WORLDWIDE
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2024 – 11:11 pm BST

PDB ID	:	1ODS
Title	:	Cephalosporin C deacetylase from Bacillus subtilis
Authors	:	Vincent, F.; Charnock, S.J.; Verschueren, K.H.G.; Turkenburg, J.P.; Scott, D.J.; Offen, W.A.; Roberts, S.; Pell, G.; Gilbert, H.J.; Brannigan, J.A.; Davies, G.J.
Deposited on	:	2003-02-20
Resolution	:	1.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

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 1.90 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.
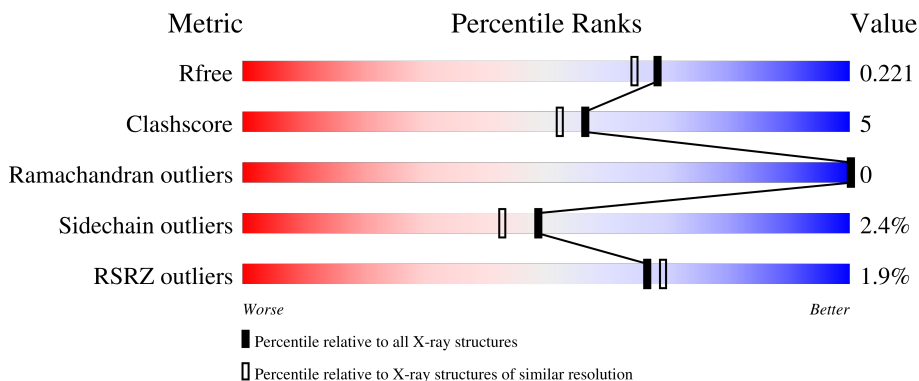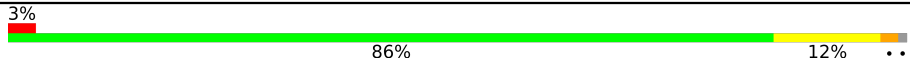

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	318	90% 9% ••
1	B	318	% 86% 13% ••
1	C	318	% 87% 11% ••
1	D	318	89% 9% ••
1	E	318	4% 86% 12% ••

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Mol	Chain	Length	Quality of chain
1	F	318	3% 86% 12%
1	G	318	5% 89% 9%
1	H	318	.% 86% 12%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 22366 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 CEPHALOSPORIN C DEACETYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total 2542	C 1645	N 413	O 478	S 6	0	5	0
1	B	316	Total 2539	C 1644	N 412	O 477	S 6	0	4	0
1	C	316	Total 2536	C 1641	N 412	O 477	S 6	0	3	0
1	D	316	Total 2543	C 1645	N 412	O 480	S 6	0	5	0
1	E	316	Total 2535	C 1641	N 413	O 475	S 6	0	3	0
1	F	316	Total 2531	C 1640	N 411	O 474	S 6	0	2	0
1	G	316	Total 2533	C 1638	N 411	O 478	S 6	0	2	0
1	H	316	Total 2542	C 1645	N 411	O 480	S 6	0	5	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLU	GLN	conflict	UNP P94388
A	255	TYR	ASP	conflict	UNP P94388
B	220	GLU	GLN	conflict	UNP P94388
B	255	TYR	ASP	conflict	UNP P94388
C	220	GLU	GLN	conflict	UNP P94388
C	255	TYR	ASP	conflict	UNP P94388
D	220	GLU	GLN	conflict	UNP P94388
D	255	TYR	ASP	conflict	UNP P94388
E	220	GLU	GLN	conflict	UNP P94388
E	255	TYR	ASP	conflict	UNP P94388
F	220	GLU	GLN	conflict	UNP P94388
F	255	TYR	ASP	conflict	UNP P94388
G	220	GLU	GLN	conflict	UNP P94388

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Chain	Residue	Modelled	Actual	Comment	Reference
G	255	TYR	ASP	conflict	UNP P94388
H	220	GLU	GLN	conflict	UNP P94388
H	255	TYR	ASP	conflict	UNP P94388

