WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 12, 2025 – 06:12 PM JST

PDB ID	:	9UJ2 / pdb_00009uj2
Title	:	14-3-3 zeta chimera with the S202R peptide of SARS-CoV-2 N (residues 200-213)
Authors	:	Boyko, K.M.; Matyuta, I.O.; Minyaev, M.E.; Perfilova, K.V.; Sluchanko, N.N.
Deposited on	:	2025-04-16
Resolution	:	1.80 Å(reported)

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

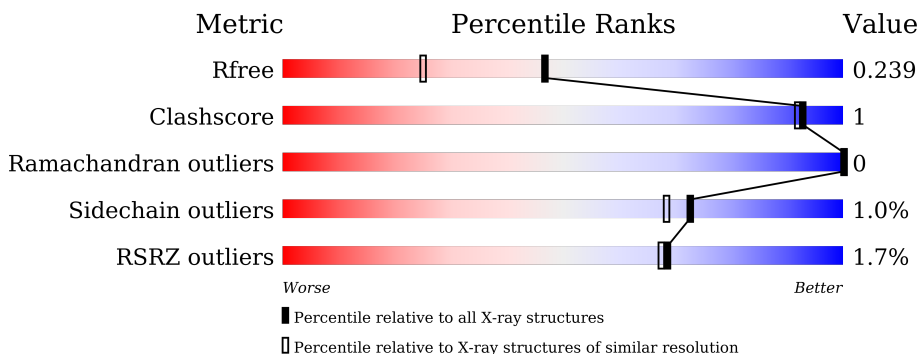|		
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 1.80 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		1.7%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	249	.% 91% 6% ·
2	A	249	2% 92% · · ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4448 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 14-3-3 protein zeta/delta,Peptide from Nucleoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	242	Total	C	N	O	P	S	0	7	0
			1948	1210	337	389	1	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P63104
B	-1	PRO	-	expression tag	UNP P63104
B	0	HIS	-	expression tag	UNP P63104
B	58	ALA	SER	engineered mutation	UNP P63104
B	73	ALA	GLU	engineered mutation	UNP P63104
B	74	ALA	LYS	engineered mutation	UNP P63104
B	75	ALA	LYS	engineered mutation	UNP P63104
B	157	ALA	LYS	engineered mutation	UNP P63104
B	158	ALA	LYS	engineered mutation	UNP P63104
B	159	ALA	GLU	engineered mutation	UNP P63104
B	230	GLY	-	linker	UNP P63104
B	231	GLY	-	linker	UNP P63104
B	232	GLY	-	linker	UNP P63104
B	235	ARG	SER	engineered mutation	UNP P0DTC9

- Molecule 2 is a protein called 14-3-3 protein zeta/delta,Peptide from Nucleoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	241	Total	C	N	O	P	S	0	9	0
			1950	1213	333	392	1	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P63104
A	-1	PRO	-	expression tag	UNP P63104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P63104
A	58	ALA	SER	engineered mutation	UNP P63104
A	73	ALA	GLU	engineered mutation	UNP P63104
A	74	ALA	LYS	engineered mutation	UNP P63104
A	75	ALA	LYS	engineered mutation	UNP P63104
A	157	ALA	LYS	engineered mutation	UNP P63104
A	158	ALA	LYS	engineered mutation	UNP P63104
A	159	ALA	GLU	engineered mutation	UNP P63104
A	230	GLY	-	linker	UNP P63104
A	231	GLY	-	linker	UNP P63104
A	232	GLY	-	linker	UNP P63104
A	235	ARG	SER	engineered mutation	UNP P0DTC9

