



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2026 – 01:53 pm BST

PDB ID : 9QT7 / pdb_00009qt7
Title : Crystal structure of affitin C10 fused to a coiled-coil domain in complex with a quinoline oligoamide foldamer
Authors : Morozov, V.; Wang, L.; Kwon, S.; Douat, C.; Huc, I.
Deposited on : 2025-04-08
Resolution : 2.80 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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

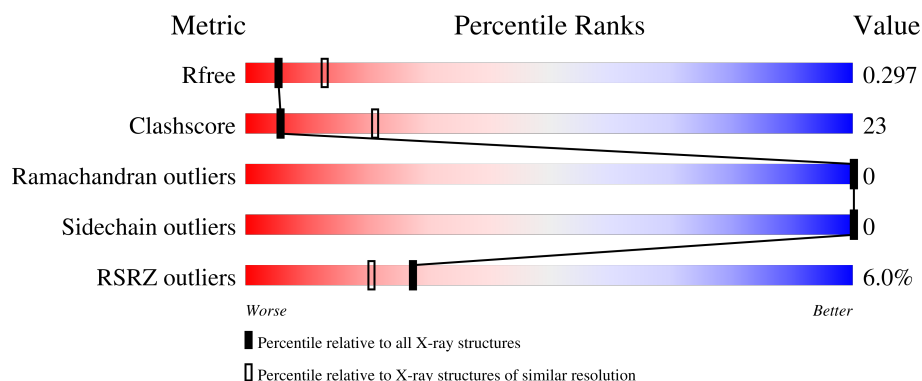
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



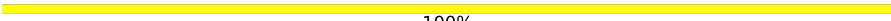
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	100	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>31%</div> <div>• 5%</div> </div> </div>
1	B	100	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>34%</div> <div>• •</div> </div> </div>
1	C	100	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>32%</div> <div>• •</div> </div> </div>
1	D	100	<div> <div>10%</div> <div> <div></div> <div>58%</div> <div>37%</div> <div>5%</div> </div> </div>
2	E	6	<div> <div></div> <div> <div>83%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	6	 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2943 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-binding protein 7d,Talin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	0	0
			677	434	119	122	2			
1	B	96	Total	C	N	O	S	0	0	0
			720	457	132	129	2			
1	C	96	Total	C	N	O	S	0	0	0
			684	434	119	129	2			
1	D	95	Total	C	N	O	S	0	0	0
			658	422	117	117	2			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P13123
A	1	PRO	-	expression tag	UNP P13123
A	21	THR	LYS	engineered mutation	UNP P13123
A	22	HIS	LYS	engineered mutation	UNP P13123
A	24	PHE	TRP	engineered mutation	UNP P13123
A	26	HIS	VAL	engineered mutation	UNP P13123
A	29	LEU	MET	engineered mutation	UNP P13123
A	31	VAL	SER	engineered mutation	UNP P13123
A	33	TYR	THR	engineered mutation	UNP P13123
A	42	HIS	ARG	engineered mutation	UNP P13123
A	44	LEU	ALA	engineered mutation	UNP P13123
A	46	PRO	SER	engineered mutation	UNP P13123
A	66	ALA	-	linker	UNP P13123
A	67	ALA	-	linker	UNP P13123
B	0	GLY	-	expression tag	UNP P13123
B	1	PRO	-	expression tag	UNP P13123
B	21	THR	LYS	engineered mutation	UNP P13123
B	22	HIS	LYS	engineered mutation	UNP P13123
B	24	PHE	TRP	engineered mutation	UNP P13123
B	26	HIS	VAL	engineered mutation	UNP P13123
B	29	LEU	MET	engineered mutation	UNP P13123

