



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:31 PM UTC

PDB ID : 9QOG / pdb\_00009qog  
Title : Crystal structure of Nanofitin C10 in complex with a a double-helical aromatic oligoamide foldamer  
Authors : Sigl, J.C.; Sachs, J.; Merlet, E.; Ferrand, Y.; Huc, I.  
Deposited on : 2025-03-26  
Resolution : 1.85 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

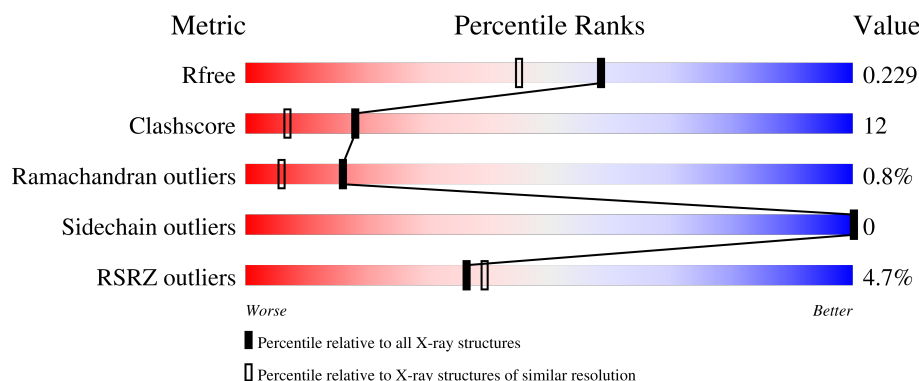
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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  $\geq 3$ , 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	66	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	66	<div> <div>6%</div> <div>76%</div> <div>20%</div> <div>5%</div> </div>
2	C	10	<div> <div>10%</div> <div>80%</div> <div>10%</div> </div>
2	D	10	<div> <div>80%</div> <div>20%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 1629 atoms, of which 19 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 Nanofitin C10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	S	0	1	0
			533	343	93	96	1			
1	B	63	Total	C	N	O	S	0	4	0
			536	344	92	99	1			

- Molecule 2 is a protein (with D amino acids) called Aromatic oligoamide foldamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	H	N	O	0	0	0
			177	119	5	23	30			
2	D	10	Total	C	H	N	O	0	0	0
			176	119	4	23	30			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C H O 17 4 10 3	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	78	Total O 78 78	0	0
6	B	45	Total O 45 45	0	0
6	C	30	Total O 30 30	0	0

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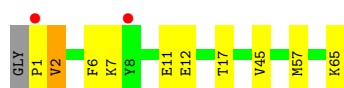
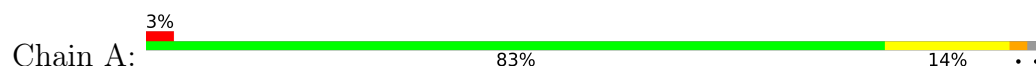
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	24	Total	O	0	0
			24	24		

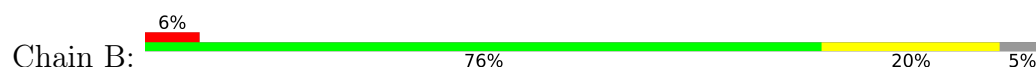
### 3 Residue-property plots [i](#)

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: Nanofitin C10



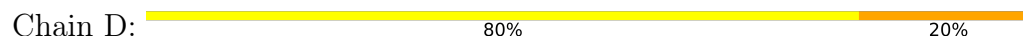
- Molecule 1: Nanofitin C10



- Molecule 2: Aromatic oligoamide foldamer



- Molecule 2: Aromatic oligoamide foldamer



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.90Å 85.90Å 56.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.27 – 1.85 17.27 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (17.27-1.85) 99.7 (17.27-1.85)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.85Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.187 , 0.229 0.187 , 0.229	Depositor DCC
$R_{free}$ test set	1860 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: QVS, ACE, QOL, QUK, SO4, A1I9S, CL, PEG, QVE

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	0.35	0/544	0.51	0/728
1	B	0.31	0/548	0.52	0/736
All	All	0.33	0/1092	0.51	0/1464

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
2	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	7	QUK	Peptide
2	D	7	QUK	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	533	0	547	11	0
1	B	536	0	534	18	0
2	C	172	5	3	0	0
2	D	172	4	3	1	0
3	A	5	0	0	1	0
4	C	7	0	10	0	0
4	D	7	10	10	0	0
5	C	1	0	0	0	0
6	A	78	0	0	7	0
6	B	45	0	0	4	0
6	C	30	0	0	0	0
6	D	24	0	0	0	1
All	All	1610	19	1107	31	1

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 12.

