wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 04:19 PM EDT

PDB ID	:	3N80
Title	:	Human mitochondrial aldehyde dehydrogenase, apo form
Authors	:	Gonzalez-Segura, L.; Hurley, T.D.
Deposited on	:	2010-05-27
Resolution	:	1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

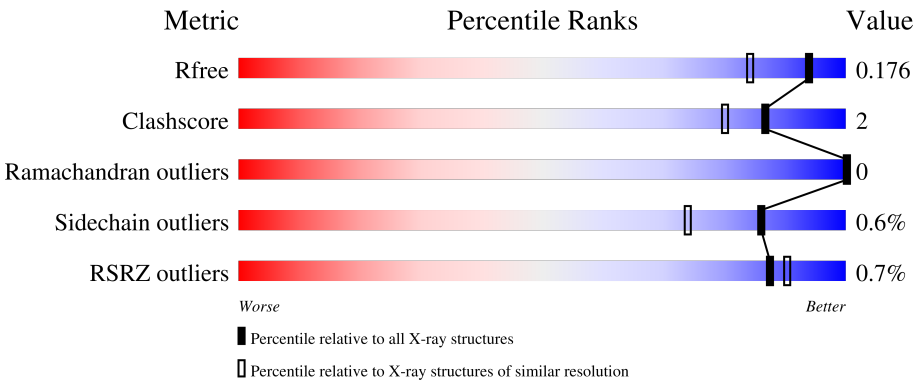
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	500	.% 94% 5% •
1	B	500	93% 6% •
1	C	500	.% 93% 6% •
1	D	500	.% 93% 6% •
1	E	500	95% • •

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Mol	Chain	Length	Quality of chain
1	F	500	95%
1	G	500	% 94%
1	H	500	% 94%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	909	-	-	X	-
3	EDO	D	914	-	-	X	-
3	EDO	H	918	-	-	X	-

2 Entry composition (i)

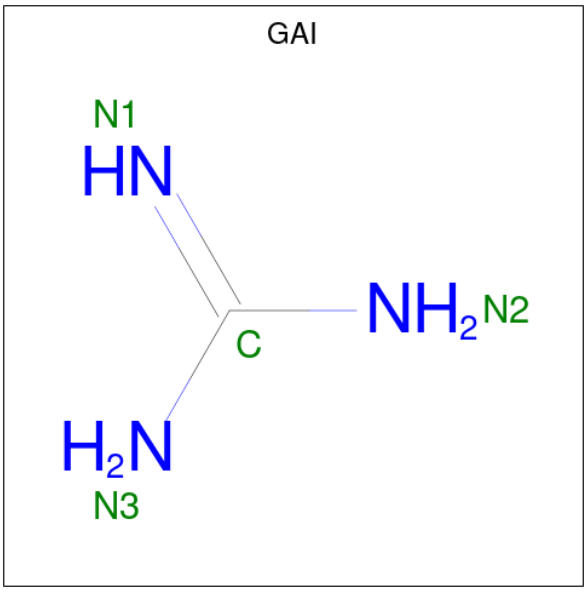
There are 6 unique types of molecules in this entry. The entry contains 36122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3845	2446	653	724	22	0	8	0
1	B	494	3871	2465	657	727	22	0	12	0
1	C	494	3864	2458	654	730	22	0	12	0
1	D	494	3858	2456	654	726	22	0	10	0
1	E	495	3887	2474	659	732	22	0	13	0
1	F	494	3884	2475	656	731	22	0	16	0
1	G	494	3905	2484	661	738	22	0	18	0
1	H	494	3882	2467	658	735	22	0	14	0

- Molecule 2 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N			
2	A	1	4	1	3		0	0
			Total	C	N			
2	A	1	4	1	3		0	0
			Total	C	N			
2	A	1	4	1	3		0	0
			Total	C	N			
2	B	1	4	1	3		0	0
			Total	C	N			
2	C	1	4	1	3		0	0
			Total	C	N			
2	C	1	4	1	3		0	0
			Total	C	N			
2	C	1	4	1	3		0	0
			Total	C	N			
2	D	1	4	1	3		0	0
			Total	C	N			
2	D	1	4	1	3		0	0
			Total	C	N			
2	D	1	4	1	3		0	0
			Total	C	N			
2	E	1	4	1	3		0	0
			Total	C	N			
2	E	1	4	1	3		0	0
			Total	C	N			
2	F	1	4	1	3		0	0
			Total	C	N			
2	F	1	4	1	3		0	0

