wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 12:52 am GMT

PDB ID	:	8B65
Title	:	Structure of rsCherry crystallized in anaerobic conditions
Authors	:	Bui, T.Y.H.; Van Meervelt, L.
Deposited on	:	2022-09-26
Resolution	:	1.55 Å(reported)

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

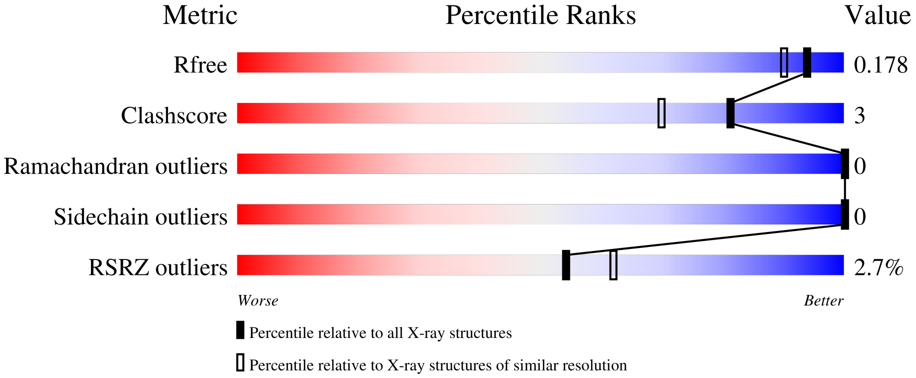
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

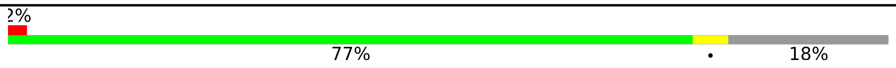
The reported resolution of this entry is 1.55 Å.

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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	270	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 2222 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 rsCherry.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	220	1917	1230	320	356	11	0	24	0

There are 91 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	initiating methionine	UNP Q9U6Y8
A	-38	ARG	-	expression tag	UNP Q9U6Y8
A	-37	GLY	-	expression tag	UNP Q9U6Y8
A	-36	SER	-	expression tag	UNP Q9U6Y8
A	-35	HIS	-	expression tag	UNP Q9U6Y8
A	-34	HIS	-	expression tag	UNP Q9U6Y8
A	-33	HIS	-	expression tag	UNP Q9U6Y8
A	-32	HIS	-	expression tag	UNP Q9U6Y8
A	-31	HIS	-	expression tag	UNP Q9U6Y8
A	-30	HIS	-	expression tag	UNP Q9U6Y8
A	-29	GLY	-	expression tag	UNP Q9U6Y8
A	-28	MET	-	expression tag	UNP Q9U6Y8
A	-27	ALA	-	expression tag	UNP Q9U6Y8
A	-26	SER	-	expression tag	UNP Q9U6Y8
A	-25	MET	-	expression tag	UNP Q9U6Y8
A	-24	THR	-	expression tag	UNP Q9U6Y8
A	-23	GLY	-	expression tag	UNP Q9U6Y8
A	-22	GLY	-	expression tag	UNP Q9U6Y8
A	-21	GLN	-	expression tag	UNP Q9U6Y8
A	-20	GLN	-	expression tag	UNP Q9U6Y8
A	-19	MET	-	expression tag	UNP Q9U6Y8
A	-18	GLY	-	expression tag	UNP Q9U6Y8
A	-17	ARG	-	expression tag	UNP Q9U6Y8
A	-16	ASP	-	expression tag	UNP Q9U6Y8
A	-15	LEU	-	expression tag	UNP Q9U6Y8
A	-14	TYR	-	expression tag	UNP Q9U6Y8
A	-13	ASP	-	expression tag	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ASP	-	expression tag	UNP Q9U6Y8
A	-11	ASP	-	expression tag	UNP Q9U6Y8
A	-10	ASP	-	expression tag	UNP Q9U6Y8
A	-9	LYS	-	expression tag	UNP Q9U6Y8
A	-8	ASP	-	expression tag	UNP Q9U6Y8
A	-7	PRO	-	expression tag	UNP Q9U6Y8
A	-6	ALA	-	expression tag	UNP Q9U6Y8
A	-5	THR	-	expression tag	UNP Q9U6Y8
A	-4	MET	-	expression tag	UNP Q9U6Y8
A	-3	VAL	-	expression tag	UNP Q9U6Y8
A	-2	SER	-	expression tag	UNP Q9U6Y8
A	-1	LYS	-	expression tag	UNP Q9U6Y8
A	0	GLY	-	expression tag	UNP Q9U6Y8
A	1	GLU	-	expression tag	UNP Q9U6Y8
A	2	GLU	-	expression tag	UNP Q9U6Y8
A	3	ASP	-	expression tag	UNP Q9U6Y8
A	4	ASN	-	expression tag	UNP Q9U6Y8
A	5	MET	-	expression tag	UNP Q9U6Y8
A	6	ALA	-	expression tag	UNP Q9U6Y8
A	7	ILE	-	expression tag	UNP Q9U6Y8
A	17	HIS	ARG	engineered mutation	UNP Q9U6Y8
A	21	SER	THR	engineered mutation	UNP Q9U6Y8
A	41	THR	HIS	engineered mutation	UNP Q9U6Y8
A	42	GLN	ASN	engineered mutation	UNP Q9U6Y8
A	44	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	66	QYX	GLN	chromophore	UNP Q9U6Y8
A	66	QYX	TYR	chromophore	UNP Q9U6Y8
A	66	QYX	GLY	chromophore	UNP Q9U6Y8
A	71	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	83	LEU	LYS	engineered mutation	UNP Q9U6Y8
A	117	GLU	CYS	engineered mutation	UNP Q9U6Y8
A	124	LEU	PHE	engineered mutation	UNP Q9U6Y8
A	125	ARG	ILE	engineered mutation	UNP Q9U6Y8
A	127	THR	VAL	engineered mutation	UNP Q9U6Y8
A	144	VAL	GLU	engineered mutation	UNP Q9U6Y8
A	147	SER	THR	engineered mutation	UNP Q9U6Y8
A	150	MET	LEU	engineered mutation	UNP Q9U6Y8
A	153	GLU	ARG	engineered mutation	UNP Q9U6Y8
A	156	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	161	SER	ILE	engineered mutation	UNP Q9U6Y8
A	162	LYS	HIS	engineered mutation	UNP Q9U6Y8
A	163	GLN	LYS	engineered mutation	UNP Q9U6Y8