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	B	1	Total 1	Cl 1	0	0
2	C	1	Total 1	Cl 1	0	0
2	D	1	Total 1	Cl 1	0	0
2	E	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0
2	G	1	Total 1	Cl 1	0	0
2	H	1	Total 1	Cl 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total 310	O 310	0	0
4	B	259	Total 259	O 259	0	0
4	C	275	Total 275	O 275	0	0
4	D	289	Total 289	O 289	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	210	Total 210	O 210	0	0
4	F	242	Total 242	O 242	0	0
4	G	194	Total 194	O 194	0	0
4	H	276	Total 276	O 276	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.
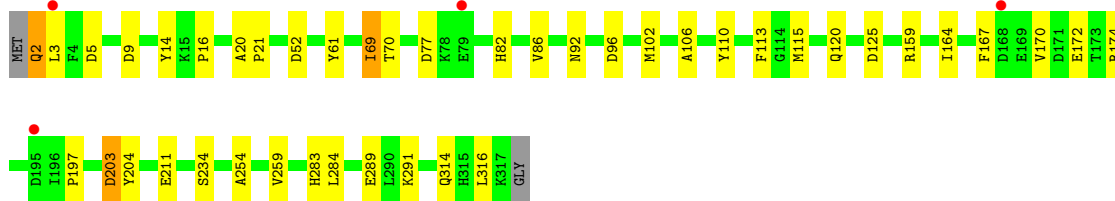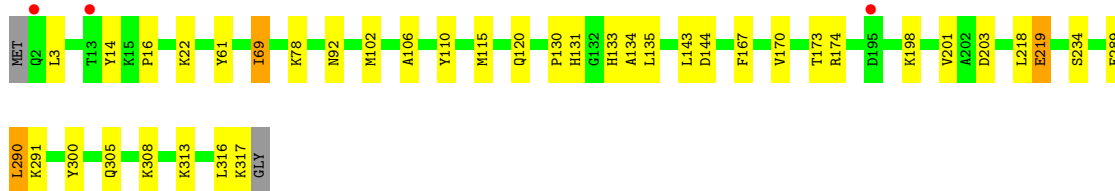
• Molecule 1: CEPHALOSPORIN C DEACETYLASE

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• Molecule 1: CEPHALOSPORIN C DEACETYLASE

L316 K317 GLY

● Molecule 1: CEPHALOSPORIN C DEACETYLASE

Chain E:

4%

86%

12%

MET Q2 L3 D9 Y14 K15 P16 K22 F27 L30 K37 V38 Q39 V54 Y61 I69 K78 E79 G80 P81 A84 N92 A106 L107 Y110 M115 Q120 L135 G136 K145 S166 F167 D168 E169 V170 D171 E172 T173 R174 I175

D195 K198 V201 A202 D203 Y204 E219 S234 D249 K258 H283 L284 E285 E289 L290 K291 K308 K313 Q314 H315 L316 K317 GLY

● Molecule 1: CEPHALOSPORIN C DEACETYLASE

Chain F:

3%

86%

12%

MET Q2 L3 F4 D5 D9 T13 K22 K29 E33 Q45 D48 Y61 K62 N66 I69 K78 E79 G80 A84 K87 N92 M102 T112 M115 Q120 S123 P130 L135 G136 D156 R159 A160 I164 F167

D168 E169 V170 D171 R174 G180 D195 D203 E289 L290 K291 K308 K313 Q314 H315 L316 K317 GLY

● Molecule 1: CEPHALOSPORIN C DEACETYLASE

Chain G:

5%

89%

9%

MET Q2 L3 T13 Y14 K15 P16 K22 Q39 D43 L44 V47 D48 V54 Y61 K62 W72 K78 E79 G80 P81 N92 A106 Y110 Q120 L135 G136 R159 F167 D168 E169 V170 R174 G180 D195 D203 Y204 L218 E219

E220 P221 R256 K270 V271 H283 L284 E285 K308 Q314 H315 L316 K317 GLY

● Molecule 1: CEPHALOSPORIN C DEACETYLASE

Chain H:

%

86%

12%

MET Q2 L3 Y14 K15 P16 E17 K18 K22 D43 V47 D48 D52 K55 Y61 K62 I69 W72 E79 K87 D96 M102 A106 Y110 A111 T112 M115 S123 P130 G136 D144 S165 S166 F167 V170 D171 E172 T173

R174 V177 G180 T187 D195 D203 S234 Y255 K258 I268 D269 K270 H283 L284 E285 L316 K317 GLY

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	315.21Å 315.21Å 68.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 1.90 14.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (100.00-1.90) 99.9 (14.99-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.152 , 0.186 0.196 , 0.221	Depositor DCC
R_{free} test set	10036 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 62.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22366	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CL, MG

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	0.54	0/2638	0.78	3/3584 (0.1%)
1	B	0.56	1/2630 (0.0%)	0.79	7/3573 (0.2%)
1	C	0.52	0/2622	0.76	3/3562 (0.1%)
1	D	0.55	0/2639	0.79	4/3584 (0.1%)
1	E	0.46	0/2621	0.73	4/3561 (0.1%)
1	F	0.51	0/2612	0.76	5/3549 (0.1%)
1	G	0.45	0/2614	0.74	1/3551 (0.0%)
1	H	0.51	0/2638	0.78	9/3584 (0.3%)
All	All	0.51	1/21014 (0.0%)	0.77	36/28548 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	MET	SD-CE	-5.23	1.48	1.77

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	69[A]	ILE	CG1-CB-CG2	7.51	127.93	111.40
1	H	69[B]	ILE	CG1-CB-CG2	7.51	127.93	111.40
1	H	144	ASP	CB-CG-OD1	6.76	124.39	118.30
1	E	171	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	5	ASP	CB-CG-OD2	6.38	124.04	118.30

