	5,5,5	0.09	0
3	EDO	C	503	-	3,3,3	0.68	0	2,2,2	0.10	0
2	SIN	D	502	-	1,7,7	0.22	0	2,8,8	0.66	0
3	EDO	D	509	-	3,3,3	0.61	0	2,2,2	0.37	0
4	PEG	A	513	-	6,6,6	0.21	0	5,5,5	0.11	0
3	EDO	D	501	-	3,3,3	0.39	0	2,2,2	0.44	0
3	EDO	A	507	-	3,3,3	0.64	0	2,2,2	0.21	0
3	EDO	C	510	-	3,3,3	0.63	0	2,2,2	0.49	0
3	EDO	B	505	-	3,3,3	0.55	0	2,2,2	0.37	0
3	EDO	C	506	-	3,3,3	0.61	0	2,2,2	0.21	0
5	GOL	D	503	-	5,5,5	0.08	0	5,5,5	0.22	0
4	PEG	D	511	-	6,6,6	0.27	0	5,5,5	0.27	0
3	EDO	C	512	-	3,3,3	0.61	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	D	507	-	3,3,3	0.59	0	2,2,2	0.22	0
3	EDO	B	509	-	3,3,3	0.65	0	2,2,2	0.22	0
3	EDO	B	504	-	3,3,3	0.62	0	2,2,2	0.27	0
3	EDO	C	511	-	3,3,3	0.60	0	2,2,2	0.27	0
3	EDO	B	516	-	3,3,3	0.61	0	2,2,2	0.27	0
2	SIN	C	501	-	1,7,7	0.29	0	2,8,8	1.37	0
4	PEG	A	511	-	6,6,6	0.12	0	5,5,5	0.11	0
3	EDO	B	515	-	3,3,3	0.61	0	2,2,2	0.27	0
3	EDO	B	503	-	3,3,3	0.73	0	2,2,2	0.39	0
3	EDO	B	506	-	3,3,3	0.77	0	2,2,2	0.06	0
3	EDO	B	508	-	3,3,3	0.51	0	2,2,2	0.37	0
3	EDO	B	510	-	3,3,3	0.74	0	2,2,2	0.13	0
2	SIN	B	501	-	1,7,7	0.16	0	2,8,8	0.31	0
5	GOL	C	502	-	5,5,5	0.05	0	5,5,5	0.16	0
3	EDO	A	505	-	3,3,3	0.49	0	2,2,2	0.44	0
3	EDO	A	504	-	3,3,3	0.58	0	2,2,2	0.36	0
2	SIN	A	501	-	1,7,7	0.13	0	2,8,8	0.85	0
3	EDO	A	510	-	3,3,3	0.63	0	2,2,2	0.17	0
4	PEG	C	514	-	6,6,6	0.12	0	5,5,5	0.06	0
3	EDO	C	507	-	3,3,3	0.59	0	2,2,2	0.38	0
3	EDO	B	512	-	3,3,3	0.53	0	2,2,2	0.38	0
3	EDO	B	518	-	3,3,3	0.64	0	2,2,2	0.26	0
3	EDO	A	502	-	3,3,3	0.57	0	2,2,2	0.30	0
3	EDO	A	506	-	3,3,3	0.58	0	2,2,2	0.35	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
3	EDO	C	505	-	-	0/1/1/1	-
3	EDO	D	505	-	-	0/1/1/1	-
3	EDO	D	508	-	-	0/1/1/1	-
3	EDO	C	509	-	-	0/1/1/1	-
4	PEG	C	513	-	-	0/4/4/4	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	B	513	-	-	0/1/1/1	-
3	EDO	A	508	-	-	0/1/1/1	-
4	PEG	B	517	-	-	1/4/4/4	-
3	EDO	C	504	-	-	0/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
4	PEG	A	512	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	508	-	-	0/1/1/1	-
5	GOL	B	502	-	-	1/4/4/4	-
3	EDO	D	506	-	-	0/1/1/1	-
3	EDO	B	514	-	-	0/1/1/1	-
3	EDO	B	511	-	-	0/1/1/1	-
3	EDO	B	507	-	-	1/1/1/1	-
3	EDO	D	510	-	-	1/1/1/1	-
5	GOL	D	504	-	-	0/4/4/4	-
3	EDO	C	503	-	-	0/1/1/1	-
2	SIN	D	502	-	-	1/1/5/5	-
3	EDO	D	509	-	-	0/1/1/1	-
4	PEG	A	513	-	-	0/4/4/4	-
3	EDO	D	501	-	-	0/1/1/1	-
