



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2024 – 04:22 pm BST

PDB ID : 8QHM
Title : DNA mimic Foldamer with sticky ends
Authors : Deepak, D.; Loos, M.; Huc, I.
Deposited on : 2023-09-08
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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 : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

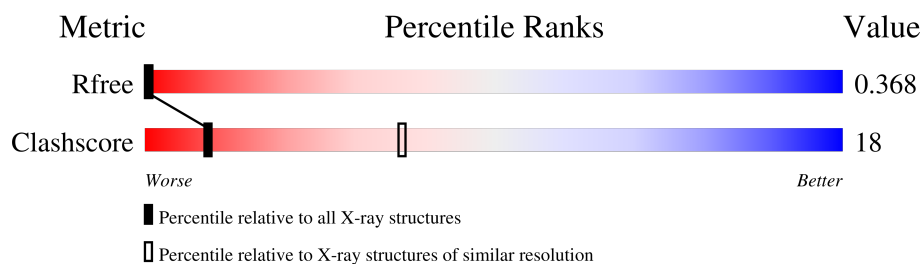
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

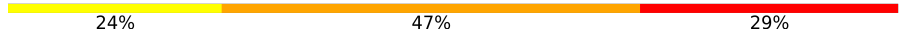

The reported resolution of this entry is 3.00 Å.

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)

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 $\leq 5\%$. 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	17	
1	F	17	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	V4F	A	12	-	X	-	-
1	V53	A	13	-	X	-	-
1	V5F	A	14	-	X	-	-
1	VNW	A	15	-	X	-	-
1	9JV	A	16	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	V4F	A	2	-	X	-	-
1	V4F	A	4	-	X	-	-
1	V4F	F	12	-	X	-	-
1	VNW	F	15	-	X	-	-
1	V4F	F	2	-	X	-	-
1	V53	F	7	-	X	-	-
1	V4F	F	8	-	X	-	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 609 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 DNA mimic Foldamer.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	17	Total	C	N	O	P	Se	0	0	0
			314	192	33	75	13	1			
1	F	16	Total	C	N	O	P	Se	0	0	0
			295	181	31	70	12	1			

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.

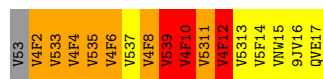
- Molecule 1: DNA mimic Foldamer

Chain A: 



- Molecule 1: DNA mimic Foldamer

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.15Å 74.15Å 83.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.00 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.97-3.00) 94.6 (19.97-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.347 , 0.381 0.348 , 0.368	Depositor DCC
R_{free} test set	262 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 97.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.66	EDS
Total number of atoms	609	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VNW, V5F, QVE, V4F, V53, 9JV

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	0	11
1	F	0	12
All	All	0	23

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	V53	Peptide
1	A	12	V4F	Peptide
1	A	13	V53	Peptide
1	A	2	V4F	Peptide
1	A	3	V53	Peptide
1	A	4	V4F	Peptide
1	A	5	V53	Peptide
1	A	6	V4F	Peptide,Mainchain
1	A	8	V4F	Peptide
1	A	9	V53	Peptide
1	F	10	V4F	Peptide,Mainchain
1	F	12	V4F	Peptide
1	F	2	V4F	Peptide

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Mol	Chain	Res	Type	Group
1	F	3	V53	Peptide
1	F	4	V4F	Peptide,Mainchain
1	F	5	V53	Peptide
1	F	6	V4F	Peptide,Mainchain
1	F	8	V4F	Peptide
1	F	9	V53	Peptide

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	314	0	0	8	0
1	F	295	0	0	3	0
All	All	609	0	0	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 18.

All (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)
1:A:13:V53:N	1:A:15:VNW:CG	2.51	0.73
1:F:9:V53:O2	1:F:11:V53:O1	2.14	0.65
1:F:10:V4F:O2	1:F:12:V4F:O3	2.16	0.63
1:A:6:V4F:N	1:A:6:V4F:NAH	2.52	0.56
1:A:3:V53:O	1:A:6:V4F:N	2.40	0.54
1:F:12:V4F:N	1:F:12:V4F:NAH	2.61	0.47
1:A:6:V4F:CAD	1:A:8:V4F:O	2.62	0.47
1:A:7:V53:C	1:A:10:V4F:N	2.78	0.46
1:A:7:V53:O	1:A:10:V4F:N	2.49	0.46
1:A:11:V53:O1	1:A:13:V53:O3	2.35	0.45
1:A:3:V53:C	1:A:6:V4F:N	2.84	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

33 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	V4F	F	10	1	21,21,22	2.32	6 (28%)	27,30,32	4.39	13 (48%)
1	V4F	A	12	1	21,21,22	2.67	11 (52%)	27,30,32	3.70	13 (48%)
1	V53	F	5	1	20,20,21	2.11	7 (35%)	25,29,31	2.87	12 (48%)
1	V4F	F	12	1	21,21,22	1.78	5 (23%)	27,30,32	5.06	18 (66%)
1	V53	F	7	1	20,20,21	1.81	9 (45%)	25,29,31	3.89	12 (48%)
1	V4F	A	6	1	21,21,22	1.71	4 (19%)	27,30,32	4.67	10 (37%)
1	VNW	A	15	1	16,16,17	1.86	4 (25%)	18,22,24	6.00	12 (66%)
1	V53	A	9	1	20,20,21	2.58	8 (40%)	25,29,31	4.67	13 (52%)
1	VNW	F	15	1	16,16,17	2.57	8 (50%)	18,22,24	5.89	10 (55%)
1	V4F	A	2	1	21,21,22	1.67	5 (23%)	27,30,32	6.83	15 (55%)
1	V4F	F	6	1	21,21,22	2.40	10 (47%)	27,30,32	5.24	12 (44%)
1	V4F	A	10	1	21,21,22	2.41	10 (47%)	27,30,32	4.35	10 (37%)
1	V5F	F	14	1	11,12,13	2.34	4 (36%)	14,15,17	3.13	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	QVE	A	17	1	20,20,20	1.98	9 (45%)	27,28,28	2.82	12 (44%)
1	V53	A	5	1	20,20,21	1.70	3 (15%)	25,29,31	2.42	10 (40%)
1	9JV	A	16	1	16,16,17	2.48	7 (43%)	19,22,24	6.09	9 (47%)
1	V4F	F	2	1	21,21,22	2.27	8 (38%)	27,30,32	5.74	15 (55%)
1	V53	A	7	1	20,20,21	1.80	6 (30%)	25,29,31	3.73	8 (32%)
1	V53	F	11	1	20,20,21	1.79	5 (25%)	25,29,31	4.56	15 (60%)
1	V4F	A	8	1	21,21,22	2.43	7 (33%)	27,30,32	5.71	12 (44%)
1	V4F	A	4	1	21,21,22	2.57	8 (38%)	27,30,32	4.31	12 (44%)
1	V53	F	3	1	20,20,21	2.52	5 (25%)	25,29,31	4.52	10 (40%)
1	QVE	F	17	1	20,20,20	1.83	7 (35%)	27,28,28	3.16	11 (40%)
1	V53	F	9	1	20,20,21	1.66	4 (20%)	25,29,31	3.02	13 (52%)
1	V53	A	13	1	20,20,21	3.00	6 (30%)	25,29,31	5.16	14 (56%)
1	9JV	F	16	1	16,16,17	2.09	3 (18%)	19,22,24	5.59	6 (31%)
1	V53	A	3	1	20,20,21	2.32	4 (20%)	25,29,31	3.62	13 (52%)
1	V4F	F	8	1	21,21,22	2.70	8 (38%)	27,30,32	4.47	13 (48%)
1	V53	A	11	1	20,20,21	1.90	5 (25%)	25,29,31	4.18	10 (40%)
1	V4F	F	4	1	21,21,22	2.32	8 (38%)	27,30,32	4.67	10 (37%)
1	V5F	A	14	1	11,12,13	1.45	2 (18%)	14,15,17	4.52	12 (85%)
1	V53	F	13	1	20,20,21	1.73	7 (35%)	25,29,31	8.04	11 (44%)
1	V53	A	1	1	20,20,21	2.72	8 (40%)	25,29,31	2.77	9 (36%)

