



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2024 – 10:18 pm BST

PDB ID : 7PCJ
Title : X-ray structure of CypA-C52AK125C/CsA/aromatic foldamer complex
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Deposited on : 2021-08-03
Resolution : 1.91 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

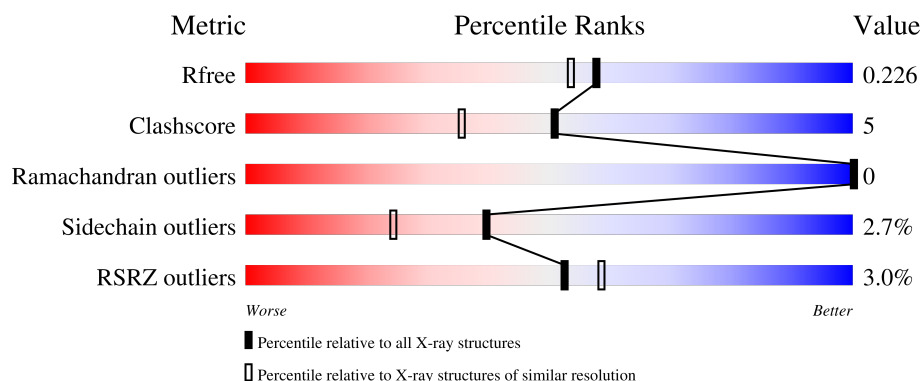
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	165	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>..</div> </div>
1	D	165	<div> <div>4%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	B	11	<div> <div>27%</div> <div>55%</div> <div>18%</div> </div>
2	E	11	<div> <div>45%</div> <div>36%</div> <div>18%</div> </div>
3	C	7	<div> <div>43%</div> <div>57%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	7	<div><div></div><div>29%</div><div>43%</div><div>29%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3009 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 Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1249	793	213	235	8			
1	D	164	Total	C	N	O	S	0	0	0
			1248	792	215	233	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	CYS	LYS	engineered mutation	UNP P62937
D	127	CYS	LYS	engineered mutation	UNP P62937

- Molecule 2 is a protein (with D amino acids) called Cyclosporin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			85	62	11	12			
2	E	11	Total	C	N	O	0	0	0
			85	62	11	12			

- Molecule 3 is a protein called Aromatic foldamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	S	0	0	0
			108	76	14	17	1			
3	C	7	Total	C	N	O	S	0	0	0
			108	76	14	17	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		

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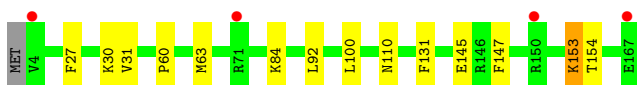
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	O 3	0	0
4	D	47	Total 47	O 47	0	0
4	E	5	Total 5	O 5	0	0
4	F	5	Total 5	O 5	0	0
4	C	2	Total 2	O 2	0	0

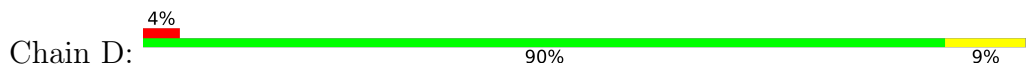
3 Residue-property plots [i](#)

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.

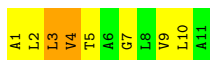
- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



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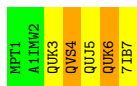
- Molecule 2: Cyclosporin A



- Molecule 2: Cyclosporin A



- Molecule 3: Aromatic foldamer



- Molecule 3: Aromatic foldamer



WPTI
A11HW2
QDK3
QVS4
QUJ5
QUK6
71B7

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.47Å 70.89Å 64.09Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	62.52 – 1.91 62.52 – 1.91	Depositor EDS
% Data completeness (in resolution range)	89.1 (62.52-1.91) 89.1 (62.52-1.91)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.177 , 0.219 0.185 , 0.226	Depositor DCC
R_{free} test set	1433 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.9	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	0.96	EDS
Total number of atoms	3009	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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: QUK, DAL, MVA, A1IMW, MLE, QUJ, QVS, ABA, BMT, 7IB, MPT, SAR

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	0.75	0/1277	0.77	0/1714
1	D	0.74	0/1276	0.76	0/1713
2	B	0.40	0/10	0.64	0/11
2	E	0.61	0/10	0.69	0/11
All	All	0.74	0/2573	0.77	0/3449

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
3	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	4	QVS	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	1249	0	1206	6	0
1	D	1248	0	1204	9	0
2	B	85	0	109	7	0
2	E	85	0	110	5	0
3	C	108	0	4	0	0
3	F	108	0	4	2	0
4	A	64	0	0	1	1
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	47	0	0	2	1
4	E	5	0	0	0	0
4	F	5	0	0	0	0
All	All	3009	0	2637	28	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 5.