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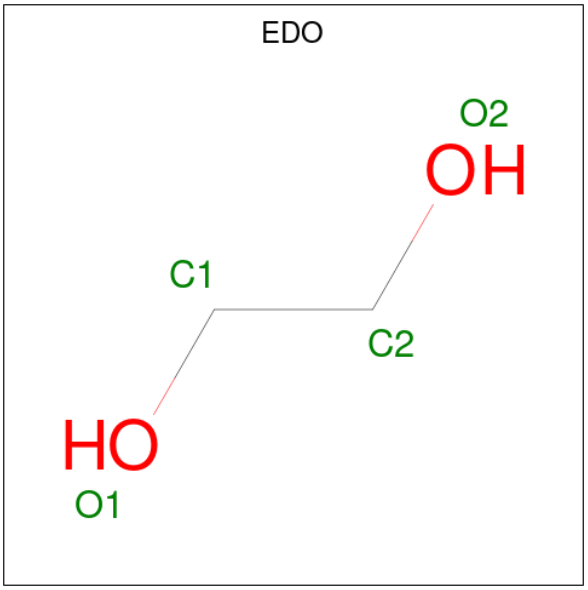
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	F	1	4	1	3	0	0
			Total	C	N		
2	F	1	4	1	3	0	0
			Total	C	N		
2	G	1	4	1	3	0	0
			Total	C	N		
2	G	1	4	1	3	0	0
			Total	C	N		
2	G	1	4	1	3	0	0
			Total	C	N		
2	H	1	4	1	3	0	0
			Total	C	N		
2	H	1	4	1	3	0	0

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



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

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

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	B	1	1	1	0	0
			Total	Na		
4	C	1	1	1	0	0
			Total	Na		
4	D	1	1	1	0	0
			Total	Na		
4	E	1	1	1	0	0
			Total	Na		
4	F	1	1	1	0	0
			Total	Na		
4	G	1	1	1	0	0
			Total	Na		
4	H	1	1	1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	H	1	1	1	0	0

- Molecule 6 is water.

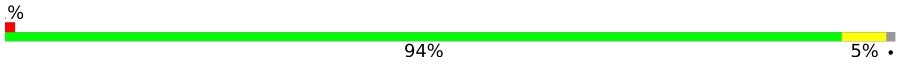
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	584	584	584	0	0
			Total	O		
6	B	617	617	617	0	0
			Total	O		
6	C	629	629	629	0	0
			Total	O		
6	D	580	580	580	0	0
			Total	O		
6	E	630	630	630	0	0
			Total	O		
6	F	637	637	637	0	0
			Total	O		
6	G	599	600	600	0	1
			Total	O		
6	H	611	613	613	0	2

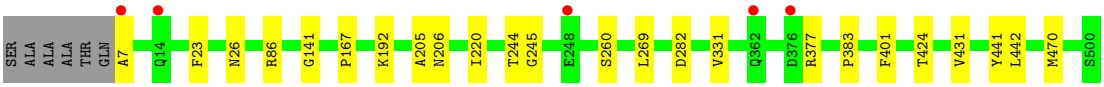
3 Residue-property plots (i)

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: Aldehyde dehydrogenase, mitochondrial

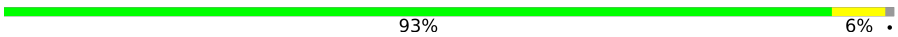
Chain A:

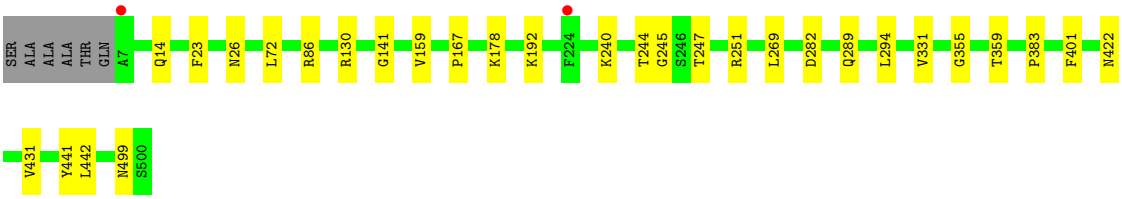




• Molecule 1: Aldehyde dehydrogenase, mitochondrial

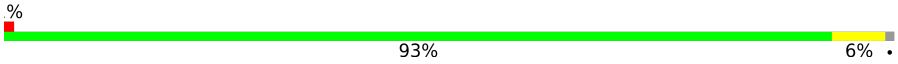
Chain B:

