Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2021 – 03:08 pm BST

PDB ID	:	6RXB
Title	:	Crystal structure of TetR-Q116A from Acinetobacter baumannii AYE in complex with minocycline
Authors	:	Tam, H.K.; Himpich, S.; Pos, K.M.
Deposited on	:	2019-06-07
Resolution	:	2.25 Å(reported)

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

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

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

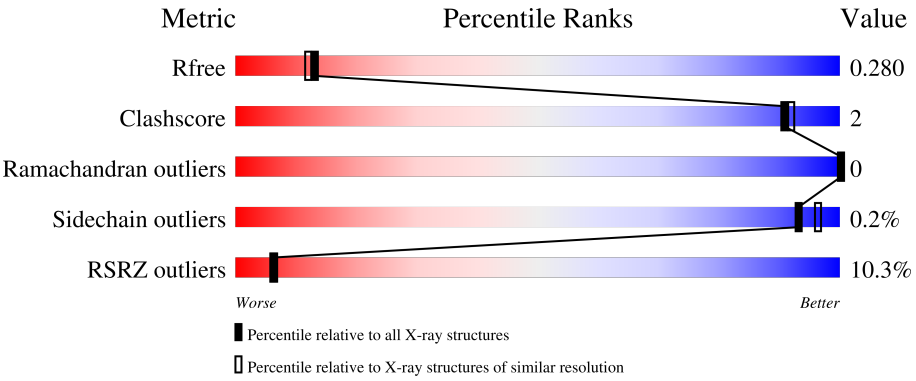
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	B	214	8% 89% · 7%
1	D	214	20% 85% · 11%
2	A	214	4% 80% · 16%
2	C	214	4% 79% · 17%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6219 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 Tetracycline repressor protein class G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	200	Total	C	N	O	S	0	1	0
			1598	998	287	305	8			
1	D	190	Total	C	N	O	S	0	1	0
			1521	955	277	283	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	116	ALA	GLN	engineered mutation	UNP B0VCI2
B	209	HIS	-	expression tag	UNP B0VCI2
B	210	HIS	-	expression tag	UNP B0VCI2
B	211	HIS	-	expression tag	UNP B0VCI2
B	212	HIS	-	expression tag	UNP B0VCI2
B	213	HIS	-	expression tag	UNP B0VCI2
B	214	HIS	-	expression tag	UNP B0VCI2
D	116	ALA	GLN	engineered mutation	UNP B0VCI2
D	209	HIS	-	expression tag	UNP B0VCI2
D	210	HIS	-	expression tag	UNP B0VCI2
D	211	HIS	-	expression tag	UNP B0VCI2
D	212	HIS	-	expression tag	UNP B0VCI2
D	213	HIS	-	expression tag	UNP B0VCI2
D	214	HIS	-	expression tag	UNP B0VCI2

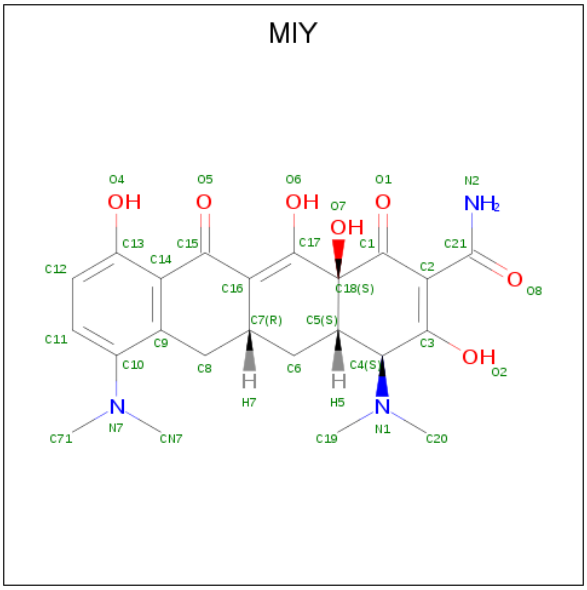
- Molecule 2 is a protein called Tetracycline repressor protein class G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	179	Total	C	N	O	S	0	3	0
			1424	894	257	267	6			
2	C	178	Total	C	N	O	S	0	0	0
			1398	879	252	262	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ALA	GLN	engineered mutation	UNP B0VCI2
A	209	HIS	-	expression tag	UNP B0VCI2
A	210	HIS	-	expression tag	UNP B0VCI2
A	211	HIS	-	expression tag	UNP B0VCI2
A	212	HIS	-	expression tag	UNP B0VCI2
A	213	HIS	-	expression tag	UNP B0VCI2
A	214	HIS	-	expression tag	UNP B0VCI2
C	116	ALA	GLN	engineered mutation	UNP B0VCI2
C	209	HIS	-	expression tag	UNP B0VCI2
C	210	HIS	-	expression tag	UNP B0VCI2
C	211	HIS	-	expression tag	UNP B0VCI2
C	212	HIS	-	expression tag	UNP B0VCI2
C	213	HIS	-	expression tag	UNP B0VCI2
C	214	HIS	-	expression tag	UNP B0VCI2