All (31) 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:16:ASP:CB	1:B:19[A]:LYS:HE3	2.15	0.77
1:A:12:GLU:OE1	6:A:201:HOH:O	2.03	0.76
1:B:0:GLY:O	1:B:53[A]:GLU:HG2	1.85	0.76
1:B:16:ASP:HB3	1:B:19[A]:LYS:HE3	1.70	0.73
1:A:2:VAL:N	6:A:203:HOH:O	2.21	0.73
3:A:101:SO4:O3	6:A:202:HOH:O	2.11	0.68
1:A:17:THR:HB	1:A:57:MET:HE1	1.76	0.68
1:B:19[A]:LYS:HD3	1:B:36:ASP:CG	2.18	0.68
1:A:6:PHE:HB3	1:A:45[B]:VAL:CG2	2.28	0.64
1:B:25:ARG:HG2	1:B:58:LEU:HD21	1.79	0.63
1:B:0:GLY:O	1:B:2:VAL:HG13	1.99	0.61
1:B:16:ASP:H	1:B:19[A]:LYS:NZ	2.00	0.59
1:B:50:ALA:HB3	1:B:55:LEU:HD21	1.84	0.59
1:B:6:PHE:CZ	1:B:13:LYS:HD3	2.38	0.58
1:B:16:ASP:HB2	1:B:19[A]:LYS:HE3	1.84	0.57
1:A:1:PRO:HG2	6:A:203:HOH:O	2.04	0.56
1:B:19[B]:LYS:HE2	6:B:122:HOH:O	2.06	0.55
1:B:13:LYS:NZ	6:B:104:HOH:O	2.41	0.53
1:B:2:VAL:HA	6:B:101:HOH:O	2.08	0.52
1:B:50:ALA:CB	1:B:55:LEU:HD21	2.40	0.52
1:A:65:LYS:HG2	6:A:264:HOH:O	2.09	0.51
1:A:1:PRO:HB2	6:A:203:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HE2	6:A:210:HOH:O	2.12	0.49
1:B:1:PRO:O	6:B:101:HOH:O	2.19	0.49
1:A:6:PHE:HB3	1:A:45[B]:VAL:HG22	1.94	0.49
1:B:25:ARG:CG	1:B:58:LEU:HD21	2.45	0.46
1:B:16:ASP:H	1:B:19[A]:LYS:HZ1	1.67	0.42
1:B:6:PHE:CZ	1:B:13:LYS:CD	3.03	0.41
1:A:7:LYS:HA	1:A:11:GLU:O	2.21	0.40
1:A:65:LYS:HA	1:A:65:LYS:HD3	1.93	0.40
2:D:1:ACE:O	2:D:2:A1I9S:C16	2.67	0.40

All (1) 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)
6:D:206:HOH:O	6:D:209:HOH:O[4_545]	1.97	0.23

## 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	A	64/66 (97%)	62 (97%)	1 (2%)	1 (2%)	7	2
1	B	65/66 (98%)	63 (97%)	2 (3%)	0	100	100
All	All	129/132 (98%)	125 (97%)	3 (2%)	1 (1%)	16	6