All (28) 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:147:PHE:O	1:A:154:THR:HA	2.06	0.56
1:A:60:PRO:HA	1:A:145:GLU:HG3	1.92	0.51
1:D:147:PHE:CE1	1:D:156:LYS:HD2	2.46	0.51
3:F:7:7IB:CG	3:F:7:7IB:C8	2.89	0.50
1:A:84:LYS:HA	1:A:110:ASN:O	2.12	0.49
1:D:86:GLU:CD	1:D:86:GLU:H	2.15	0.49
1:D:7:THR:HA	1:D:24:PHE:O	2.15	0.46
2:E:3:MLE:HB2	2:E:4:MVA:HN1	1.97	0.46
1:D:151:ASN:ND2	4:D:303:HOH:O	2.49	0.45
1:D:147:PHE:CD1	1:D:156:LYS:HD2	2.52	0.44
3:F:6:QUK:O	3:F:7:7IB:C3	2.65	0.43
2:B:4:MVA:HA	2:B:5:BMT:HN1	1.83	0.43
1:D:120:LYS:O	4:D:301:HOH:O	2.22	0.43
2:E:4:MVA:HA	2:E:5:BMT:HN1	1.76	0.43
1:A:100:LEU:HG	1:A:131:PHE:CZ	2.54	0.43
1:D:14:VAL:HG22	1:D:158:ILE:HD12	2.01	0.43
2:E:3:MLE:O	2:E:3:MLE:HN3	2.18	0.42
2:B:1:DAL:C	2:B:3:MLE:HN1	2.48	0.42
2:E:9:VAL:HA	2:E:10:MLE:HN1	1.75	0.42
2:B:5:BMT:HN2	2:B:5:BMT:OG1	2.20	0.41
2:B:3:MLE:HA	2:B:4:MVA:HN1	1.89	0.41
1:D:104:ASN:O	2:E:5:BMT:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HD2	4:A:339:HOH:O	2.19	0.41
2:B:10:MLE:HN2	2:B:10:MLE:HB3	1.79	0.41
1:D:107:PRO:O	1:D:109:THR:HG23	2.21	0.41
1:A:27:PHE:CD2	1:A:92:LEU:HD13	2.56	0.41
2:B:9:VAL:HA	2:B:10:MLE:HN1	1.68	0.40
2:B:1:DAL:HA	2:B:2:MLE:HN1	1.75	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)
4:A:342:HOH:O	4:D:301:HOH:O[2_657]	1.52	0.68

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/165 (98%)	157 (97%)	5 (3%)	0	100	100
1	D	162/165 (98%)	156 (96%)	6 (4%)	0	100	100
2	B	1/11 (9%)	1 (100%)	0	0	100	100
2	E	1/11 (9%)	1 (100%)	0	0	100	100
All	All	326/352 (93%)	315 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/133 (98%)	126 (97%)	4 (3%)	35	18
1	D	129/133 (97%)	126 (98%)	3 (2%)	45	30
2	B	1/1 (100%)	1 (100%)	0	100	100
2	E	1/1 (100%)	1 (100%)	0	100	100
All	All	261/268 (97%)	254 (97%)	7 (3%)	40	24

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	31	VAL
1	A	63	MET
1	A	153	LYS
1	D	31	VAL
1	D	63	MET
1	D	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