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).
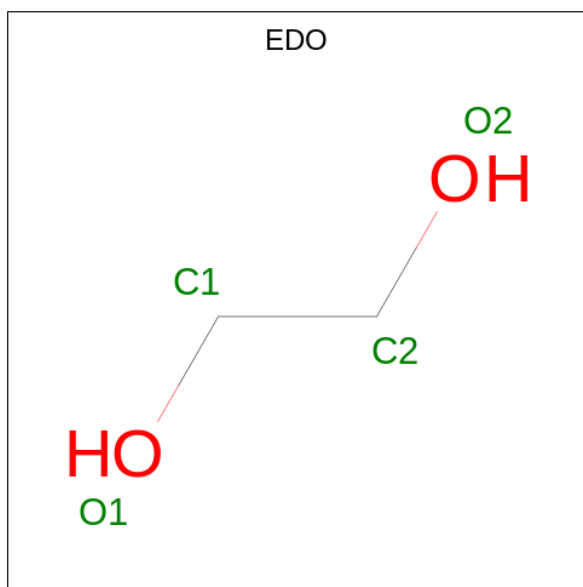
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).
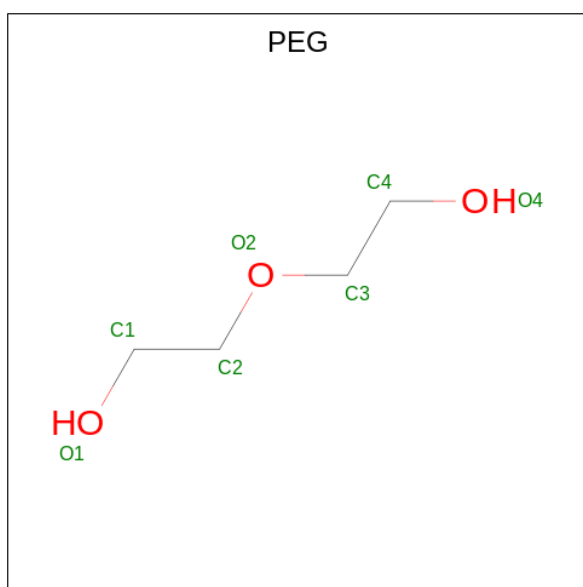
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 7	C 4	O 3	0	0
4	A	1	Total 7	C 4	O 3	0	0
4	A	1	Total 7	C 4	O 3	0	0
4	A	1	Total 7	C 4	O 3	0	0
4	A	1	Total 7	C 4	O 3	0	0
4	A	1	Total 7	C 4	O 3	0	0
4	A	1	Total 7	C 4	O 3	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	225	Total 225	O 225	0	2
5	A	212	Total 212	O 212	0	3

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: 14-3-3 protein zeta/delta,Peptide from Nucleoprotein
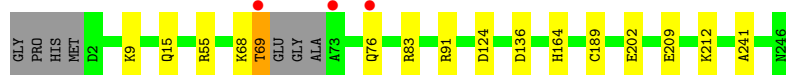
• Molecule 2: 14-3-3 protein zeta/delta,Peptide from Nucleoprotein
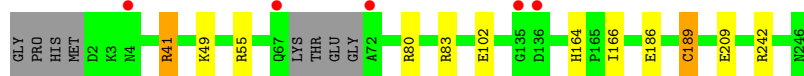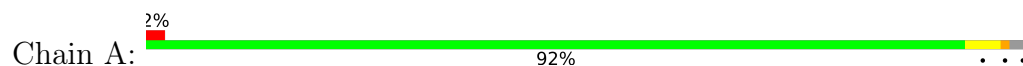
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.55Å 84.45Å 139.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.76 – 1.80 21.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (21.76-1.80) 99.4 (21.76-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.195 , 0.233 0.203 , 0.239	Depositor DCC
R_{free} test set	3243 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.0	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4448	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 5.05% 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: TPO, EDO, CME, PEG, OCY

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	0.78	1/1957 (0.1%)	1.39	7/2627 (0.3%)
2	A	0.77	0/1970	1.35	5/2645 (0.2%)
All	All	0.77	1/3927 (0.0%)	1.37	12/5272 (0.2%)

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	2
2	A	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	HIS	CG-CD2	-5.50	1.29	1.35

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	THR	CA-CB-OG1	-6.77	99.45	109.60
2	A	83	ARG	CD-NE-CZ	6.35	133.29	124.40
1	B	209	GLU	CB-CG-CD	6.26	123.23	112.60
2	A	80	ARG	CD-NE-CZ	6.05	132.87	124.40
1	B	9	LYS	CB-CG-CD	6.03	125.17	111.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	242	ARG	Sidechain
2	A	55	ARG	Sidechain
1	B	55	ARG	Sidechain
1	B	91[A]	ARG	Sidechain

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	1948	0	1926	3	0
2	A	1950	0	1924	8	0
3	A	36	0	54	0	0
3	B	28	0	42	0	0
4	A	42	0	59	5	0
4	B	7	0	10	2	0
5	A	212	0	0	1	0
5	B	225	0	0	0	0
All	All	4448	0	4015	11	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.