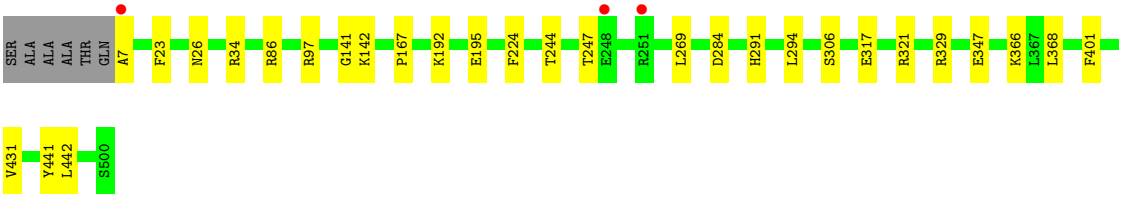




• Molecule 1: Aldehyde dehydrogenase, mitochondrial

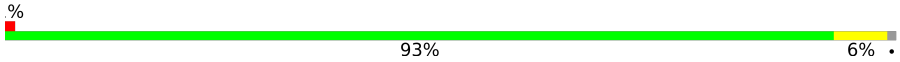
Chain C:

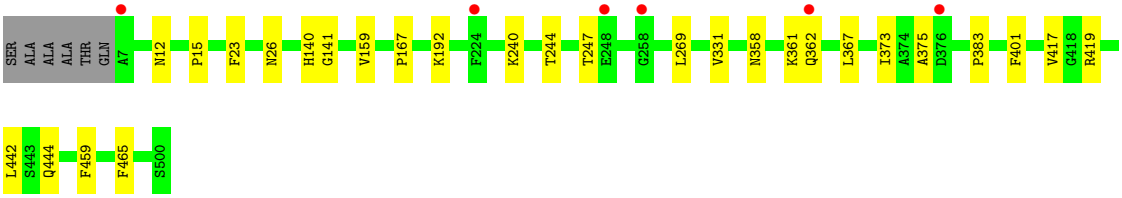




• Molecule 1: Aldehyde dehydrogenase, mitochondrial

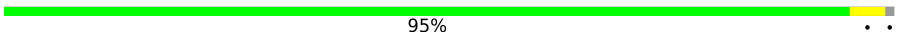
Chain D:

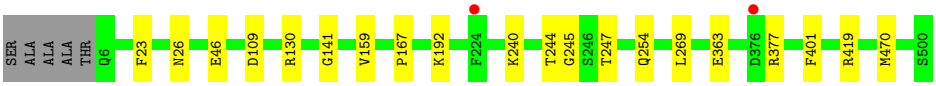




• Molecule 1: Aldehyde dehydrogenase, mitochondrial

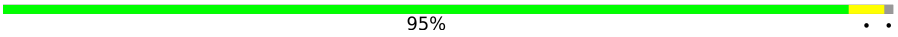
Chain E:

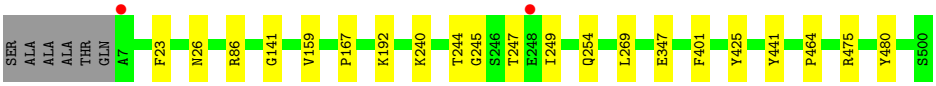




• Molecule 1: Aldehyde dehydrogenase, mitochondrial

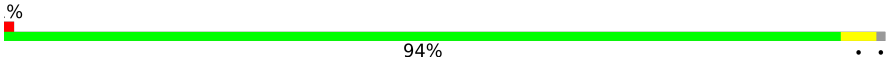
Chain F:





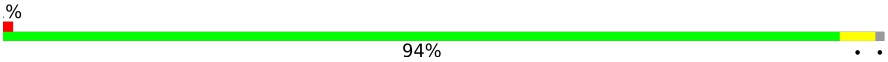
• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain G:



• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.66Å 152.29Å 177.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 20.97 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.50) 99.0 (20.97-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.149 , 0.175 0.150 , 0.176	Depositor DCC
R_{free} test set	30070 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	9.7	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	36122	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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 44.03 % 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 1.6183e-04. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GAI, MG, NA, EDO, CSO

