Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 10:44 pm GMT

PDB ID	:	7PZG
Title	:	Phocaeicola vulgatus sialic acid esterase at 1.44 Angstrom resolution
Authors	:	Scott, H.; Armstrong, Z.; Davies, G.J.
Deposited on	:	2021-10-12
Resolution	:	1.44 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 (1)) were used in the production of this report:

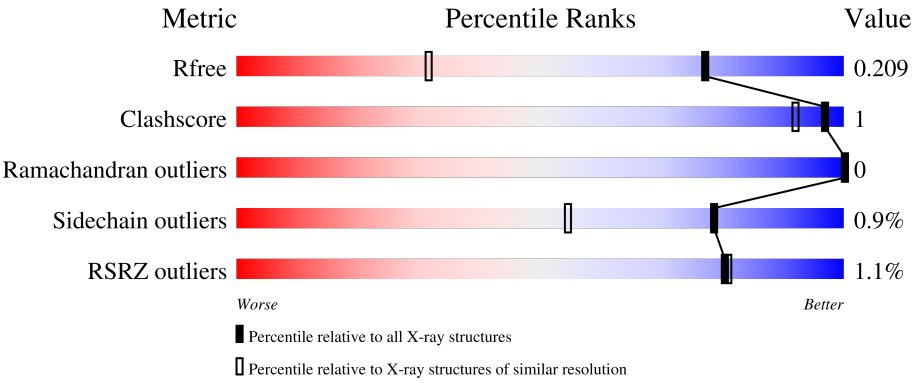
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.44 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	AAA	221	90% · 10%
1	BBB	221	88% · 10%
1	CCC	221	86% · 10%
1	DDD	221	86% · 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13712 atoms, of which 6548 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 Lysophospholipase L1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	200	Total	C	H	N	O	S	79	4	0
			3278	1045	1651	273	301	8			
1	BBB	199	Total	C	H	N	O	S	78	1	0
			3211	1026	1617	265	295	8			
1	CCC	199	Total	C	H	N	O	S	79	2	0
			3223	1032	1622	267	294	8			
1	DDD	199	Total	C	H	N	O	S	77	1	0
			3224	1029	1626	266	295	8			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	MET	-	initiating methionine	UNP A0A174J845
AAA	3	GLY	-	expression tag	UNP A0A174J845
AAA	4	SER	-	expression tag	UNP A0A174J845
AAA	5	SER	-	expression tag	UNP A0A174J845
AAA	6	HIS	-	expression tag	UNP A0A174J845
AAA	7	HIS	-	expression tag	UNP A0A174J845
AAA	8	HIS	-	expression tag	UNP A0A174J845
AAA	9	HIS	-	expression tag	UNP A0A174J845
AAA	10	HIS	-	expression tag	UNP A0A174J845
AAA	11	HIS	-	expression tag	UNP A0A174J845
AAA	12	GLY	-	expression tag	UNP A0A174J845
AAA	13	THR	-	expression tag	UNP A0A174J845
AAA	14	ALA	-	expression tag	UNP A0A174J845
AAA	15	GLU	-	expression tag	UNP A0A174J845
AAA	16	ASN	-	expression tag	UNP A0A174J845
AAA	17	LEU	-	expression tag	UNP A0A174J845
AAA	18	TYR	-	expression tag	UNP A0A174J845
AAA	19	PHE	-	expression tag	UNP A0A174J845
AAA	20	GLN	-	expression tag	UNP A0A174J845
AAA	21	GLY	-	expression tag	UNP A0A174J845
BBB	2	MET	-	initiating methionine	UNP A0A174J845

