



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:54 AM BST

PDB ID : 5DI0
Title : Crystal structure of Dln1
Authors : Jia, N.; Jiang, Y.L.; Cheng, W.; Wang, H.W.; Zhou, C.Z.; Chen, Y.
Deposited on : 2015-08-31
Resolution : 1.70 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 : 2.13.1
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) : 2.13.1

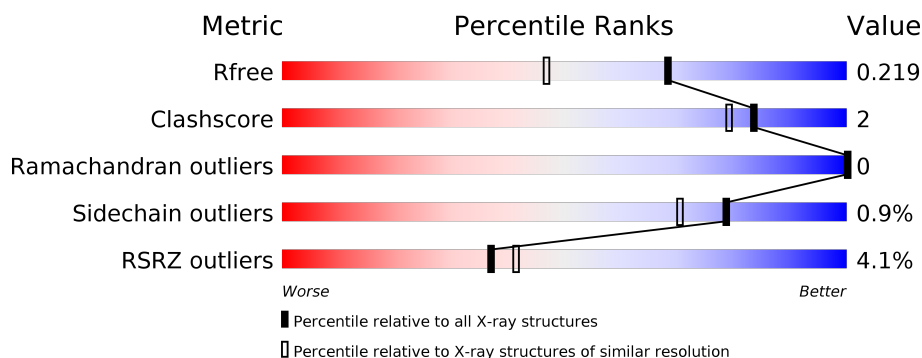
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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	335	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	B	335	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6071 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 Natterin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	7	0
			2466	1563	401	492	10			
1	B	318	Total	C	N	O	S	0	14	0
			2499	1589	406	494	10			

There are 40 discrepancies between the modelled and reference sequences:

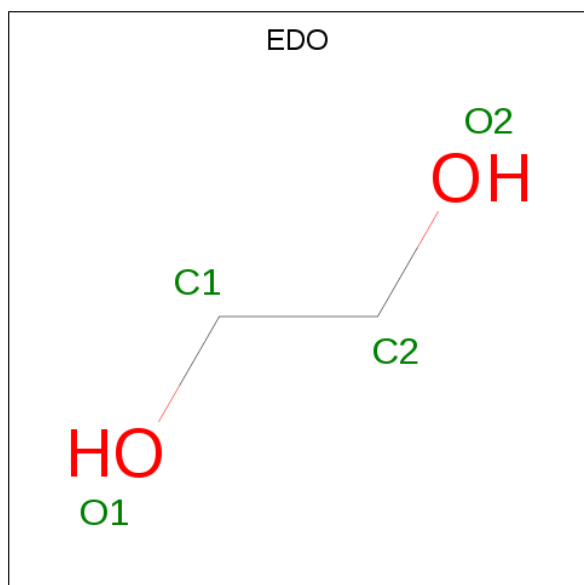
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q5CZR5
A	-18	GLY	-	expression tag	UNP Q5CZR5
A	-17	SER	-	expression tag	UNP Q5CZR5
A	-16	SER	-	expression tag	UNP Q5CZR5
A	-15	HIS	-	expression tag	UNP Q5CZR5
A	-14	HIS	-	expression tag	UNP Q5CZR5
A	-13	HIS	-	expression tag	UNP Q5CZR5
A	-12	HIS	-	expression tag	UNP Q5CZR5
A	-11	HIS	-	expression tag	UNP Q5CZR5
A	-10	HIS	-	expression tag	UNP Q5CZR5
A	-9	SER	-	expression tag	UNP Q5CZR5
A	-8	SER	-	expression tag	UNP Q5CZR5
A	-7	GLY	-	expression tag	UNP Q5CZR5
A	-6	LEU	-	expression tag	UNP Q5CZR5
A	-5	VAL	-	expression tag	UNP Q5CZR5
A	-4	PRO	-	expression tag	UNP Q5CZR5
A	-3	ARG	-	expression tag	UNP Q5CZR5
A	-2	GLY	-	expression tag	UNP Q5CZR5
A	-1	SER	-	expression tag	UNP Q5CZR5
A	0	HIS	-	expression tag	UNP Q5CZR5
B	-19	MET	-	expression tag	UNP Q5CZR5
B	-18	GLY	-	expression tag	UNP Q5CZR5
B	-17	SER	-	expression tag	UNP Q5CZR5
B	-16	SER	-	expression tag	UNP Q5CZR5
B	-15	HIS	-	expression tag	UNP Q5CZR5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q5CZR5
B	-13	HIS	-	expression tag	UNP Q5CZR5
B	-12	HIS	-	expression tag	UNP Q5CZR5
B	-11	HIS	-	expression tag	UNP Q5CZR5
B	-10	HIS	-	expression tag	UNP Q5CZR5
B	-9	SER	-	expression tag	UNP Q5CZR5
B	-8	SER	-	expression tag	UNP Q5CZR5
B	-7	GLY	-	expression tag	UNP Q5CZR5
B	-6	LEU	-	expression tag	UNP Q5CZR5
B	-5	VAL	-	expression tag	UNP Q5CZR5
B	-4	PRO	-	expression tag	UNP Q5CZR5
B	-3	ARG	-	expression tag	UNP Q5CZR5
B	-2	GLY	-	expression tag	UNP Q5CZR5
B	-1	SER	-	expression tag	UNP Q5CZR5
B	0	HIS	-	expression tag	UNP Q5CZR5