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	VAL	SER	engineered mutation	UNP P13123
B	33	TYR	THR	engineered mutation	UNP P13123
B	42	HIS	ARG	engineered mutation	UNP P13123
B	44	LEU	ALA	engineered mutation	UNP P13123
B	46	PRO	SER	engineered mutation	UNP P13123
B	66	ALA	-	linker	UNP P13123
B	67	ALA	-	linker	UNP P13123
C	0	GLY	-	expression tag	UNP P13123
C	1	PRO	-	expression tag	UNP P13123
C	21	THR	LYS	engineered mutation	UNP P13123
C	22	HIS	LYS	engineered mutation	UNP P13123
C	24	PHE	TRP	engineered mutation	UNP P13123
C	26	HIS	VAL	engineered mutation	UNP P13123
C	29	LEU	MET	engineered mutation	UNP P13123
C	31	VAL	SER	engineered mutation	UNP P13123
C	33	TYR	THR	engineered mutation	UNP P13123
C	42	HIS	ARG	engineered mutation	UNP P13123
C	44	LEU	ALA	engineered mutation	UNP P13123
C	46	PRO	SER	engineered mutation	UNP P13123
C	66	ALA	-	linker	UNP P13123
C	67	ALA	-	linker	UNP P13123
D	0	GLY	-	expression tag	UNP P13123
D	1	PRO	-	expression tag	UNP P13123
D	21	THR	LYS	engineered mutation	UNP P13123
D	22	HIS	LYS	engineered mutation	UNP P13123
D	24	PHE	TRP	engineered mutation	UNP P13123
D	26	HIS	VAL	engineered mutation	UNP P13123
D	29	LEU	MET	engineered mutation	UNP P13123
D	31	VAL	SER	engineered mutation	UNP P13123
D	33	TYR	THR	engineered mutation	UNP P13123
D	42	HIS	ARG	engineered mutation	UNP P13123
D	44	LEU	ALA	engineered mutation	UNP P13123
D	46	PRO	SER	engineered mutation	UNP P13123
D	66	ALA	-	linker	UNP P13123
D	67	ALA	-	linker	UNP P13123

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

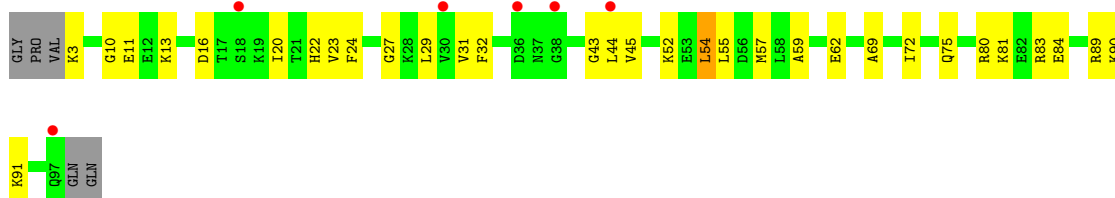
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total 102	C 66	N 11	O 23	P 2	0	0	0
2	F	6	Total 102	C 66	N 11	O 23	P 2	0	0	0

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.

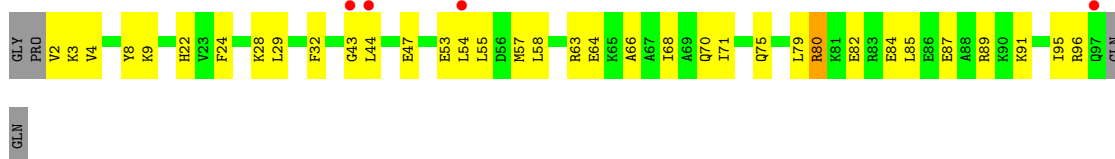
- Molecule 1: DNA-binding protein 7d,Talin-1

Chain A: 



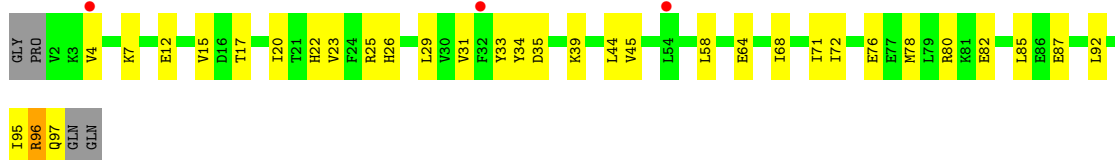
- Molecule 1: DNA-binding protein 7d,Talin-1

Chain B: 