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	VAL

### 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	A	57/57 (100%)	57 (100%)	0	100	100
1	B	57/57 (100%)	57 (100%)	0	100	100
All	All	114/114 (100%)	114 (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. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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	A1I9S	C	3	2	21,21,22	1.06	1 (4%)	27,28,30	1.83	7 (25%)
2	QVE	D	6	2	19,19,20	1.21	2 (10%)	25,26,28	2.36	5 (20%)
2	A1I9S	C	5	2	21,21,22	1.11	3 (14%)	27,28,30	1.97	8 (29%)
2	A1I9S	D	4	2	21,21,22	1.05	2 (9%)	27,28,30	1.88	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	A1I9S	D	5	2	21,21,22	1.04	2 (9%)	27,28,30	1.91	6 (22%)
2	A1I9S	C	2	2	21,21,22	1.08	1 (4%)	27,28,30	1.91	6 (22%)
2	QVE	C	6	2	19,19,20	1.29	2 (10%)	25,26,28	1.96	7 (28%)
2	QOL	C	9	2	21,21,22	1.31	3 (14%)	25,28,30	1.89	5 (20%)
2	QOL	D	9	2	21,21,22	1.35	4 (19%)	25,28,30	1.82	4 (16%)
2	QUK	C	7	2	19,19,20	1.12	3 (15%)	24,25,27	1.78	5 (20%)
2	A1I9S	D	3	2	21,21,22	1.11	3 (14%)	27,28,30	1.42	2 (7%)
2	QVE	D	10	2	20,20,20	1.14	2 (10%)	28,28,28	1.17	2 (7%)
2	A1I9S	D	2	2	21,21,22	1.09	2 (9%)	27,28,30	1.76	7 (25%)
2	QUK	D	7	2	19,19,20	1.22	2 (10%)	24,25,27	1.91	4 (16%)
2	A1I9S	C	4	2	21,21,22	1.12	1 (4%)	27,28,30	1.73	4 (14%)
2	QVS	C	8	2	15,15,16	1.40	3 (20%)	20,21,23	1.94	4 (20%)
2	QVS	D	8	2	15,15,16	1.28	2 (13%)	20,21,23	1.74	4 (20%)
2	QVE	C	10	2	20,20,20	1.09	1 (5%)	28,28,28	1.12	2 (7%)

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	A1I9S	C	3	2	-	0/9/9/11	0/2/2/2
2	QVE	D	6	2	-	1/7/7/9	0/2/2/2
2	A1I9S	C	5	2	-	1/9/9/11	0/2/2/2
2	A1I9S	D	4	2	-	2/9/9/11	0/2/2/2
2	A1I9S	D	5	2	-	0/9/9/11	0/2/2/2
2	A1I9S	C	2	2	-	2/9/9/11	0/2/2/2
2	QVE	C	6	2	-	2/7/7/9	0/2/2/2
2	QOL	C	9	2	-	3/11/11/13	0/2/2/2
2	QOL	D	9	2	-	3/11/11/13	0/2/2/2
2	QUK	C	7	2	-	0/7/7/9	0/2/2/2
2	A1I9S	D	3	2	-	2/9/9/11	0/2/2/2
2	QVE	D	10	2	-	0/9/9/9	0/2/2/2
2	A1I9S	D	2	2	-	2/9/9/11	0/2/2/2
2	QUK	D	7	2	-	1/7/7/9	0/2/2/2
2	A1I9S	C	4	2	-	0/9/9/11	0/2/2/2
2	QVS	C	8	2	-	0/2/2/4	0/2/2/2
2	QVS	D	8	2	-	0/2/2/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	QVE	C	10	2	-	2/9/9/9	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	QVS	OB-C8	-2.75	1.28	1.36
2	C	5	A1I9S	C15-C12	-2.58	1.37	1.42
2	D	9	QOL	OZ1-CE1	-2.54	1.31	1.42
2	D	5	A1I9S	C15-C12	-2.51	1.37	1.42
2	C	8	QVS	OB-C8	-2.46	1.29	1.36
2	D	3	A1I9S	C11-C10	2.40	1.46	1.40
2	C	9	QOL	OZ1-CE1	-2.37	1.32	1.42
2	D	7	QUK	C10-C	2.37	1.51	1.48
2	C	6	QVE	CA-C	2.37	1.51	1.48
2	D	9	QOL	OZ2-CE2	-2.35	1.32	1.42
2	D	10	QVE	C4-C5	2.33	1.41	1.36
2	D	8	QVS	C8-C6	2.31	1.47	1.42
2	C	7	QUK	C10-C	2.26	1.51	1.48
2	C	7	QUK	C10-N11	2.23	1.35	1.33
2	D	3	A1I9S	CA-C	2.21	1.51	1.48
2	C	8	QVS	C5-C6	-2.20	1.37	1.42
2	D	9	QOL	C10-C	2.18	1.51	1.48
2	C	2	A1I9S	O23-C14	2.15	1.43	1.36
2	D	2	A1I9S	O23-C14	2.15	1.43	1.36
2	D	7	QUK	OB-C8	2.12	1.43	1.36
2	D	4	A1I9S	O23-C14	2.12	1.43	1.36
2	C	6	QVE	OB-C8	2.12	1.43	1.36
2	D	10	QVE	OB-C8	2.11	1.43	1.36
2	D	5	A1I9S	O23-C14	2.11	1.43	1.36
2	D	2	A1I9S	C15-C12	-2.10	1.38	1.42
2	C	3	A1I9S	O23-C14	2.10	1.43	1.36
2	D	6	QVE	CA-C	2.09	1.51	1.48
2	D	6	QVE	OB-C8	2.09	1.43	1.36
2	C	4	A1I9S	O23-C14	2.09	1.43	1.36
2	C	5	A1I9S	O23-C14	2.08	1.43	1.36
2	C	10	QVE	OB-C8	2.08	1.43	1.36
2	C	7	QUK	OB-C8	2.08	1.43	1.36
2	C	8	QVS	C8-C6	2.07	1.46	1.42
2	C	9	QOL	OB-C8	2.07	1.43	1.36
2	D	4	A1I9S	CA-C	2.05	1.50	1.48
2	D	3	A1I9S	O23-C14	2.04	1.42	1.36
2	C	9	QOL	C10-C	2.03	1.50	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	QOL	OB-C8	2.02	1.42	1.36
2	C	5	A1I9S	CA-C	2.01	1.50	1.48