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	V4F	F	10	1	-	3/10/10/12	0/2/2/2
1	V4F	A	12	1	-	5/10/10/12	0/2/2/2
1	V53	F	5	1	-	0/8/8/10	0/2/2/2
1	V4F	F	12	1	-	5/10/10/12	0/2/2/2
1	V53	F	7	1	-	6/8/8/10	0/2/2/2
1	V4F	A	6	1	-	6/10/10/12	0/2/2/2
1	VNW	A	15	1	-	2/4/4/6	0/2/2/2
1	V53	A	9	1	-	2/8/8/10	0/2/2/2
1	VNW	F	15	1	-	2/4/4/6	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	V4F	A	2	1	-	8/10/10/12	0/2/2/2
1	V4F	F	6	1	-	3/10/10/12	0/2/2/2
1	V4F	A	10	1	-	0/10/10/12	0/2/2/2
1	V5F	F	14	1	-	1/4/6/8	0/1/1/1
1	QVE	A	17	1	-	2/9/9/9	0/2/2/2
1	V53	A	5	1	-	5/8/8/10	0/2/2/2
1	9JV	A	16	1	-	3/4/4/6	0/2/2/2
1	V4F	F	2	1	-	8/10/10/12	0/2/2/2
1	V53	A	7	1	-	0/8/8/10	0/2/2/2
1	V53	F	11	1	-	3/8/8/10	0/2/2/2
1	V4F	A	8	1	-	6/10/10/12	0/2/2/2
1	V4F	A	4	1	-	6/10/10/12	0/2/2/2
1	V53	F	3	1	-	2/8/8/10	0/2/2/2
1	QVE	F	17	1	-	5/9/9/9	0/2/2/2
1	V53	F	9	1	-	0/8/8/10	0/2/2/2
1	V53	A	13	1	-	4/8/8/10	0/2/2/2
1	9JV	F	16	1	-	4/4/4/6	0/2/2/2
1	V53	A	3	1	-	3/8/8/10	0/2/2/2
1	V4F	F	8	1	-	9/10/10/12	0/2/2/2
1	V53	A	11	1	-	0/8/8/10	0/2/2/2
1	V4F	F	4	1	-	7/10/10/12	0/2/2/2
1	V5F	A	14	1	-	1/4/6/8	0/1/1/1
1	V53	F	13	1	-	2/8/8/10	0/2/2/2
1	V53	A	1	1	-	0/8/8/10	0/2/2/2