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



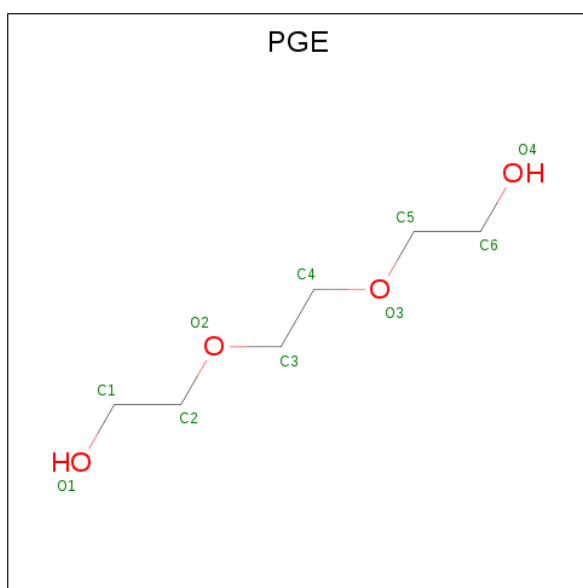
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



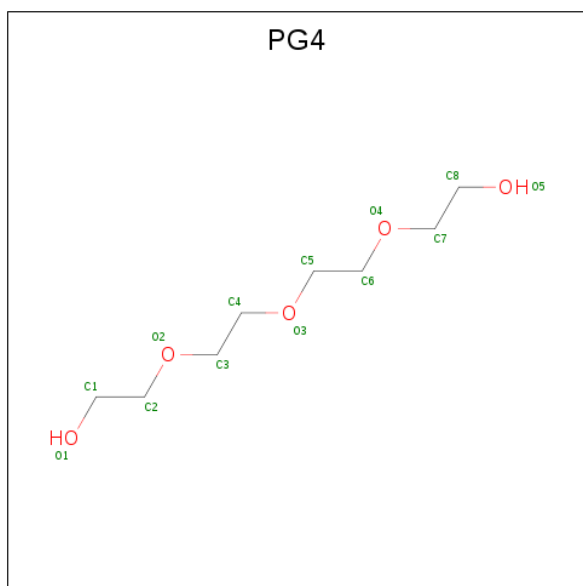
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	400	Total 400	O 400	0	0
7	B	452	Total 452	O 452	0	0

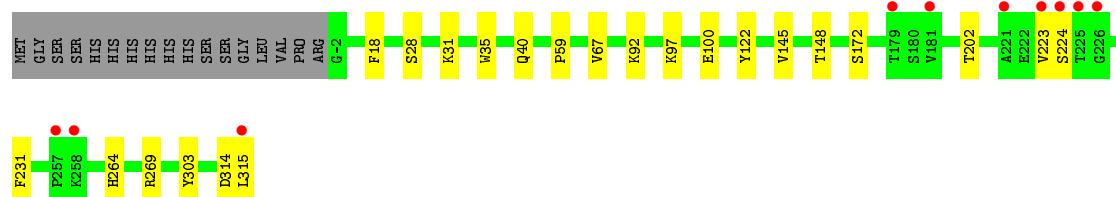
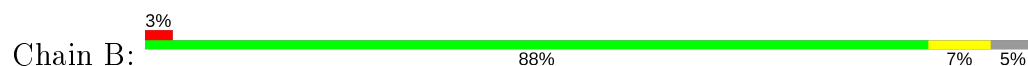
3 Residue-property plots [i](#)

