



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 02:32 am BST

PDB ID : 6BYW
Title : Structure of GoxA from Pseudoalteromonas luteoviolacea
Authors : Yukl, E.T.; Avalos, D.
Deposited on : 2017-12-21
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.11
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) : 2.11

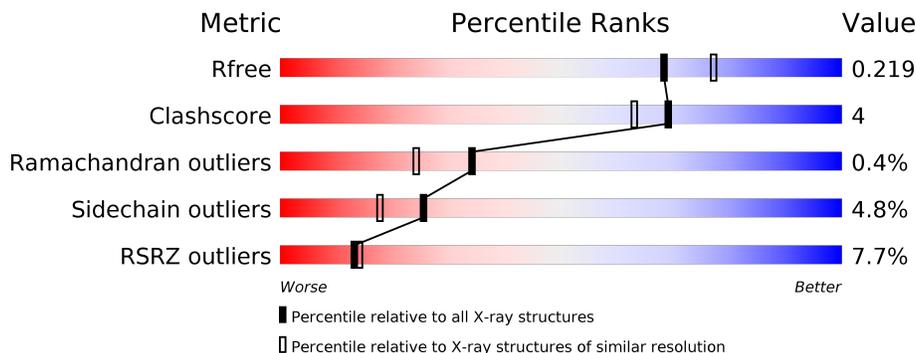
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	816	 9% 86% 9% • •
1	B	816	 6% 86% 8% • •
1	C	816	 7% 84% 10% • 5%
1	D	816	 7% 85% 9% • 5%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 49970 atoms, of which 23533 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.

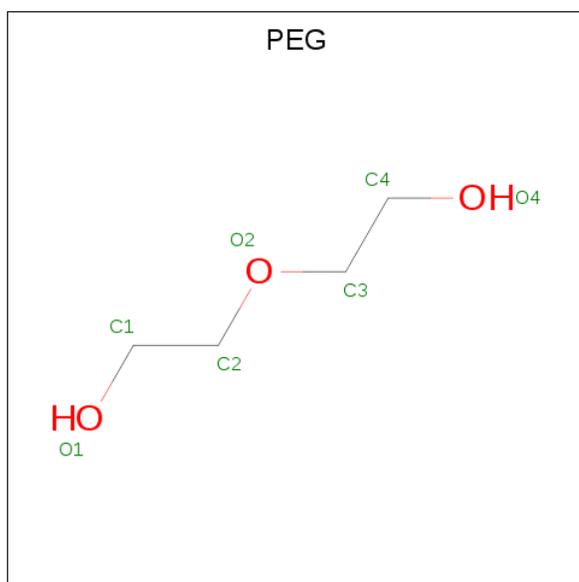
- Molecule 1 is a protein called GoxA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	B	781	12046	3915	5858	1051	1202	20	0	2	0
1	A	787	12157	3946	5913	1063	1215	20	0	3	0
1	C	778	12043	3902	5875	1050	1197	19	0	1	0
1	D	776	11973	3885	5831	1046	1191	20	0	2	0

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

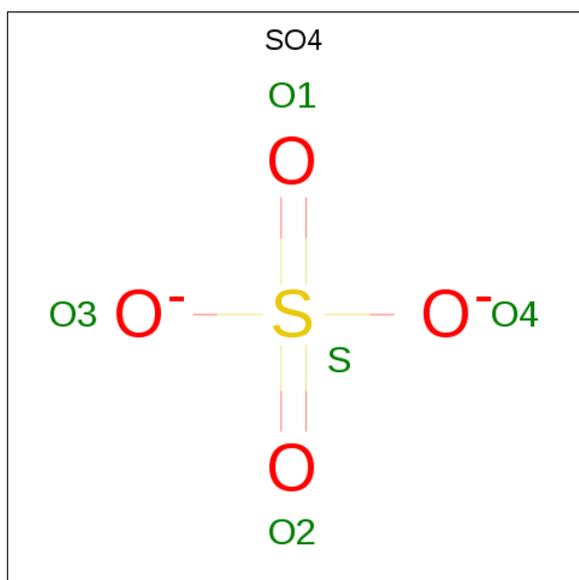
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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



