Full wwPDB X-ray Structure Validation Report (i)

Jan 24, 2023 – 06:05 AM EST

PDB ID	:	3HVY
Title	:	Crystal structure of putative cystathionine beta-lyase involved in aluminum resistance (NP_348457.1) from Clostridium acetobutylicum at 2.00 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2009-06-16
Resolution	:	2.00 Å(reported)

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

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

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

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

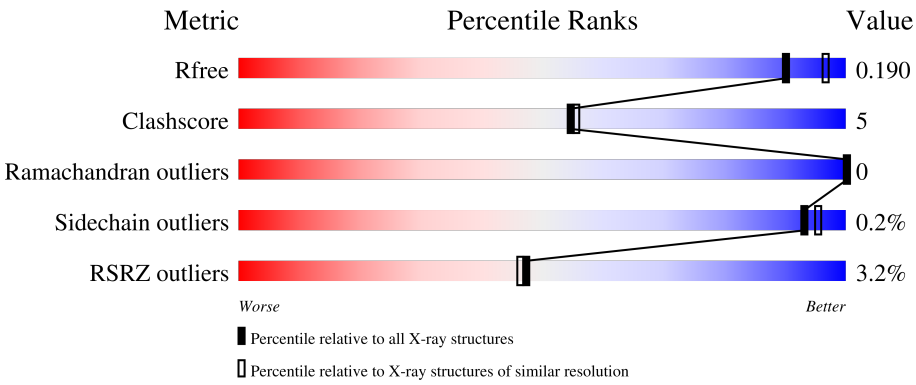
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	428	4% 90% 7% • •
1	B	428	2% 88% 8% • •
1	C	428	3% 91% 7% • •
1	D	428	3% 90% 8% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13952 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 Cystathionine beta-lyase family protein, YNBB B.subtilis ortholog.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S	Se			
1	A	417	3237	2064	540	614	1	5	13	0	4	0
1	B	417	3271	2078	549	625	1	5	13	0	6	0
1	C	420	3241	2062	541	619	1	5	13	0	3	0
1	D	423	3261	2077	544	621	1	5	13	0	4	0

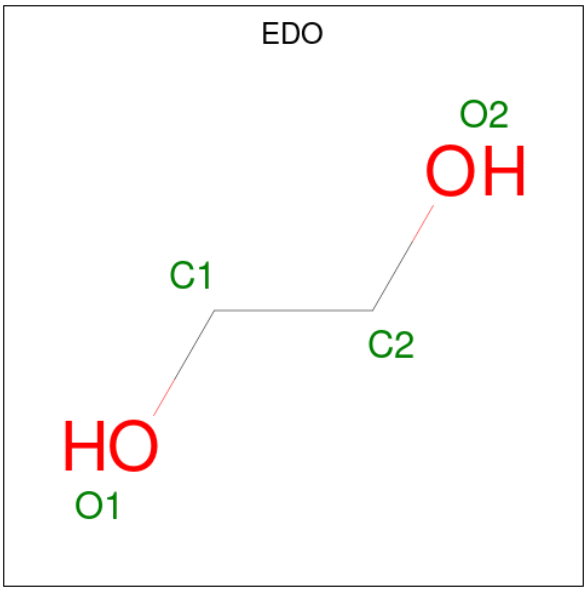
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q97I22
B	0	GLY	-	expression tag	UNP Q97I22
C	0	GLY	-	expression tag	UNP Q97I22
D	0	GLY	-	expression tag	UNP Q97I22

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

- Molecule 4 is water.

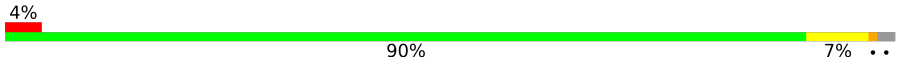
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	181	182	182	0	1
			Total	O		
4	B	231	231	231	0	0
			Total	O		
4	C	206	206	206	0	0
			Total	O		
4	D	247	247	247	0	0

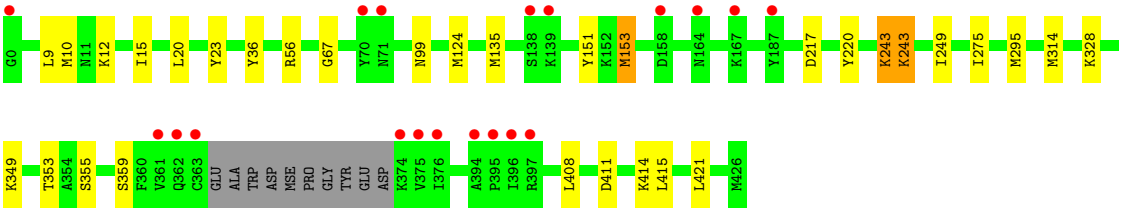
3 Residue-property plots (i)