- Molecule 3 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: $C_{23}H_{27}N_3O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			33	23	3	7		
3	D	1	Total	C	N	O	0	0
			33	23	3	7		
3	A	1	Total	C	N	O	0	0
			33	23	3	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 33 23 3 7	0	0

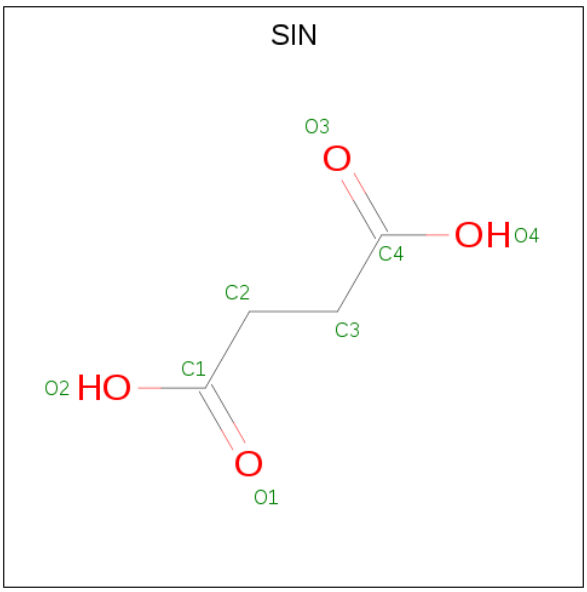
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

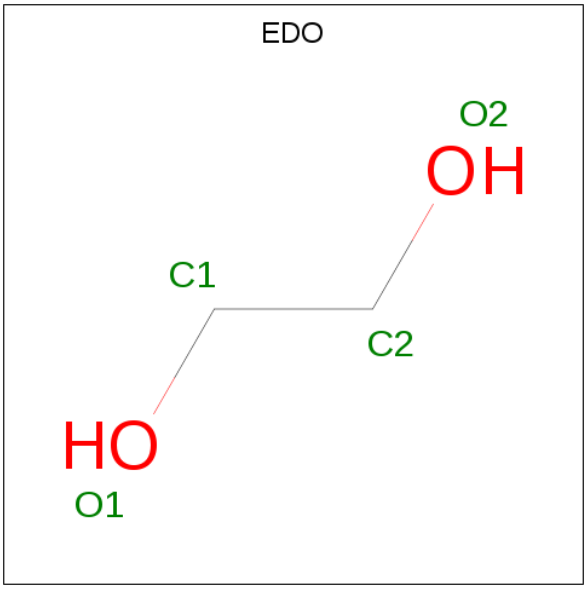
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Cl 1 1	0	0
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 8 4 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

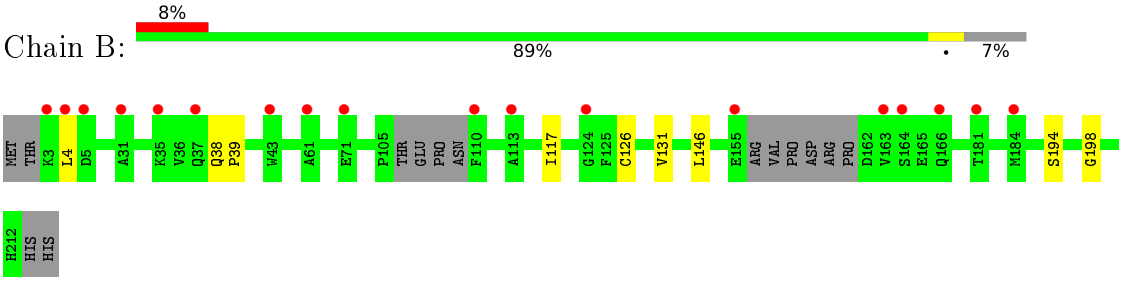
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	47	Total O 47 47	0	0
8	D	21	Total O 21 21	0	0
8	A	34	Total O 34 34	0	0
8	C	26	Total O 26 26	0	0