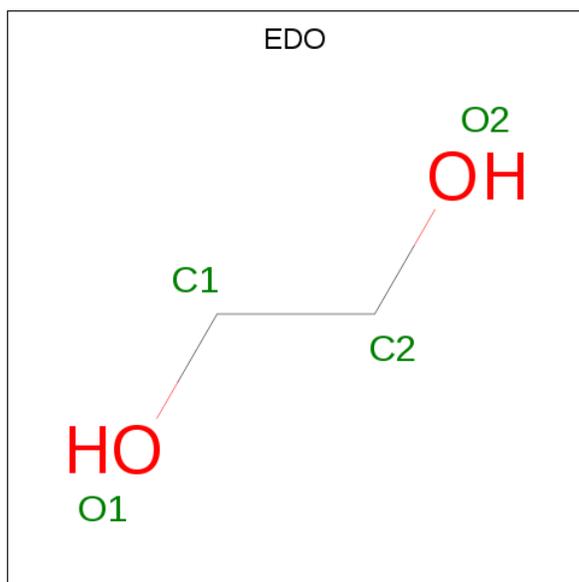
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	B	1	17	4	10	3	0	0
3	A	1	17	4	10	3	0	0
3	A	1	17	4	10	3	0	0
3	C	1	17	4	10	3	0	0
3	D	1	17	4	10	3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C H O 10 2 6 2	0	0

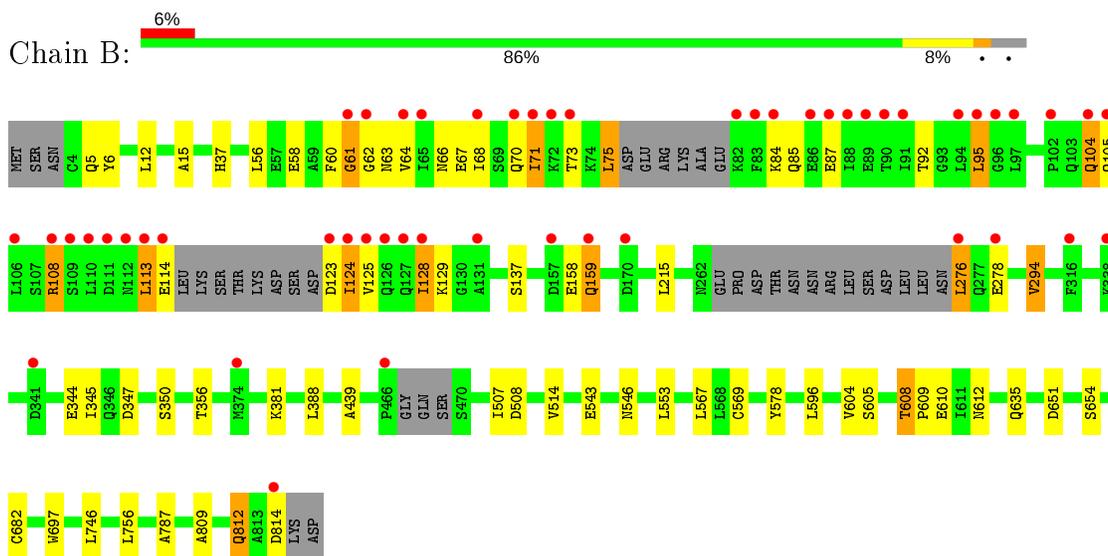
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	453	Total O 453 453	0	0
6	A	355	Total O 355 355	0	0
6	C	440	Total O 440 440	0	0
6	D	393	Total O 394 394	0	1

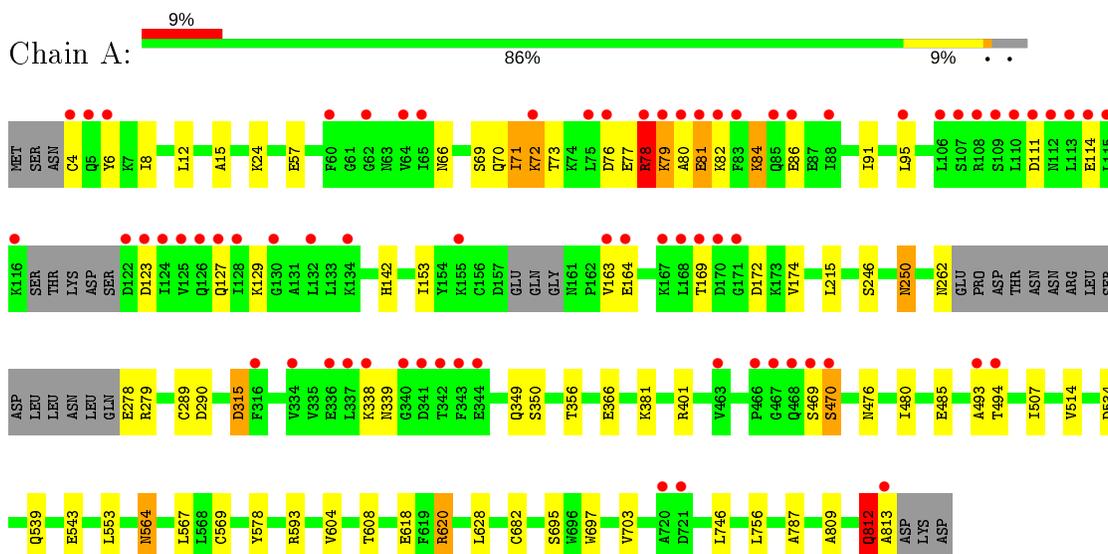
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