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	V53	CAJ-C	10.44	1.59	1.48
1	A	4	V4F	CAE-NAH	-8.82	1.23	1.33
1	F	3	V53	CAJ-C	8.20	1.57	1.48
1	A	1	V53	CAJ-C	8.03	1.57	1.48
1	A	8	V4F	CAE-C	7.98	1.57	1.48
1	F	8	V4F	CAE-C	7.63	1.56	1.48
1	F	10	V4F	CAE-NAH	-7.53	1.24	1.33
1	A	9	V53	CAJ-C	6.56	1.55	1.48
1	A	10	V4F	CAE-C	6.43	1.55	1.48
1	A	16	9JV	CA-C	6.34	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	V4F	O01-C01	-5.95	1.33	1.43
1	A	3	V53	CAJ-NAH	5.73	1.39	1.33
1	F	16	9JV	O15-C76	5.58	1.46	1.36
1	F	14	V5F	O1-C6	-5.42	1.37	1.47
1	A	11	V53	CAJ-C	5.26	1.54	1.48
1	F	2	V4F	CAE-NAH	-5.20	1.27	1.33
1	A	13	V53	CA-N	5.05	1.54	1.38
1	A	3	V53	P-C01	5.03	1.93	1.80
1	F	15	VNW	SE1-C12	4.94	1.98	1.92
1	F	15	VNW	CA-NB	-4.90	1.27	1.33
1	F	6	V4F	O01-CAF	4.82	1.51	1.36
1	F	4	V4F	CAE-NAH	-4.82	1.27	1.33
1	A	16	9JV	O15-C76	4.75	1.45	1.36
1	F	4	V4F	O01-C01	-4.69	1.35	1.43
1	A	9	V53	O01-C01	-4.58	1.36	1.43
1	A	12	V4F	CAK-CAJ	4.57	1.46	1.37
1	A	6	V4F	CAE-NAH	-4.49	1.28	1.33
1	F	8	V4F	O01-C01	-4.49	1.36	1.43
1	A	15	VNW	SE1-C12	4.46	1.97	1.92
1	F	16	9JV	CA-C	-4.45	1.43	1.48
1	F	3	V53	O01-C01	-4.40	1.36	1.43
1	F	2	V4F	P-C01	4.38	1.91	1.80
1	A	5	V53	CAJ-NAH	4.37	1.37	1.33
1	F	6	V4F	CAE-NAH	-4.27	1.28	1.33
1	A	9	V53	CAJ-NAH	4.25	1.37	1.33
1	A	12	V4F	CAE-C	4.23	1.53	1.48
1	F	11	V53	CAJ-C	4.03	1.52	1.48
1	F	4	V4F	CAE-C	4.03	1.52	1.48
1	A	10	V4F	O01-C01	-3.93	1.37	1.43
1	F	3	V53	CAL-CAM	-3.93	1.32	1.42
1	F	2	V4F	O01-CAF	3.92	1.48	1.36
1	A	7	V53	CAJ-C	3.89	1.52	1.48
1	A	1	V53	CAL-CAM	-3.87	1.32	1.42
1	A	2	V4F	CAE-C	3.79	1.52	1.48
1	F	5	V53	CA-CAM	3.75	1.49	1.42
1	F	8	V4F	P-O1	3.74	1.58	1.50
1	F	17	QVE	C9-CA	-3.71	1.30	1.40
1	A	8	V4F	CAE-NAH	-3.70	1.29	1.33
1	F	10	V4F	O01-C01	-3.69	1.37	1.43
1	A	17	QVE	C6-C7	-3.69	1.33	1.42
1	F	5	V53	CAJ-C	3.61	1.52	1.48
1	F	6	V4F	O-C	3.59	1.33	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	15	VNW	CG-NB	-3.58	1.30	1.37
1	F	14	V5F	O1-C1	3.51	1.43	1.37
1	F	12	V4F	O01-CAF	3.49	1.47	1.36
1	F	4	V4F	O01-CAF	3.47	1.47	1.36
1	F	6	V4F	CAK-CAJ	3.47	1.44	1.37
1	A	11	V53	CAL-CAM	-3.42	1.33	1.42
1	F	8	V4F	CAK-CAJ	3.40	1.43	1.37
1	A	1	V53	CAM-NAH	-3.40	1.30	1.37
1	F	5	V53	O01-CAF	3.40	1.47	1.36
1	A	1	V53	CA-CAM	-3.39	1.36	1.42
1	A	12	V4F	CAI-CAL	3.37	1.49	1.42
1	F	6	V4F	CAE-C	3.37	1.52	1.48
1	A	12	V4F	CAG-CAK	3.36	1.46	1.38
1	F	9	V53	P-C01	3.35	1.88	1.80
1	F	15	VNW	C12-C06	-3.32	1.38	1.42
1	A	4	V4F	O01-C01	-3.31	1.38	1.43
1	F	13	V53	CAG-CAI	3.30	1.44	1.36
1	F	12	V4F	CAK-CAJ	3.28	1.43	1.37
1	A	9	V53	CAL-CAM	-3.26	1.34	1.42
1	A	3	V53	P-O2	-3.24	1.47	1.54
1	F	9	V53	CAI-CAL	-3.24	1.35	1.42
1	F	5	V53	P-C01	3.23	1.88	1.80
1	F	12	V4F	P-C01	3.23	1.88	1.80
1	A	8	V4F	O01-CAF	3.21	1.46	1.36
1	F	15	VNW	C06-CG	-3.20	1.34	1.42
1	A	6	V4F	CAF-CAL	-3.19	1.33	1.42
1	A	3	V53	CAG-CAI	3.18	1.43	1.36
1	F	8	V4F	CAG-CAK	3.16	1.45	1.38
1	F	10	V4F	O01-CAF	3.12	1.46	1.36
1	A	10	V4F	O01-CAF	3.11	1.46	1.36
1	F	2	V4F	CAK-CAJ	3.10	1.43	1.37
1	A	17	QVE	C5-C6	-3.10	1.35	1.42
1	A	7	V53	CA-N	3.09	1.48	1.38
1	A	13	V53	CAI-CAL	-3.06	1.36	1.42
1	F	11	V53	CAL-CAM	-3.05	1.34	1.42
1	F	8	V4F	P-O3	-3.05	1.47	1.54
1	F	7	V53	P-C01	3.05	1.88	1.80
1	A	13	V53	P-O3	-3.03	1.48	1.54
1	A	15	VNW	CA-NB	-3.01	1.29	1.33
1	A	9	V53	P-O1	3.00	1.56	1.50
1	F	7	V53	CAJ-C	2.99	1.51	1.48
1	A	2	V4F	O01-C01	-2.97	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	17	QVE	C6-C7	-2.97	1.35	1.42
1	A	17	QVE	C2-C7	2.97	1.47	1.42
1	F	9	V53	CAL-CAM	-2.94	1.35	1.42
1	A	5	V53	P-C01	2.92	1.87	1.80
1	A	4	V4F	O01-CAF	2.89	1.45	1.36
1	A	9	V53	CAD-CAF	2.86	1.46	1.37
1	F	6	V4F	O01-C01	-2.84	1.39	1.43
1	F	17	QVE	CA-C	-2.82	1.46	1.50
1	A	10	V4F	CAM-NAH	-2.82	1.31	1.37
1	F	12	V4F	CAF-CAL	-2.81	1.34	1.42
1	F	5	V53	CAG-CAI	2.80	1.43	1.36
1	F	2	V4F	CA-CAJ	2.80	1.61	1.51
1	A	1	V53	P-C01	2.80	1.87	1.80
1	F	8	V4F	O01-CAF	2.78	1.45	1.36
1	F	6	V4F	CAL-CAM	-2.77	1.35	1.42
1	A	6	V4F	P-C01	2.77	1.87	1.80
1	A	12	V4F	CAM-NAH	-2.77	1.31	1.37
1	A	1	V53	O01-C01	-2.76	1.39	1.43
1	F	5	V53	P-O1	2.76	1.56	1.50
1	A	12	V4F	P-O1	2.75	1.55	1.50
1	A	10	V4F	CAJ-CAM	-2.75	1.37	1.43
1	A	7	V53	CA-CAM	2.74	1.47	1.42
1	F	11	V53	O-C	2.74	1.31	1.21
1	F	6	V4F	CA-CAJ	2.73	1.61	1.51
1	F	5	V53	CA-N	2.73	1.47	1.38
1	F	13	V53	O01-CAF	2.69	1.44	1.36
1	F	17	QVE	OB-C8	2.69	1.44	1.36
1	A	10	V4F	CAL-CAM	-2.68	1.35	1.42
1	F	4	V4F	CAM-NAH	-2.68	1.31	1.37
1	A	2	V4F	CAM-NAH	-2.63	1.32	1.37
1	A	16	9JV	C77-CA	2.62	1.44	1.39
1	F	9	V53	CA-N	2.62	1.46	1.38
1	F	2	V4F	O01-C01	-2.61	1.39	1.43
1	A	11	V53	CAJ-NAH	2.61	1.35	1.33
1	A	17	QVE	C8-C6	-2.59	1.35	1.42
1	A	8	V4F	CAM-NAH	-2.57	1.32	1.37
1	F	13	V53	CAI-CAL	-2.57	1.37	1.42
1	F	7	V53	CA-N	2.56	1.46	1.38
1	A	11	V53	CAI-CAL	-2.56	1.37	1.42
1	F	15	VNW	C08-C07	2.55	1.42	1.36
1	A	12	V4F	P-O3	-2.54	1.49	1.54
1	F	6	V4F	CAM-NAH	-2.54	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	V4F	CA-CAJ	2.52	1.60	1.51
1	F	4	V4F	CA-CAJ	2.52	1.60	1.51
1	A	9	V53	P-C01	2.52	1.86	1.80
1	A	1	V53	CA-N	2.52	1.46	1.38
1	F	14	V5F	CA-C1	-2.51	1.37	1.40
1	F	7	V53	CAJ-NAH	2.50	1.35	1.33
1	A	10	V4F	CAK-CAJ	2.49	1.42	1.37
1	F	4	V4F	CAK-CAJ	2.47	1.42	1.37
1	A	10	V4F	CAG-CAI	2.46	1.42	1.36
1	A	12	V4F	P-O2	-2.46	1.49	1.54
1	F	11	V53	O01-CAF	2.44	1.44	1.36
1	A	4	V4F	P-C01	2.42	1.86	1.80
1	F	13	V53	P-O3	-2.42	1.49	1.54
1	F	3	V53	CAD-CAF	2.41	1.45	1.37
1	F	14	V5F	CA-N	2.41	1.45	1.37
1	A	6	V4F	CAJ-CAM	-2.41	1.38	1.43
1	A	17	QVE	C9-C8	2.39	1.44	1.37
1	A	14	V5F	O-C	2.39	1.29	1.19
1	F	12	V4F	P-O2	-2.39	1.49	1.54
1	A	5	V53	P-O1	2.38	1.55	1.50
1	A	4	V4F	CAJ-CAM	-2.37	1.38	1.43
1	A	12	V4F	O01-CAF	2.36	1.43	1.36
1	A	9	V53	O01-CAF	2.36	1.43	1.36
1	F	13	V53	CAD-CAJ	2.36	1.43	1.39
1	F	13	V53	CAJ-NAH	2.35	1.35	1.33
1	A	16	9JV	C79-C80	-2.33	1.37	1.42
1	A	14	V5F	O1-C6	-2.32	1.43	1.47
1	F	17	QVE	C4-C5	2.32	1.42	1.36
1	F	7	V53	O01-CAF	2.30	1.43	1.36
1	F	6	V4F	P-C01	2.29	1.86	1.80
1	F	16	9JV	C77-C76	2.29	1.44	1.37
1	F	3	V53	CAF-CAL	-2.29	1.36	1.42
1	A	2	V4F	P-C01	2.28	1.86	1.80
1	A	15	VNW	C12-C06	-2.27	1.39	1.42
1	A	1	V53	CAG-CAI	2.27	1.41	1.36
1	A	8	V4F	O01-C01	-2.27	1.40	1.43
1	A	11	V53	P-C01	2.25	1.86	1.80
1	A	17	QVE	O-C	2.24	1.29	1.22
1	F	15	VNW	C15-C12	-2.24	1.35	1.40
1	A	17	QVE	C4-C5	2.23	1.41	1.36
1	A	8	V4F	CAL-CAM	-2.23	1.36	1.42
1	F	8	V4F	CAF-CAL	-2.23	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	V4F	CAM-NAH	-2.23	1.32	1.37
1	F	7	V53	CAL-CAM	-2.21	1.36	1.42
1	F	10	V4F	CAI-CAL	-2.21	1.37	1.42
1	F	10	V4F	CAM-NAH	-2.20	1.32	1.37
1	F	7	V53	O-C	2.20	1.29	1.21
1	A	7	V53	CAG-CAI	2.19	1.41	1.36
1	F	15	VNW	CD-N	2.19	1.45	1.38
1	A	15	VNW	C15-CA	2.19	1.43	1.39
1	A	13	V53	CA-CAM	2.18	1.46	1.42
1	A	4	V4F	CAE-C	2.18	1.50	1.48
1	F	4	V4F	CAL-CAM	-2.17	1.36	1.42
1	A	13	V53	O01-C01	-2.17	1.40	1.43
1	F	2	V4F	CAE-C	-2.16	1.46	1.48
1	A	17	QVE	OXT-C	-2.15	1.24	1.30
1	F	10	V4F	CAL-CAM	-2.14	1.37	1.42
1	A	16	9JV	C82-C81	-2.14	1.38	1.42
1	A	10	V4F	CAG-CAK	2.14	1.43	1.38
1	F	17	QVE	OXT-C	-2.13	1.24	1.30
1	A	17	QVE	OE2-CD	2.13	1.29	1.22
1	A	12	V4F	CAL-CAM	-2.12	1.37	1.42
1	F	13	V53	CAG-CAK	2.11	1.43	1.38
1	A	16	9JV	C84-C83	-2.10	1.34	1.38
1	F	7	V53	O01-C01	-2.08	1.40	1.43
1	A	8	V4F	CAG-CAK	2.07	1.43	1.38
1	A	10	V4F	P-O3	-2.07	1.50	1.54
1	A	16	9JV	C80-C81	-2.06	1.37	1.42
1	F	7	V53	CAD-CAF	2.05	1.43	1.37
1	A	4	V4F	CAG-CAI	2.04	1.41	1.36
1	F	2	V4F	CAL-CAM	-2.04	1.37	1.42
1	F	11	V53	CA-N	2.04	1.44	1.38
1	A	7	V53	O01-C01	-2.04	1.40	1.43
1	F	17	QVE	OE2-CD	2.03	1.28	1.22
1	A	7	V53	P-O3	-2.01	1.50	1.54

