



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:00 AM UTC

PDB ID : 3HVV / pdb_00003hvv
Title : Crystal structure of putative cystathionine beta-lyase involved in aluminum resistance (NP_348457.1) from *Clostridium acetobutylicum* at 2.00 Å 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

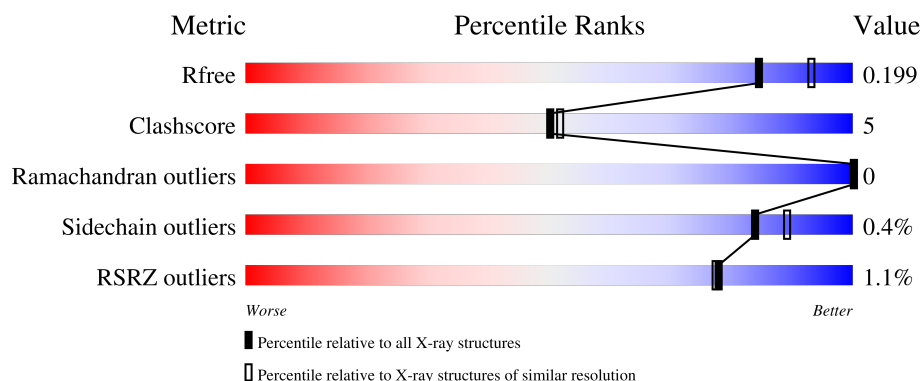
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	% 89% 8% ..
1	B	428	% 88% 9% ..
1	C	428	% 90% 8% ..
1	D	428	% 90% 8% ..

2 Entry composition

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

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 (CCD ID: NA) (formula: Na).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

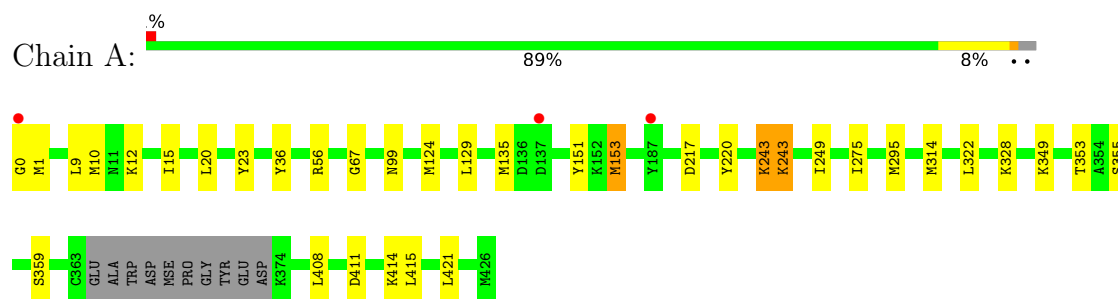
- Molecule 4 is water.

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

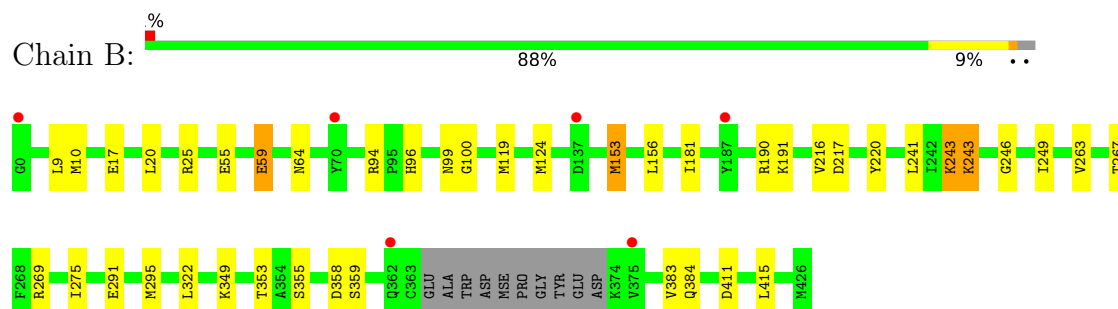
3 Residue-property plots

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.