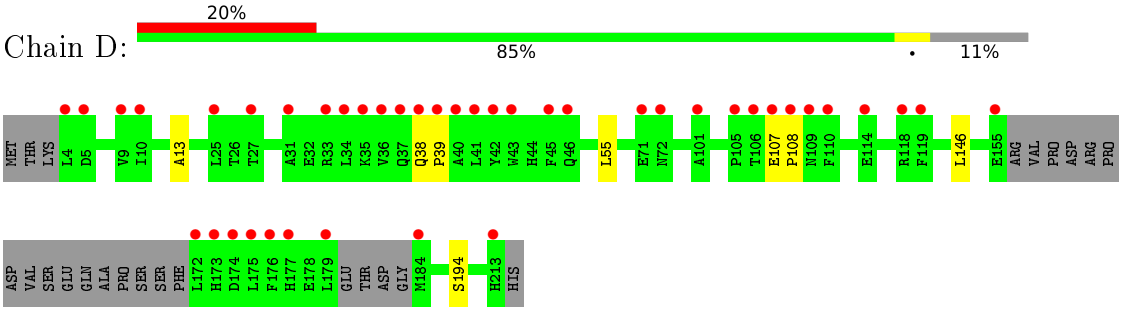
3 Residue-property plots (i)

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.

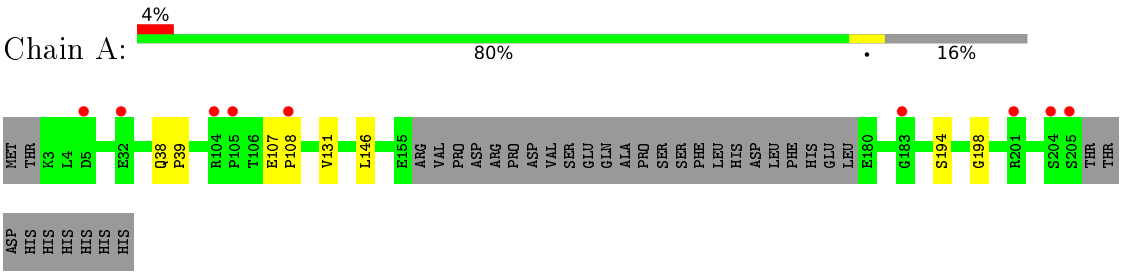
- Molecule 1: Tetracycline repressor protein class G



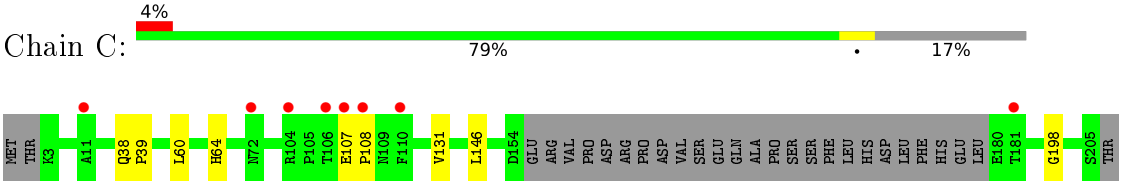
- Molecule 1: Tetracycline repressor protein class G



- Molecule 2: Tetracycline repressor protein class G



- Molecule 2: Tetracycline repressor protein class G



THR
ASP
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.54Å 64.23Å 220.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.25 48.41 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.41-2.25) 100.0 (48.41-2.25)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.240 , 0.276 0.243 , 0.280	Depositor DCC
R_{free} test set	2151 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6219	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MIY, CSU, MG, CL, EDO, SIN

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	B	0.66	0/1609	0.69	0/2171
1	D	0.66	0/1545	0.70	0/2086
2	A	0.66	0/1455	0.69	0/1965
2	C	0.66	0/1423	0.71	0/1922
All	All	0.66	0/6032	0.70	0/8144

There are no bond length outliers.

There are no bond angle outliers.