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	0.59	0/3928	0.77	2/5325 (0.0%)
1	B	0.63	0/3964	0.79	3/5373 (0.1%)
1	C	0.62	0/3959	0.78	3/5365 (0.1%)
1	D	0.60	0/3948	0.77	1/5351 (0.0%)
1	E	0.62	0/3986	0.78	3/5401 (0.1%)
1	F	0.63	0/3991	0.78	4/5409 (0.1%)
1	G	0.62	0/4006	0.80	0/5428
1	H	0.62	0/3974	0.77	1/5387 (0.0%)
All	All	0.62	0/31756	0.78	17/43039 (0.0%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	282	ASP	CB-CG-OD1	7.96	125.47	118.30
1	H	86	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	F	86	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	A	282	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	130	ARG	NE-CZ-NH1	-5.99	117.30	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3845	0	3805	12	0
1	B	3871	0	3838	19	0
1	C	3864	0	3829	22	0
1	D	3858	0	3818	17	0
1	E	3887	0	3851	12	0
1	F	3884	0	3868	12	0
1	G	3905	0	3872	14	0
1	H	3882	0	3836	19	0
2	A	12	0	12	0	0
2	B	4	0	4	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
2	E	8	0	8	0	0
2	F	16	0	16	0	0
2	G	12	0	12	0	0
2	H	8	0	8	0	0
3	A	20	0	30	5	0
3	B	20	0	30	6	0
3	C	20	0	30	2	0
3	D	12	0	18	4	0
3	E	16	0	24	2	0
3	F	28	0	42	4	0
3	G	12	0	18	0	0
3	H	16	0	24	8	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	H	1	0	0	0	0
6	A	584	0	0	2	0
6	B	617	0	0	6	1
6	C	629	0	0	5	2
6	D	580	0	0	4	1
6	E	630	0	0	3	2
6	F	637	0	0	1	0
6	G	600	0	0	4	1
6	H	613	0	0	5	1
All	All	36122	0	31017	129	4

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.

The worst 5 of 129 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:46:GLU:HB2	3:H:918:EDO:H21	1.17	1.10
1:E:363[B]:GLU:HG3	6:E:4434:HOH:O	1.71	0.90
1:E:363[A]:GLU:HG3	6:E:4639:HOH:O	1.74	0.87
1:H:46:GLU:HB2	3:H:918:EDO:C2	2.03	0.87
1:E:363[A]:GLU:CG	6:E:4639:HOH:O	2.24	0.84

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:3202:HOH:O	6:E:2423:HOH:O[3_645]	2.09	0.11
6:C:4579:HOH:O	6:D:4636:HOH:O[4_556]	2.16	0.04
6:C:650:HOH:O	6:G:4035:HOH:O[3_646]	2.18	0.02
6:E:4734:HOH:O	6:H:2040:HOH:O[4_466]	2.19	0.01

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	498/500 (100%)	485 (97%)	13 (3%)	0	100	100
1	B	502/500 (100%)	490 (98%)	12 (2%)	0	100	100
1	C	502/500 (100%)	489 (97%)	13 (3%)	0	100	100
1	D	500/500 (100%)	486 (97%)	14 (3%)	0	100	100
1	E	504/500 (101%)	492 (98%)	12 (2%)	0	100	100
1	F	506/500 (101%)	492 (97%)	14 (3%)	0	100	100
1	G	508/500 (102%)	495 (97%)	13 (3%)	0	100	100
1	H	504/500 (101%)	491 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4024/4000 (101%)	3920 (97%)	104 (3%)	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	A	405/401 (101%)	401 (99%)	4 (1%)	76 57
1	B	409/401 (102%)	406 (99%)	3 (1%)	84 69
1	C	409/401 (102%)	407 (100%)	2 (0%)	88 78
1	D	407/401 (102%)	405 (100%)	2 (0%)	88 78
1	E	411/401 (102%)	409 (100%)	2 (0%)	88 78
1	F	413/401 (103%)	411 (100%)	2 (0%)	88 78
1	G	414/401 (103%)	412 (100%)	2 (0%)	88 78
1	H	411/401 (102%)	409 (100%)	2 (0%)	88 78
All	All	3279/3208 (102%)	3260 (99%)	19 (1%)	86 74

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	401	PHE
1	H	192	LYS
1	H	401	PHE
1	G	401	PHE
1	C	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	358	ASN
1	H	291	HIS