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: Cystathionine beta-lyase family protein, YNBB B.subtilis ortholog

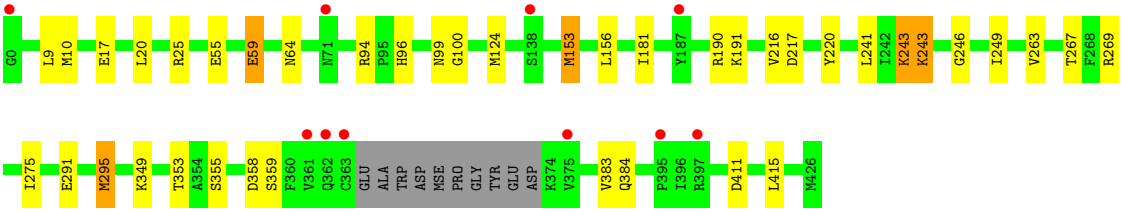
Chain A:





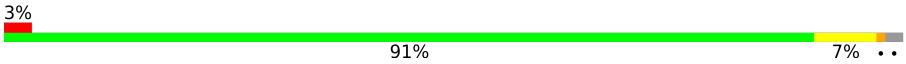
• Molecule 1: Cystathionine beta-lyase family protein, YNBB B.subtilis ortholog

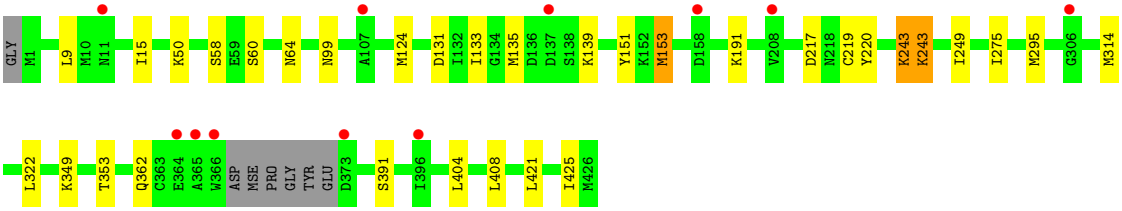
Chain B:



• Molecule 1: Cystathionine beta-lyase family protein, YNBB B.subtilis ortholog

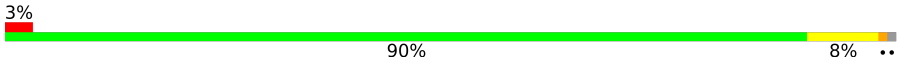
Chain C:

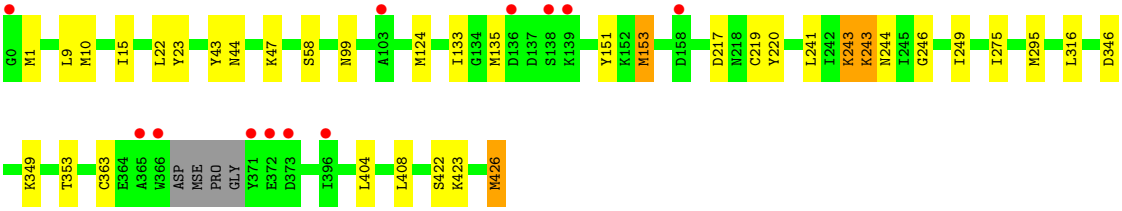




• Molecule 1: Cystathionine beta-lyase family protein, YNBB B.subtilis ortholog

Chain D:




G0
M1
L9
M10
I15
L22
Y23
Y43
N44
K47
S58
N99
A103
M124
I133
G134
M135
D136
D137
S138
K139
Y151
K152
M153
D158
D217
N218
C219
Y220
L241
I242
K243
K243
N244
I245
G246
I249
I275
M295
L316
D346
K349
T353
C363
E364
A365
W366
ASP
MSE
PRO
GLY
Y371
E372
D373
I396
L404
L408
S422
K423
M426

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.83Å 186.62Å 93.71Å 90.00° 103.06° 90.00°	Depositor
Resolution (Å)	30.03 – 2.00 30.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.03-2.00) 99.3 (30.03-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.145 , 0.187 0.154 , 0.190	Depositor DCC
R_{free} test set	6601 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13952	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 (i)