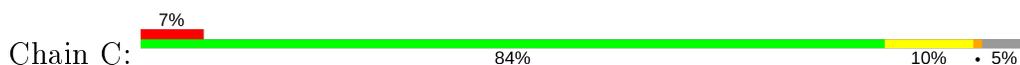
- Molecule 1: GoxA

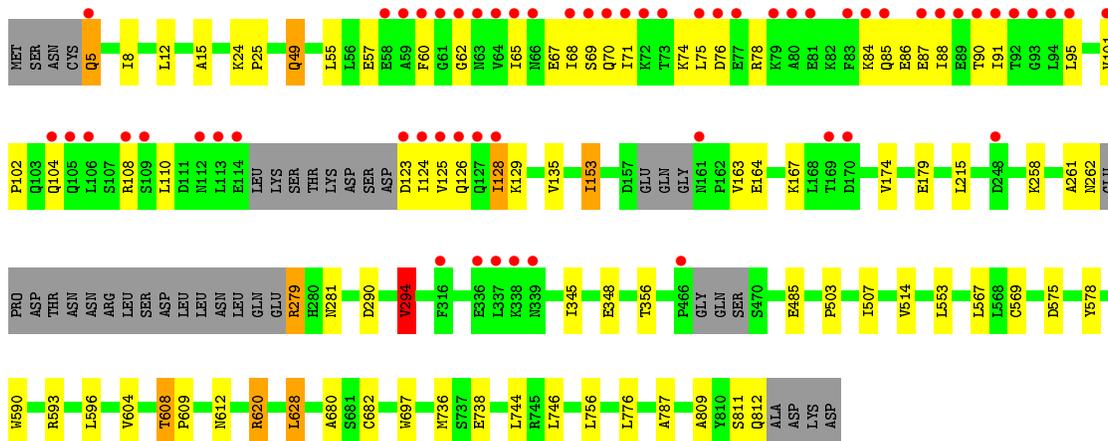


- Molecule 1: GoxA

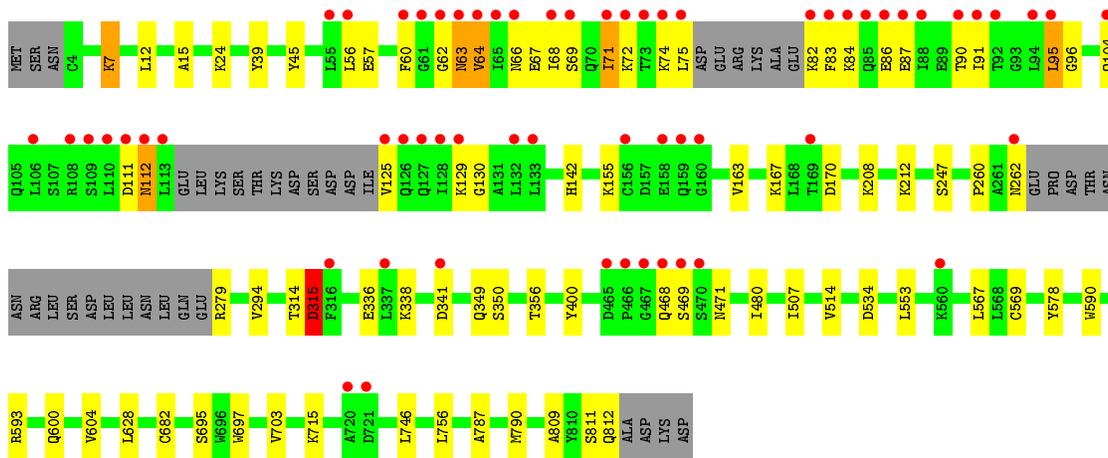
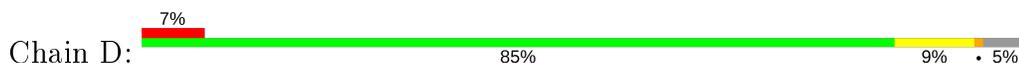