All (381) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	V53	C-CAJ-NAH	24.82	138.98	114.66
1	F	13	V53	CAD-CAJ-C	-23.43	100.97	121.23
1	A	2	V4F	O-C-CAE	-20.08	105.19	124.22
1	A	2	V4F	CAD-CAE-C	-19.03	104.78	121.23
1	F	13	V53	O-C-CAJ	-18.76	106.44	124.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	V4F	C-CAE-NAH	18.08	132.37	114.66
1	F	2	V4F	CAD-CAE-C	-17.91	105.74	121.23
1	A	6	V4F	O-C-CAE	-16.74	108.36	124.22
1	F	2	V4F	C-CAE-NAH	16.08	130.41	114.66
1	F	16	9JV	O-C-CA	-15.60	109.44	124.22
1	A	9	V53	CAJ-NAH-CAM	15.29	129.71	118.11
1	F	6	V4F	CAD-CAE-C	-15.26	108.03	121.23
1	F	12	V4F	C-CAE-NAH	15.07	129.43	114.66
1	A	8	V4F	O-C-CAE	-15.02	109.98	124.22
1	A	16	9JV	C-CA-N2	14.87	129.23	114.66
1	F	3	V53	CAJ-NAH-CAM	14.81	129.35	118.11
1	F	4	V4F	O-C-CAE	-14.40	110.58	124.22
1	F	10	V4F	O-C-CAE	-14.39	110.58	124.22
1	A	15	VNW	C15-CA-C	-14.37	108.81	121.23
1	A	10	V4F	C-CAE-NAH	14.25	128.63	114.66
1	A	13	V53	CAJ-NAH-CAM	13.87	128.63	118.11
1	A	16	9JV	O-C-CA	-13.76	111.18	124.22
1	A	16	9JV	C77-CA-C	-13.63	109.45	121.23
1	F	15	VNW	O-C-CA	-13.57	111.36	124.22
1	A	15	VNW	O-C-CA	-13.51	111.42	124.22
1	F	8	V4F	C-CAE-NAH	13.50	127.89	114.66
1	F	6	V4F	C-CAE-NAH	13.49	127.88	114.66
1	A	8	V4F	CAE-NAH-CAM	13.45	128.31	118.11
1	F	7	V53	CAJ-NAH-CAM	13.37	128.25	118.11
1	F	15	VNW	C15-CA-C	-13.32	109.71	121.23
1	A	7	V53	CAJ-NAH-CAM	13.20	128.12	118.11
1	F	11	V53	CAJ-NAH-CAM	13.01	127.98	118.11
1	F	6	V4F	O-C-CAE	-12.81	112.08	124.22
1	A	4	V4F	O-C-CAE	-12.80	112.09	124.22
1	A	8	V4F	C-CAE-NAH	12.22	126.64	114.66
1	F	12	V4F	CAD-CAE-C	-12.14	110.73	121.23
1	A	11	V53	C-CAJ-NAH	12.07	126.49	114.66
1	A	15	VNW	C-CA-NB	11.75	126.17	114.66
1	F	15	VNW	C-CA-NB	11.64	126.06	114.66
1	A	9	V53	CA-CAM-NAH	11.61	130.12	118.64
1	F	12	V4F	O-C-CAE	-11.19	113.61	124.22
1	A	6	V4F	CAD-CAE-C	-11.11	111.62	121.23
1	F	16	9JV	C77-CA-C	-11.09	111.64	121.23
1	A	3	V53	CAJ-NAH-CAM	11.08	126.51	118.11
1	A	4	V4F	C01-O01-CAF	10.93	132.93	118.19
1	A	13	V53	C-CAJ-NAH	10.76	125.20	114.66
1	F	2	V4F	O-C-CAE	-10.17	114.58	124.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	V4F	CAE-NAH-CAM	10.07	125.75	118.11
1	A	11	V53	CAJ-NAH-CAM	10.03	125.72	118.11
1	F	4	V4F	C-CAE-NAH	9.96	124.42	114.66
1	A	10	V4F	CAD-CAE-C	-9.92	112.65	121.23
1	F	4	V4F	CAE-NAH-CAM	9.89	125.61	118.11
1	A	13	V53	O-C-CAJ	-9.80	114.93	124.22
1	A	8	V4F	CAD-CAE-C	-9.78	112.77	121.23
1	F	10	V4F	CAD-CAE-C	-9.71	112.84	121.23
1	F	16	9JV	C103-O15-C76	9.62	131.20	117.75
1	F	16	9JV	C-CA-N2	9.55	124.02	114.66
1	A	6	V4F	C-CAE-NAH	9.39	123.86	114.66
1	F	8	V4F	CAE-NAH-CAM	9.33	125.19	118.11
1	F	3	V53	C-CAJ-NAH	9.29	123.77	114.66
1	A	12	V4F	O-C-CAE	-9.25	115.45	124.22
1	F	11	V53	C-CAJ-NAH	9.23	123.70	114.66
1	A	13	V53	C01-O01-CAF	-9.20	105.78	118.19
1	F	4	V4F	C01-O01-CAF	-9.17	105.81	118.19
1	F	17	QVE	C-CA-N11	9.13	130.84	116.28
1	F	10	V4F	C-CAE-NAH	9.01	123.49	114.66
1	A	1	V53	CAJ-NAH-CAM	8.99	124.92	118.11
1	A	14	V5F	O1-C1-CA	8.89	125.71	114.75
1	F	9	V53	O-C-CAJ	-8.77	115.91	124.22
1	A	10	V4F	CAE-NAH-CAM	8.57	124.61	118.11
1	A	14	V5F	C1-CA-N	8.50	126.74	119.46
1	A	4	V4F	C-CAE-NAH	8.24	122.73	114.66
1	F	8	V4F	CAD-CAE-C	-8.22	114.12	121.23
1	F	8	V4F	O-C-CAE	-8.19	116.46	124.22
1	F	14	V5F	O1-C6-C	7.82	121.96	108.23
1	F	17	QVE	CG-OB-C8	-7.67	108.22	116.95
1	F	5	V53	CAJ-NAH-CAM	7.57	123.85	118.11
1	F	11	V53	O-C-CAJ	-7.50	117.12	124.22
1	A	8	V4F	CA-CAJ-CAM	7.28	130.46	118.84
1	A	2	V4F	CAE-NAH-CAM	7.23	123.59	118.11
1	F	3	V53	O-C-CAJ	-7.11	117.48	124.22
1	A	3	V53	O-C-CAJ	-7.04	117.55	124.22
1	A	11	V53	CAD-CAJ-C	-7.04	115.14	121.23
1	F	2	V4F	C01-O01-CAF	7.04	127.68	118.19
1	A	3	V53	CA-CAM-NAH	7.03	125.59	118.64
1	F	7	V53	C01-O01-CAF	7.02	127.66	118.19
1	A	5	V53	O1-P-C01	-7.00	88.08	112.92
1	A	10	V4F	C01-O01-CAF	-6.92	108.85	118.19
1	F	7	V53	CA-CAM-NAH	6.91	125.47	118.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	11	V53	O3-P-O1	-6.91	94.13	112.39
1	A	7	V53	CA-CAM-NAH	6.87	125.44	118.64
1	F	10	V4F	CAE-NAH-CAM	6.79	123.25	118.11
1	A	11	V53	O-C-CAJ	-6.77	117.80	124.22
1	A	12	V4F	O2-P-O1	6.53	129.65	112.39
1	F	6	V4F	CAE-NAH-CAM	6.53	123.06	118.11
1	F	15	VNW	C14-SE1-C12	6.51	106.82	99.54
1	A	15	VNW	C07-C06-C12	-6.51	116.83	123.53
1	A	11	V53	CA-CAM-NAH	6.40	124.97	118.64
1	A	8	V4F	CAJ-CAM-NAH	6.40	125.54	118.52
1	A	14	V5F	O1-C6-C	6.28	119.26	108.23
1	A	12	V4F	C-CAE-NAH	6.23	120.76	114.66
1	A	8	V4F	C01-O01-CAF	-6.06	110.01	118.19
1	F	11	V53	CAD-CAJ-C	-6.02	116.02	121.23
1	F	4	V4F	CAD-CAE-C	-6.02	116.03	121.23
1	A	7	V53	O-C-CAJ	-6.01	118.53	124.22
1	A	17	QVE	OB-CG-CD	-5.98	92.41	110.24
1	F	5	V53	CA-CAM-NAH	5.92	124.49	118.64
1	F	3	V53	CA-CAM-NAH	5.82	124.39	118.64
1	A	17	QVE	CG-OB-C8	-5.77	110.38	116.95
1	A	8	V4F	CA-CAJ-CAK	-5.72	108.83	120.11
1	F	8	V4F	CAJ-CAM-NAH	5.63	124.70	118.52
1	A	9	V53	CAM-CA-N	5.62	128.78	118.07
1	A	13	V53	CA-CAM-NAH	5.61	124.19	118.64
1	A	3	V53	CAL-CAM-NAH	-5.37	111.70	122.78
1	F	13	V53	O01-CAF-CAL	5.34	129.94	115.01
1	F	14	V5F	C2-C1-CA	-5.34	116.75	120.88
1	F	12	V4F	C01-O01-CAF	5.34	125.39	118.19
1	A	17	QVE	C2-C7-N11	5.34	123.92	118.64
1	F	6	V4F	O01-CAF-CAL	5.32	129.88	115.01
1	F	2	V4F	O3-P-O1	-5.32	98.33	112.39
1	F	17	QVE	C9-CA-C	-5.30	108.11	119.57
1	A	10	V4F	O-C-CAE	-5.18	119.31	124.22
1	A	9	V53	CAD-CAJ-C	5.15	125.68	121.23
1	F	17	QVE	OB-C8-C6	5.13	129.36	115.01
1	F	3	V53	CAG-CAK-CA	-5.11	111.36	121.19
1	A	16	9JV	C82-C81-N2	5.04	123.62	118.64
1	A	4	V4F	CAD-CAE-C	-5.02	116.89	121.23
1	F	12	V4F	CAJ-CAM-NAH	4.98	123.99	118.52
1	F	9	V53	CAJ-NAH-CAM	4.91	121.83	118.11
1	F	2	V4F	O01-CAF-CAL	4.88	128.65	115.01
1	A	13	V53	CAG-CAI-CAL	-4.85	114.16	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	V53	CAD-CAJ-C	4.81	125.38	121.23
1	A	4	V4F	O3-P-O1	-4.78	99.74	112.39
1	F	3	V53	CAK-CA-CAM	4.76	127.53	120.06
1	F	5	V53	C01-O01-CAF	4.75	124.59	118.19
1	A	6	V4F	CAG-CAI-CAL	-4.68	114.41	120.89
1	A	4	V4F	CAJ-CAM-CAL	4.67	124.55	119.79
1	F	11	V53	CA-CAM-NAH	4.59	123.18	118.64
1	F	15	VNW	C07-C06-C12	-4.58	118.82	123.53
1	F	15	VNW	CA-NB-CG	4.57	121.57	118.11
1	A	13	V53	CAD-CAJ-C	-4.46	117.37	121.23
1	A	16	9JV	C103-O15-C76	4.43	123.95	117.75
1	F	16	9JV	O15-C76-C80	4.43	118.78	114.46
1	A	12	V4F	O2-P-O3	-4.42	95.18	108.08
1	F	3	V53	C01-O01-CAF	-4.40	112.25	118.19
1	F	13	V53	CAG-CAK-CA	-4.40	112.72	121.19
1	A	4	V4F	CAE-NAH-CAM	4.39	121.44	118.11
1	A	8	V4F	CAL-CAM-NAH	-4.35	113.81	122.78
1	A	17	QVE	C3-C2-N	-4.34	111.68	120.36
1	A	13	V53	CAK-CA-CAM	-4.32	113.28	120.06
1	F	15	VNW	C12-C06-CG	4.23	122.00	115.33
1	A	1	V53	O1-P-C01	-4.21	98.00	112.92
1	F	14	V5F	C1-CA-N	-4.20	115.86	119.46
1	F	9	V53	CAG-CAI-CAL	-4.20	115.07	120.89
1	F	2	V4F	O2-P-O3	4.20	120.33	108.08
1	F	11	V53	CAK-CA-N	-4.19	111.98	120.36
1	F	2	V4F	CAI-CAG-CAK	-4.19	114.31	120.99
1	A	5	V53	CAJ-NAH-CAM	4.19	121.29	118.11
1	F	5	V53	CAM-CA-N	4.19	126.06	118.07
1	F	8	V4F	CAI-CAG-CAK	-4.19	114.31	120.99
1	A	7	V53	CAL-CAM-NAH	-4.18	114.15	122.78
1	A	1	V53	O-C-CAJ	-4.17	120.27	124.22
1	A	9	V53	CAL-CAM-NAH	-4.17	114.19	122.78
1	F	12	V4F	CAE-NAH-CAM	4.14	121.25	118.11
1	A	15	VNW	CD-CG-NB	4.12	122.72	118.64
1	A	9	V53	CAK-CA-N	-4.11	112.14	120.36
1	A	9	V53	O01-CAF-CAL	-4.11	103.53	115.01
1	F	6	V4F	O2-P-O3	4.10	120.06	108.08
1	F	8	V4F	O2-P-C01	4.07	119.18	106.68
1	A	13	V53	O1-P-C01	-4.02	98.66	112.92
1	A	17	QVE	C-CA-N11	4.01	122.68	116.28
1	A	13	V53	CAL-CAM-NAH	-4.01	114.50	122.78
1	F	12	V4F	CAI-CAL-CAF	-4.01	113.35	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	9	V53	CAI-CAG-CAK	4.01	127.38	120.99
1	A	1	V53	CAI-CAG-CAK	-4.00	114.61	120.99
1	A	1	V53	C-CAJ-NAH	3.94	118.53	114.66
1	A	6	V4F	C01-O01-CAF	-3.94	112.88	118.19
1	A	13	V53	CAM-CA-N	3.92	125.55	118.07
1	A	12	V4F	O3-P-C01	3.91	118.69	106.68
1	A	16	9JV	O15-C76-C80	3.87	118.24	114.46
1	F	5	V53	CAL-CAM-NAH	-3.87	114.79	122.78
1	F	12	V4F	CA-CAJ-CAM	3.86	125.00	118.84
1	F	8	V4F	CAJ-CAM-CAL	-3.84	115.87	119.79
1	A	17	QVE	CA-N11-C7	3.83	125.32	117.24
1	A	10	V4F	O01-CAF-CAL	3.82	125.69	115.01
1	F	8	V4F	CAI-CAL-CAM	3.81	126.87	118.98
1	F	11	V53	CAM-CA-N	3.81	125.33	118.07
1	F	9	V53	CAG-CAK-CA	-3.80	113.89	121.19
1	F	7	V53	CAK-CA-N	-3.80	112.78	120.36
1	A	9	V53	CAI-CAL-CAF	-3.77	113.90	122.58
1	A	3	V53	O1-P-C01	-3.77	99.56	112.92
1	A	14	V5F	CB-C6-C	-3.74	99.31	113.19
1	A	15	VNW	C12-C06-CG	3.73	121.22	115.33
1	F	3	V53	CAD-CAJ-C	3.71	124.43	121.23
1	A	16	9JV	C83-C82-C81	3.70	125.86	120.06
1	A	14	V5F	C5-CA-N	-3.67	113.02	120.13
1	A	2	V4F	O01-CAF-CAL	3.66	125.25	115.01
1	F	5	V53	CAK-CA-N	-3.64	113.08	120.36
1	F	2	V4F	CA-CAJ-CAM	3.62	124.62	118.84
1	F	11	V53	O01-CAF-CAL	3.60	125.08	115.01
1	F	6	V4F	O01-CAF-CAD	-3.60	112.93	124.69
1	F	12	V4F	O2-P-O1	-3.59	102.89	112.39
1	F	3	V53	O3-P-C01	-3.59	95.65	106.68
1	A	14	V5F	O1-C1-C2	-3.58	115.45	123.87
1	F	7	V53	O2-P-O1	-3.58	102.94	112.39
1	F	9	V53	C-CAJ-NAH	3.56	118.15	114.66
1	A	14	V5F	C3-C4-C5	-3.55	114.78	120.19
1	F	17	QVE	OB-C8-C9	-3.54	113.13	124.69
1	F	10	V4F	CAG-CAK-CAJ	-3.51	115.26	121.48
1	A	2	V4F	CAJ-CAM-NAH	3.50	122.36	118.52
1	A	7	V53	CAM-CA-N	3.49	124.73	118.07
1	F	11	V53	CAL-CAM-NAH	-3.42	115.72	122.78
1	A	15	VNW	C14-SE1-C12	3.42	103.36	99.54
1	A	2	V4F	CA-CAJ-CAM	3.41	124.29	118.84
1	A	12	V4F	O1-P-C01	-3.41	100.82	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	V53	O2-P-C01	3.40	117.11	106.68
1	A	4	V4F	CAJ-CAM-NAH	-3.40	114.79	118.52
1	A	10	V4F	CAJ-CAM-CAL	3.40	123.25	119.79
1	F	6	V4F	O2-P-O1	-3.39	103.42	112.39
1	A	17	QVE	C7-C2-N	3.39	124.53	118.07
1	A	4	V4F	CAD-CAF-CAL	-3.38	112.39	120.01
1	A	16	9JV	C83-C82-N	-3.38	113.61	120.36
1	A	9	V53	CAI-CAL-CAM	3.38	125.98	118.98
1	F	7	V53	C-CAJ-NAH	3.37	117.97	114.66
1	F	4	V4F	O2-P-O3	3.36	117.91	108.08
1	A	5	V53	CAG-CAI-CAL	-3.35	116.25	120.89
1	F	4	V4F	CAJ-CAM-CAL	3.35	123.20	119.79
1	A	5	V53	CA-CAM-NAH	3.35	121.95	118.64
1	A	6	V4F	CA-CAJ-CAK	3.33	126.67	120.11
1	A	2	V4F	O01-CAF-CAD	-3.33	113.83	124.69
1	F	12	V4F	CA-CAJ-CAK	-3.30	113.61	120.11
1	F	7	V53	CAM-CA-N	3.25	124.27	118.07
1	A	6	V4F	CA-CAJ-CAM	-3.25	113.65	118.84
1	F	15	VNW	C15-C12-C06	-3.24	117.68	120.44
1	A	2	V4F	CAL-CAM-NAH	-3.23	116.11	122.78
1	F	7	V53	CAL-CAM-NAH	-3.22	116.13	122.78
1	F	2	V4F	O2-P-O1	-3.19	103.96	112.39
1	F	8	V4F	CAI-CAL-CAF	-3.17	115.28	122.58
1	A	12	V4F	O01-CAF-CAD	-3.14	114.44	124.69
1	A	1	V53	O2-P-C01	3.13	116.29	106.68
1	A	13	V53	CAI-CAL-CAM	3.13	125.47	118.98
1	A	13	V53	CAI-CAL-CAF	-3.12	115.39	122.58
1	F	9	V53	CAD-CAJ-C	-3.10	118.54	121.23
1	F	11	V53	O3-P-O2	3.10	117.13	108.08
1	F	10	V4F	C01-O01-CAF	-3.08	114.03	118.19
1	A	17	QVE	C9-CA-N11	-3.08	117.00	124.50
1	A	14	V5F	C4-C3-C2	3.07	124.87	120.19
1	F	5	V53	CAF-CAL-CAM	3.07	124.28	117.19
1	A	15	VNW	C15-C12-C06	-3.06	117.84	120.44
1	F	9	V53	CA-CAM-NAH	3.05	121.66	118.64
1	F	10	V4F	O2-P-O1	-3.05	104.33	112.39
1	A	2	V4F	O2-P-O3	3.04	116.95	108.08
1	A	8	V4F	O2-P-O1	-3.04	104.36	112.39
1	A	5	V53	CAI-CAL-CAF	-3.03	115.59	122.58
1	A	4	V4F	O01-CAF-CAL	3.02	123.46	115.01
1	A	2	V4F	C01-O01-CAF	-3.00	114.14	118.19
1	F	12	V4F	O2-P-C01	3.00	115.89	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	11	V53	O01-CAF-CAD	-3.00	114.90	124.69
1	A	14	V5F	C1-O1-C6	-2.99	112.56	118.05
1	A	9	V53	CAI-CAG-CAK	-2.98	116.23	120.99
1	A	7	V53	O2-P-O1	-2.98	104.52	112.39
1	F	10	V4F	O01-CAF-CAL	2.93	123.20	115.01
1	F	17	QVE	CA-N11-C7	2.92	123.40	117.24
1	A	1	V53	O3-P-C01	2.92	115.64	106.68
1	A	12	V4F	CA-CAJ-CAK	2.90	125.84	120.11
1	F	10	V4F	O2-P-C01	2.90	115.57	106.68
1	A	10	V4F	O01-CAF-CAD	-2.90	115.23	124.69
1	A	11	V53	CAL-CAM-NAH	-2.88	116.84	122.78
1	F	10	V4F	O3-P-O1	2.87	119.98	112.39
1	A	14	V5F	O1-C6-CB	2.86	111.75	106.59
1	F	6	V4F	CAG-CAI-CAL	2.86	124.86	120.89
1	A	17	QVE	C4-C3-C2	-2.85	115.70	121.19
1	F	10	V4F	CAI-CAG-CAK	2.84	125.52	120.99
1	A	3	V53	O2-P-C01	2.84	115.39	106.68
1	F	4	V4F	O01-CAF-CAL	2.82	122.89	115.01
1	F	12	V4F	CAJ-CAM-CAL	-2.80	116.93	119.79
1	A	10	V4F	O3-P-O1	-2.78	105.03	112.39
1	A	11	V53	CAG-CAK-CA	-2.77	115.87	121.19
1	F	8	V4F	C01-O01-CAF	-2.76	114.47	118.19
1	F	9	V53	O3-P-C01	2.76	115.14	106.68
1	F	7	V53	O3-P-O1	-2.75	105.11	112.39
1	A	8	V4F	O3-P-C01	2.75	115.12	106.68
1	F	11	V53	C01-O01-CAF	2.75	121.90	118.19
1	F	6	V4F	CAL-CAM-NAH	-2.74	117.12	122.78
1	A	17	QVE	OXT-C-O	-2.73	117.29	123.35
1	F	12	V4F	O3-P-O1	2.73	119.60	112.39
1	A	11	V53	O1-P-C01	-2.72	103.27	112.92
1	A	6	V4F	CAI-CAG-CAK	2.72	125.33	120.99
1	A	11	V53	CAK-CA-N	-2.72	114.93	120.36
1	F	13	V53	O01-CAF-CAD	-2.70	115.89	124.69
1	A	8	V4F	O2-P-O3	2.69	115.92	108.08
1	F	4	V4F	O2-P-C01	-2.66	98.52	106.68
1	F	7	V53	CAD-CAJ-C	2.64	123.51	121.23
1	A	7	V53	O2-P-C01	2.64	114.79	106.68
1	A	14	V5F	C2-C1-CA	-2.64	118.84	120.88
1	F	9	V53	CAI-CAL-CAF	-2.63	116.53	122.58
1	A	2	V4F	CAG-CAI-CAL	-2.62	117.25	120.89
1	A	12	V4F	O3-P-O1	-2.62	105.45	112.39
1	F	13	V53	O2-P-C01	2.62	114.72	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5	V53	O-C-CAJ	-2.61	121.75	124.22
1	A	4	V4F	CAG-CAI-CAL	-2.61	117.28	120.89
1	F	13	V53	CAD-CAF-CAL	-2.59	114.17	120.01
1	A	5	V53	CAI-CAL-CAM	2.57	124.30	118.98
1	F	2	V4F	CAD-CAF-CAL	-2.56	114.23	120.01
1	F	6	V4F	CAJ-CAM-CAL	2.54	122.38	119.79
1	F	11	V53	CAG-CAK-CA	-2.53	116.32	121.19
1	A	13	V53	O2-P-C01	2.51	114.38	106.68
1	A	1	V53	O3-P-O2	-2.51	100.76	108.08
1	F	12	V4F	CAF-CAL-CAM	2.50	122.98	117.19
1	F	17	QVE	C3-C2-N	-2.48	115.40	120.36
1	F	7	V53	CAG-CAK-CA	-2.47	116.44	121.19
1	F	12	V4F	CAG-CAI-CAL	-2.46	117.48	120.89
1	F	17	QVE	OB-CG-CD	-2.46	102.92	110.24
1	F	17	QVE	O-C-CA	2.45	126.20	121.24
1	F	14	V5F	C5-CA-N	2.45	124.87	120.13
1	A	15	VNW	CA-NB-CG	2.45	119.96	118.11
1	F	11	V53	CAG-CAI-CAL	2.42	124.26	120.89
1	A	12	V4F	O01-CAF-CAL	2.42	121.79	115.01
1	A	10	V4F	CAG-CAK-CAJ	-2.41	117.20	121.48
1	F	2	V4F	CAJ-CA-N	-2.41	103.22	115.58
1	F	5	V53	O3-P-C01	2.41	114.07	106.68
1	F	16	9JV	C77-C76-C80	-2.40	114.60	120.01
1	A	2	V4F	CAG-CAK-CAJ	-2.40	117.23	121.48
1	F	2	V4F	CAG-CAI-CAL	2.38	124.20	120.89
1	F	5	V53	CAI-CAL-CAF	-2.38	117.11	122.58
1	A	15	VNW	CG-CD-N	2.37	122.59	118.07
1	A	17	QVE	C3-C2-C7	2.37	123.78	120.06
1	F	2	V4F	O01-CAF-CAD	-2.37	116.95	124.69
1	F	7	V53	O3-P-O2	2.36	114.96	108.08
1	A	5	V53	O2-P-O1	2.35	118.61	112.39
1	A	4	V4F	CAG-CAK-CAJ	-2.34	117.33	121.48
1	A	5	V53	C-CAJ-NAH	2.34	116.96	114.66
1	F	10	V4F	CAJ-CAM-CAL	2.34	122.17	119.79
1	A	3	V53	CAI-CAL-CAM	-2.34	114.12	118.98
1	F	9	V53	CAL-CAM-NAH	-2.34	117.95	122.78
1	A	11	V53	CAK-CA-CAM	2.34	123.73	120.06
1	A	3	V53	CAG-CAK-CA	-2.33	116.70	121.19
1	F	8	V4F	O3-P-C01	-2.33	99.52	106.68
1	A	12	V4F	CA-CAJ-CAM	-2.31	115.15	118.84
1	F	5	V53	CAD-CAJ-C	2.31	123.22	121.23
1	A	14	V5F	C5-CA-C1	2.30	120.23	118.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	V4F	CAJ-CAM-NAH	-2.29	116.01	118.52
1	A	3	V53	CAG-CAI-CAL	2.27	124.04	120.89
1	F	12	V4F	CAG-CAK-CAJ	-2.26	117.48	121.48
1	F	12	V4F	CAI-CAL-CAM	2.25	123.64	118.98
1	A	3	V53	CAD-CAF-CAL	2.24	125.05	120.01
1	F	6	V4F	CA-CAJ-CAM	2.22	122.39	118.84
1	F	10	V4F	CAL-CAM-NAH	-2.22	118.20	122.78
1	A	2	V4F	CAI-CAG-CAK	2.22	124.53	120.99
1	A	3	V53	CAM-CA-N	2.22	122.29	118.07
1	A	6	V4F	CAG-CAK-CAJ	-2.21	117.57	121.48
1	F	15	VNW	C06-CG-NB	-2.21	118.22	122.78
1	F	3	V53	O2-P-C01	2.20	113.42	106.68
1	A	15	VNW	SE1-C12-C15	2.19	126.14	122.87
1	A	9	V53	O01-CAF-CAD	2.18	131.80	124.69
1	A	3	V53	CAK-CA-N	-2.17	116.03	120.36
1	F	17	QVE	OE2-CD-CG	-2.17	114.30	122.44
1	A	5	V53	CAD-CAJ-C	-2.17	119.35	121.23
1	A	1	V53	CAG-CAI-CAL	2.17	123.90	120.89
1	F	17	QVE	C4-C3-C2	-2.16	117.03	121.19
1	F	14	V5F	O1-C1-C2	2.16	128.94	123.87
1	F	4	V4F	O3-P-O1	-2.16	106.68	112.39
1	F	9	V53	C01-O01-CAF	2.16	121.10	118.19
1	F	13	V53	CAK-CA-CAM	2.15	123.43	120.06
1	F	13	V53	O2-P-O1	-2.14	106.74	112.39
1	F	2	V4F	CAG-CAK-CAJ	2.14	125.27	121.48
1	F	5	V53	CAG-CAK-CA	-2.12	117.12	121.19
1	A	9	V53	O2-P-C01	-2.12	100.19	106.68
1	A	15	VNW	C07-C08-C09	-2.10	117.64	120.99
1	A	16	9JV	C79-C80-C76	-2.07	117.80	122.58
1	A	9	V53	CAD-CAF-CAL	2.07	124.67	120.01
1	F	9	V53	O2-P-O1	-2.06	106.94	112.39
1	F	13	V53	CA-CAM-NAH	-2.05	116.61	118.64
1	A	12	V4F	CAG-CAI-CAL	-2.05	118.05	120.89
1	A	2	V4F	CA-CAJ-CAK	-2.04	116.08	120.11
1	F	8	V4F	CAG-CAK-CAJ	2.04	125.09	121.48
1	F	15	VNW	C08-C07-C06	-2.03	118.08	120.89
1	A	17	QVE	OE2-CD-CG	2.03	130.06	122.44
1	F	12	V4F	CAJ-CA-N	-2.02	105.23	115.58
1	F	14	V5F	C3-C4-C5	-2.01	117.12	120.19
1	A	3	V53	CAF-CAL-CAM	2.01	121.83	117.19