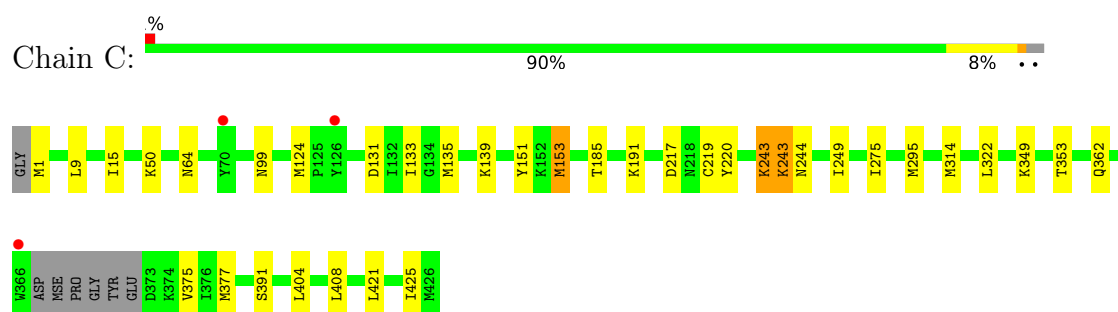
- Molecule 1: Cystathionine beta-lyase family protein, YNBB B.subtilis ortholog



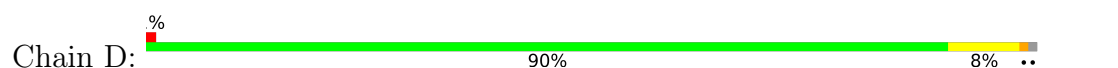
- Molecule 1: Cystathionine beta-lyase family protein, YNBB B.subtilis ortholog

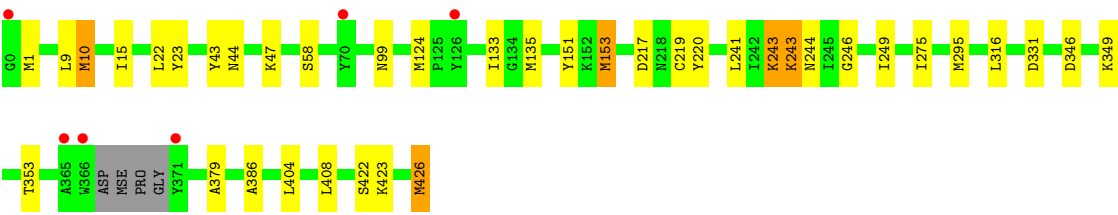


- Molecule 1: Cystathionine beta-lyase family protein, YNBB B.subtilis ortholog



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





4 Data and refinement statistics

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) 99.2 (30.03-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.145 , 0.187 (Not available) , 0.199	Depositor DCC
R_{free} test set	6601 reflections (4.99%)	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 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: LLP, NA, 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	0.93	1/3253 (0.0%)	0.91	1/4365 (0.0%)
1	B	1.02	2/3287 (0.1%)	0.92	2/4410 (0.0%)
1	C	0.95	2/3258 (0.1%)	0.96	3/4379 (0.1%)
1	D	1.02	2/3277 (0.1%)	0.97	3/4401 (0.1%)
All	All	0.98	7/13075 (0.1%)	0.94	9/17555 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	MSE	SE-CE	7.37	2.17	1.95
1	D	10	MSE	SE-CE	7.19	2.17	1.95
1	B	383	VAL	CA-CB	-6.19	1.47	1.54
1	B	119	MSE	SE-CE	6.13	2.13	1.95
1	C	1	MSE	SE-CE	5.95	2.13	1.95
1	D	379	ALA	CA-CB	5.41	1.58	1.53
1	C	377	MSE	SE-CE	5.24	2.11	1.95

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	MSE	CG-SE-CE	-10.04	76.84	98.92
1	D	153	MSE	CG-SE-CE	-7.58	82.25	98.92
1	C	153	MSE	CG-SE-CE	-6.95	83.63	98.92
1	B	153	MSE	CG-SE-CE	-6.81	83.93	98.92
1	D	386	ALA	CA-C-N	-5.46	113.92	122.65
1	D	386	ALA	C-N-CA	-5.46	113.92	122.65
1	C	375	VAL	N-CA-C	5.44	115.69	107.75
1	C	185	THR	N-CA-C	-5.43	102.85	110.50
1	B	59	GLU	N-CA-CB	5.31	118.40	110.22