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	QVE	CG-OB-C8	-7.39	100.96	116.68
2	C	2	A1I9S	O-C-CA	-6.51	118.21	124.22
2	D	2	A1I9S	O-C-CA	-6.35	118.36	124.22
2	D	4	A1I9S	O-C-CA	-5.88	118.79	124.22
2	C	3	A1I9S	O-C-CA	-5.73	118.93	124.22
2	D	7	QUK	O-C-C10	-5.70	118.96	124.22
2	D	9	QOL	O-C-C10	-5.33	119.30	124.22
2	C	4	A1I9S	O-C-CA	-5.13	119.49	124.22
2	C	9	QOL	O-C-C10	-5.11	119.50	124.22
2	D	5	A1I9S	O-C-CA	-4.84	119.75	124.22
2	D	6	QVE	O-C-CA	-4.83	119.77	124.22
2	C	8	QVS	O-C-CA	-4.82	119.77	124.22
2	D	3	A1I9S	O-C-CA	-4.66	119.92	124.22
2	D	4	A1I9S	C10-C11-N	-4.45	113.01	120.36
2	D	8	QVS	O-C-CA	-4.39	120.17	124.22
2	C	7	QUK	O-C-C10	-4.36	120.19	124.22
2	C	5	A1I9S	C15-C16-C11	-4.31	117.87	121.36
2	C	5	A1I9S	C10-C11-N	-4.21	113.41	120.36
2	C	6	QVE	O-C-CA	-4.20	120.34	124.22
2	D	4	A1I9S	C16-C11-N	4.18	128.29	120.11
2	D	6	QVE	C3-C2-N	4.15	128.62	120.39
2	C	6	QVE	C3-C2-N	4.08	128.48	120.39
2	C	9	QOL	C7-CA-N	-4.00	110.73	118.16
2	D	5	A1I9S	C15-C16-C11	-3.93	118.18	121.36
2	C	4	A1I9S	C10-C11-N	-3.83	114.03	120.36
2	C	9	QOL	C3-CA-N	3.81	127.96	120.39
2	D	3	A1I9S	C18-O23-C14	-3.81	106.54	117.74
2	C	4	A1I9S	C16-C11-N	3.79	127.54	120.11
2	C	7	QUK	CG-OB-C8	-3.77	106.64	117.74
2	C	5	A1I9S	C18-O23-C14	-3.73	106.75	117.74
2	C	7	QUK	C3-CA-N	3.72	127.78	120.39
2	C	6	QVE	CG-OB-C8	-3.70	108.81	116.68
2	C	9	QOL	C9-C10-N11	3.60	127.33	123.18
2	D	7	QUK	CG-OB-C8	-3.60	107.15	117.74
2	D	7	QUK	C3-CA-N	3.58	127.49	120.39
2	D	5	A1I9S	C10-C11-N	-3.57	114.47	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	QOL	C9-C10-N11	3.56	127.29	123.18
2	D	5	A1I9S	C18-O23-C14	-3.56	107.27	117.74
2	C	5	A1I9S	O-C-CA	-3.54	120.96	124.22
2	C	7	QUK	C7-CA-N	-3.50	111.67	118.16
2	D	7	QUK	C7-CA-N	-3.50	111.67	118.16
2	C	8	QVS	C7-C2-N	-3.41	111.83	118.16
2	D	10	QVE	C3-C2-N	3.41	127.15	120.39