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	3	GLY	-	expression tag	UNP A0A174J845
BBB	4	SER	-	expression tag	UNP A0A174J845
BBB	5	SER	-	expression tag	UNP A0A174J845
BBB	6	HIS	-	expression tag	UNP A0A174J845
BBB	7	HIS	-	expression tag	UNP A0A174J845
BBB	8	HIS	-	expression tag	UNP A0A174J845
BBB	9	HIS	-	expression tag	UNP A0A174J845
BBB	10	HIS	-	expression tag	UNP A0A174J845
BBB	11	HIS	-	expression tag	UNP A0A174J845
BBB	12	GLY	-	expression tag	UNP A0A174J845
BBB	13	THR	-	expression tag	UNP A0A174J845
BBB	14	ALA	-	expression tag	UNP A0A174J845
BBB	15	GLU	-	expression tag	UNP A0A174J845
BBB	16	ASN	-	expression tag	UNP A0A174J845
BBB	17	LEU	-	expression tag	UNP A0A174J845
BBB	18	TYR	-	expression tag	UNP A0A174J845
BBB	19	PHE	-	expression tag	UNP A0A174J845
BBB	20	GLN	-	expression tag	UNP A0A174J845
BBB	21	GLY	-	expression tag	UNP A0A174J845
CCC	2	MET	-	initiating methionine	UNP A0A174J845
CCC	3	GLY	-	expression tag	UNP A0A174J845
CCC	4	SER	-	expression tag	UNP A0A174J845
CCC	5	SER	-	expression tag	UNP A0A174J845
CCC	6	HIS	-	expression tag	UNP A0A174J845
CCC	7	HIS	-	expression tag	UNP A0A174J845
CCC	8	HIS	-	expression tag	UNP A0A174J845
CCC	9	HIS	-	expression tag	UNP A0A174J845
CCC	10	HIS	-	expression tag	UNP A0A174J845
CCC	11	HIS	-	expression tag	UNP A0A174J845
CCC	12	GLY	-	expression tag	UNP A0A174J845
CCC	13	THR	-	expression tag	UNP A0A174J845
CCC	14	ALA	-	expression tag	UNP A0A174J845
CCC	15	GLU	-	expression tag	UNP A0A174J845
CCC	16	ASN	-	expression tag	UNP A0A174J845
CCC	17	LEU	-	expression tag	UNP A0A174J845
CCC	18	TYR	-	expression tag	UNP A0A174J845
CCC	19	PHE	-	expression tag	UNP A0A174J845
CCC	20	GLN	-	expression tag	UNP A0A174J845
CCC	21	GLY	-	expression tag	UNP A0A174J845
DDD	2	MET	-	initiating methionine	UNP A0A174J845
DDD	3	GLY	-	expression tag	UNP A0A174J845
DDD	4	SER	-	expression tag	UNP A0A174J845

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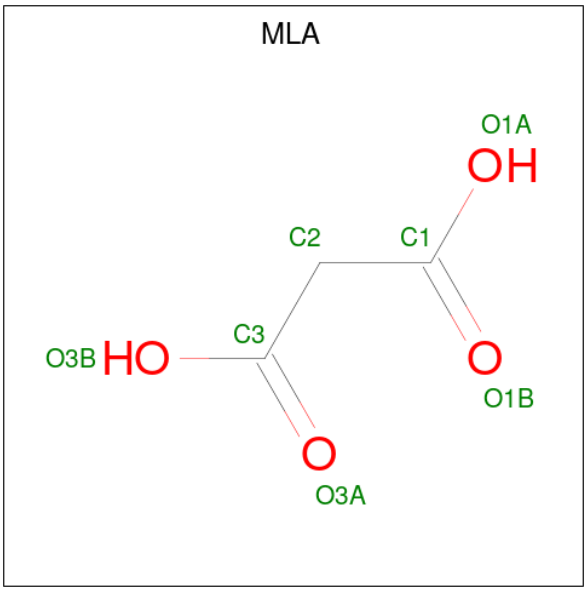
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	5	SER	-	expression tag	UNP A0A174J845
DDD	6	HIS	-	expression tag	UNP A0A174J845
DDD	7	HIS	-	expression tag	UNP A0A174J845
DDD	8	HIS	-	expression tag	UNP A0A174J845
DDD	9	HIS	-	expression tag	UNP A0A174J845
DDD	10	HIS	-	expression tag	UNP A0A174J845
DDD	11	HIS	-	expression tag	UNP A0A174J845
DDD	12	GLY	-	expression tag	UNP A0A174J845
DDD	13	THR	-	expression tag	UNP A0A174J845
DDD	14	ALA	-	expression tag	UNP A0A174J845
DDD	15	GLU	-	expression tag	UNP A0A174J845
DDD	16	ASN	-	expression tag	UNP A0A174J845
DDD	17	LEU	-	expression tag	UNP A0A174J845
DDD	18	TYR	-	expression tag	UNP A0A174J845
DDD	19	PHE	-	expression tag	UNP A0A174J845
DDD	20	GLN	-	expression tag	UNP A0A174J845
DDD	21	GLY	-	expression tag	UNP A0A174J845