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: Natterin-like protein



- Molecule 1: Natterin-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.11Å 95.10Å 147.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 1.70 47.55 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.60-1.70) 98.2 (47.55-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.172 , 0.209 0.182 , 0.219	Depositor DCC
R_{free} test set	4400 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6071	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.18% 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: PEG, PG4, PGE, EDO, CL

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	0/2537	0.71	0/3434
1	B	0.56	0/2595	0.72	0/3513
All	All	0.55	0/5132	0.72	0/6947

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	GLN	Peptide

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	2466	0	2427	4	1
1	B	2499	0	2486	17	1
2	A	20	0	30	3	0
2	B	28	0	42	1	0
3	A	42	0	60	0	0
3	B	14	0	20	0	0
4	A	40	0	56	0	0
4	B	30	0	42	3	0
5	A	26	0	36	0	0
5	B	52	0	72	3	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
7	A	400	0	0	1	1
7	B	452	0	0	3	1
All	All	6071	0	5271	25	2

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 (25) 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:B:18:PHE:HB3	4:B:410:PGE:H3	1.75	0.68
1:B:145[A]:VAL:HG11	1:B:148:THR:HG23	1.81	0.62
1:B:314:ASP:O	1:B:315:LEU:HB2	2.06	0.55
1:A:195:LYS:HE2	1:A:303:TYR:HB2	1.87	0.54
1:B:92:LYS:HE3	1:B:100:GLU:OE2	2.10	0.51
4:B:410:PGE:H32	7:B:547:HOH:O	2.12	0.50
1:B:97:LYS:HB3	2:B:407:EDO:H11	1.94	0.49
1:A:11:GLY:O	2:A:405:EDO:H21	2.13	0.49
1:B:202:THR:HG23	7:B:753:HOH:O	2.13	0.48
1:B:223:VAL:HG12	1:B:224:SER:N	2.28	0.48
1:A:35:TRP:CE2	1:A:59:PRO:HB3	2.49	0.47
1:B:172[A]:SER:OG	1:B:264[A]:HIS:ND1	2.39	0.47
2:A:403:EDO:O2	6:A:418:CL:CL	2.62	0.47
1:B:314:ASP:O	1:B:315:LEU:CB	2.62	0.47
1:B:31:LYS:CD	1:B:67[A]:VAL:HG12	2.45	0.47
1:B:172[A]:SER:HG	1:B:264[A]:HIS:HD1	1.56	0.46
1:A:152[B]:ASN:ND2	7:A:509:HOH:O	2.46	0.45
4:B:410:PGE:H52	7:B:547:HOH:O	2.16	0.45
1:B:269[B]:ARG:HD2	1:B:303:TYR:OH	2.16	0.44
1:B:35:TRP:CE2	1:B:59:PRO:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LYS:HE2	5:B:416:PG4:H11	2.02	0.42
2:A:404:EDO:H11	2:A:405:EDO:O1	2.20	0.42
1:B:97:LYS:NZ	5:B:415:PG4:H32	2.35	0.42
1:B:28:SER:HB3	1:B:122:TYR:CZ	2.55	0.42
1:B:97:LYS:HE2	5:B:415:PG4:H51	2.03	0.41

All (2) 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)
7:A:655:HOH:O	7:B:794:HOH:O[1_455]	2.02	0.18
1:A:62[A]:SER:OG	1:B:100:GLU:OE1[4_455]	2.19	0.01

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	323/335 (96%)	317 (98%)	6 (2%)	0	100	100
1	B	330/335 (98%)	324 (98%)	6 (2%)	0	100	100
All	All	653/670 (98%)	641 (98%)	12 (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	A	278/286 (97%)	274 (99%)	4 (1%)	67	53
1	B	285/286 (100%)	284 (100%)	1 (0%)	91	87
All	All	563/572 (98%)	558 (99%)	5 (1%)	78	70