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Mol	Chain	Res	Type
1	D	390	GLN
1	H	349	GLN
1	F	358	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	D	302[A]	-	3,6,7	0.77	0	0,6,8	-	-
1	CSO	F	302[A]	-	3,6,7	0.95	0	0,6,8	-	-
1	CSO	F	302[B]	-	3,6,7	0.65	0	0,6,8	-	-
1	CSO	G	302[A]	-	3,6,7	0.84	0	0,6,8	-	-
1	CSO	C	302[B]	-	3,6,7	0.69	0	0,6,8	-	-
1	CSO	G	302[B]	-	3,6,7	0.51	0	0,6,8	-	-
1	CSO	D	302[B]	-	3,6,7	0.48	0	0,6,8	-	-
1	CSO	A	302[A]	-	3,6,7	0.81	0	0,6,8	-	-
1	CSO	E	302[A]	-	3,6,7	1.09	0	0,6,8	-	-
1	CSO	B	302[B]	-	3,6,7	0.45	0	0,6,8	-	-
1	CSO	B	302[A]	-	3,6,7	0.98	0	0,6,8	-	-
1	CSO	A	302[B]	-	3,6,7	0.47	0	0,6,8	-	-
1	CSO	H	302[A]	-	3,6,7	0.90	0	0,6,8	-	-
1	CSO	E	302[B]	-	3,6,7	0.59	0	0,6,8	-	-
1	CSO	H	302[B]	-	3,6,7	0.64	0	0,6,8	-	-
1	CSO	C	302[A]	-	3,6,7	0.64	0	0,6,8	-	-