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	B	1598	0	1536	6	0
1	D	1521	0	1476	5	0
2	A	1424	0	1409	6	0
2	C	1398	0	1381	7	0
3	A	33	0	24	1	0
3	B	33	0	24	2	0
3	C	33	0	24	1	0
3	D	33	0	24	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	D	8	0	4	0	0
7	A	4	0	6	0	0
8	A	34	0	0	0	0
8	B	47	0	0	0	0
8	C	26	0	0	0	0
8	D	21	0	0	0	0
All	All	6219	0	5908	20	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (20) 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)
2:C:131:VAL:HG13	3:C:301:MIY:H712	1.88	0.56
1:B:131:VAL:HG13	3:B:301:MIY:H712	1.89	0.55
2:A:131:VAL:HG13	3:A:301:MIY:H712	1.90	0.54
1:B:146:LEU:HD22	2:A:146:LEU:HD22	1.91	0.52
1:D:146:LEU:HD22	2:C:146:LEU:HD22	1.93	0.50
1:B:117:ILE:HD11	3:B:301:MIY:H711	1.94	0.49
2:C:107:GLU:N	2:C:108:PRO:HD2	2.30	0.46
1:B:38:GLN:N	1:B:39:PRO:CD	2.79	0.46
2:C:38:GLN:N	2:C:39:PRO:CD	2.78	0.46
2:A:38:GLN:N	2:A:39:PRO:CD	2.79	0.45
1:B:198:GLY:HA3	2:A:194:SER:O	2.17	0.45
1:D:107:GLU:HB2	1:D:108:PRO:HD3	2.00	0.44
3:D:301:MIY:H713	3:D:301:MIY:H81	2.00	0.43
1:D:38:GLN:N	1:D:39:PRO:CD	2.82	0.43
2:A:107:GLU:HB3	2:A:108:PRO:HD3	2.01	0.43
2:C:107:GLU:N	2:C:108:PRO:CD	2.82	0.42
1:B:194:SER:O	2:A:198:GLY:HA3	2.20	0.42
2:C:60:LEU:O	2:C:64:HIS:HB3	2.20	0.41
1:D:13:ALA:HB3	1:D:55:LEU:HD21	2.03	0.41
1:D:194:SER:O	2:C:198:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

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	B	193/214 (90%)	191 (99%)	2 (1%)	0	100	100
1	D	184/214 (86%)	184 (100%)	0	0	100	100
2	A	178/214 (83%)	175 (98%)	3 (2%)	0	100	100
2	C	174/214 (81%)	171 (98%)	3 (2%)	0	100	100
All	All	729/856 (85%)	721 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	B	163/177 (92%)	162 (99%)	1 (1%)	86	91
1	D	156/177 (88%)	156 (100%)	0	100	100
2	A	147/178 (83%)	147 (100%)	0	100	100
2	C	143/178 (80%)	143 (100%)	0	100	100
All	All	609/710 (86%)	608 (100%)	1 (0%)	93	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 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	CSU	D	126	1	6,9,10	0.86	0	3,12,14	1.08	0
1	CSU	B	126[B]	1	6,9,10	1.48	1 (16%)	3,12,14	1.45	1 (33%)
1	CSU	B	126[A]	1	6,9,10	1.46	1 (16%)	3,12,14	1.42	1 (33%)

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	CSU	D	126	1	-	1/4/8/10	-
1	CSU	B	126[B]	1	-	4/4/8/10	-
1	CSU	B	126[A]	1	-	4/4/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126[B]	CSU	OD3-S	3.13	1.55	1.45
1	B	126[A]	CSU	OD3-S	3.12	1.54	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	126[B]	CSU	OD2-S-OD1	2.11	120.43	112.78
1	B	126[A]	CSU	OD2-S-OD1	2.06	120.26	112.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	126[A]	CSU	N-CA-CB-SG
1	B	126[A]	CSU	OD1-S-SG-CB
1	B	126[A]	CSU	OD2-S-SG-CB
1	B	126[A]	CSU	OD3-S-SG-CB
1	B	126[B]	CSU	N-CA-CB-SG
1	B	126[B]	CSU	OD1-S-SG-CB
1	B	126[B]	CSU	OD2-S-SG-CB
1	B	126[B]	CSU	OD3-S-SG-CB
1	D	126	CSU	OD3-S-SG-CB

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
7	EDO	A	303	-	3,3,3	0.06	0	2,2,2	0.16	0
3	MIY	C	301	4	35,36,36	1.14	2 (5%)	41,58,58	1.08	3 (7%)
3	MIY	D	301	4	35,36,36	1.13	2 (5%)	41,58,58	1.09	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SIN	D	304	-	1,7,7	0.23	0	2,8,8	1.17	0
3	MIY	B	301	4	35,36,36	1.14	2 (5%)	41,58,58	1.07	2 (4%)
3	MIY	A	301	4	35,36,36	1.14	2 (5%)	41,58,58	1.10	3 (7%)