2	D	6	QVE	C9-CA-N11	3.39	127.09	123.18
2	C	2	A1I9S	C13-CA-N5	3.38	127.08	123.18
2	C	6	QVE	C9-CA-N11	3.33	127.02	123.18
2	D	6	QVE	C7-C2-N	-3.31	112.02	118.16
2	C	3	A1I9S	C10-C11-N	-3.30	114.91	120.36
2	C	8	QVS	C3-C2-N	3.27	126.88	120.39
2	C	8	QVS	C9-C8-C6	-3.24	114.63	120.45
2	D	9	QOL	C7-CA-N	-3.24	112.14	118.16
2	D	8	QVS	C7-C2-N	-3.24	112.16	118.16
2	D	10	QVE	C7-C2-N	-3.20	112.22	118.16
2	D	2	A1I9S	C13-CA-N5	3.18	126.84	123.18
2	D	9	QOL	C3-CA-N	3.09	126.52	120.39
2	C	5	A1I9S	C16-C11-N	3.07	126.12	120.11
2	C	6	QVE	C7-C2-N	-3.06	112.47	118.16
2	C	2	A1I9S	C10-C11-N	-2.91	115.55	120.36
2	C	2	A1I9S	C16-C11-N	2.80	125.59	120.11
2	D	8	QVS	C9-C8-C6	-2.73	115.55	120.45
2	D	8	QVS	C3-C2-N	2.63	125.62	120.39
2	C	3	A1I9S	C18-O23-C14	-2.63	110.00	117.74
2	C	10	QVE	C3-C2-N	2.60	125.56	120.39
2	D	5	A1I9S	C16-C11-N	2.55	125.11	120.11
2	D	2	A1I9S	C20-C19-C18	-2.53	104.80	113.53
2	C	7	QUK	C9-C10-N11	2.47	126.03	123.18
2	C	6	QVE	C-CA-N11	-2.41	112.30	114.66
2	C	5	A1I9S	C20-C19-C18	-2.39	105.29	113.53
2	C	2	A1I9S	C13-CA-C	-2.38	116.83	121.11
2	C	9	QOL	C-C10-N11	-2.38	112.33	114.66
2	C	5	A1I9S	O23-C18-C19	-2.32	99.75	108.30
2	C	3	A1I9S	C16-C11-N	2.27	124.56	120.11
2	D	2	A1I9S	C10-C11-N	-2.26	116.63	120.36
2	C	4	A1I9S	C17-O22-C10	-2.20	108.96	114.88
2	C	3	A1I9S	C16-C11-C10	2.18	120.50	118.15
2	C	5	A1I9S	C16-C11-C10	2.14	120.46	118.15
2	C	6	QVE	C4-C5-C6	-2.12	118.05	120.91
2	C	2	A1I9S	CA-N5-C9	-2.12	116.31	118.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	A1I9S	C16-C11-N	2.10	124.23	120.11
2	C	10	QVE	C7-C2-N	-2.09	114.29	118.16
2	C	3	A1I9S	C-CA-N5	2.06	116.68	114.66
2	C	3	A1I9S	CA-N5-C9	-2.04	116.38	118.06
2	D	5	A1I9S	C16-C11-C10	2.03	120.34	118.15
2	D	2	A1I9S	C18-O23-C14	-2.03	111.78	117.74
2	D	2	A1I9S	CA-N5-C9	-2.01	116.40	118.06
2	D	4	A1I9S	C13-CA-N5	2.00	125.49	123.18