- Molecule 1: GoxA





• Molecule 1: GoxA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.84Å 93.24Å 188.46Å 90.00° 94.88° 90.00°	Depositor
Resolution (Å)	48.28 – 2.05 48.28 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.28-2.05) 98.8 (48.28-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.05Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.185 , 0.219 0.186 , 0.219	Depositor DCC
R_{free} test set	11722 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtrriage
Anisotropy	0.459	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49970	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: TRQ, MG, PEG, EDO, SO4

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	0.28	0/6376	0.50	0/8678
1	B	0.28	0/6319	0.53	4/8602 (0.0%)
1	C	0.27	0/6299	0.52	3/8573 (0.0%)
1	D	0.27	0/6274	0.50	0/8542
All	All	0.28	0/25268	0.51	7/34395 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	VAL	CG1-CB-CG2	7.47	122.86	110.90
1	C	294	VAL	CG1-CB-CG2	6.63	121.51	110.90
1	B	276	LEU	CB-CG-CD2	6.61	122.24	111.00
1	B	75	LEU	CB-CG-CD1	6.41	121.89	111.00
1	C	55	LEU	C-N-CA	6.09	136.92	121.70

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	6244	5913	6010	49	0
1	B	6188	5858	5954	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6168	5875	5941	49	2
1	D	6142	5831	5913	42	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	14	20	20	1	0
3	B	7	10	10	0	0
3	C	7	10	10	2	0
3	D	7	10	10	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
5	D	4	6	6	0	0
6	A	355	0	0	5	0
6	B	453	0	0	5	0
6	C	440	0	0	5	0
6	D	394	0	0	2	0
All	All	26437	23533	23874	179	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 4.

The worst 5 of 179 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:D:82:LYS:NZ	1:D:111:ASP:O	1.94	0.98
1:A:246:SER:O	6:A:1001:HOH:O	1.90	0.89
1:C:78:ARG:NH2	1:C:87:GLU:OE2	2.06	0.89
1:A:80:ALA:HA	1:A:81:GLU:CB	2.05	0.86
1:C:485:GLU:OE2	6:C:1001:HOH:O	1.99	0.80

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)
1:C:84:LYS:HZ3	1:D:170:ASP:OD2[1_455]	1.55	0.05
1:C:84:LYS:NZ	1:D:170:ASP:OD2[1_455]	2.17	0.03

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	781/816 (96%)	749 (96%)	28 (4%)	4 (0%)	29	18
1	B	772/816 (95%)	752 (97%)	18 (2%)	2 (0%)	41	31
1	C	768/816 (94%)	743 (97%)	25 (3%)	0	100	100
1	D	769/816 (94%)	737 (96%)	26 (3%)	6 (1%)	19	10
All	All	3090/3264 (95%)	2981 (96%)	97 (3%)	12 (0%)	34	24

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	VAL
1	D	315[A]	ASP
1	D	315[B]	ASP
1	B	61	GLY
1	A	78	ARG

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	685/711 (96%)	647 (94%)	38 (6%)	21	13
1	B	679/711 (96%)	641 (94%)	38 (6%)	21	12
1	C	677/711 (95%)	645 (95%)	32 (5%)	26	18
1	D	674/711 (95%)	648 (96%)	26 (4%)	32	25
All	All	2715/2844 (96%)	2581 (95%)	134 (5%)	25	17

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315[A]	ASP
1	A	812	GLN
1	D	336	GLU
1	A	381	LYS
1	A	578	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	D	471	ASN
1	D	600	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TRQ	D	697	1	13,17,18	4.84	7 (53%)	14,24,26	3.60	4 (28%)
1	TRQ	A	697	1	13,17,18	4.85	6 (46%)	14,24,26	3.55	3 (21%)
1	TRQ	C	697	1	13,17,18	4.72	5 (38%)	14,24,26	3.74	5 (35%)
1	TRQ	B	697	1	13,17,18	4.78	7 (53%)	14,24,26	3.56	4 (28%)