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	C	510	-	-	0/1/1/1	-
3	EDO	B	505	-	-	0/1/1/1	-
3	EDO	C	506	-	-	1/1/1/1	-
5	GOL	D	503	-	-	0/4/4/4	-
4	PEG	D	511	-	-	1/4/4/4	-
3	EDO	C	512	-	-	1/1/1/1	-
3	EDO	D	507	-	-	0/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	C	511	-	-	0/1/1/1	-
3	EDO	B	516	-	-	0/1/1/1	-
2	SIN	C	501	-	-	0/1/5/5	-
4	PEG	A	511	-	-	1/4/4/4	-
3	EDO	B	515	-	-	0/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	B	508	-	-	0/1/1/1	-
3	EDO	B	510	-	-	1/1/1/1	-
2	SIN	B	501	-	-	1/1/5/5	-
5	GOL	C	502	-	-	1/4/4/4	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
2	SIN	A	501	-	-	1/1/5/5	-
3	EDO	A	510	-	-	1/1/1/1	-
4	PEG	C	514	-	-	3/4/4/4	-
3	EDO	C	507	-	-	0/1/1/1	-
3	EDO	B	512	-	-	0/1/1/1	-
3	EDO	B	518	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	502	SIN	C1-C2-C3-C4
2	A	501	SIN	C1-C2-C3-C4
5	B	502	GOL	O1-C1-C2-C3
3	B	507	EDO	O1-C1-C2-O2
3	C	506	EDO	O1-C1-C2-O2
3	B	510	EDO	O1-C1-C2-O2
4	C	514	PEG	O2-C3-C4-O4
3	D	510	EDO	O1-C1-C2-O2
4	A	511	PEG	C1-C2-O2-C3
4	B	517	PEG	C1-C2-O2-C3
3	A	509	EDO	O1-C1-C2-O2
4	C	514	PEG	C4-C3-O2-C2
4	D	511	PEG	C1-C2-O2-C3
3	A	507	EDO	O1-C1-C2-O2
3	C	512	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
5	C	502	GOL	C1-C2-C3-O3
4	C	514	PEG	C1-C2-O2-C3
3	A	503	EDO	O1-C1-C2-O2
3	B	509	EDO	O1-C1-C2-O2
3	B	504	EDO	O1-C1-C2-O2
3	A	510	EDO	O1-C1-C2-O2
3	A	506	EDO	O1-C1-C2-O2
4	A	512	PEG	C1-C2-O2-C3
2	B	501	SIN	C1-C2-C3-C4

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	509	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	512	PEG	3	0
5	D	504	GOL	1	0
3	C	510	EDO	2	0
3	C	512	EDO	1	0
3	B	509	EDO	1	0
3	B	510	EDO	1	0
5	C	502	GOL	1	0
3	A	506	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	481/515 (93%)	-0.34	4 (0%)	86	85	22, 34, 52, 75	0
1	B	480/515 (93%)	-0.33	2 (0%)	92	91	22, 33, 49, 67	0
1	C	481/515 (93%)	-0.36	4 (0%)	86	85	25, 34, 52, 83	0
1	D	481/515 (93%)	-0.20	5 (1%)	82	81	22, 37, 56, 80	0
All	All	1923/2060 (93%)	-0.31	15 (0%)	86	85	22, 34, 53, 83	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	ASP	4.0
1	D	17	VAL	3.7
1	A	33	GLY	3.7
1	A	34	ASP	3.4
1	C	33	GLY	3.1
1	D	296	TYR	3.1
1	C	17	VAL	2.8
1	A	32	ASP	2.5
1	C	137	TYR	2.4
1	D	18	THR	2.4
1	D	378	ILE	2.3
1	D	371	GLY	2.2
1	B	18	THR	2.1
1	A	17	VAL	2.1
1	B	137	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	PEG	B	517	7/7	0.68	0.28	59,64,67,68	0