5.1 Standard geometry (i)

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

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	0.74	0/3253	0.76	1/4365 (0.0%)
1	B	0.84	5/3287 (0.2%)	0.79	1/4410 (0.0%)
1	C	0.75	0/3258	0.78	1/4379 (0.0%)
1	D	0.82	1/3277 (0.0%)	0.81	1/4401 (0.0%)
All	All	0.79	6/13075 (0.0%)	0.79	4/17555 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295[A]	MSE	SE-CE	-7.46	1.51	1.95
1	B	295[B]	MSE	SE-CE	-7.46	1.51	1.95
1	B	59	GLU	CB-CG	6.67	1.64	1.52
1	B	59	GLU	CD-OE1	6.56	1.32	1.25
1	D	363	CYS	CB-SG	-6.09	1.72	1.82
1	B	383	VAL	CB-CG2	5.74	1.65	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	MSE	CG-SE-CE	-10.03	76.84	98.90
1	D	153	MSE	CG-SE-CE	-7.57	82.25	98.90
1	C	153	MSE	CG-SE-CE	-6.94	83.63	98.90
1	B	153	MSE	CG-SE-CE	-6.80	83.93	98.90

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	3237	0	3177	33	0
1	B	3271	0	3207	43	0
1	C	3241	0	3165	37	0
1	D	3261	0	3186	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	20	0	30	2	0
3	B	20	0	30	1	0
3	C	24	0	36	1	0
3	D	8	0	12	1	0
4	A	182	0	0	1	0
4	B	231	0	0	1	0
4	C	206	0	0	2	0
4	D	247	0	0	3	0
All	All	13952	0	12843	133	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 (133) 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:153:MSE:SE	1:A:153:MSE:CE	2.17	1.42
1:D:10:MSE:CE	1:D:10:MSE:SE	2.17	1.42
1:D:249:ILE:HD11	1:D:295[A]:MSE:SE	1.73	1.38
1:D:124:MSE:CE	1:D:153:MSE:HE1	1.65	1.26
1:D:249:ILE:CD1	1:D:295[A]:MSE:SE	2.41	1.18
1:B:249:ILE:HG13	1:B:295[A]:MSE:CE	1.79	1.11
1:D:124:MSE:HE2	1:D:153:MSE:HE1	1.31	1.10
1:C:249:ILE:HD11	1:C:295[A]:MSE:SE	2.07	1.04
1:C:275:ILE:HD13	1:D:99:ASN:HD21	1.30	0.96
1:C:124:MSE:CE	1:C:153:MSE:HE1	1.97	0.94
1:B:249:ILE:CG1	1:B:295[A]:MSE:CE	2.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HD13	1:B:99:ASN:HD21	1.36	0.90
1:D:124:MSE:HE1	1:D:153:MSE:HE1	1.53	0.89
1:A:10:MSE:HE3	1:A:20:LEU:CD1	2.05	0.87
1:B:249:ILE:CG1	1:B:295[A]:MSE:HE3	2.06	0.85
1:A:10:MSE:HE3	1:A:20:LEU:HD12	1.57	0.84
1:C:275:ILE:CD1	1:D:99:ASN:HD21	1.90	0.84
1:A:153:MSE:CE	1:A:153:MSE:CG	2.57	0.82
1:C:124:MSE:HE2	1:C:153:MSE:HE1	1.61	0.81
1:B:10:MSE:HE3	1:B:20:LEU:HD12	1.63	0.79
1:A:10:MSE:CE	1:A:20:LEU:HD12	2.15	0.76
1:B:249:ILE:HG13	1:B:295[A]:MSE:HE1	1.67	0.75
1:A:124:MSE:CE	1:A:153:MSE:HE1	2.16	0.75
1:D:124:MSE:CE	1:D:153:MSE:CE	2.58	0.75
1:A:249:ILE:HD11	1:A:295[A]:MSE:SE	2.38	0.74
1:A:275:ILE:CD1	1:B:99:ASN:HD21	2.02	0.73
1:D:124:MSE:HE2	1:D:153:MSE:CE	2.14	0.71
1:C:249:ILE:CD1	1:C:295[A]:MSE:SE	2.87	0.70
1:C:99:ASN:HD21	1:D:275:ILE:HD13	1.56	0.69
1:B:249:ILE:CG1	1:B:295[A]:MSE:HE1	2.23	0.68
1:B:249:ILE:HG12	1:B:295[A]:MSE:HE3	1.74	0.68
1:A:124:MSE:HA	1:A:153:MSE:HE2	1.76	0.65
1:C:243[A]:LLP:OP4	1:C:243[A]:LLP:C4'	2.45	0.65
1:D:43:TYR:OH	3:D:429:EDO:H12	1.98	0.63
1:B:220:TYR:HE2	1:B:243[A]:LLP:O3	1.82	0.62
1:A:99:ASN:HD21	1:B:275:ILE:HD13	1.64	0.61
1:B:25[B]:ARG:HG2	1:B:25[B]:ARG:HH11	1.66	0.61
1:A:124:MSE:HE2	1:A:153:MSE:HE1	1.82	0.61
1:D:249:ILE:HD12	1:D:295[A]:MSE:SE	2.48	0.61
1:C:275:ILE:HD13	1:D:99:ASN:ND2	2.10	0.60
1:C:124:MSE:HA	1:C:153:MSE:HE2	1.84	0.59
1:A:135:MSE:HE3	1:A:151:TYR:CE2	2.37	0.59
3:A:428:EDO:H11	1:B:269:ARG:HA	1.85	0.59
1:D:349:LYS:O	1:D:353:THR:HG23	2.03	0.59
1:B:249:ILE:CD1	1:B:295[A]:MSE:HE1	2.32	0.58
1:D:1:MSE:HE3	1:D:23:TYR:CE2	2.39	0.58
1:B:291:GLU:O	1:B:295[A]:MSE:HG3	2.05	0.56
1:C:353:THR:HG21	4:C:557:HOH:O	2.05	0.55
1:B:220:TYR:CE2	1:B:243[A]:LLP:O3	2.60	0.55
1:C:314:MSE:SE	1:C:421:LEU:HD13	2.57	0.55
1:A:153:MSE:CE	1:A:153:MSE:HG3	2.36	0.54
1:C:135:MSE:HE2	1:C:151:TYR:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ILE:HG13	1:B:295[A]:MSE:HE2	1.83	0.53
1:D:220:TYR:CE2	1:D:243[A]:LLP:O3	2.61	0.53
1:B:249:ILE:HD11	1:B:295[A]:MSE:HE1	1.90	0.53
1:D:220:TYR:HE2	1:D:243[A]:LLP:O3	1.92	0.53
1:B:295[B]:MSE:CE	4:D:871:HOH:O	2.56	0.52
1:A:36:TYR:CE1	1:A:328:LYS:HD2	2.44	0.52
1:A:23:TYR:CE1	1:A:414:LYS:HD2	2.44	0.52
1:A:295[B]:MSE:SE	1:C:408:LEU:HB3	2.60	0.52
1:C:99:ASN:HD21	1:D:275:ILE:CD1	2.22	0.52
1:D:422[A]:SER:O	1:D:426:MSE:HE3	2.10	0.52