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
1	CSO	D	302[A]	-	-	0/1/5/7	-
1	CSO	F	302[A]	-	-	0/1/5/7	-
1	CSO	F	302[B]	-	-	0/1/5/7	-
1	CSO	G	302[A]	-	-	0/1/5/7	-
1	CSO	C	302[B]	-	-	0/1/5/7	-
1	CSO	G	302[B]	-	-	1/1/5/7	-
1	CSO	D	302[B]	-	-	0/1/5/7	-
1	CSO	A	302[A]	-	-	0/1/5/7	-
1	CSO	E	302[A]	-	-	0/1/5/7	-
1	CSO	B	302[B]	-	-	0/1/5/7	-
1	CSO	B	302[A]	-	-	0/1/5/7	-
1	CSO	A	302[B]	-	-	0/1/5/7	-
1	CSO	H	302[A]	-	-	0/1/5/7	-
1	CSO	E	302[B]	-	-	0/1/5/7	-
1	CSO	H	302[B]	-	-	0/1/5/7	-
1	CSO	C	302[A]	-	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	302[B]	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 8 are monoatomic - leaving 57 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	$\#\|Z\| > 2$
3	EDO	H	948	-	3,3,3	0.49	0	2,2,2	0.67	0
2	GAI	A	801	-	3,3,3	1.14	0	3,3,3	1.12	0
2	GAI	H	808	-	3,3,3	0.87	0	3,3,3	1.75	1 (33%)
3	EDO	E	915	-	3,3,3	0.40	0	2,2,2	0.70	0
3	EDO	B	909	-	3,3,3	0.42	0	2,2,2	0.27	0
3	EDO	C	913	-	3,3,3	0.46	0	2,2,2	0.13	0
3	EDO	C	963	-	3,3,3	0.45	0	2,2,2	0.52	0
3	EDO	B	902	-	3,3,3	0.45	0	2,2,2	0.13	0
3	EDO	E	920	-	3,3,3	0.52	0	2,2,2	0.32	0
2	GAI	C	803	-	3,3,3	1.57	0	3,3,3	0.46	0
3	EDO	G	907	-	3,3,3	0.54	0	2,2,2	0.71	0
2	GAI	E	815	-	3,3,3	1.87	1 (33%)	3,3,3	1.04	0
2	GAI	F	806	-	3,3,3	0.87	0	3,3,3	0.44	0
3	EDO	A	911	-	3,3,3	0.43	0	2,2,2	0.44	0
2	GAI	D	804	-	3,3,3	1.29	0	3,3,3	1.86	1 (33%)
3	EDO	E	905	-	3,3,3	0.52	0	2,2,2	0.20	0
3	EDO	H	908	-	3,3,3	0.40	0	2,2,2	0.28	0
2	GAI	G	838	-	3,3,3	1.27	0	3,3,3	0.73	0
3	EDO	F	906	-	3,3,3	0.67	0	2,2,2	0.44	0
2	GAI	C	823	-	3,3,3	1.12	0	3,3,3	1.02	0
3	EDO	A	910	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	B	942	-	3,3,3	0.56	0	2,2,2	0.48	0
2	GAI	E	805	-	3,3,3	0.76	0	3,3,3	0.68	0
3	EDO	F	919	-	3,3,3	0.49	0	2,2,2	0.72	0
3	EDO	B	922	-	3,3,3	0.38	0	2,2,2	0.66	0
2	GAI	D	833	-	3,3,3	1.76	1 (33%)	3,3,3	1.33	0
2	GAI	C	813	-	3,3,3	1.37	0	3,3,3	0.74	0
2	GAI	G	807	-	3,3,3	1.55	0	3,3,3	0.04	0
3	EDO	F	916	-	3,3,3	0.54	0	2,2,2	0.19	0
3	EDO	A	941	-	3,3,3	0.50	0	2,2,2	0.47	0
3	EDO	E	925	-	3,3,3	0.31	0	2,2,2	0.81	0
2	GAI	A	811	-	3,3,3	1.59	1 (33%)	3,3,3	0.85	0
3	EDO	B	912	-	3,3,3	0.54	0	2,2,2	0.34	0
3	EDO	G	927	-	3,3,3	0.39	0	2,2,2	0.60	0
2	GAI	F	839	-	3,3,3	1.36	0	3,3,3	0.51	0
3	EDO	F	946	-	3,3,3	0.60	0	2,2,2	0.25	0
3	EDO	C	903	-	3,3,3	0.51	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GAI	B	802	-	3,3,3	1.28	0	3,3,3	0.59	0
3	EDO	A	901	-	3,3,3	0.45	0	2,2,2	0.46	0
2	GAI	F	826	-	3,3,3	1.25	0	3,3,3	0.62	0
3	EDO	D	944	-	3,3,3	0.43	0	2,2,2	0.73	0
2	GAI	H	818	-	3,3,3	1.58	1 (33%)	3,3,3	1.33	0
3	EDO	C	943	-	3,3,3	0.52	0	2,2,2	0.46	0
3	EDO	F	926	-	3,3,3	0.53	0	2,2,2	0.23	0
3	EDO	D	904	-	3,3,3	0.46	0	2,2,2	0.15	0
2	GAI	D	814	-	3,3,3	1.56	0	3,3,3	0.89	0
3	EDO	F	966	-	3,3,3	0.45	0	2,2,2	0.42	0
3	EDO	H	928	-	3,3,3	0.40	0	2,2,2	0.16	0
2	GAI	A	812	-	3,3,3	1.54	0	3,3,3	1.19	0
2	GAI	F	816	-	3,3,3	1.84	2 (66%)	3,3,3	0.80	0
3	EDO	A	921	-	3,3,3	0.35	0	2,2,2	0.67	0
3	EDO	C	923	-	3,3,3	0.28	0	2,2,2	0.79	0
3	EDO	F	956	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	H	918	-	3,3,3	0.40	0	2,2,2	0.26	0
3	EDO	D	914	-	3,3,3	0.53	0	2,2,2	0.63	0
3	EDO	G	917	-	3,3,3	0.54	0	2,2,2	0.07	0
2	GAI	G	817	-	3,3,3	1.27	0	3,3,3	0.79	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	H	948	-	-	1/1/1/1	-
3	EDO	E	915	-	-	0/1/1/1	-
3	EDO	B	909	-	-	1/1/1/1	-
3	EDO	C	913	-	-	0/1/1/1	-
3	EDO	C	963	-	-	0/1/1/1	-
3	EDO	B	902	-	-	0/1/1/1	-
3	EDO	E	920	-	-	1/1/1/1	-
3	EDO	G	907	-	-	0/1/1/1	-
3	EDO	E	905	-	-	0/1/1/1	-
3	EDO	A	911	-	-	0/1/1/1	-
3	EDO	H	908	-	-	0/1/1/1	-
3	EDO	F	906	-	-	0/1/1/1	-
3	EDO	A	910	-	-	1/1/1/1	-
3	EDO	B	942	-	-	0/1/1/1	-
3	EDO	F	919	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	922	-	-	0/1/1/1	-
3	EDO	F	916	-	-	0/1/1/1	-
3	EDO	A	941	-	-	0/1/1/1	-
3	EDO	B	912	-	-	0/1/1/1	-
3	EDO	G	927	-	-	0/1/1/1	-
3	EDO	F	946	-	-	0/1/1/1	-
3	EDO	C	903	-	-	0/1/1/1	-
3	EDO	A	901	-	-	0/1/1/1	-
3	EDO	D	944	-	-	0/1/1/1	-
3	EDO	C	943	-	-	0/1/1/1	-
3	EDO	F	926	-	-	0/1/1/1	-
3	EDO	D	904	-	-	0/1/1/1	-
3	EDO	F	966	-	-	0/1/1/1	-
3	EDO	H	928	-	-	1/1/1/1	-
3	EDO	C	923	-	-	0/1/1/1	-
3	EDO	F	956	-	-	0/1/1/1	-
3	EDO	A	921	-	-	0/1/1/1	-
3	EDO	H	918	-	-	1/1/1/1	-
3	EDO	D	914	-	-	0/1/1/1	-
3	EDO	G	917	-	-	0/1/1/1	-
3	EDO	E	925	-	-	0/1/1/1	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	815	GAI	C-N1	-2.53	1.25	1.30
2	D	833	GAI	C-N1	-2.38	1.25	1.30
2	A	811	GAI	C-N1	-2.20	1.26	1.30
2	F	816	GAI	C-N3	-2.10	1.32	1.36
2	F	816	GAI	C-N1	-2.08	1.26	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	804	GAI	N3-C-N2	2.73	122.63	116.13
2	H	808	GAI	N3-C-N2	2.45	121.96	116.13