The worst 5 of 11 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:A:189:CME:SD	2:A:189:CME:SG	2.33	1.27
2:A:49[A]:LYS:NZ	4:A:315[A]:PEG:H21	2.02	0.74
2:A:49[C]:LYS:NZ	5:A:401[C]:HOH:O	2.28	0.61
1:B:241:ALA:H	4:B:307:PEG:H21	1.68	0.59
2:A:166:ILE:HD11	4:A:312:PEG:H42	1.89	0.54

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	243/249 (98%)	242 (100%)	1 (0%)	0	100	100
2	A	245/249 (98%)	244 (100%)	1 (0%)	0	100	100
All	All	488/498 (98%)	486 (100%)	2 (0%)	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	203/201 (101%)	200 (98%)	3 (2%)	60	53
2	A	203/201 (101%)	202 (100%)	1 (0%)	86	86
All	All	406/402 (101%)	402 (99%)	4 (1%)	73	68

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	B	68	LYS
1	B	212	LYS
2	A	209	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	67	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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	#$|Z| > 2$
2	TPO	A	238	2	8,10,11	0.75	0	10,14,16	0.90	0
1	TPO	B	238	1	8,10,11	0.50	0	10,14,16	0.65	0
2	CME	A	189	2	8,9,10	1.48	1 (12%)	5,9,11	0.68	0
1	OCY	B	189	1	7,8,9	0.50	0	4,8,10	1.72	1 (25%)

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
2	TPO	A	238	2	-	1/9/11/13	-
1	TPO	B	238	1	-	1/9/11/13	-
2	CME	A	189	2	-	0/5/8/10	-
1	OCY	B	189	1	-	0/5/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	189	CME	SD-SG	3.91	2.33	2.03

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	OCY	CE-CD-SG	-3.08	102.56	112.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	238	TPO	CB-OG1-P-O2P
2	A	238	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	189	CME	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 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	PEG	A	308	-	6,6,6	0.32	0	5,5,5	0.69	0
4	PEG	A	315[A]	-	6,6,6	1.29	1 (16%)	5,5,5	0.60	0
4	PEG	A	306	-	6,6,6	0.19	0	5,5,5	0.42	0
3	EDO	B	303	-	3,3,3	0.25	0	2,2,2	0.14	0
4	PEG	A	309	-	6,6,6	0.52	0	5,5,5	0.78	0
4	PEG	A	312	-	6,6,6	0.55	0	5,5,5	0.72	0
3	EDO	A	310	-	3,3,3	0.88	0	2,2,2	1.41	0
3	EDO	A	307	-	3,3,3	0.33	0	2,2,2	0.55	0
3	EDO	B	306	-	3,3,3	0.15	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	EDO	A	304	-	3,3,3	0.23	0	2,2,2	0.44	0
3	EDO	B	308	-	3,3,3	0.54	0	2,2,2	0.62	0
3	EDO	B	301	-	3,3,3	0.17	0	2,2,2	0.05	0
3	EDO	A	314	-	3,3,3	0.27	0	2,2,2	0.44	0
4	PEG	B	307	-	6,6,6	0.54	0	5,5,5	0.64	0
3	EDO	B	302	-	3,3,3	0.39	0	2,2,2	0.43	0
3	EDO	A	305	-	3,3,3	0.11	0	2,2,2	0.17	0
4	PEG	A	313	-	6,6,6	0.18	0	5,5,5	0.50	0
3	EDO	B	304	-	3,3,3	0.49	0	2,2,2	0.38	0
3	EDO	A	303	-	3,3,3	0.14	0	2,2,2	0.05	0
3	EDO	B	305	-	3,3,3	0.81	0	2,2,2	0.82	0
3	EDO	A	302	-	3,3,3	0.09	0	2,2,2	0.41	0
3	EDO	A	311	-	3,3,3	0.93	0	2,2,2	1.08	0
3	EDO	A	301	-	3,3,3	0.41	0	2,2,2	0.56	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	PEG	A	308	-	-	2/4/4/4	-
4	PEG	A	315[A]	-	-	2/4/4/4	-
4	PEG	A	306	-	-	2/4/4/4	-
3	EDO	B	303	-	-	0/1/1/1	-
4	PEG	A	309	-	-	3/4/4/4	-
4	PEG	A	312	-	-	3/4/4/4	-
3	EDO	A	310	-	-	1/1/1/1	-
3	EDO	A	307	-	-	1/1/1/1	-
3	EDO	B	306	-	-	1/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	B	308	-	-	1/1/1/1	-
3	EDO	B	301	-	-	0/1/1/1	-
3	EDO	A	314	-	-	1/1/1/1	-
4	PEG	B	307	-	-	2/4/4/4	-
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	A	305	-	-	0/1/1/1	-
4	PEG	A	313	-	-	2/4/4/4	-
3	EDO	B	304	-	-	0/1/1/1	-
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	B	305	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	A	311	-	-	1/1/1/1	-
3	EDO	A	301	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	315[A]	PEG	C3-C4	-2.90	1.34	1.49