26 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	MLE	E	8	2	7,8,9	0.45	0	6,9,11	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLE	B	2	2	7,8,9	0.67	0	6,9,11	0.56	0
2	BMT	E	5	2	11,12,13	0.61	0	12,14,16	1.12	1 (8%)
3	QUK	F	3	3	19,19,20	2.18	1 (5%)	22,25,27	1.72	3 (13%)
3	QUJ	C	5	3	19,19,20	1.87	2 (10%)	23,26,28	1.98	6 (26%)
3	QUJ	F	5	3	19,19,20	2.05	1 (5%)	23,26,28	2.19	7 (30%)
2	MLE	E	2	2	7,8,9	0.59	0	6,9,11	0.69	0
2	MLE	B	8	2	7,8,9	0.55	0	6,9,11	0.98	0
2	MVA	E	4	2	6,7,8	0.66	0	7,8,10	0.80	0
2	MLE	B	3	2	7,8,9	0.37	0	6,9,11	1.03	1 (16%)
2	MVA	B	4	2	6,7,8	0.70	0	7,8,10	1.29	1 (14%)
2	SAR	B	7	2	4,4,5	1.36	1 (25%)	1,3,5	1.73	0
2	ABA	B	6	2	4,5,6	0.64	0	1,5,7	0.27	0
3	QVS	C	4	3	15,15,16	2.12	3 (20%)	19,21,23	2.23	6 (31%)
3	QUK	C	6	3	19,19,20	1.94	2 (10%)	22,25,27	2.02	4 (18%)
3	QUK	F	6	3	19,19,20	2.06	2 (10%)	22,25,27	1.97	5 (22%)
2	ABA	E	6	2	4,5,6	0.48	0	1,5,7	0.07	0
2	MLE	E	3	2	7,8,9	0.40	0	6,9,11	1.00	1 (16%)
2	SAR	E	7	2	4,4,5	1.50	1 (25%)	1,3,5	1.70	0
2	MLE	E	10	2	7,8,9	0.74	0	6,9,11	0.74	0
3	QVS	F	4	3	15,15,16	2.37	2 (13%)	19,21,23	2.02	5 (26%)
3	QUK	C	3	3	19,19,20	1.82	2 (10%)	22,25,27	3.14	9 (40%)
2	BMT	B	5	2	11,12,13	0.65	0	12,14,16	0.69	0
2	MLE	B	10	2	7,8,9	0.59	0	6,9,11	0.69	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
2	MLE	E	8	2	-	1/5/8/10	-
2	MLE	B	2	2	-	0/5/8/10	-
2	BMT	E	5	2	-	3/13/16/18	-
3	QUK	F	3	3	-	3/7/7/9	0/2/2/2
3	QUJ	C	5	3	-	0/7/7/9	0/2/2/2
3	QUJ	F	5	3	-	2/7/7/9	0/2/2/2
2	MLE	E	2	2	-	0/5/8/10	-
2	MLE	B	8	2	-	1/5/8/10	-
2	MVA	E	4	2	-	1/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	B	3	2	-	0/5/8/10	-
2	MVA	B	4	2	-	3/6/8/10	-
2	SAR	B	7	2	-	1/1/2/3	-
2	ABA	B	6	2	-	0/3/4/6	-
3	QVS	C	4	3	-	2/2/2/4	0/2/2/2
3	QUK	C	6	3	-	3/7/7/9	0/2/2/2
3	QUK	F	6	3	-	1/7/7/9	0/2/2/2
2	ABA	E	6	2	-	0/3/4/6	-
2	MLE	E	3	2	-	0/5/8/10	-
2	SAR	E	7	2	-	1/1/2/3	-
2	MLE	E	10	2	-	0/5/8/10	-
3	QVS	F	4	3	-	0/2/2/4	0/2/2/2
3	QUK	C	3	3	-	3/7/7/9	0/2/2/2
2	BMT	B	5	2	-	1/13/16/18	-
2	MLE	B	10	2	-	2/5/8/10	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	QUK	C10-C	-8.81	1.39	1.48
3	F	4	QVS	CA-C	-8.00	1.40	1.48
3	F	6	QUK	C10-C	-7.97	1.40	1.48
3	F	5	QUJ	CA-C	-7.72	1.40	1.48
3	C	6	QUK	C10-C	-7.65	1.40	1.48
3	C	5	QUJ	CA-C	-6.99	1.41	1.48
3	C	4	QVS	CA-C	-6.29	1.42	1.48
3	C	3	QUK	C10-C	-6.08	1.42	1.48
3	C	3	QUK	C10-N11	4.44	1.37	1.33
3	C	4	QVS	C2-C7	-3.16	1.37	1.42
2	E	7	SAR	CA-N	2.66	1.49	1.46
3	F	6	QUK	C10-N11	2.50	1.35	1.33
2	B	7	SAR	CA-N	2.37	1.49	1.46
3	C	6	QUK	C10-N11	2.28	1.35	1.33
3	C	4	QVS	CA-N11	2.14	1.35	1.33
3	C	5	QUJ	CA-N11	2.12	1.35	1.33
3	F	4	QVS	CA-N11	2.09	1.35	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	QUK	C-C10-N11	7.22	121.74	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	QUJ	CA-N11-C7	6.83	123.29	118.11
3	F	5	QUJ	CA-N11-C7	6.80	123.27	118.11
3	C	6	QUK	C10-N11-C7	6.60	123.12	118.11
3	C	3	QUK	C7-CA-N	6.44	130.35	118.07
3	F	6	QUK	C10-N11-C7	6.34	122.91	118.11
3	F	4	QVS	CA-N11-C7	6.16	122.78	118.11
3	C	4	QVS	CA-N11-C7	6.12	122.75	118.11
3	F	3	QUK	C10-N11-C7	5.96	122.63	118.11
3	C	3	QUK	CA-C7-N11	5.53	124.11	118.64
3	C	3	QUK	C10-N11-C7	5.29	122.12	118.11
3	C	3	QUK	C3-CA-N	-4.60	111.17	120.36
3	C	4	QVS	C3-C2-N	3.86	128.08	120.36
3	C	4	QVS	C7-C2-N	-3.62	111.17	118.07
3	F	5	QUJ	C3-C2-N	3.48	127.31	120.36
3	F	5	QUJ	CG-OB-C8	3.33	129.14	118.25
3	C	4	QVS	C9-CA-C	3.24	124.02	121.23
3	C	3	QUK	O-C-C10	-3.20	121.19	124.22
3	F	5	QUJ	C9-CA-C	3.18	123.98	121.23
3	F	5	QUJ	C7-C2-N	-3.15	112.06	118.07
3	C	6	QUK	O-C-C10	-3.15	121.24	124.22
3	F	5	QUJ	O-C-CA	-3.11	121.28	124.22
3	C	3	QUK	C9-C10-C	-3.09	118.55	121.23
3	F	6	QUK	O-C-C10	-3.05	121.33	124.22
3	C	6	QUK	C-C10-N11	2.98	117.58	114.66
3	F	3	QUK	C-C10-N11	2.97	117.57	114.66
3	F	4	QVS	C9-CA-C	2.94	123.77	121.23
3	C	5	QUJ	C3-C2-N	2.88	126.12	120.36
3	C	5	QUJ	O-C-CA	-2.84	121.53	124.22
3	C	5	QUJ	C9-CA-C	2.79	123.63	121.23
3	F	6	QUK	C3-CA-N	2.77	125.91	120.36
3	C	6	QUK	C3-CA-N	2.77	125.90	120.36
2	E	5	BMT	CB-CA-N	2.76	116.90	111.41
3	F	6	QUK	C-C10-N11	2.75	117.35	114.66
3	F	4	QVS	C3-C2-N	2.69	125.73	120.36
3	C	4	QVS	O-C-CA	-2.68	121.68	124.22
2	B	4	MVA	CB-CA-C	-2.68	109.68	113.04
3	C	5	QUJ	C-CA-N11	2.67	117.28	114.66
3	C	5	QUJ	C7-C2-N	-2.63	113.05	118.07
3	F	4	QVS	C7-C2-N	-2.44	113.42	118.07
3	C	3	QUK	C6-C7-N11	-2.42	117.79	122.78
3	C	3	QUK	C5-C6-C8	-2.40	117.05	122.58
3	F	6	QUK	OB-C8-C6	2.36	121.62	115.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	QVS	C-CA-N11	2.30	116.91	114.66
2	B	3	MLE	O-C-CA	-2.17	119.08	124.78
3	F	5	QUJ	C-CA-N11	2.15	116.77	114.66
3	F	3	QUK	O-C-C10	-2.08	122.25	124.22
2	E	3	MLE	O-C-CA	-2.07	119.34	124.78
3	F	4	QVS	C-CA-N11	2.01	116.63	114.66