1:C:9:LEU:HD22	1:C:15:ILE:HD12	1.91	0.52
1:B:100:GLY:N	1:B:243[A]:LLP:OP2	2.42	0.51
1:B:156:LEU:HD13	1:B:190:ARG:HD2	1.92	0.50
1:D:422[B]:SER:O	1:D:426:MSE:HE3	2.12	0.50
1:B:295[B]:MSE:HE1	4:D:871:HOH:O	2.10	0.50
1:D:249:ILE:HD11	1:D:295[A]:MSE:CE	2.41	0.50
1:B:243[A]:LLP:C4'	1:B:243[A]:LLP:OP4	2.60	0.50
1:A:314:MSE:SE	1:A:421:LEU:HD13	2.62	0.49
1:B:10:MSE:HE1	1:B:17:GLU:HG2	1.95	0.48
1:A:349:LYS:O	1:A:353:THR:HG23	2.14	0.48
1:D:217:ASP:OD2	1:D:243[A]:LLP:N1	2.47	0.48
1:B:355:SER:O	1:B:359:SER:HB3	2.13	0.47
1:D:22:LEU:HD22	1:D:316:LEU:HB3	1.95	0.47
1:C:131:ASP:OD2	1:C:139:LYS:NZ	2.47	0.47
1:D:124:MSE:HA	1:D:153:MSE:HE2	1.96	0.47
1:D:135:MSE:HE2	1:D:151:TYR:CE2	2.49	0.47
1:B:124:MSE:HA	1:B:153:MSE:HE2	1.96	0.47
1:B:181:ILE:HB	1:B:216:VAL:HG22	1.96	0.47
1:A:249:ILE:HD13	1:A:249:ILE:HG21	1.64	0.46
1:B:124:MSE:SE	1:B:153:MSE:CE	3.13	0.46
1:C:219:CYS:O	1:C:220:TYR:HB2	2.16	0.46
1:D:9:LEU:HD22	1:D:15:ILE:HD12	1.97	0.46
1:C:124:MSE:HE1	1:C:153:MSE:HE1	1.90	0.46
1:C:349:LYS:O	1:C:353:THR:HG23	2.15	0.46
1:A:124:MSE:SE	1:A:153:MSE:HE1	2.66	0.46
1:B:217:ASP:OD2	1:B:243[A]:LLP:N1	2.49	0.46
1:C:243[A]:LLP:OP2	4:C:487:HOH:O	2.20	0.45
1:B:411:ASP:O	1:B:415:LEU:HG	2.17	0.45
1:A:220:TYR:CE2	1:A:243[A]:LLP:O3	2.69	0.45
1:B:9:LEU:HD21	1:B:415:LEU:HD22	1.98	0.45
1:A:411:ASP:HA	1:A:414:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:TYR:CE2	1:C:243[A]:LLP:O3	2.70	0.45
1:D:346:ASP:O	1:D:423:LYS:HE2	2.17	0.45
1:A:408:LEU:HB3	1:C:295[B]:MSE:SE	2.67	0.45
1:A:411:ASP:O	1:A:415:LEU:HG	2.17	0.44
1:C:349:LYS:NZ	1:C:362:GLN:OE1	2.40	0.44
4:B:685:HOH:O	1:D:295[A]:MSE:SE	2.85	0.44
1:C:58:SER:HG	1:C:60:SER:HG	1.64	0.44
1:C:191:LYS:HD2	3:C:430:EDO:H12	1.98	0.43
1:A:12:LYS:HD3	1:C:50:LYS:HG2	2.00	0.43
1:A:217:ASP:OD2	1:A:243[A]:LLP:N1	2.52	0.43
1:A:355:SER:O	1:A:359:SER:HB3	2.19	0.43
1:B:94:ARG:HB3	1:B:96:HIS:HD2	1.84	0.43
1:C:217:ASP:OD2	1:C:243[A]:LLP:N1	2.51	0.43
1:D:133:ILE:HD13	1:D:135:MSE:HE3	2.01	0.42
1:A:99:ASN:HD21	1:B:275:ILE:CD1	2.29	0.42
3:A:428:EDO:H11	1:B:269:ARG:CA	2.48	0.42
1:D:44:ASN:OD1	1:D:47:LYS:HE2	2.19	0.42
1:B:241:LEU:O	1:B:246:GLY:HA3	2.20	0.42
1:B:263:VAL:O	1:B:267:THR:HG23	2.20	0.42
1:B:295[B]:MSE:SE	1:D:408:LEU:HB3	2.70	0.42
1:D:404:LEU:HD23	4:D:594:HOH:O	2.19	0.41
1:A:56:ARG:NH1	4:A:556:HOH:O	2.46	0.41
1:D:241:LEU:O	1:D:246:GLY:HA3	2.20	0.41
1:C:9:LEU:HD22	1:C:15:ILE:CD1	2.50	0.41
1:C:9:LEU:HB3	1:C:15:ILE:HD12	2.03	0.41
1:C:133:ILE:HD13	1:C:135:MSE:HE3	2.02	0.41
1:A:9:LEU:HB3	1:A:15:ILE:HD12	2.02	0.41
1:A:67:GLY:HA3	1:B:384:GLN:O	2.20	0.41
1:A:249:ILE:HG13	1:A:295[A]:MSE:HE2	2.03	0.41
1:B:64:ASN:HB2	1:C:64:ASN:HB2	2.02	0.41
1:B:349:LYS:O	1:B:353:THR:HG23	2.20	0.41
1:B:358:ASP:OD1	1:D:58:SER:HB2	2.21	0.41
1:C:133:ILE:CD1	1:C:135:MSE:HE3	2.50	0.41
1:C:220:TYR:HE2	1:C:243[A]:LLP:O3	2.04	0.41
1:C:391:SER:O	1:C:404:LEU:HD12	2.21	0.41
1:B:55:GLU:O	1:B:55:GLU:HG3	2.21	0.40
1:B:191:LYS:HD2	3:B:432:EDO:H21	2.04	0.40
1:C:322:LEU:C	1:C:322:LEU:HD23	2.41	0.40
1:C:425:ILE:O	1:C:425:ILE:HG13	2.21	0.40
1:D:219:CYS:O	1:D:220:TYR:HB2	2.21	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	414/428 (97%)	399 (96%)	15 (4%)	0	100	100
1	B	417/428 (97%)	407 (98%)	10 (2%)	0	100	100
1	C	417/428 (97%)	401 (96%)	16 (4%)	0	100	100
1	D	421/428 (98%)	408 (97%)	13 (3%)	0	100	100
All	All	1669/1712 (98%)	1615 (97%)	54 (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	332/346 (96%)	332 (100%)	0	100	100
1	B	337/346 (97%)	336 (100%)	1 (0%)	92	95
1	C	332/346 (96%)	332 (100%)	0	100	100
1	D	332/346 (96%)	330 (99%)	2 (1%)	86	90
All	All	1333/1384 (96%)	1330 (100%)	3 (0%)	93	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	GLU
1	D	244	ASN
1	D	426	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	B	96	HIS
1	C	96	HIS
1	D	96	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	LLP	D	243[A]	1	23,24,25	1.98	6 (26%)	25,32,34	1.26	3 (12%)
1	LLP	A	243[A]	1	23,24,25	1.96	7 (30%)	25,32,34	1.74	6 (24%)
1	LLP	C	243[A]	1	23,24,25	1.97	4 (17%)	25,32,34	1.32	3 (12%)
1	LLP	B	243[A]	1	23,24,25	1.98	6 (26%)	25,32,34	1.50	5 (20%)