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
7	EDO	A	303	-	-	0/1/1/1	-
3	MIY	C	301	4	-	1/12/70/70	0/4/4/4
3	MIY	D	301	4	-	0/12/70/70	0/4/4/4
6	SIN	D	304	-	-	0/1/5/5	-
3	MIY	B	301	4	-	0/12/70/70	0/4/4/4
3	MIY	A	301	4	-	0/12/70/70	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	MIY	C21-N2	5.61	1.48	1.33
3	C	301	MIY	C21-N2	5.61	1.48	1.33
3	B	301	MIY	C21-N2	5.59	1.48	1.33
3	D	301	MIY	C21-N2	5.58	1.48	1.33
3	B	301	MIY	O5-C15	2.26	1.28	1.23
3	D	301	MIY	O5-C15	2.25	1.28	1.23
3	C	301	MIY	O5-C15	2.25	1.28	1.23
3	A	301	MIY	O5-C15	2.24	1.28	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	MIY	C15-C16-C17	2.40	120.70	118.80
3	C	301	MIY	C18-C5-C4	2.34	114.84	111.64
3	D	301	MIY	C18-C5-C4	2.31	114.80	111.64
3	A	301	MIY	C18-C5-C4	2.27	114.74	111.64
3	D	301	MIY	O7-C18-C17	-2.25	106.54	110.14
3	D	301	MIY	C15-C16-C17	2.23	120.56	118.80
3	C	301	MIY	O7-C18-C17	-2.20	106.62	110.14
3	B	301	MIY	C18-C5-C4	2.19	114.64	111.64
3	A	301	MIY	C15-C16-C17	2.16	120.51	118.80
3	B	301	MIY	O7-C18-C17	-2.11	106.77	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	MIY	O7-C18-C17	-2.09	106.79	110.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	MIY	C9-C10-N7-CN7

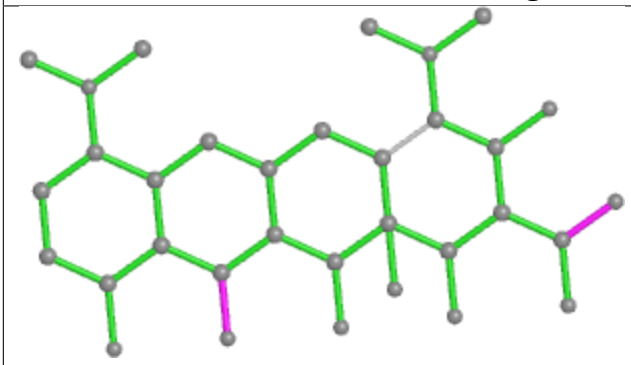
There are no ring outliers.

4 monomers are involved in 5 short contacts:

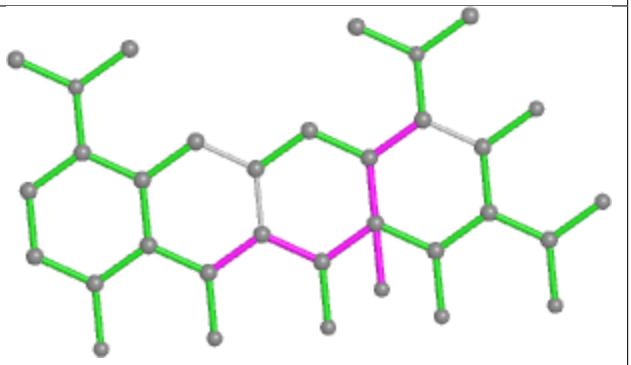
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	MIY	1	0
3	D	301	MIY	1	0
3	B	301	MIY	2	0
3	A	301	MIY	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