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	3237	0	3177	35	0
1	B	3271	0	3207	44	0
1	C	3241	0	3165	36	0
1	D	3261	0	3186	37	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	136	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 (136) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:322:LEU:C	1:C:322:LEU:HD23	2.41	0.45
1:A:322:LEU:C	1:A:322:LEU:HD23	2.42	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: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:D:331:ASP:C	1:D:331:ASP:OD1	2.62	0.42
1:A:99:ASN:HD21	1:B:275:ILE:CD1	2.29	0.42
1:A:0:GLY:O	1:A:1:MSE:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:322:LEU:HD23	1:B:322:LEU:C	2.46	0.40
1:B:191:LYS:HD2	3:B:432:EDO:H21	2.04	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%)	331 (100%)	1 (0%)	86	91
1	B	337/346 (97%)	336 (100%)	1 (0%)	86	91
1	C	332/346 (96%)	331 (100%)	1 (0%)	86	91
1	D	332/346 (96%)	330 (99%)	2 (1%)	78	85
All	All	1333/1384 (96%)	1328 (100%)	5 (0%)	84	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LEU
1	B	59	GLU
1	C	244	ASN
1	D	244	ASN
1	D	426	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	99	ASN
1	B	96	HIS
1	B	99	ASN
1	D	96	HIS
1	D	99	ASN
1	D	339	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	243[A]	1	23,24,25	1.96	7 (30%)	25,32,34	1.76	8 (32%)
1	LLP	C	243[A]	1	23,24,25	1.97	4 (17%)	25,32,34	1.33	3 (12%)
1	LLP	D	243[A]	1	23,24,25	1.96	6 (26%)	25,32,34	1.29	4 (16%)
1	LLP	B	243[A]	1	23,24,25	1.98	7 (30%)	25,32,34	1.53	6 (24%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243[A]	LLP	O3-C3	-6.24	1.22	1.36
1	B	243[A]	LLP	O3-C3	-6.13	1.22	1.36
1	A	243[A]	LLP	O3-C3	-6.08	1.23	1.36
1	D	243[A]	LLP	O3-C3	-5.61	1.24	1.36
1	D	243[A]	LLP	C4-C4'	3.58	1.54	1.46
1	D	243[A]	LLP	CE-NZ	3.29	1.54	1.46
1	C	243[A]	LLP	CE-NZ	3.06	1.53	1.46
1	B	243[A]	LLP	C4-C4'	2.79	1.52	1.46
1	C	243[A]	LLP	C4'-NZ	2.71	1.36	1.27
1	C	243[A]	LLP	C4-C4'	2.59	1.52	1.46
1	D	243[A]	LLP	C4'-NZ	2.59	1.35	1.27
1	B	243[A]	LLP	C4'-NZ	2.59	1.35	1.27
1	A	243[A]	LLP	C2-N1	2.51	1.38	1.33
1	B	243[A]	LLP	CE-NZ	2.49	1.52	1.46
1	A	243[A]	LLP	CE-NZ	2.49	1.52	1.46
1	D	243[A]	LLP	C6-N1	2.48	1.39	1.34
1	A	243[A]	LLP	C4-C4'	2.45	1.51	1.46
1	D	243[A]	LLP	P-OP2	-2.28	1.46	1.54
1	A	243[A]	LLP	C4'-NZ	2.22	1.34	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243[A]	LLP	P-OP2	-2.21	1.46	1.54
1	A	243[A]	LLP	C6-N1	2.20	1.38	1.34
1	B	243[A]	LLP	C4-C5	-2.17	1.38	1.42
1	A	243[A]	LLP	C4-C5	-2.17	1.39	1.42
1	B	243[A]	LLP	C2-N1	2.06	1.37	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243[A]	LLP	OP4-C5'-C5	4.25	117.33	109.36
1	A	243[A]	LLP	C4-C4'-NZ	-3.77	106.63	124.04
1	C	243[A]	LLP	C4-C4'-NZ	-3.27	108.94	124.04
1	D	243[A]	LLP	C4-C4'-NZ	-3.20	109.28	124.04
1	A	243[A]	LLP	OP3-P-OP2	3.07	119.31	107.80
1	B	243[A]	LLP	C4-C4'-NZ	-2.86	110.84	124.04
1	B	243[A]	LLP	C5-C6-N1	-2.66	119.51	123.83
1	A	243[A]	LLP	OP2-P-OP4	-2.56	100.00	106.67
1	B	243[A]	LLP	OP3-P-OP4	-2.32	100.63	106.67
1	C	243[A]	LLP	C5-C6-N1	-2.28	120.12	123.83
1	D	243[A]	LLP	OP4-C5'-C5	2.27	113.61	109.36
1	D	243[A]	LLP	C4-C3-C2	2.26	121.41	120.14
1	A	243[A]	LLP	C2'-C2-N1	2.20	121.78	117.64
1	D	243[A]	LLP	C5-C6-N1	-2.17	120.31	123.83
1	A	243[A]	LLP	CD-CE-NZ	-2.14	105.16	110.83
1	B	243[A]	LLP	C6-C5-C4	2.11	121.83	118.21
1	A	243[A]	LLP	C4-C3-C2	2.10	121.33	120.14
1	B	243[A]	LLP	OP2-P-OP4	-2.06	101.31	106.67
1	A	243[A]	LLP	C5-C6-N1	-2.05	120.50	123.83
1	C	243[A]	LLP	OP3-P-OP2	2.02	115.37	107.80
1	B	243[A]	LLP	OP4-C5'-C5	2.01	113.11	109.36