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	LLP	D	243[A]	1	-	7/16/17/19	0/1/1/1
1	LLP	A	243[A]	1	-	5/16/17/19	0/1/1/1
1	LLP	C	243[A]	1	-	6/16/17/19	0/1/1/1
1	LLP	B	243[A]	1	-	7/16/17/19	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243[A]	LLP	O3-C3	-6.18	1.22	1.37
1	B	243[A]	LLP	O3-C3	-6.08	1.22	1.37
1	A	243[A]	LLP	O3-C3	-6.03	1.23	1.37
1	D	243[A]	LLP	O3-C3	-5.56	1.24	1.37
1	D	243[A]	LLP	C4-C4'	4.01	1.54	1.46
1	D	243[A]	LLP	CE-NZ	3.38	1.54	1.46
1	C	243[A]	LLP	CE-NZ	3.15	1.53	1.46
1	B	243[A]	LLP	C4-C4'	3.12	1.52	1.46
1	C	243[A]	LLP	C4-C4'	2.90	1.52	1.46
1	A	243[A]	LLP	C4-C4'	2.74	1.51	1.46
1	C	243[A]	LLP	C4'-NZ	2.67	1.36	1.27
1	B	243[A]	LLP	CE-NZ	2.56	1.52	1.46
1	A	243[A]	LLP	CE-NZ	2.55	1.52	1.46
1	D	243[A]	LLP	C4'-NZ	2.55	1.35	1.27
1	B	243[A]	LLP	C4'-NZ	2.55	1.35	1.27
1	B	243[A]	LLP	C4-C5	-2.40	1.38	1.42
1	A	243[A]	LLP	C4-C5	-2.40	1.39	1.42
1	D	243[A]	LLP	C6-N1	2.39	1.39	1.34
1	A	243[A]	LLP	C2-N1	2.36	1.38	1.33
1	D	243[A]	LLP	P-OP2	-2.21	1.46	1.54
1	A	243[A]	LLP	C4'-NZ	2.19	1.34	1.27
1	B	243[A]	LLP	P-OP2	-2.14	1.46	1.54
1	A	243[A]	LLP	C6-N1	2.12	1.38	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243[A]	LLP	OP4-C5'-C5	4.19	117.33	109.35
1	A	243[A]	LLP	C4-C4'-NZ	-3.85	106.63	124.31
1	C	243[A]	LLP	C4-C4'-NZ	-3.35	108.94	124.31
1	D	243[A]	LLP	C4-C4'-NZ	-3.27	109.28	124.31
1	A	243[A]	LLP	OP3-P-OP2	3.05	119.31	107.64
1	B	243[A]	LLP	C4-C4'-NZ	-2.93	110.84	124.31
1	B	243[A]	LLP	C5-C6-N1	-2.59	119.51	123.82
1	A	243[A]	LLP	OP2-P-OP4	-2.53	100.00	106.73
1	A	243[A]	LLP	CD-CE-NZ	-2.36	105.16	110.93
1	B	243[A]	LLP	OP3-P-OP4	-2.29	100.63	106.73
1	D	243[A]	LLP	OP4-C5'-C5	2.23	113.61	109.35
1	C	243[A]	LLP	C5-C6-N1	-2.22	120.12	123.82
1	D	243[A]	LLP	C5-C6-N1	-2.11	120.31	123.82
1	A	243[A]	LLP	C2'-C2-N1	2.10	121.78	117.67
1	B	243[A]	LLP	OP2-P-OP4	-2.04	101.31	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	243[A]	LLP	OP3-P-OP2	2.02	115.37	107.64
1	B	243[A]	LLP	C6-C5-C4	2.00	121.83	118.15