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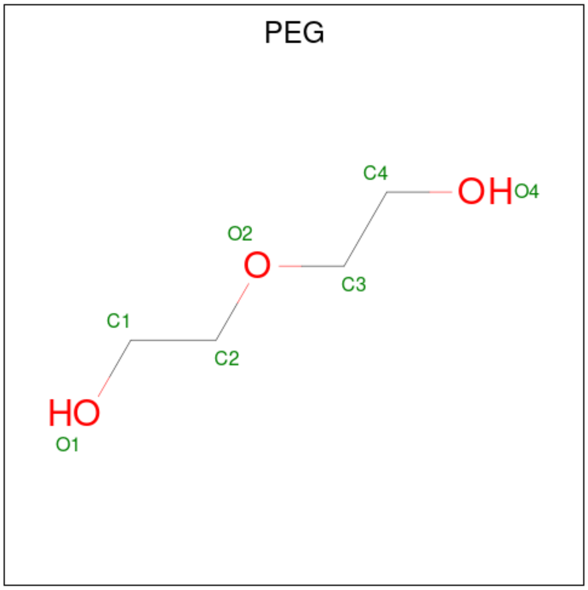
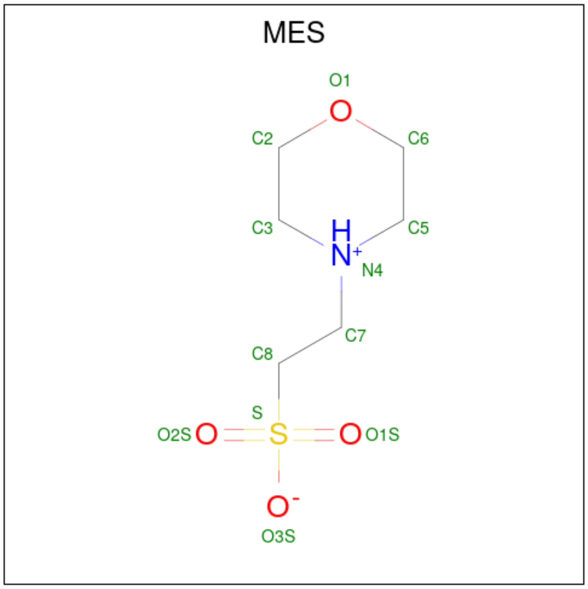
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	ARG	ALA	engineered mutation	UNP Q9U6Y8
A	174	ASP	LEU	engineered mutation	UNP Q9U6Y8
A	175	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	178	TRP	LYS	engineered mutation	UNP Q9U6Y8
A	179	THR	SER	engineered mutation	UNP Q9U6Y8
A	180	THR	ILE	engineered mutation	UNP Q9U6Y8
A	182	LYS	MET	engineered mutation	UNP Q9U6Y8
A	192	ALA	TYR	engineered mutation	UNP Q9U6Y8
A	194	ASN	TYR	engineered mutation	UNP Q9U6Y8
A	196	ASN	ASP	engineered mutation	UNP Q9U6Y8
A	197	ILE	SER	engineered mutation	UNP Q9U6Y8
A	217	ALA	THR	engineered mutation	UNP Q9U6Y8
A	222	SER	-	expression tag	UNP Q9U6Y8
A	223	THR	-	expression tag	UNP Q9U6Y8
A	224	GLY	-	expression tag	UNP Q9U6Y8
A	225	GLY	-	expression tag	UNP Q9U6Y8
A	226	MET	-	expression tag	UNP Q9U6Y8
A	227	ASP	-	expression tag	UNP Q9U6Y8
A	228	GLU	-	expression tag	UNP Q9U6Y8
A	229	LEU	-	expression tag	UNP Q9U6Y8
A	230	TYR	-	expression tag	UNP Q9U6Y8
A	231	LYS	-	expression tag	UNP Q9U6Y8