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2	V4F	O-C-CAE-CAD
1	A	2	V4F	O-C-CAE-NAH
1	A	2	V4F	N-CA-CAJ-CAM
1	A	2	V4F	O01-C01-P-O3
1	A	2	V4F	O01-C01-P-O2
1	A	2	V4F	O01-C01-P-O1
1	F	2	V4F	O-C-CAE-NAH
1	F	2	V4F	O01-C01-P-O3
1	F	2	V4F	O01-C01-P-O2
1	F	2	V4F	O01-C01-P-O1
1	A	3	V53	O01-C01-P-O1
1	A	3	V53	O01-C01-P-O2
1	A	3	V53	O01-C01-P-O3
1	A	4	V4F	O-C-CAE-NAH
1	A	4	V4F	O01-C01-P-O3
1	A	4	V4F	O01-C01-P-O2
1	F	4	V4F	O-C-CAE-CAD
1	F	4	V4F	O-C-CAE-NAH
1	F	4	V4F	O01-C01-P-O3
1	F	4	V4F	O01-C01-P-O2
1	A	5	V53	O01-C01-P-O1
1	A	5	V53	O01-C01-P-O2
1	A	5	V53	O01-C01-P-O3
1	A	6	V4F	O-C-CAE-CAD
1	A	6	V4F	O-C-CAE-NAH
1	A	6	V4F	O01-C01-P-O3
1	A	6	V4F	O01-C01-P-O2
1	A	6	V4F	O01-C01-P-O1
1	F	6	V4F	O-C-CAE-NAH
1	F	7	V53	O01-C01-P-O1
1	F	7	V53	O01-C01-P-O2
1	F	7	V53	O01-C01-P-O3
1	A	8	V4F	O-C-CAE-CAD
1	A	8	V4F	O-C-CAE-NAH
1	A	8	V4F	N-CA-CAJ-CAM
1	A	8	V4F	O01-C01-P-O3
1	A	8	V4F	O01-C01-P-O2
1	F	8	V4F	O-C-CAE-NAH
1	F	8	V4F	N-CA-CAJ-CAM
1	F	8	V4F	O01-C01-P-O3
1	F	8	V4F	O01-C01-P-O2
1	F	8	V4F	O01-C01-P-O1