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	243[A]	LLP	C4-C5-C5'-OP4
1	A	243[A]	LLP	C6-C5-C5'-OP4
1	A	243[A]	LLP	O-C-CA-CB
1	B	243[A]	LLP	C4-C5-C5'-OP4
1	B	243[A]	LLP	C6-C5-C5'-OP4
1	B	243[A]	LLP	O-C-CA-CB
1	C	243[A]	LLP	C4-C5-C5'-OP4
1	C	243[A]	LLP	C6-C5-C5'-OP4
1	C	243[A]	LLP	O-C-CA-CB
1	D	243[A]	LLP	C4-C5-C5'-OP4
1	D	243[A]	LLP	C6-C5-C5'-OP4
1	C	243[A]	LLP	C4-C4'-NZ-CE
1	B	243[A]	LLP	C4-C4'-NZ-CE
1	D	243[A]	LLP	C4-C4'-NZ-CE
1	A	243[A]	LLP	C3-C4-C4'-NZ
1	C	243[A]	LLP	C3-C4-C4'-NZ
1	B	243[A]	LLP	C3-C4-C4'-NZ
1	D	243[A]	LLP	C3-C4-C4'-NZ
1	D	243[A]	LLP	C5'-OP4-P-OP1
1	B	243[A]	LLP	C5-C4-C4'-NZ
1	C	243[A]	LLP	C5-C4-C4'-NZ
1	D	243[A]	LLP	C5-C4-C4'-NZ
1	A	243[A]	LLP	CD-CE-NZ-C4'
1	B	243[A]	LLP	CG-CD-CE-NZ
1	D	243[A]	LLP	C5'-OP4-P-OP3