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MVA	N-CA-CB-CG2
2	B	5	BMT	CB-CA-N-CN
2	B	8	MLE	O-C-CA-CB
2	E	8	MLE	O-C-CA-CB
3	F	3	QUK	O-C-C10-C9
3	C	3	QUK	O-C-C10-N11
3	C	3	QUK	O-C-C10-C9
3	C	4	QVS	O-C-CA-C9
3	C	6	QUK	CE-CD-CG-OB
3	F	5	QUJ	C6-C8-OB-CG
2	B	10	MLE	CA-CB-CG-CD1
3	F	5	QUJ	C9-C8-OB-CG
2	B	10	MLE	CA-CB-CG-CD2
3	C	3	QUK	CG-CD-CE-N1
3	F	6	QUK	CG-CD-CE-N1
3	C	6	QUK	C6-C8-OB-CG
3	C	6	QUK	C9-C8-OB-CG
2	B	4	MVA	N-CA-CB-CG1
3	C	4	QVS	O-C-CA-N11
2	E	5	BMT	CE-CD2-CG2-CB
2	E	5	BMT	CB-CA-N-CN
2	B	4	MVA	CB-CA-N-CN
2	E	4	MVA	CB-CA-N-CN
3	F	3	QUK	CE-CD-CG-OB
2	E	5	BMT	CE-CD2-CG2-CD1
2	B	7	SAR	C-CA-N-CN
2	E	7	SAR	C-CA-N-CN
3	F	3	QUK	O-C-C10-N11