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Mol	Chain	Res	Type	Atoms
1	A	9	V53	O01-C01-P-O1
1	A	9	V53	O01-C01-P-O2
1	F	10	V4F	O-C-CAE-CAD
1	F	10	V4F	O-C-CAE-NAH
1	F	11	V53	CAL-CAF-O01-C01
1	A	12	V4F	O01-C01-P-O3
1	A	12	V4F	O01-C01-P-O2
1	F	12	V4F	N-CA-CAJ-CAM
1	A	13	V53	O01-C01-P-O1
1	A	15	VNW	O-C-CA-NB
1	A	15	VNW	O-C-CA-C15
1	F	15	VNW	O-C-CA-NB
1	F	15	VNW	O-C-CA-C15
1	F	16	9JV	O-C-CA-C77
1	F	16	9JV	O-C-CA-N2
1	F	17	QVE	OE1-CD-CG-OB
1	A	16	9JV	C77-C76-O15-C103
1	A	16	9JV	C80-C76-O15-C103
1	F	16	9JV	C77-C76-O15-C103
1	F	3	V53	CAL-CAF-O01-C01
1	A	12	V4F	CAL-CAF-O01-C01
1	F	11	V53	CAD-CAF-O01-C01
1	F	16	9JV	C80-C76-O15-C103
1	A	4	V4F	CAL-CAF-O01-C01
1	F	12	V4F	CAL-CAF-O01-C01
1	A	2	V4F	CAL-CAF-O01-C01
1	A	5	V53	CAL-CAF-O01-C01
1	F	8	V4F	CAL-CAF-O01-C01
1	F	17	QVE	C6-C8-OB-CG
1	F	2	V4F	CAL-CAF-O01-C01
1	F	6	V4F	CAL-CAF-O01-C01
1	F	13	V53	CAL-CAF-O01-C01
1	F	17	QVE	OE2-CD-CG-OB
1	F	7	V53	CAL-CAF-O01-C01
1	A	13	V53	CAL-CAF-O01-C01
1	F	17	QVE	C9-C8-OB-CG
1	A	17	QVE	OE1-CD-CG-OB
1	A	17	QVE	OE2-CD-CG-OB
1	F	4	V4F	CAL-CAF-O01-C01
1	A	12	V4F	CAD-CAF-O01-C01
1	A	4	V4F	CAD-CAF-O01-C01
1	F	2	V4F	CAD-CAF-O01-C01