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	243[A]	LLP	3	0
1	A	243[A]	LLP	2	0
1	C	243[A]	LLP	5	0
1	B	243[A]	LLP	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	D	429	-	3,3,3	0.64	0	2,2,2	0.41	0
3	EDO	C	429	-	3,3,3	0.36	0	2,2,2	0.51	0
3	EDO	C	433	-	3,3,3	0.63	0	2,2,2	0.23	0
3	EDO	C	428	-	3,3,3	0.54	0	2,2,2	0.36	0
3	EDO	A	429	-	3,3,3	0.13	0	2,2,2	1.03	0
3	EDO	A	430	-	3,3,3	0.45	0	2,2,2	0.29	0
3	EDO	C	432	-	3,3,3	0.71	0	2,2,2	0.22	0
3	EDO	A	431	-	3,3,3	0.65	0	2,2,2	0.09	0
3	EDO	B	429	-	3,3,3	0.60	0	2,2,2	0.08	0
3	EDO	C	430	-	3,3,3	0.52	0	2,2,2	0.40	0
3	EDO	C	431	-	3,3,3	0.39	0	2,2,2	0.49	0
3	EDO	B	431	-	3,3,3	0.57	0	2,2,2	0.33	0
3	EDO	A	432	2	3,3,3	0.85	0	2,2,2	0.63	0
3	EDO	B	428	-	3,3,3	0.59	0	2,2,2	0.31	0
3	EDO	A	428	-	3,3,3	0.91	0	2,2,2	0.87	0
3	EDO	B	432	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	D	428	-	3,3,3	0.35	0	2,2,2	0.34	0
3	EDO	B	430	-	3,3,3	0.70	0	2,2,2	0.63	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	D	429	-	-	1/1/1/1	-
3	EDO	C	429	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	433	-	-	0/1/1/1	-
3	EDO	C	428	-	-	1/1/1/1	-
3	EDO	A	429	-	-	0/1/1/1	-
3	EDO	A	430	-	-	0/1/1/1	-
3	EDO	C	432	-	-	0/1/1/1	-
3	EDO	A	431	-	-	0/1/1/1	-
3	EDO	B	429	-	-	1/1/1/1	-
3	EDO	C	430	-	-	0/1/1/1	-
3	EDO	C	431	-	-	1/1/1/1	-
3	EDO	B	431	-	-	1/1/1/1	-
3	EDO	A	432	2	-	1/1/1/1	-
3	EDO	B	428	-	-	0/1/1/1	-
3	EDO	A	428	-	-	0/1/1/1	-
3	EDO	B	432	-	-	0/1/1/1	-
3	EDO	D	428	-	-	1/1/1/1	-
3	EDO	B	430	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	428	EDO	O1-C1-C2-O2
3	C	429	EDO	O1-C1-C2-O2
3	C	431	EDO	O1-C1-C2-O2
3	D	429	EDO	O1-C1-C2-O2
3	B	429	EDO	O1-C1-C2-O2
3	B	431	EDO	O1-C1-C2-O2
3	D	428	EDO	O1-C1-C2-O2
3	B	430	EDO	O1-C1-C2-O2
3	A	432	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	429	EDO	1	0
3	C	430	EDO	1	0
3	A	428	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	432	EDO	1	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	404/428 (94%)	-0.11	19 (4%)	31	30	27, 34, 49, 72	0
1	B	404/428 (94%)	-0.24	10 (2%)	57	56	27, 34, 51, 72	0
1	C	407/428 (95%)	-0.08	11 (2%)	54	53	25, 33, 49, 76	0
1	D	410/428 (95%)	-0.20	12 (2%)	51	50	27, 33, 51, 80	0
All	All	1625/1712 (94%)	-0.16	52 (3%)	47	46	25, 34, 50, 80	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	366	TRP	7.2
1	D	365	ALA	6.0
1	C	365	ALA	5.2
1	D	371	TYR	5.2
1	B	363	CYS	4.7
1	C	373	ASP	4.6
1	D	138	SER	4.3
1	B	375	VAL	4.2
1	A	375	VAL	4.1
1	D	366	TRP	4.1
1	A	396	ILE	3.9
1	A	363	CYS	3.8
1	A	0	GLY	3.8
1	B	0	GLY	3.7
1	D	0	GLY	3.5
1	D	372	GLU	3.3
1	A	187	TYR	3.2
1	A	158	ASP	3.1
1	A	138	SER	3.0
1	A	374	LYS	2.9
1	B	362	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	361	VAL	2.8
1	D	373	ASP	2.7
1	D	136	ASP	2.7
1	A	362	GLN	2.7
1	A	361	VAL	2.7
1	B	138	SER	2.6
1	A	397	ARG	2.6
1	A	71	ASN	2.6
1	A	164	ASN	2.6
1	C	107	ALA	2.6
1	A	376	ILE	2.6
1	C	208	VAL	2.5
1	C	137	ASP	2.5
1	D	158	ASP	2.5
1	B	187	TYR	2.4
1	B	395	PRO	2.3
1	B	397	ARG	2.3
1	C	364	GLU	2.3
1	A	70	TYR	2.3
1	C	158	ASP	2.2
1	C	396	ILE	2.2
1	A	167	LYS	2.2
1	A	139	LYS	2.2
1	C	11	ASN	2.2
1	D	103	ALA	2.1
1	D	139	LYS	2.1
1	C	306	GLY	2.1
1	D	396	ILE	2.1
1	B	71	ASN	2.1
1	A	394	ALA	2.0
1	A	395	PRO	2.0