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	2542	0	2486	23	0
1	B	2539	0	2481	28	0
1	C	2536	0	2474	20	0
1	D	2543	0	2481	24	0
1	E	2535	0	2479	26	0
1	F	2531	0	2475	32	0
1	G	2533	0	2465	25	0
1	H	2542	0	2479	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	1	0
2	E	1	0	0	0	0
2	F	1	0	0	1	0
2	G	1	0	0	0	0
2	H	1	0	0	1	0
3	A	2	0	0	0	0
4	A	310	0	0	7	1
4	B	259	0	0	3	1
4	C	275	0	0	1	0
4	D	289	0	0	2	0
4	E	210	0	0	2	0
4	F	242	0	0	3	0
4	G	194	0	0	3	0
4	H	276	0	0	1	0
All	All	22366	0	19820	200	1

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.

The worst 5 of 200 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:69:ILE:HB	4:A:2183:HOH:O	1.60	1.01
1:H:102:MET:HE2	1:H:112:THR:HG22	1.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:LYS:HE2	4:F:2076:HOH:O	1.63	0.98
1:E:174:ARG:HD2	1:E:316:LEU:O	1.66	0.94
1:D:174:ARG:HD2	1:D:316:LEU:O	1.70	0.90

All (1) 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)
4:A:2169:HOH:O	4:B:2147:HOH:O[2_655]	2.01	0.19

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	319/318 (100%)	306 (96%)	13 (4%)	0	100	100
1	B	318/318 (100%)	306 (96%)	12 (4%)	0	100	100
1	C	317/318 (100%)	305 (96%)	12 (4%)	0	100	100
1	D	319/318 (100%)	306 (96%)	13 (4%)	0	100	100
1	E	317/318 (100%)	302 (95%)	15 (5%)	0	100	100
1	F	316/318 (99%)	301 (95%)	15 (5%)	0	100	100
1	G	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
1	H	319/318 (100%)	305 (96%)	14 (4%)	0	100	100
All	All	2541/2544 (100%)	2430 (96%)	111 (4%)	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	271/267 (102%)	265 (98%)	6 (2%)	52	47
1	B	270/267 (101%)	264 (98%)	6 (2%)	52	47
1	C	269/267 (101%)	261 (97%)	8 (3%)	41	33
1	D	271/267 (102%)	264 (97%)	7 (3%)	46	39
1	E	269/267 (101%)	262 (97%)	7 (3%)	46	39
1	F	268/267 (100%)	259 (97%)	9 (3%)	37	28
1	G	268/267 (100%)	262 (98%)	6 (2%)	52	47
1	H	271/267 (102%)	264 (97%)	7 (3%)	46	39
All	All	2157/2136 (101%)	2101 (97%)	56 (3%)	49	39

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	69	ILE
1	H	270	LYS
1	F	45	GLN
1	H	234	SER
1	H	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	314	GLN
1	H	12	GLN
1	G	2	GLN
1	G	182	GLN
1	H	182	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	316/318 (99%)	-0.07	0	100	100	5, 9, 14, 19	5 (1%)
1	B	316/318 (99%)	0.03	4 (1%)	77	79	5, 9, 14, 21	9 (2%)
1	C	316/318 (99%)	-0.03	3 (0%)	84	85	5, 9, 14, 21	6 (1%)
1	D	316/318 (99%)	-0.08	0	100	100	6, 9, 14, 19	7 (2%)
1	E	316/318 (99%)	0.24	13 (4%)	37	40	4, 10, 14, 19	7 (2%)
1	F	316/318 (99%)	0.09	10 (3%)	47	50	6, 10, 14, 20	5 (1%)
1	G	316/318 (99%)	0.22	15 (4%)	31	34	4, 10, 14, 24	3 (0%)
1	H	316/318 (99%)	-0.10	2 (0%)	89	90	5, 10, 15, 20	5 (1%)
All	All	2528/2544 (99%)	0.04	47 (1%)	66	69	4, 9, 14, 24	47 (1%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	285	GLU	4.0
1	G	80	GLY	3.9
1	E	195	ASP	3.8
1	E	30	LEU	3.8
1	F	195	ASP	3.5

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

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

6.3 Carbohydrates ⓘ

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	MG	A	1319	1/1	0.94	0.05	31,31,31,31	0
3	MG	A	1320	1/1	0.98	0.07	21,21,21,21	0
2	CL	D	1318	1/1	0.99	0.19	18,18,18,18	0
2	CL	E	1318	1/1	0.99	0.15	24,24,24,24	0
2	CL	F	1318	1/1	0.99	0.19	18,18,18,18	0
2	CL	G	1318	1/1	0.99	0.15	24,24,24,24	0
2	CL	H	1318	1/1	0.99	0.14	17,17,17,17	0
2	CL	B	1318	1/1	0.99	0.18	16,16,16,16	0
2	CL	C	1318	1/1	0.99	0.17	19,19,19,19	0
2	CL	A	1318	1/1	1.00	0.14	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.