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	A1I9S	O-C-CA-C13
2	C	2	A1I9S	O-C-CA-N5
2	D	2	A1I9S	O-C-CA-C13
2	D	2	A1I9S	O-C-CA-N5
2	D	6	QVE	O-C-CA-C9
2	C	9	QOL	CG-CD-CE1-OZ1
2	C	9	QOL	CE1-CD-CE2-OZ2
2	C	9	QOL	CE1-CD-CG-OB
2	D	9	QOL	CG-CD-CE1-OZ1
2	D	9	QOL	CE1-CD-CE2-OZ2
2	D	9	QOL	CE1-CD-CG-OB
2	D	4	A1I9S	O23-C18-C19-C20
2	D	4	A1I9S	C18-C19-C20-N21
2	D	3	A1I9S	C19-C18-O23-C14
2	C	10	QVE	OE1-CD-CG-OB
2	D	7	QUK	CE-CD-CG-OB
2	C	10	QVE	OE2-CD-CG-OB
2	D	3	A1I9S	O23-C18-C19-C20
2	C	5	A1I9S	O23-C18-C19-C20
2	C	6	QVE	O-C-CA-C9
2	C	6	QVE	C9-C8-OB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	A1I9S	1	0



## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	PEG	D	101	-	6,6,6	0.10	0	5,5,5	0.13	0
3	SO4	A	101	-	4,4,4	0.30	0	6,6,6	0.33	0
4	PEG	C	101	-	6,6,6	0.17	0	5,5,5	0.10	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	D	101	-	-	2/4/4/4	-
4	PEG	C	101	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	101	PEG	O1-C1-C2-O2
4	D	101	PEG	O2-C3-C4-O4
4	D	101	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	101	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	65/66 (98%)	-0.05	2 (3%) 51 55	12, 30, 59, 73	1 (1%)
1	B	63/66 (95%)	0.18	4 (6%) 26 28	12, 30, 69, 76	4 (6%)
2	C	0/10	-	-	-	-
2	D	0/10	-	-	-	-
All	All	128/152 (84%)	0.06	6 (4%) 36 39	12, 30, 66, 76	5 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	TYR	3.4
1	B	0	GLY	3.3
1	A	1	PRO	3.0
1	B	61	ALA	3.0
1	B	8	TYR	2.7
1	B	1	PRO	2.4

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	QVE	C	6	18/19	0.93	0.08	20,25,35,36	0
2	QVE	D	6	18/19	0.94	0.08	20,23,49,50	0
2	A1I9S	D	5	20/21	0.95	0.07	22,25,40,50	0
2	A1I9S	C	2	20/21	0.95	0.07	19,24,31,37	0
2	A1I9S	D	2	20/21	0.95	0.07	20,27,33,47	0
2	QUK	C	7	18/19	0.95	0.08	19,22,49,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1I9S	D	4	20/21	0.96	0.07	17,24,43,53	0
2	A1I9S	C	5	20/21	0.96	0.07	19,23,41,50	0
2	A1I9S	C	4	20/21	0.96	0.07	17,23,44,53	0
2	QUK	D	7	18/19	0.96	0.07	19,22,49,59	0
2	QVS	C	8	14/15	0.96	0.06	22,26,31,34	0
2	QVS	D	8	14/15	0.96	0.06	19,25,31,32	0
2	QOL	C	9	20/21	0.96	0.06	18,21,41,47	0
2	QOL	D	9	20/21	0.96	0.06	15,21,37,46	0
2	A1I9S	C	3	20/21	0.97	0.05	19,21,36,43	0
2	A1I9S	D	3	20/21	0.97	0.07	19,25,50,51	0
2	QVE	C	10	19/19	0.97	0.05	18,22,35,38	0
2	QVE	D	10	19/19	0.97	0.05	18,23,36,45	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	PEG	C	101	7/7	0.77	0.12	43,49,53,55	0
4	PEG	D	101	7/7	0.87	0.10	37,49,57,67	0
3	SO4	A	101	5/5	0.90	0.11	46,50,58,61	0
5	CL	C	102	1/1	0.99	0.27	44,44,44,44	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.