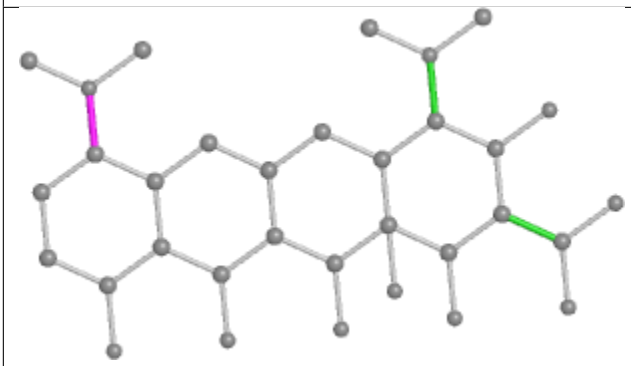
Ligand MIY C 301



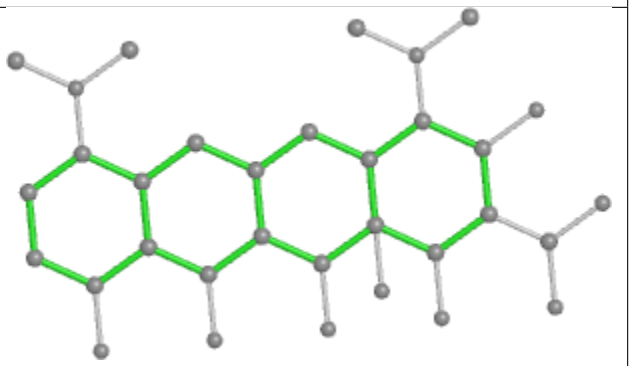
Bond lengths



Bond angles

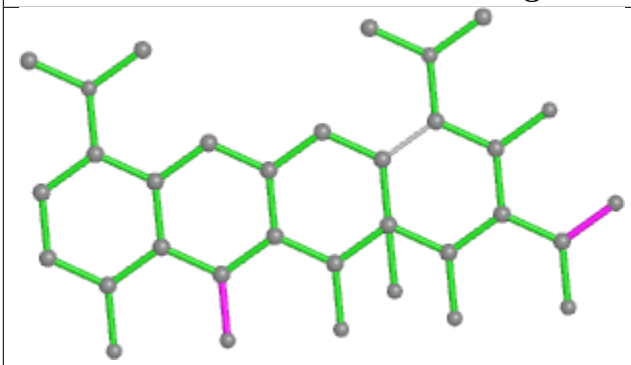


Torsions

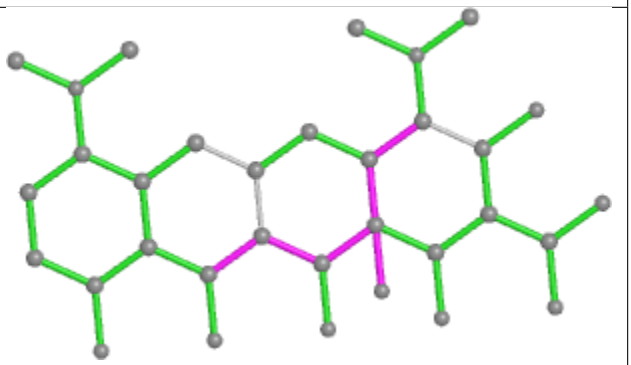


Rings

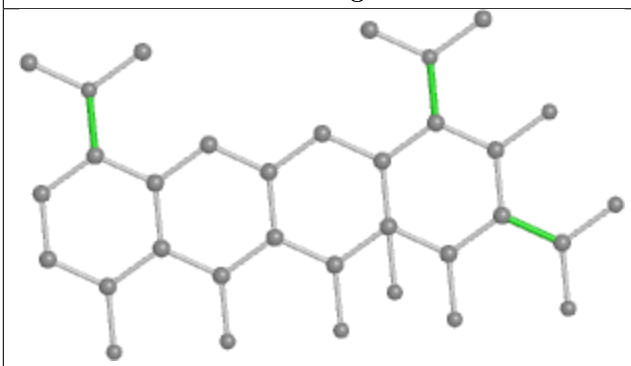
Ligand MIY D 301



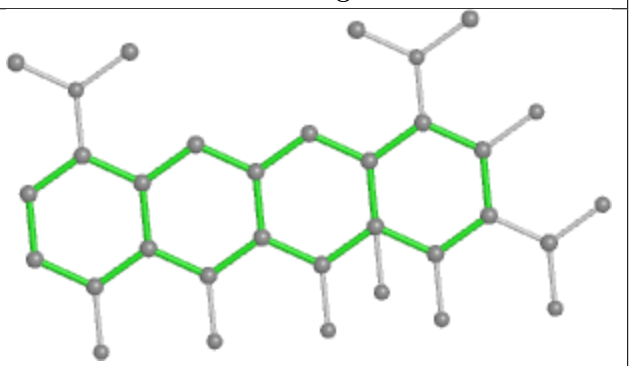
Bond lengths



Bond angles

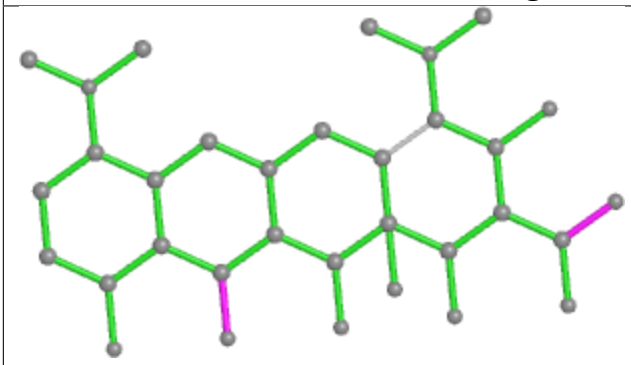


Torsions

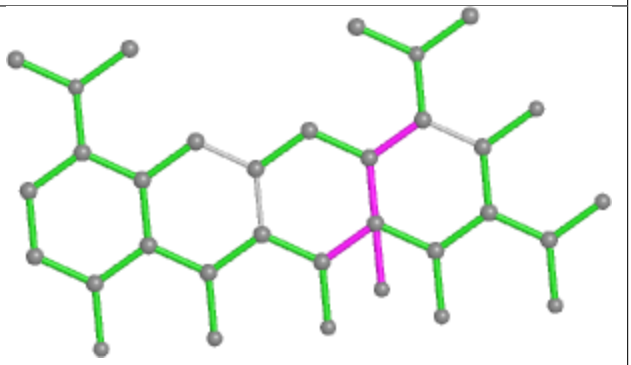


Rings

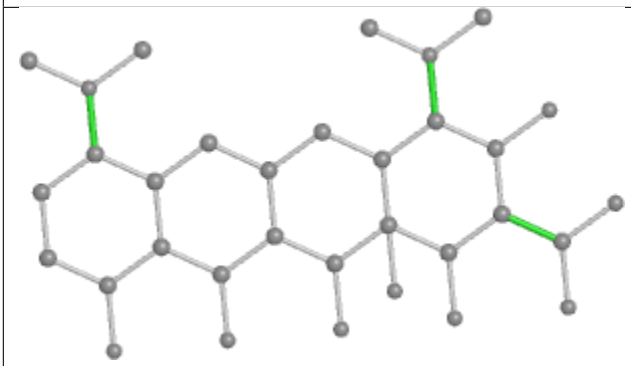
Ligand MIY B 301



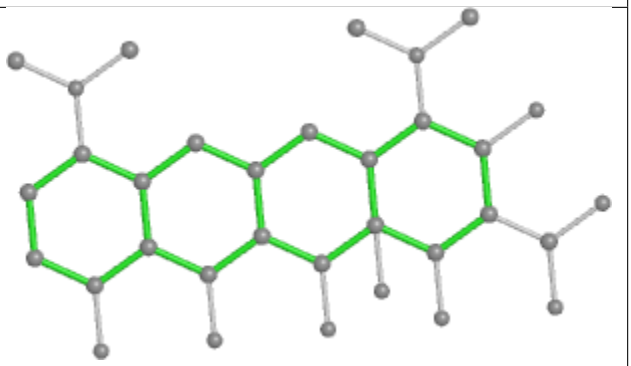
Bond lengths



Bond angles

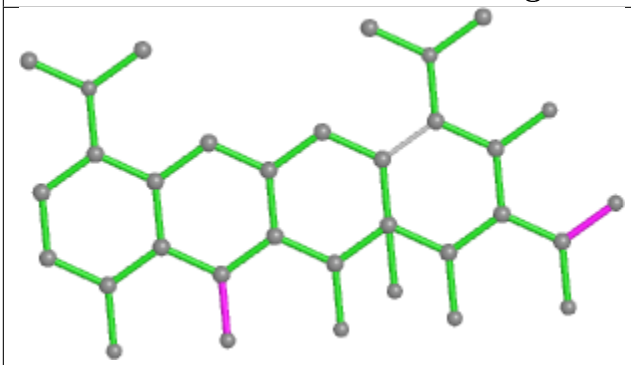


Torsions

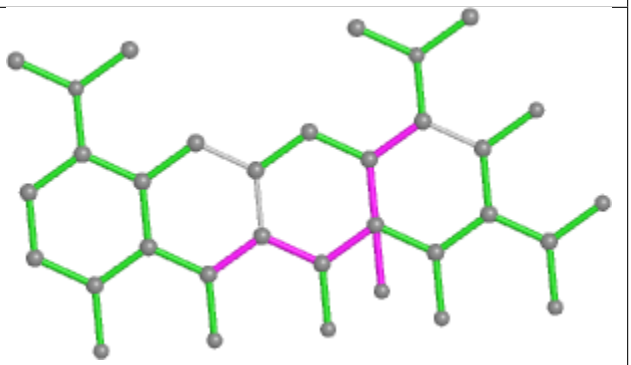


Rings

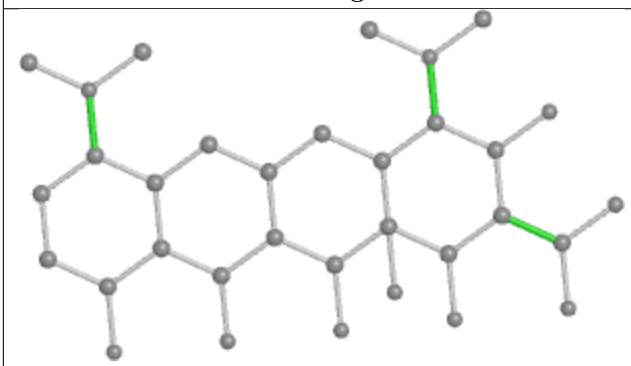
Ligand MIY A 301



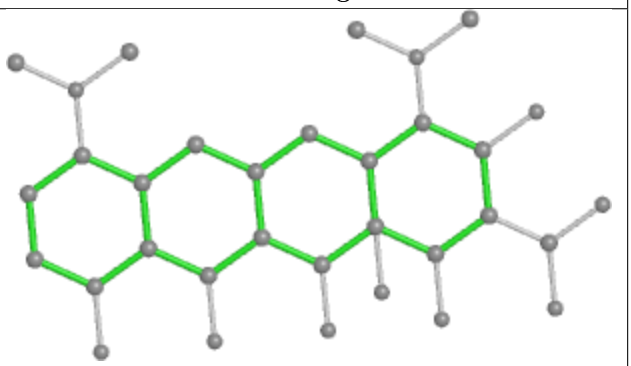
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	199/214 (92%)	0.75	18 (9%) 9 10	34, 52, 76, 85	0
1	D	189/214 (88%)	1.22	42 (22%) 0 0	41, 65, 108, 127	0
2	A	179/214 (83%)	0.46	9 (5%) 28 31	36, 48, 62, 75	0
2	C	178/214 (83%)	0.62	8 (4%) 33 36	38, 56, 73, 84	0