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

Mol	Chain	Res	Type
1	A	40	GLN
1	A	178	LYS
1	A	231	PHE
1	A	271	SER
1	B	231	PHE

Some 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 ⓘ

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 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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
4	PGE	B	412	-	9,9,9	0.48	0	8,8,8	0.17	0
3	PEG	A	410	-	6,6,6	0.42	0	5,5,5	0.24	0
3	PEG	A	407	-	6,6,6	0.40	0	5,5,5	0.58	0
3	PEG	B	409	-	6,6,6	0.36	0	5,5,5	0.39	0
2	EDO	B	403	-	3,3,3	0.41	0	2,2,2	0.39	0
2	EDO	B	402	-	3,3,3	0.40	0	2,2,2	0.36	0
3	PEG	A	406	-	6,6,6	0.36	0	5,5,5	0.27	0
3	PEG	A	408	-	6,6,6	0.40	0	5,5,5	0.31	0
5	PG4	B	414	-	12,12,12	0.58	0	11,11,11	0.56	0
2	EDO	A	401	-	3,3,3	0.47	0	2,2,2	0.36	0
2	EDO	A	404	-	3,3,3	0.37	0	2,2,2	0.40	0
2	EDO	B	404	-	3,3,3	0.46	0	2,2,2	0.11	0
4	PGE	A	414	-	9,9,9	0.49	0	8,8,8	0.60	0
3	PEG	A	409	-	6,6,6	0.53	0	5,5,5	0.38	0
4	PGE	A	413	-	9,9,9	0.48	0	8,8,8	0.57	0
3	PEG	B	408	-	6,6,6	0.54	0	5,5,5	0.36	0
2	EDO	B	406	-	3,3,3	0.49	0	2,2,2	0.13	0
5	PG4	B	416	-	12,12,12	0.67	0	11,11,11	0.59	0
2	EDO	B	405	-	3,3,3	0.50	0	2,2,2	0.24	0
5	PG4	B	415	-	12,12,12	0.54	0	11,11,11	0.54	0
4	PGE	A	415	-	9,9,9	0.53	0	8,8,8	0.31	0
2	EDO	A	403	-	3,3,3	0.40	0	2,2,2	0.71	0
5	PG4	B	413	-	12,12,12	0.52	0	11,11,11	0.46	0
2	EDO	B	407	-	3,3,3	0.46	0	2,2,2	0.08	0
5	PG4	A	417	-	12,12,12	0.47	0	11,11,11	0.65	0
4	PGE	B	411	-	9,9,9	0.41	0	8,8,8	0.60	0
3	PEG	A	411	-	6,6,6	0.59	0	5,5,5	0.26	0
2	EDO	A	402	-	3,3,3	0.58	0	2,2,2	0.07	0
4	PGE	A	412	-	9,9,9	0.61	0	8,8,8	0.62	0
2	EDO	B	401	-	3,3,3	0.45	0	2,2,2	0.26	0
4	PGE	B	410	-	9,9,9	0.41	0	8,8,8	0.51	0
5	PG4	A	416	-	12,12,12	0.46	0	11,11,11	0.62	0
2	EDO	A	405	-	3,3,3	0.53	0	2,2,2	0.17	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
4	PGE	B	412	-	-	3/7/7/7	-
3	PEG	A	410	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	407	-	-	1/4/4/4	-
3	PEG	B	409	-	-	2/4/4/4	-
2	EDO	B	403	-	-	1/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
3	PEG	A	406	-	-	0/4/4/4	-
3	PEG	A	408	-	-	2/4/4/4	-
5	PG4	B	414	-	-	6/10/10/10	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	A	404	-	-	1/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-
4	PGE	A	414	-	-	3/7/7/7	-
3	PEG	A	409	-	-	2/4/4/4	-
4	PGE	A	413	-	-	1/7/7/7	-
3	PEG	B	408	-	-	0/4/4/4	-