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	LLP	A	243[A]	24/25	0.88	0.28	32,40,48,50	24
1	LLP	D	243[A]	24/25	0.92	0.25	26,35,47,49	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	C	243[A]	24/25	0.93	0.21	27,34,42,46	24
1	LLP	B	243[A]	24/25	0.93	0.23	33,40,49,49	24

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
3	EDO	A	432	4/4	0.71	0.35	49,55,63,66	0
2	NA	C	427	1/1	0.82	0.13	43,43,43,43	0
3	EDO	D	429	4/4	0.86	0.14	42,51,51,63	0
3	EDO	B	431	4/4	0.88	0.30	36,50,52,56	0
3	EDO	A	428	4/4	0.90	0.17	36,44,48,55	0
3	EDO	C	429	4/4	0.90	0.18	38,44,46,47	0
2	NA	B	427	1/1	0.90	0.11	36,36,36,36	0
3	EDO	C	432	4/4	0.91	0.13	43,51,54,61	0
3	EDO	B	430	4/4	0.93	0.21	36,45,51,56	0
3	EDO	A	430	4/4	0.94	0.36	55,58,64,65	0
3	EDO	A	429	4/4	0.95	0.14	41,44,45,47	0
3	EDO	C	431	4/4	0.95	0.09	52,53,57,59	0
3	EDO	B	429	4/4	0.95	0.12	34,37,45,52	0
3	EDO	B	432	4/4	0.95	0.09	41,45,46,51	0
3	EDO	C	430	4/4	0.96	0.13	42,47,47,52	0
2	NA	D	427	1/1	0.96	0.12	37,37,37,37	0
3	EDO	C	428	4/4	0.96	0.09	33,40,42,45	0
2	NA	A	427	1/1	0.96	0.25	40,40,40,40	0
3	EDO	A	431	4/4	0.97	0.10	38,44,46,52	0
3	EDO	C	433	4/4	0.97	0.07	34,45,45,49	0
3	EDO	D	428	4/4	0.97	0.08	30,32,38,49	0
3	EDO	B	428	4/4	0.97	0.09	33,45,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.