All	All	745/856 (87%)	0.77	77 (10%) 6 6	34, 54, 85, 127	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	43	TRP	8.8
1	D	108	PRO	7.6
1	D	42	TYR	5.2
1	D	110	PHE	5.1
1	B	166	GLN	5.0
1	D	46	GLN	5.0
1	D	37	GLN	5.0
1	B	184	MET	4.9
1	D	184	MET	4.9
1	D	35	LYS	4.9
1	D	5	ASP	4.8
1	B	163	VAL	4.7
1	D	174	ASP	4.6
1	D	106	THR	4.5
1	D	10	ILE	4.4
1	B	164	SER	4.3
1	D	34	LEU	4.3
2	C	110	PHE	4.3
1	D	213	HIS	4.2
1	D	177	HIS	4.2
1	D	41	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	109	ASN	4.1
2	C	106	THR	4.0
1	D	40	ALA	4.0
1	D	173	HIS	3.8
1	B	43	TRP	3.7
1	D	72	ASN	3.6
1	B	110	PHE	3.4
1	D	38	GLN	3.4
1	D	4	LEU	3.4
1	D	172	LEU	3.4
1	D	39	PRO	3.3
2	C	107	GLU	3.3
1	D	45	PHE	3.3
1	D	27	THR	3.3
1	D	176	PHE	3.2
2	A	108	PRO	3.1
1	D	118	ARG	3.0
1	B	71	GLU	3.0
1	B	113	ALA	2.8
1	B	124	GLY	2.8
1	D	31	ALA	2.8
2	A	5	ASP	2.8
1	D	105	PRO	2.7
1	D	25	LEU	2.7
1	D	107	GLU	2.7
1	D	36	VAL	2.7
2	A	104	ARG	2.7
1	B	37	GLN	2.7
2	A	105	PRO	2.6
2	A	205	SER	2.6
2	A	183	GLY	2.6
1	B	3	LYS	2.6
1	B	5	ASP	2.5
2	A	204	SER	2.4
2	C	72	ASN	2.4
1	D	9	VAL	2.4
1	D	119	PHE	2.4
1	D	71	GLU	2.4
1	D	175	LEU	2.4
1	D	114	GLU	2.4