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



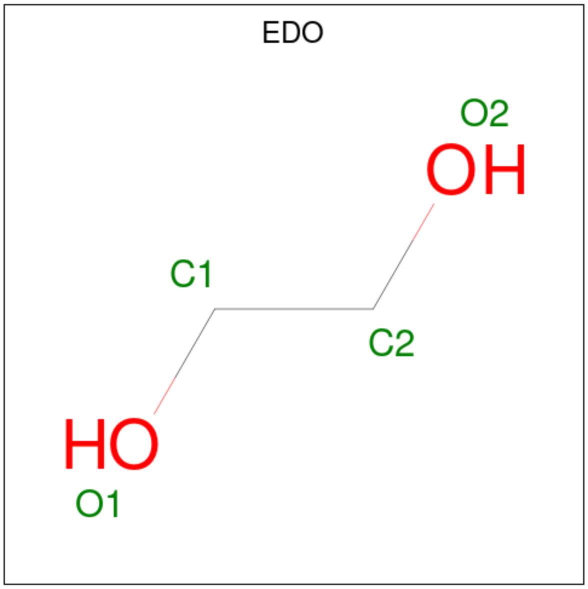
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	7	4	3	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



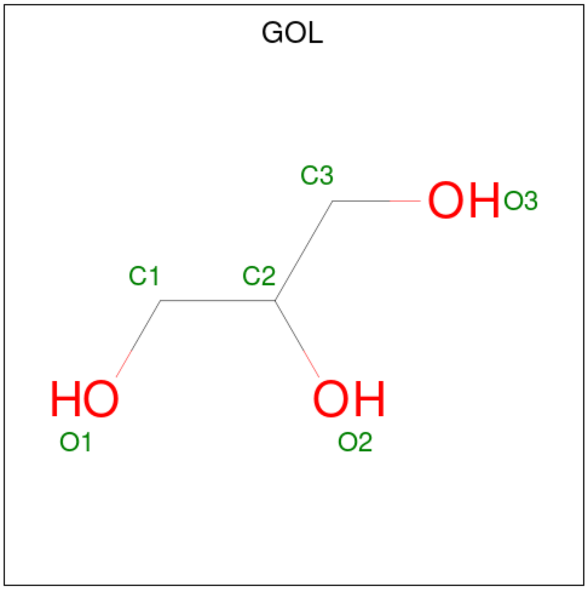
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	8	2	2	0	1

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	1

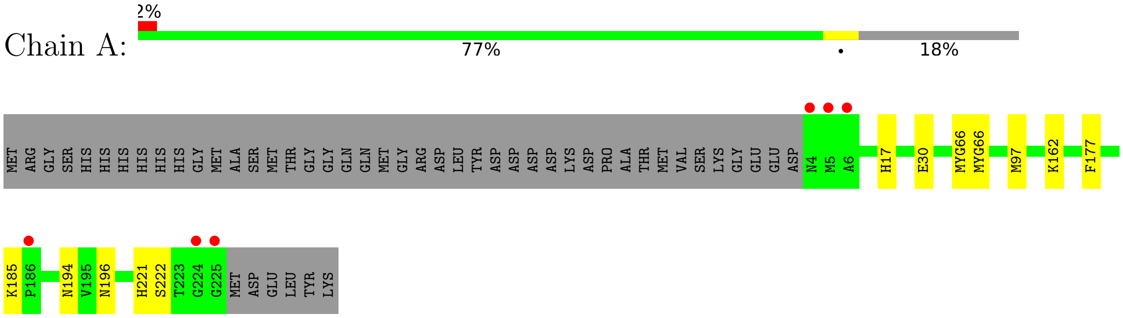
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	269	Total O 272 272	0	22

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: rsCherry



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	61.17Å 42.90Å 108.57Å 90.00° 105.76° 90.00°	Depositor
Resolution (Å)	46.20 – 1.55 46.20 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.20-1.55) 95.8 (46.20-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.151 , 0.179 0.151 , 0.178	Depositor DCC
R_{free} test set	1963 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.3	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	2222	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GOL, Q2K, EDO, QYX, PEG

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	0.64	0/1965	0.82	0/2638

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	A	1917	0	1845	7	0
2	A	7	0	10	2	0
3	A	12	0	16	1	0
4	A	8	0	12	1	0
5	A	6	0	8	1	0
6	A	272	0	0	4	0
All	All	2222	0	1891	10	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 3.