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

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Mol	Chain	Res	Type	Atoms
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	B	243[A]	LLP	C4-C4'-NZ-CE
1	C	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	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	C	243[A]	LLP	C5-C4-C4'-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	A	243[A]	LLP	2	0
1	C	243[A]	LLP	5	0
1	D	243[A]	LLP	3	0
1	B	243[A]	LLP	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	430	-	3,3,3	0.42	0	2,2,2	0.33	0
3	EDO	B	432	-	3,3,3	0.42	0	2,2,2	0.37	0
3	EDO	B	428	-	3,3,3	0.56	0	2,2,2	0.33	0
3	EDO	A	429	-	3,3,3	0.12	0	2,2,2	1.04	0
3	EDO	C	430	-	3,3,3	0.47	0	2,2,2	0.44	0
3	EDO	D	428	-	3,3,3	0.33	0	2,2,2	0.34	0
3	EDO	D	429	-	3,3,3	0.63	0	2,2,2	0.37	0
3	EDO	A	432	2	3,3,3	0.83	0	2,2,2	0.55	0
3	EDO	A	428	-	3,3,3	0.87	0	2,2,2	0.77	0
3	EDO	B	431	-	3,3,3	0.54	0	2,2,2	0.37	0
3	EDO	C	429	-	3,3,3	0.36	0	2,2,2	0.53	0
3	EDO	A	431	-	3,3,3	0.63	0	2,2,2	0.03	0
3	EDO	C	428	-	3,3,3	0.51	0	2,2,2	0.37	0
3	EDO	B	429	-	3,3,3	0.59	0	2,2,2	0.14	0
3	EDO	B	430	-	3,3,3	0.67	0	2,2,2	0.56	0
3	EDO	C	433	-	3,3,3	0.61	0	2,2,2	0.21	0
3	EDO	C	432	-	3,3,3	0.69	0	2,2,2	0.26	0
3	EDO	C	431	-	3,3,3	0.36	0	2,2,2	0.53	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	A	430	-	-	0/1/1/1	-
3	EDO	B	432	-	-	0/1/1/1	-
3	EDO	B	428	-	-	0/1/1/1	-
3	EDO	A	429	-	-	0/1/1/1	-
3	EDO	C	430	-	-	0/1/1/1	-
3	EDO	D	428	-	-	1/1/1/1	-
3	EDO	D	429	-	-	1/1/1/1	-
3	EDO	A	432	2	-	1/1/1/1	-
3	EDO	A	428	-	-	0/1/1/1	-
3	EDO	B	431	-	-	1/1/1/1	-
3	EDO	C	429	-	-	1/1/1/1	-
3	EDO	A	431	-	-	0/1/1/1	-
3	EDO	C	428	-	-	1/1/1/1	-
3	EDO	B	429	-	-	1/1/1/1	-
3	EDO	B	430	-	-	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	432	-	-	1/1/1/1	-
3	EDO	C	431	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) 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	B	429	EDO	O1-C1-C2-O2
3	D	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
3	C	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	B	432	EDO	1	0
3	C	430	EDO	1	0
3	D	429	EDO	1	0
3	A	428	EDO	2	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