2	EDO	B	406	-	-	0/1/1/1	-
5	PG4	B	416	-	-	3/10/10/10	-
2	EDO	B	405	-	-	1/1/1/1	-
5	PG4	B	415	-	-	7/10/10/10	-
4	PGE	A	415	-	-	0/7/7/7	-
2	EDO	A	403	-	-	1/1/1/1	-
5	PG4	B	413	-	-	4/10/10/10	-
2	EDO	B	407	-	-	1/1/1/1	-
5	PG4	A	417	-	-	6/10/10/10	-
4	PGE	B	411	-	-	3/7/7/7	-
3	PEG	A	411	-	-	1/4/4/4	-
2	EDO	A	402	-	-	1/1/1/1	-
4	PGE	A	412	-	-	5/7/7/7	-
2	EDO	B	401	-	-	0/1/1/1	-
4	PGE	B	410	-	-	3/7/7/7	-
5	PG4	A	416	-	-	4/10/10/10	-
2	EDO	A	405	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	408	PEG	O2-C3-C4-O4
5	B	414	PG4	O2-C3-C4-O3
5	B	416	PG4	O2-C3-C4-O3
3	B	409	PEG	O1-C1-C2-O2
3	A	408	PEG	O1-C1-C2-O2
5	B	414	PG4	O1-C1-C2-O2
5	B	415	PG4	O4-C7-C8-O5
5	B	413	PG4	O4-C7-C8-O5
4	B	411	PGE	O1-C1-C2-O2
4	A	412	PGE	O3-C5-C6-O4
5	A	416	PG4	O1-C1-C2-O2
5	B	414	PG4	O3-C5-C6-O4
5	B	415	PG4	O3-C5-C6-O4
3	A	409	PEG	O2-C3-C4-O4
5	B	415	PG4	O1-C1-C2-O2
4	B	410	PGE	O3-C5-C6-O4
5	A	416	PG4	O2-C3-C4-O3
5	A	417	PG4	O3-C5-C6-O4
4	A	412	PGE	O1-C1-C2-O2
5	B	415	PG4	O2-C3-C4-O3
3	A	410	PEG	O2-C3-C4-O4
5	A	417	PG4	O4-C7-C8-O5
2	A	404	EDO	O1-C1-C2-O2
2	B	407	EDO	O1-C1-C2-O2
2	A	402	EDO	O1-C1-C2-O2
3	A	410	PEG	O1-C1-C2-O2
4	A	414	PGE	O1-C1-C2-O2
5	A	417	PG4	O1-C1-C2-O2
3	B	409	PEG	O2-C3-C4-O4
4	B	412	PGE	O1-C1-C2-O2
2	B	403	EDO	O1-C1-C2-O2
4	B	412	PGE	O3-C5-C6-O4
5	B	413	PG4	C4-C3-O2-C2
4	A	412	PGE	C6-C5-O3-C4
4	B	411	PGE	C4-C3-O2-C2
5	A	417	PG4	C8-C7-O4-C6
4	A	412	PGE	C3-C4-O3-C5
4	A	412	PGE	C4-C3-O2-C2
5	A	416	PG4	C5-C6-O4-C7
5	B	415	PG4	C6-C5-O3-C4
3	A	407	PEG	O1-C1-C2-O2
5	A	416	PG4	C3-C4-O3-C5
5	B	414	PG4	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	411	PGE	C3-C4-O3-C5
5	B	415	PG4	C1-C2-O2-C3
5	A	417	PG4	C3-C4-O3-C5
5	A	417	PG4	O2-C3-C4-O3
5	B	416	PG4	O1-C1-C2-O2
5	B	413	PG4	C5-C6-O4-C7
5	B	413	PG4	C8-C7-O4-C6
5	B	414	PG4	C1-C2-O2-C3
4	A	413	PGE	O2-C3-C4-O3
4	B	410	PGE	C1-C2-O2-C3
2	A	403	EDO	O1-C1-C2-O2
2	A	405	EDO	O1-C1-C2-O2
3	A	411	PEG	C4-C3-O2-C2
5	B	415	PG4	C4-C3-O2-C2
3	A	409	PEG	C4-C3-O2-C2
4	A	414	PGE	O2-C3-C4-O3
3	A	410	PEG	C4-C3-O2-C2
5	B	416	PG4	C4-C3-O2-C2
4	B	412	PGE	O2-C3-C4-O3
5	B	414	PG4	C4-C3-O2-C2
4	B	410	PGE	O2-C3-C4-O3
4	A	414	PGE	C4-C3-O2-C2
2	B	405	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	EDO	1	0
5	B	416	PG4	1	0
5	B	415	PG4	2	0
2	A	403	EDO	1	0
2	B	407	EDO	1	0
4	B	410	PGE	3	0
2	A	405	EDO	2	0