The worst 5 of 10 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:HB3	2:A:301:PEG:H32	1.67	0.76
1:A:162:LYS:CD	6:A:584:HOH:O	2.37	0.72
1:A:194:ASN:OD1	1:A:222[A]:SER:HA	2.04	0.58
1:A:221[B]:HIS:O	5:A:304[B]:GOL:H12	2.06	0.56
1:A:185:LYS:HG2	6:A:435:HOH:O	2.12	0.49

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	A	236/270 (87%)	231 (98%)	5 (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	202/226 (89%)	202 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

2 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	Q2K	A	66[B]	1	15,16,17	0.96	1 (6%)	8,21,23	1.33	1 (12%)
1	QYX	A	66[A]	1	22,24,25	2.83	6 (27%)	16,32,34	2.84	3 (18%)

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	Q2K	A	66[B]	1	-	1/5/27/28	0/1/1/1
1	QYX	A	66[A]	1	-	3/9/31/32	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66[A]	QYX	CB2-CA2	-11.03	1.38	1.50
1	A	66[A]	QYX	CA2-N2	4.33	1.43	1.35
1	A	66[A]	QYX	C1-N2	-3.13	1.31	1.35
1	A	66[A]	QYX	C1-N3	3.05	1.40	1.37
1	A	66[A]	QYX	CB2-CG2	-2.41	1.47	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66[A]	QYX	CG2-CB2-CA2	7.74	132.01	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66[A]	QYX	O2-C2-CA2	7.41	135.73	120.67
1	A	66[A]	QYX	O3-C3-CA3	-2.56	119.05	126.32
1	A	66[B]	Q2K	O3-C3-CA3	-2.27	119.54	126.39

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66[A]	QYX	N2-CA2-CB2-CG2
1	A	66[A]	QYX	C3-CA3-N3-C2
1	A	66[B]	Q2K	CB1-CG1-SD-CE
1	A	66[A]	QYX	C2-CA2-CB2-CG2

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)

6 ligands 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	$\#\|Z\| > 2$
4	EDO	A	303	-	3,3,3	0.06	0	2,2,2	0.30	0
4	EDO	A	305	-	3,3,3	0.08	0	2,2,2	0.03	0
2	PEG	A	301	-	6,6,6	0.52	0	5,5,5	0.52	0
3	MES	A	302[B]	-	6,6,12	0.49	0	6,6,16	0.35	0
5	GOL	A	304[B]	-	5,5,5	0.09	0	5,5,5	0.45	0
3	MES	A	302[A]	-	6,6,12	0.48	0	6,6,16	0.32	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	EDO	A	303	-	-	0/1/1/1	-
4	EDO	A	305	-	-	0/1/1/1	-
2	PEG	A	301	-	-	2/4/4/4	-
3	MES	A	302[B]	-	-	-	0/1/1/1
5	GOL	A	304[B]	-	-	3/4/4/4	-
3	MES	A	302[A]	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304[B]	GOL	C1-C2-C3-O3
2	A	301	PEG	C4-C3-O2-C2
5	A	304[B]	GOL	O2-C2-C3-O3
5	A	304[B]	GOL	O1-C1-C2-O2
2	A	301	PEG	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	EDO	1	0
2	A	301	PEG	2	0
3	A	302[B]	MES	1	0
5	A	304[B]	GOL	1	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 (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	219/270 (81%)	-0.37	6 (2%)	54	62	14, 19, 30, 57	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	MET	7.0
1	A	6	ALA	5.2
1	A	225[A]	GLY	3.7
1	A	4	ASN	2.9
1	A	224[A]	GLY	2.6

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	QYX	A	66[A]	23/24	0.96	0.07	15,18,21,24	23
1	Q2K	A	66[B]	16/17	0.98	0.06	15,19,21,25	16

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
4	EDO	A	303	4/4	0.65	0.16	42,47,48,50	0
2	PEG	A	301	7/7	0.81	0.18	30,35,49,51	0
4	EDO	A	305	4/4	0.85	0.24	40,47,53,54	0
3	MES	A	302[A]	6/12	0.93	0.11	27,28,33,33	6
3	MES	A	302[B]	6/12	0.93	0.11	27,29,32,34	6
5	GOL	A	304[B]	6/6	0.94	0.19	18,21,23,25	6

6.5 Other polymers (i)

There are no such residues in this entry.