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	910	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	E	920	EDO	O1-C1-C2-O2
3	B	909	EDO	O1-C1-C2-O2
3	F	919	EDO	O1-C1-C2-O2
3	H	918	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	948	EDO	1	0
3	B	909	EDO	4	0
3	C	963	EDO	1	0
3	E	920	EDO	2	0
3	A	910	EDO	2	0
3	B	942	EDO	1	0
3	F	919	EDO	3	0
3	B	922	EDO	1	0
3	A	941	EDO	3	0
3	F	946	EDO	1	0
3	C	943	EDO	1	0
3	H	918	EDO	7	0
3	D	914	EDO	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	493/500 (98%)	-0.37	5 (1%)	82	85	6, 12, 22, 32	0
1	B	493/500 (98%)	-0.50	2 (0%)	92	94	6, 10, 19, 30	0
1	C	493/500 (98%)	-0.50	3 (0%)	89	91	5, 10, 18, 31	0
1	D	493/500 (98%)	-0.38	6 (1%)	79	82	5, 11, 21, 33	0
1	E	494/500 (98%)	-0.52	2 (0%)	92	94	5, 9, 17, 31	1 (0%)
1	F	493/500 (98%)	-0.56	2 (0%)	92	94	4, 9, 16, 28	0
1	G	493/500 (98%)	-0.38	3 (0%)	89	91	5, 11, 21, 32	0
1	H	493/500 (98%)	-0.47	4 (0%)	86	89	5, 10, 18, 31	0
All	All	3945/4000 (98%)	-0.46	27 (0%)	87	90	4, 10, 19, 33	1 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	7	ALA	6.5
1	H	7	ALA	6.5
1	A	7	ALA	6.2
1	D	7	ALA	6.0
1	B	7	ALA	5.8

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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
1	CSO	A	302[A]	7/8	0.87	0.14	11,11,19,21	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	A	302[B]	7/8	0.87	0.14	9,11,14,15	4
1	CSO	B	302[A]	7/8	0.87	0.14	9,10,18,21	4
1	CSO	B	302[B]	7/8	0.87	0.14	8,9,12,13	4
1	CSO	C	302[A]	7/8	0.88	0.14	8,9,16,20	4
1	CSO	C	302[B]	7/8	0.88	0.14	7,8,10,12	4
1	CSO	F	302[A]	7/8	0.88	0.14	8,9,17,19	4
1	CSO	F	302[B]	7/8	0.88	0.14	7,8,12,18	4
1	CSO	E	302[A]	7/8	0.89	0.14	7,9,18,19	4
1	CSO	E	302[B]	7/8	0.89	0.14	6,8,10,12	4
1	CSO	D	302[A]	7/8	0.89	0.13	10,10,18,19	4
1	CSO	D	302[B]	7/8	0.89	0.13	8,10,12,14	4
1	CSO	H	302[A]	7/8	0.89	0.13	9,9,18,19	4
1	CSO	H	302[B]	7/8	0.89	0.13	8,9,12,15	4
1	CSO	G	302[A]	7/8	0.91	0.11	9,10,19,20	4
1	CSO	G	302[B]	7/8	0.91	0.11	8,9,13,14	4