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, 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%)	0.05	3 (0%) 84 84	17, 34, 49, 72	2 (0%)
1	B	404/428 (94%)	-0.05	6 (1%) 72 71	16, 34, 51, 72	4 (0%)
1	C	407/428 (95%)	-0.10	3 (0%) 84 84	18, 33, 49, 76	1 (0%)
1	D	410/428 (95%)	-0.18	6 (1%) 72 71	14, 33, 51, 80	2 (0%)
All	All	1625/1712 (94%)	-0.07	18 (1%) 78 77	14, 33, 50, 80	9 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	366	TRP	4.9
1	D	366	TRP	4.7
1	D	371	TYR	4.2
1	B	0	GLY	3.3
1	A	0	GLY	3.1
1	A	187	TYR	2.7
1	B	187	TYR	2.7
1	B	70	TYR	2.6
1	D	0	GLY	2.6
1	C	126	TYR	2.6
1	C	70	TYR	2.4
1	B	375	VAL	2.3
1	B	362	GLN	2.2
1	D	70	TYR	2.2
1	D	126	TYR	2.2
1	B	137	ASP	2.2
1	A	137	ASP	2.0
1	D	365	ALA	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	0.82	0.19	32,40,48,50	24
1	LLP	B	243[A]	24/25	0.83	0.18	33,40,49,49	24
1	LLP	D	243[A]	24/25	0.84	0.17	26,35,47,49	24
1	LLP	C	243[A]	24/25	0.85	0.15	27,34,42,46	24

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	C	429	4/4	0.87	0.15	38,44,46,47	0
3	EDO	C	431	4/4	0.87	0.14	52,53,57,59	0
3	EDO	A	432	4/4	0.88	0.16	49,55,63,66	0
3	EDO	C	432	4/4	0.89	0.14	43,51,54,61	0
3	EDO	D	429	4/4	0.89	0.14	42,51,51,63	0
3	EDO	B	430	4/4	0.90	0.18	36,45,51,56	0
3	EDO	B	431	4/4	0.90	0.20	36,50,52,56	0
3	EDO	A	428	4/4	0.91	0.21	36,44,48,55	0
3	EDO	B	428	4/4	0.91	0.15	33,45,46,47	0
3	EDO	A	429	4/4	0.91	0.12	41,44,45,47	0
3	EDO	A	430	4/4	0.91	0.16	55,58,64,65	0
2	NA	C	427	1/1	0.92	0.10	43,43,43,43	0
2	NA	B	427	1/1	0.93	0.12	36,36,36,36	0
3	EDO	A	431	4/4	0.93	0.13	38,44,46,52	0
3	EDO	D	428	4/4	0.94	0.14	30,32,38,49	0
3	EDO	C	430	4/4	0.94	0.15	42,47,47,52	0
3	EDO	B	429	4/4	0.95	0.14	34,37,45,52	0
3	EDO	B	432	4/4	0.95	0.13	41,45,46,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	C	428	4/4	0.95	0.12	33,40,42,45	0
3	EDO	C	433	4/4	0.96	0.13	34,45,45,49	0
2	NA	D	427	1/1	0.96	0.09	37,37,37,37	0
2	NA	A	427	1/1	0.96	0.14	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.