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Mol	Chain	Res	Type	Atoms
1	F	6	V4F	CAD-CAF-O01-C01
1	A	6	V4F	N-CA-CAJ-CAM
1	F	10	V4F	N-CA-CAJ-CAM
1	F	7	V53	CAD-CAF-O01-C01
1	F	12	V4F	CAD-CAF-O01-C01
1	F	3	V53	CAD-CAF-O01-C01
1	A	16	9JV	O-C-CA-N2
1	F	13	V53	CAD-CAF-O01-C01
1	A	4	V4F	O01-C01-P-O1
1	F	4	V4F	O01-C01-P-O1
1	F	11	V53	O01-C01-P-O1
1	A	12	V4F	O01-C01-P-O1
1	A	2	V4F	CAD-CAF-O01-C01
1	F	14	V5F	CB-C6-O1-C1
1	F	8	V4F	CAD-CAF-O01-C01
1	A	5	V53	CAD-CAF-O01-C01
1	F	8	V4F	N-CA-CAJ-CAK
1	A	13	V53	CAD-CAF-O01-C01
1	F	2	V4F	N-CA-CAJ-CAM
1	F	2	V4F	P-C01-O01-CAF
1	F	7	V53	P-C01-O01-CAF
1	F	8	V4F	P-C01-O01-CAF
1	F	17	QVE	CD-CG-OB-C8
1	F	12	V4F	O01-C01-P-O3
1	A	13	V53	O01-C01-P-O3
1	A	14	V5F	CB-C6-O1-C1
1	F	4	V4F	CAD-CAF-O01-C01
1	F	12	V4F	O-C-CAE-NAH
1	A	8	V4F	O01-C01-P-O1