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

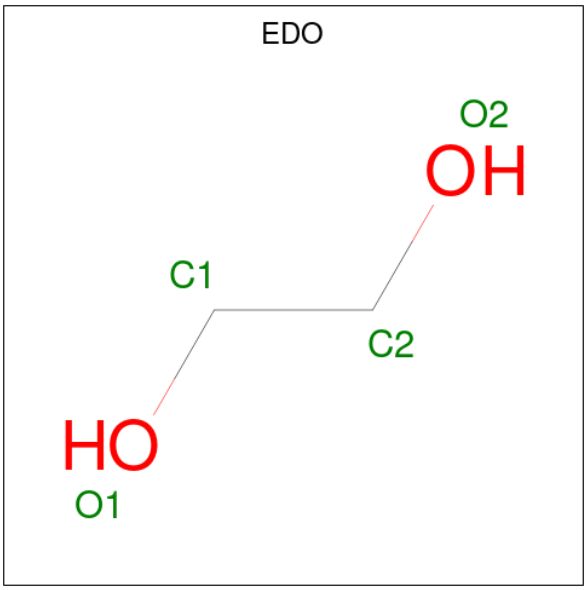
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Mg 1 1	0	0
2	BBB	1	Total Mg 1 1	0	0
2	CCC	1	Total Mg 1 1	0	0
2	DDD	1	Total Mg 1 1	0	0

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C H O 9 3 2 4	0	0
3	BBB	1	Total C H O 9 3 2 4	0	0
3	CCC	1	Total C H O 9 3 2 4	0	0
3	DDD	1	Total C H O 9 3 2 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
4	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
4	DDD	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 5 is water.

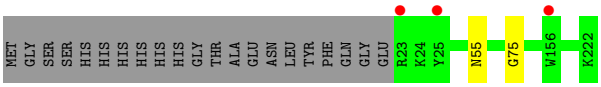
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	201	Total	O	0	0
			201	201		
5	BBB	196	Total	O	0	0
			196	196		
5	CCC	132	Total	O	0	0
			132	132		
5	DDD	167	Total	O	0	0
			167	167		

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.

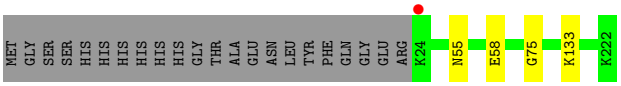
• Molecule 1: Lysophospholipase L1

Chain AAA:



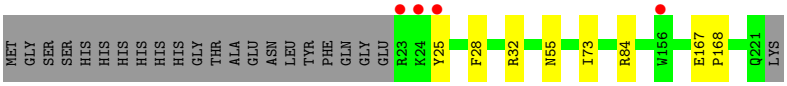
• Molecule 1: Lysophospholipase L1

Chain BBB:



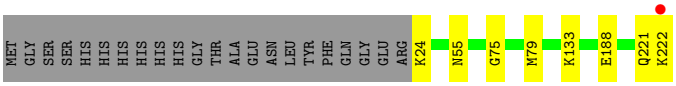
• Molecule 1: Lysophospholipase L1

Chain CCC:



• Molecule 1: Lysophospholipase L1

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.27Å 90.15Å 76.58Å 90.00° 99.29° 90.00°	Depositor
Resolution (Å)	70.43 – 1.44 70.33 – 1.44	Depositor EDS
% Data completeness (in resolution range)	97.6 (70.43-1.44) 97.6 (70.33-1.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.177 , 0.203 0.184 , 0.209	Depositor DCC
R_{free} test set	8262 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13712	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: MLA, MG, 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	AAA	0.77	0/1660	0.91	0/2244
1	BBB	0.79	1/1627 (0.1%)	0.92	0/2200
1	CCC	0.79	0/1635	0.93	4/2212 (0.2%)
1	DDD	0.76	0/1631	0.87	0/2204
All	All	0.78	1/6553 (0.0%)	0.91	4/8860 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	58	GLU	CD-OE1	5.29	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	84	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	CCC	25[A]	TYR	CB-CA-C	-6.03	98.34	110.40
1	CCC	25[B]	TYR	CB-CA-C	-6.03	98.34	110.40
1	CCC	32	ARG	NE-CZ-NH1	5.38	122.99	120.30

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	AAA	1627	1651	1638	1	0
1	BBB	1594	1617	1608	2	0
1	CCC	1601	1622	1607	4	0
1	DDD	1598	1626	1619	5	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	7	2	2	1	0
3	BBB	7	2	2	1	0
3	CCC	7	2	2	0	0
3	DDD	7	2	2	1	0
4	AAA	4	6	6	0	0
4	BBB	4	6	6	0	0
4	CCC	4	6	6	0	0
4	DDD	4	6	6	0	0
5	AAA	201	0	0	0	0
5	BBB	196	0	0	1	0
5	CCC	132	0	0	3	0
5	DDD	167	0	0	0	0
All	All	7164	6548	6504	12	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 1.

All (12) 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:CCC:28:PHE:O	5:CCC:401:HOH:O	2.03	0.74
1:BBB:75:GLY:HA2	3:BBB:302:MLA:HC21	1.77	0.67
1:CCC:73:ILE:HG23	5:CCC:401:HOH:O	1.95	0.65
1:DDD:133:LYS:NZ	1:DDD:222:LYS:O	2.34	0.61
1:DDD:75:GLY:HA2	3:DDD:302:MLA:HC22	1.89	0.55
1:CCC:28:PHE:C	5:CCC:401:HOH:O	2.45	0.54
1:DDD:188:GLU:CD	1:DDD:188:GLU:H	2.12	0.52
1:DDD:188:GLU:CD	1:DDD:188:GLU:N	2.69	0.45
1:CCC:167:GLU:HB3	1:CCC:168:PRO:HD3	1.99	0.44
1:AAA:75:GLY:HA2	3:AAA:302:MLA:HC22	1.98	0.44
1:BBB:133:LYS:NZ	5:BBB:403:HOH:O	2.51	0.43
1:DDD:79:MET:HB2	1:DDD:79:MET:HE3	1.92	0.43

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	AAA	202/221 (91%)	196 (97%)	6 (3%)	0	100	100
1	BBB	198/221 (90%)	195 (98%)	3 (2%)	0	100	100
1	CCC	199/221 (90%)	195 (98%)	4 (2%)	0	100	100
1	DDD	198/221 (90%)	195 (98%)	3 (2%)	0	100	100
All	All	797/884 (90%)	781 (98%)	16 (2%)	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	AAA	180/196 (92%)	179 (99%)	1 (1%)	86	68
1	BBB	177/196 (90%)	176 (99%)	1 (1%)	86	68
1	CCC	176/196 (90%)	175 (99%)	1 (1%)	86	68
1	DDD	178/196 (91%)	175 (98%)	3 (2%)	60	28
All	All	711/784 (91%)	705 (99%)	6 (1%)	78	61