5	GOL	D	503	6/6	0.69	0.31	74,75,75,76	0
3	EDO	A	506	4/4	0.69	0.20	56,57,58,58	0
5	GOL	C	502	6/6	0.70	0.34	65,66,67,68	0
3	EDO	A	508	4/4	0.74	0.14	58,59,59,59	0
3	EDO	C	512	4/4	0.74	0.16	63,63,63,64	0
3	EDO	D	509	4/4	0.76	0.23	60,60,61,61	0
3	EDO	B	515	4/4	0.77	0.17	53,55,55,56	0
3	EDO	A	507	4/4	0.77	0.23	47,51,53,55	0
3	EDO	C	511	4/4	0.77	0.19	68,68,70,71	0
3	EDO	C	503	4/4	0.79	0.39	42,43,45,46	0
3	EDO	C	509	4/4	0.79	0.15	54,55,56,57	0
3	EDO	B	516	4/4	0.80	0.26	55,55,56,56	0
5	GOL	B	502	6/6	0.80	0.24	64,64,65,65	0
4	PEG	A	512	7/7	0.82	0.27	36,39,43,43	0
2	SIN	D	502	8/8	0.82	0.24	56,60,70,71	0
4	PEG	D	511	7/7	0.82	0.17	53,54,55,55	0
3	EDO	C	508	4/4	0.83	0.16	60,60,60,60	0
5	GOL	D	504	6/6	0.83	0.28	58,61,61,63	0
3	EDO	B	506	4/4	0.83	0.58	59,61,63,63	0
2	SIN	B	501	8/8	0.83	0.17	47,49,58,60	0
3	EDO	B	513	4/4	0.83	0.17	55,55,56,57	0
3	EDO	D	506	4/4	0.83	0.15	61,61,62,62	0
2	SIN	C	501	8/8	0.84	0.20	66,67,70,71	0
3	EDO	B	507	4/4	0.84	0.16	43,44,47,47	0
3	EDO	C	507	4/4	0.84	0.14	59,59,59,59	0
3	EDO	B	514	4/4	0.84	0.12	62,64,64,65	0
4	PEG	A	513	7/7	0.85	0.13	63,65,67,68	0
3	EDO	B	508	4/4	0.86	0.27	56,57,59,60	0
3	EDO	B	511	4/4	0.86	0.13	67,68,69,71	0
3	EDO	C	510	4/4	0.86	0.22	36,39,42,44	0
3	EDO	B	509	4/4	0.86	0.14	54,54,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	D	510	4/4	0.86	0.15	42,43,43,45	0
3	EDO	A	505	4/4	0.87	0.46	43,45,46,49	0
4	PEG	C	514	7/7	0.87	0.23	53,54,55,55	0
3	EDO	D	508	4/4	0.88	0.25	58,59,60,60	0
3	EDO	B	510	4/4	0.88	0.20	45,45,47,48	0
3	EDO	A	510	4/4	0.89	0.15	52,53,55,55	0
3	EDO	B	504	4/4	0.90	0.14	48,50,50,51	0
2	SIN	A	501	8/8	0.90	0.17	53,57,62,63	0
3	EDO	B	512	4/4	0.90	0.21	63,63,63,64	0
3	EDO	A	509	4/4	0.90	0.19	29,34,39,39	0
3	EDO	C	504	4/4	0.91	0.10	43,44,44,45	0
3	EDO	D	507	4/4	0.91	0.34	51,55,59,61	0
3	EDO	A	504	4/4	0.91	0.16	56,57,57,57	0
3	EDO	D	501	4/4	0.92	0.23	54,56,59,61	0
3	EDO	B	503	4/4	0.92	0.10	33,36,39,42	0
4	PEG	A	511	7/7	0.92	0.12	47,51,54,56	0
4	PEG	C	513	7/7	0.93	0.13	36,38,40,40	0
3	EDO	A	503	4/4	0.93	0.16	39,42,43,43	0
3	EDO	B	505	4/4	0.93	0.42	39,41,41,42	0
3	EDO	B	518	4/4	0.93	0.14	48,51,54,54	0
3	EDO	A	502	4/4	0.93	0.09	39,41,45,49	0
3	EDO	D	505	4/4	0.93	0.35	39,40,42,43	0
3	EDO	C	506	4/4	0.94	0.13	43,43,44,46	0
3	EDO	C	505	4/4	0.96	0.07	33,35,37,41	0

6.5 Other polymers

There are no such residues in this entry.