There are no bond angle outliers.

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	309	PEG	C4-C3-O2-C2
4	A	315[A]	PEG	O1-C1-C2-O2
4	A	312	PEG	O1-C1-C2-O2
3	A	301	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	315[A]	PEG	3	0
4	A	312	PEG	2	0
4	B	307	PEG	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(Å²)	Q<0.9
1	B	240/249 (96%)	-0.22	3 (1%)	74	74	8, 24, 51, 75	7 (2%)
2	A	239/249 (95%)	-0.24	5 (2%)	63	62	7, 23, 48, 69	9 (3%)
All	All	479/498 (96%)	-0.23	8 (1%)	69	67	7, 24, 49, 75	16 (3%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	THR	4.0
1	B	73	ALA	3.8
2	A	72	ALA	3.6
2	A	136	ASP	3.2
2	A	135	GLY	2.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å²)	Q<0.9
1	OCY	B	189	9/10	0.96	0.08	18,20,29,36	0
2	CME	A	189	10/11	0.97	0.07	18,24,30,31	0
1	TPO	B	238	11/12	0.99	0.04	12,13,15,15	0
2	TPO	A	238	11/12	0.99	0.03	13,14,15,15	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

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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, 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
4	PEG	A	315[A]	7/7	0.74	0.20	19,22,30,30	7
3	EDO	A	301	4/4	0.76	0.19	43,45,49,52	0
3	EDO	A	303	4/4	0.79	0.15	45,46,48,49	0
3	EDO	B	308	4/4	0.79	0.17	51,53,53,53	0
4	PEG	A	313	7/7	0.80	0.17	46,47,53,54	0
3	EDO	B	303	4/4	0.81	0.18	49,49,51,56	0
4	PEG	A	306	7/7	0.82	0.16	44,45,48,48	7
4	PEG	A	309	7/7	0.82	0.17	47,49,55,58	0
3	EDO	B	302	4/4	0.83	0.14	40,43,44,48	0
4	PEG	A	308	7/7	0.84	0.16	33,37,40,40	7
3	EDO	A	305	4/4	0.85	0.16	48,53,54,57	0
3	EDO	A	304	4/4	0.85	0.13	49,53,54,60	0
3	EDO	A	310	4/4	0.86	0.15	20,28,28,30	4
3	EDO	A	302	4/4	0.88	0.12	38,43,44,51	0
3	EDO	A	307	4/4	0.89	0.13	35,37,40,41	0
4	PEG	B	307	7/7	0.90	0.18	23,26,51,52	0
3	EDO	B	301	4/4	0.90	0.12	42,42,43,43	0
3	EDO	B	305	4/4	0.92	0.11	23,24,26,27	0
4	PEG	A	312	7/7	0.92	0.11	32,34,35,36	7
3	EDO	A	314	4/4	0.93	0.12	37,42,42,45	0
3	EDO	B	304	4/4	0.93	0.10	24,32,33,38	0
3	EDO	B	306	4/4	0.94	0.12	36,40,42,49	0
3	EDO	A	311	4/4	0.94	0.10	18,25,26,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.