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	318/335 (94%)	0.04	16 (5%) 28 32	12, 22, 61, 88	0
1	B	318/335 (94%)	-0.11	10 (3%) 49 53	13, 21, 41, 75	0
All	All	636/670 (94%)	-0.03	26 (4%) 37 41	12, 22, 51, 88	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	THR	6.1
1	A	221	ALA	5.7
1	B	225	THR	5.7
1	A	224	SER	5.3
1	A	226	GLY	5.1
1	A	180	SER	5.1
1	B	315	LEU	4.7
1	B	223	VAL	4.6
1	B	181	VAL	3.9
1	A	315	LEU	3.7
1	A	223	VAL	3.5
1	A	181	VAL	3.3
1	A	227	PHE	3.3
1	A	164	LYS	2.8
1	A	179	THR	2.8
1	B	224	SER	2.7
1	A	228	SER	2.7
1	A	182	LYS	2.6
1	A	271	SER	2.5
1	B	226	GLY	2.4
1	B	221	ALA	2.3
1	A	178	LYS	2.3
1	A	-2	GLY	2.2
1	B	179	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	258	LYS	2.0
1	B	257	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	402	4/4	0.47	0.27	51,56,57,60	0
3	PEG	A	409	7/7	0.59	0.26	51,58,61,62	0
2	EDO	B	406	4/4	0.65	0.28	69,70,71,75	0
2	EDO	A	405	4/4	0.72	0.30	39,40,40,41	0
4	PGE	B	412	10/10	0.75	0.24	61,66,71,72	0
2	EDO	B	407	4/4	0.75	0.22	45,46,48,53	0
5	PG4	B	414	13/13	0.78	0.14	48,51,54,55	0
2	EDO	A	404	4/4	0.79	0.14	42,43,45,47	0
2	EDO	B	404	4/4	0.81	0.24	64,66,66,67	0
3	PEG	A	410	7/7	0.81	0.17	50,51,54,54	0
2	EDO	B	405	4/4	0.82	0.13	50,51,51,51	0
4	PGE	A	414	10/10	0.82	0.13	47,50,54,55	0
3	PEG	A	411	7/7	0.84	0.21	33,41,46,46	0
2	EDO	B	403	4/4	0.84	0.11	54,55,56,57	0
4	PGE	A	412	10/10	0.84	0.13	33,36,42,46	0
4	PGE	B	411	10/10	0.84	0.13	41,45,49,51	0
5	PG4	A	417	13/13	0.85	0.14	46,47,50,50	0
5	PG4	B	415	13/13	0.85	0.13	43,47,52,53	0
5	PG4	B	416	13/13	0.86	0.13	29,48,50,51	0
4	PGE	B	410	10/10	0.86	0.21	36,38,42,43	0
3	PEG	B	409	7/7	0.86	0.23	28,38,44,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	401	4/4	0.87	0.20	39,43,44,49	0
3	PEG	A	407	7/7	0.88	0.12	30,31,33,38	0
5	PG4	A	416	13/13	0.88	0.12	39,40,45,45	0
4	PGE	A	413	10/10	0.88	0.15	25,39,47,53	0
5	PG4	B	413	13/13	0.89	0.20	26,46,62,62	0
3	PEG	A	408	7/7	0.90	0.14	47,47,52,54	0
4	PGE	A	415	10/10	0.90	0.10	41,45,54,57	0
2	EDO	B	402	4/4	0.91	0.17	26,30,32,33	0
3	PEG	B	408	7/7	0.91	0.12	32,34,37,38	0
2	EDO	B	401	4/4	0.91	0.10	45,45,46,47	0
2	EDO	A	403	4/4	0.92	0.17	25,32,36,39	0
3	PEG	A	406	7/7	0.92	0.15	31,33,40,42	0
6	CL	A	418	1/1	0.97	0.04	24,24,24,24	0
6	CL	B	417	1/1	0.99	0.07	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.