1	B	31	ALA	2.3
2	C	11	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	61	ALA	2.3
2	C	108	PRO	2.3
1	D	179	LEU	2.3
1	B	181	THR	2.2
1	D	101	ALA	2.2
1	B	35	LYS	2.1
1	D	33	ARG	2.1
1	B	4	LEU	2.1
1	B	155	GLU	2.1
1	D	155	GLU	2.1
2	A	32	GLU	2.0
2	C	104	ARG	2.0
2	A	201	ARG	2.0
2	C	181	THR	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSU	B	126[A]	10/11	0.73	0.27	55,61,66,67	10
1	CSU	B	126[B]	10/11	0.73	0.27	55,59,62,63	10
1	CSU	D	126	10/11	0.92	0.16	58,60,62,64	0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SIN	D	304	8/8	0.78	0.22	65,65,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	A	304	1/1	0.79	0.07	85,85,85,85	0
4	MG	B	302	1/1	0.81	0.15	33,33,33,33	0
7	EDO	A	303	4/4	0.85	0.18	50,50,50,50	0
4	MG	D	302	1/1	0.87	0.22	46,46,46,46	0
3	MIY	A	301	33/33	0.88	0.16	49,50,51,51	0
4	MG	C	302	1/1	0.89	0.24	39,39,39,39	0
4	MG	A	302	1/1	0.89	0.16	40,40,40,40	0
3	MIY	B	301	33/33	0.92	0.14	43,44,44,45	0
3	MIY	D	301	33/33	0.92	0.13	51,52,52,52	0
3	MIY	C	301	33/33	0.93	0.15	44,45,45,46	0
5	CL	D	303	1/1	0.96	0.08	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.