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, 95th 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	GAI	D	814	4/4	0.70	0.20	29,29,30,31	0
2	GAI	F	826	4/4	0.72	0.16	28,28,28,29	0
2	GAI	C	823	4/4	0.74	0.17	26,26,27,27	0
2	GAI	C	813	4/4	0.75	0.17	26,27,28,30	0
2	GAI	A	812	4/4	0.76	0.18	26,27,27,28	0
2	GAI	G	817	4/4	0.77	0.18	27,29,29,29	0
2	GAI	G	838	4/4	0.81	0.20	23,24,25,26	0
3	EDO	E	925	4/4	0.82	0.14	29,29,31,35	0
2	GAI	A	811	4/4	0.85	0.14	28,28,29,30	0
3	EDO	G	927	4/4	0.85	0.15	36,36,37,38	0
2	GAI	H	818	4/4	0.86	0.23	25,25,26,28	0
2	GAI	F	839	4/4	0.87	0.14	19,21,21,21	0
3	EDO	F	919	4/4	0.87	0.18	18,19,24,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAI	E	805	4/4	0.87	0.13	12,15,15,15	0
3	EDO	H	928	4/4	0.87	0.12	21,21,22,24	0
2	GAI	F	816	4/4	0.88	0.18	27,27,28,30	0
3	EDO	G	917	4/4	0.89	0.17	20,25,27,28	0
3	EDO	A	910	4/4	0.89	0.15	18,18,23,24	0
3	EDO	E	920	4/4	0.89	0.19	20,21,24,24	0
2	GAI	E	815	4/4	0.90	0.24	26,27,27,29	0
2	GAI	H	808	4/4	0.90	0.10	12,14,15,15	0
3	EDO	A	911	4/4	0.90	0.13	23,26,26,28	0
2	GAI	B	802	4/4	0.91	0.09	13,14,15,16	0
3	EDO	C	963	4/4	0.91	0.10	22,24,27,28	0
3	EDO	A	921	4/4	0.92	0.09	37,37,38,38	0
3	EDO	B	912	4/4	0.92	0.12	18,21,21,24	0
2	GAI	D	833	4/4	0.92	0.10	20,22,22,24	0
3	EDO	B	942	4/4	0.93	0.16	12,21,22,25	0
3	EDO	C	943	4/4	0.93	0.15	11,19,20,23	0
3	EDO	B	909	4/4	0.93	0.22	21,22,24,27	0
3	EDO	E	915	4/4	0.93	0.13	19,23,24,26	0
2	GAI	G	807	4/4	0.93	0.09	10,12,13,13	0
3	EDO	D	944	4/4	0.94	0.14	18,23,23,25	0
3	EDO	F	926	4/4	0.94	0.07	11,12,16,16	0
3	EDO	F	966	4/4	0.94	0.11	21,23,23,23	0
3	EDO	B	922	4/4	0.94	0.16	15,26,28,31	0
3	EDO	C	923	4/4	0.94	0.08	17,19,20,25	0
3	EDO	H	918	4/4	0.94	0.18	13,15,24,25	0
3	EDO	D	914	4/4	0.94	0.12	15,17,18,20	0
3	EDO	H	948	4/4	0.94	0.17	10,19,21,24	0
5	MG	H	609	1/1	0.94	0.30	38,38,38,38	0
3	EDO	F	946	4/4	0.95	0.11	11,20,21,26	0
2	GAI	A	801	4/4	0.95	0.07	13,14,14,15	0
3	EDO	G	907	4/4	0.96	0.07	12,14,15,15	0
3	EDO	F	906	4/4	0.96	0.08	11,13,14,15	0
2	GAI	F	806	4/4	0.96	0.08	10,10,11,12	0
2	GAI	C	803	4/4	0.96	0.07	10,11,12,13	0
2	GAI	D	804	4/4	0.96	0.09	12,13,13,16	0
3	EDO	F	956	4/4	0.96	0.10	13,15,17,18	0
4	NA	G	607	1/1	0.96	0.06	13,13,13,13	0
3	EDO	A	941	4/4	0.96	0.15	10,20,22,23	0
3	EDO	C	913	4/4	0.97	0.08	15,18,19,21	0
3	EDO	H	908	4/4	0.97	0.06	13,15,16,16	0
3	EDO	D	904	4/4	0.97	0.06	13,16,16,18	0
3	EDO	B	902	4/4	0.97	0.07	13,16,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	903	4/4	0.97	0.06	13,15,16,17	0
3	EDO	F	916	4/4	0.97	0.07	15,19,19,23	0
3	EDO	E	905	4/4	0.97	0.06	14,17,17,17	0
4	NA	H	608	1/1	0.98	0.06	10,10,10,10	0
3	EDO	A	901	4/4	0.98	0.06	12,15,16,18	0
4	NA	E	605	1/1	0.99	0.04	9,9,9,9	0
4	NA	F	606	1/1	0.99	0.04	10,10,10,10	0
4	NA	B	602	1/1	0.99	0.04	10,10,10,10	0
4	NA	C	603	1/1	0.99	0.03	10,10,10,10	0
4	NA	D	604	1/1	0.99	0.05	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.