There are no ring outliers.

12 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	10	V4F	1	0
1	F	12	V4F	2	0
1	A	6	V4F	4	0
1	A	15	VNW	1	0
1	A	10	V4F	2	0
1	A	7	V53	2	0
1	F	11	V53	1	0
1	A	8	V4F	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	9	V53	1	0
1	A	13	V53	2	0
1	A	3	V53	2	0
1	A	11	V53	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	0/17	-	-	-	-
1	F	0/17	-	-	-	-
All	All	0/34	-	-	-	-

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
1	V53	A	9	19/20	0.87	0.19	12,23,32,38	0
1	V4F	A	2	20/21	0.88	0.15	6,15,25,31	0
1	9JV	A	16	15/16	0.88	0.18	12,17,30,38	0
1	V53	F	9	19/20	0.90	0.17	9,17,29,38	0
1	QVE	F	17	19/19	0.90	0.19	11,18,28,35	0
1	V53	A	7	19/20	0.91	0.15	14,19,34,45	0
1	V4F	F	10	20/21	0.91	0.15	12,22,41,52	0
1	V53	F	13	19/20	0.91	0.14	8,19,41,56	0
1	V4F	A	8	20/21	0.91	0.16	8,18,26,45	0
1	V4F	F	2	20/21	0.91	0.14	4,19,41,65	0
1	V53	A	5	19/20	0.92	0.13	4,11,29,63	0
1	V53	F	5	19/20	0.92	0.14	7,17,31,44	0
1	V4F	A	6	20/21	0.92	0.13	9,15,24,38	0
1	V53	F	11	19/20	0.92	0.15	11,16,37,41	0
1	V4F	A	12	20/21	0.92	0.14	10,17,32,47	0
1	V4F	F	6	20/21	0.92	0.13	12,21,52,64	0
1	V53	A	1	19/20	0.92	0.13	7,11,16,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	V4F	F	4	20/21	0.92	0.14	10,19,35,55	0
1	V4F	A	4	20/21	0.93	0.13	9,12,38,44	0
1	V53	A	3	19/20	0.93	0.12	5,10,30,33	0
1	V4F	F	12	20/21	0.93	0.13	10,24,55,65	0
1	V53	A	13	19/20	0.93	0.13	10,19,32,36	0
1	V4F	A	10	20/21	0.93	0.14	11,17,31,33	0
1	V5F	A	14	12/13	0.93	0.15	6,15,21,33	0
1	V4F	F	8	20/21	0.93	0.13	12,22,35,52	0
1	QVE	A	17	19/19	0.93	0.14	7,14,25,26	0
1	V53	A	11	19/20	0.93	0.13	10,18,41,49	0
1	VNW	F	15	15/16	0.94	0.14	0,17,27,48	0
1	V53	F	7	19/20	0.94	0.12	12,15,46,48	0
1	9JV	F	16	15/16	0.94	0.14	6,11,17,43	0
1	V53	F	3	19/20	0.94	0.14	8,13,30,36	0
1	V5F	F	14	12/13	0.94	0.12	7,13,15,21	0
1	VNW	A	15	15/16	0.96	0.12	8,12,21,45	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.