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	TRQ	D	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	A	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	C	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	B	697	1	-	0/4/19/21	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CH2-CZ2	-12.05	1.40	1.54
1	D	697	TRQ	CH2-CZ2	-11.81	1.40	1.54
1	B	697	TRQ	CH2-CZ2	-11.74	1.40	1.54
1	C	697	TRQ	CH2-CZ2	-11.25	1.41	1.54
1	C	697	TRQ	CE2-CZ2	-7.99	1.39	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	TRQ	CZ2-CE2-NE1	11.74	138.69	119.94
1	D	697	TRQ	CZ2-CE2-NE1	11.48	138.27	119.94
1	B	697	TRQ	CZ2-CE2-NE1	11.46	138.24	119.94
1	C	697	TRQ	CZ2-CE2-NE1	11.39	138.13	119.94
1	B	697	TRQ	CD2-CE2-NE1	-4.64	102.14	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	697	TRQ	1	0
1	A	697	TRQ	1	0
1	C	697	TRQ	1	0
1	B	697	TRQ	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	PEG	D	902	-	6,6,6	0.46	0	5,5,5	0.43	0
3	PEG	A	903	-	6,6,6	0.46	0	5,5,5	0.27	0
5	EDO	D	903	-	3,3,3	0.49	0	2,2,2	0.27	0
3	PEG	A	902	-	6,6,6	0.49	0	5,5,5	1.11	0
4	SO4	C	903	-	4,4,4	0.16	0	6,6,6	0.18	0
3	PEG	C	902	-	6,6,6	0.56	0	5,5,5	0.43	0
3	PEG	B	902	-	6,6,6	0.48	0	5,5,5	0.23	0
4	SO4	B	903	-	4,4,4	0.11	0	6,6,6	0.20	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	PEG	D	902	-	-	2/4/4/4	-
3	PEG	A	903	-	-	1/4/4/4	-
5	EDO	D	903	-	-	0/1/1/1	-
3	PEG	A	902	-	-	3/4/4/4	-
3	PEG	C	902	-	-	2/4/4/4	-
3	PEG	B	902	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	C	902	PEG	O1-C1-C2-O2
3	A	902	PEG	O2-C3-C4-O4
3	D	902	PEG	O1-C1-C2-O2
3	A	903	PEG	O2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	PEG	1	0
3	C	902	PEG	2	0
4	B	903	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	786/816 (96%)	0.31	70 (8%) 9 10	19, 37, 83, 116	0
1	B	780/816 (95%)	0.21	51 (6%) 18 20	15, 28, 79, 122	0
1	C	777/816 (95%)	0.23	59 (7%) 13 14	16, 29, 74, 109	0
1	D	775/816 (94%)	0.28	61 (7%) 12 13	17, 33, 86, 139	0
All	All	3118/3264 (95%)	0.26	241 (7%) 13 14	15, 32, 81, 139	0

The worst 5 of 241 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	8.4
1	B	110	LEU	7.7
1	B	83	PHE	7.7
1	D	75	LEU	7.6
1	C	62	GLY	7.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TRQ	A	697	16/17	0.95	0.18	19,20,30,47	0
1	TRQ	D	697	16/17	0.96	0.17	19,20,29,32	0
1	TRQ	C	697	16/17	0.97	0.16	16,17,34,44	0
1	TRQ	B	697	16/17	0.97	0.17	15,16,31,32	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	PEG	D	902	7/7	0.53	0.31	50,63,76,76	0
3	PEG	A	903	7/7	0.71	0.26	46,61,93,93	0
3	PEG	C	902	7/7	0.85	0.21	34,55,72,80	0
3	PEG	A	902	7/7	0.88	0.19	52,63,77,77	0
3	PEG	B	902	7/7	0.91	0.11	33,46,57,64	0
5	EDO	D	903	4/4	0.92	0.11	49,59,65,78	0
4	SO4	C	903	5/5	0.92	0.28	56,66,76,88	0
4	SO4	B	903	5/5	0.95	0.25	72,76,104,107	0
2	MG	C	901	1/1	0.98	0.06	20,20,20,20	0
2	MG	A	901	1/1	0.98	0.13	24,24,24,24	0
2	MG	D	901	1/1	0.98	0.16	23,23,23,23	0
2	MG	B	901	1/1	0.98	0.10	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.