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	MLE	1	0
2	E	5	BMT	2	0
2	E	4	MVA	2	0
2	B	3	MLE	2	0
2	B	4	MVA	2	0
3	F	6	QUK	1	0
2	E	3	MLE	2	0
2	E	10	MLE	1	0
2	B	5	BMT	2	0
2	B	10	MLE	2	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	164/165 (99%)	0.38	4 (2%) 59 65	24, 35, 55, 72	0
1	D	164/165 (99%)	0.50	6 (3%) 45 52	26, 38, 54, 66	0
2	B	2/11 (18%)	0.59	0 100 100	31, 31, 31, 34	0
2	E	2/11 (18%)	0.25	0 100 100	31, 31, 31, 32	0
3	C	0/7	-	-	-	-
3	F	0/7	-	-	-	-
All	All	332/366 (90%)	0.44	10 (3%) 52 58	24, 37, 55, 72	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	VAL	5.2
1	A	4	VAL	3.9
1	D	167	GLU	3.7
1	A	167	GLU	2.5
1	D	16	GLY	2.3
1	D	154	THR	2.1
1	A	71	ARG	2.1
1	A	150	ARG	2.1
1	D	19	LEU	2.1
1	D	151	ASN	2.1

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(\AA^2)	Q<0.9
3	QUJ	F	5	18/19	0.83	0.15	45,51,68,72	0
3	QUK	C	3	18/19	0.86	0.13	51,56,70,72	0
3	QVS	C	4	14/15	0.88	0.11	42,45,54,56	0
3	QUK	F	6	18/19	0.88	0.11	38,45,71,74	0
3	QUJ	C	5	18/19	0.89	0.13	40,50,68,69	0
3	QUK	F	3	18/19	0.90	0.11	49,54,74,80	0
2	DAL	B	1	5/6	0.91	0.12	29,31,32,34	0
3	QVS	F	4	14/15	0.91	0.09	46,48,52,60	0
3	QUK	C	6	18/19	0.91	0.10	41,45,57,61	0
2	MLE	B	8	9/10	0.93	0.11	32,37,45,46	0
2	ABA	E	6	6/7	0.93	0.10	29,34,35,37	0
2	SAR	E	7	5/6	0.93	0.08	35,35,37,37	0
2	BMT	E	5	13/14	0.94	0.10	23,27,37,40	0
2	MVA	E	4	8/9	0.94	0.08	23,25,26,26	0
2	MLE	E	8	9/10	0.94	0.12	31,36,58,60	0
2	MLE	B	10	9/10	0.94	0.10	31,34,44,45	0
2	ABA	B	6	6/7	0.95	0.07	28,30,32,33	0
2	MLE	B	2	9/10	0.95	0.08	26,28,29,30	0
2	SAR	B	7	5/6	0.95	0.07	34,34,37,37	0
2	BMT	B	5	13/14	0.95	0.09	23,26,35,38	0
2	MLE	B	3	9/10	0.95	0.08	24,27,32,33	0
2	MLE	E	10	9/10	0.96	0.08	28,31,44,46	0
2	DAL	E	1	5/6	0.96	0.08	29,29,30,32	0
2	MVA	B	4	8/9	0.96	0.07	23,25,26,26	0
2	MLE	E	2	9/10	0.97	0.06	24,29,31,33	0
2	MLE	E	3	9/10	0.97	0.06	22,24,29,31	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.