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	55	ASN
1	BBB	55	ASN

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Mol	Chain	Res	Type
1	CCC	55	ASN
1	DDD	24	LYS
1	DDD	55	ASN
1	DDD	221	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	MLA	CCC	302	-	6,6,6	1.05	0	7,7,7	1.65	1 (14%)
3	MLA	AAA	302	-	6,6,6	1.39	0	7,7,7	1.43	1 (14%)
3	MLA	DDD	302	-	6,6,6	1.35	1 (16%)	7,7,7	0.52	0
4	EDO	BBB	303	-	3,3,3	0.55	0	2,2,2	0.72	0
4	EDO	DDD	303	-	3,3,3	0.36	0	2,2,2	0.25	0
4	EDO	CCC	303	-	3,3,3	0.15	0	2,2,2	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	AAA	303	-	3,3,3	0.35	0	2,2,2	0.28	0
3	MLA	BBB	302	-	6,6,6	1.45	1 (16%)	7,7,7	0.65	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	MLA	CCC	302	-	-	1/4/4/4	-
3	MLA	AAA	302	-	-	0/4/4/4	-
3	MLA	DDD	302	-	-	1/4/4/4	-
4	EDO	BBB	303	-	-	1/1/1/1	-
4	EDO	DDD	303	-	-	1/1/1/1	-
4	EDO	CCC	303	-	-	1/1/1/1	-
4	EDO	AAA	303	-	-	1/1/1/1	-
3	MLA	BBB	302	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	302	MLA	O3A-C3	2.33	1.29	1.22
3	BBB	302	MLA	O1B-C1	2.25	1.29	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CCC	302	MLA	O3B-C3-C2	2.99	124.09	114.54
3	AAA	302	MLA	C3-C2-C1	2.42	121.34	112.87

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	302	MLA	C1-C2-C3-O3A
3	BBB	302	MLA	C1-C2-C3-O3B
3	BBB	302	MLA	O1B-C1-C2-C3
4	DDD	303	EDO	O1-C1-C2-O2
4	CCC	303	EDO	O1-C1-C2-O2
3	BBB	302	MLA	O1A-C1-C2-C3
4	AAA	303	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	BBB	303	EDO	O1-C1-C2-O2
3	CCC	302	MLA	O1A-C1-C2-C3
3	DDD	302	MLA	O1B-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	302	MLA	1	0
3	DDD	302	MLA	1	0
3	BBB	302	MLA	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

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	AAA	200/221 (90%)	-0.25	3 (1%)	73	73	14, 20, 34, 54	0
1	BBB	199/221 (90%)	-0.33	1 (0%)	91	92	15, 19, 33, 64	0
1	CCC	199/221 (90%)	0.08	4 (2%)	65	65	15, 25, 40, 62	0
1	DDD	199/221 (90%)	-0.30	1 (0%)	91	92	15, 22, 36, 70	0
All	All	797/884 (90%)	-0.20	9 (1%)	80	81	14, 21, 37, 70	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	25[A]	TYR	6.4
1	AAA	25	TYR	6.1
1	DDD	222	LYS	2.9
1	CCC	23	ARG	2.5
1	BBB	24	LYS	2.4
1	CCC	24	LYS	2.3
1	CCC	156	TRP	2.1
1	AAA	23	ARG	2.1
1	AAA	156	TRP	2.1

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

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
4	EDO	CCC	303	4/4	0.80	0.10	35,39,42,42	1
4	EDO	AAA	303	4/4	0.83	0.13	29,35,38,40	1
4	EDO	DDD	303	4/4	0.83	0.13	28,34,44,44	1
3	MLA	BBB	302	7/7	0.86	0.13	23,34,44,50	0
2	MG	CCC	301	1/1	0.86	0.38	56,56,56,56	0
3	MLA	AAA	302	7/7	0.90	0.17	23,33,41,41	0
3	MLA	DDD	302	7/7	0.91	0.15	25,39,49,60	0
4	EDO	BBB	303	4/4	0.91	0.14	20,30,34,35	1
3	MLA	CCC	302	7/7	0.93	0.14	24,34,46,48	0
2	MG	AAA	301	1/1	0.95	0.09	35,35,35,35	0
2	MG	BBB	301	1/1	0.99	0.08	17,17,17,17	0
2	MG	DDD	301	1/1	0.99	0.06	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.