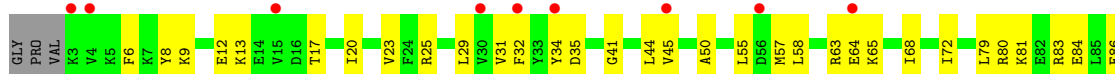
- Molecule 1: DNA-binding protein 7d,Talin-1

Chain C: 



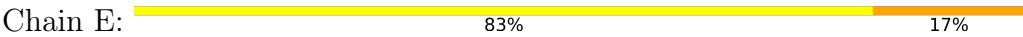
- Molecule 1: DNA-binding protein 7d,Talin-1

Chain D: 

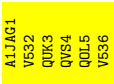
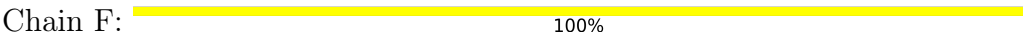




● Molecule 2: Quinoline oligoamide foldamer



● Molecule 2: Quinoline oligoamide foldamer



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.46Å 105.54Å 65.52Å 90.00° 99.30° 90.00°	Depositor
Resolution (Å)	64.66 – 2.80 64.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (64.66-2.80) 96.6 (64.66-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.245 , 0.296 0.246 , 0.297	Depositor DCC
R_{free} test set	681 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2943	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QUK, V53, QVS, A1JAG, QOL

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	0.82	0/687	1.21	2/931 (0.2%)
1	B	0.75	0/730	0.98	0/983
1	C	0.81	0/694	1.17	0/943
1	D	0.78	0/667	1.15	1/904 (0.1%)
All	All	0.79	0/2778	1.13	3/3761 (0.1%)

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	2
1	B	0	3
1	C	0	2
2	E	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	24	PHE	CA-CB-CG	6.73	120.53	113.80
1	D	12	GLU	N-CA-C	5.46	118.36	110.28
1	A	54	LEU	N-CA-C	-5.37	106.79	113.55

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	ARG	Sidechain
1	A	89	ARG	Sidechain
1	B	63	ARG	Sidechain
1	B	80	ARG	Sidechain
1	B	96	ARG	Sidechain
1	C	80	ARG	Sidechain
1	C	96	ARG	Sidechain
2	E	3	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	677	0	621	30	0
1	B	720	0	696	29	0
1	C	684	0	612	33	0
1	D	658	0	595	45	0
2	E	102	0	0	0	0
2	F	102	0	0	0	0
All	All	2943	0	2524	127	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 23.

All (127) 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:C:23:VAL:HG22	1:C:58:LEU:HD12	1.33	1.08
1:D:79:LEU:CD2	1:D:83:ARG:HH12	1.68	1.06
1:A:20:ILE:CD1	1:A:54:LEU:HD11	1.92	1.00
1:A:20:ILE:HD12	1:A:54:LEU:CD1	1.95	0.96
1:D:79:LEU:HD21	1:D:83:ARG:HH12	1.31	0.95
1:A:20:ILE:CD1	1:A:54:LEU:CD1	2.45	0.95
1:A:31:VAL:HG22	1:A:44:LEU:HG	1.50	0.94
1:A:75:GLN:NE2	1:D:92:LEU:HD11	1.83	0.93
1:D:50:ALA:HB3	1:D:55:LEU:CD2	1.99	0.92
1:C:78:MET:O	1:C:82:GLU:HG3	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:HA	1:A:16:ASP:HA	1.51	0.90
1:A:20:ILE:HD13	1:A:54:LEU:HD11	1.53	0.90
1:A:54:LEU:HA	1:A:57:MET:HG3	1.60	0.83
1:D:79:LEU:CD2	1:D:83:ARG:NH1	2.42	0.83
1:B:95:ILE:CG2	1:C:71:ILE:HD13	2.12	0.80
1:D:17:THR:O	1:D:57:MET:HE1	1.82	0.79
1:C:23:VAL:HG22	1:C:58:LEU:CD1	2.10	0.77
1:A:75:GLN:HA	1:D:92:LEU:HD12	1.66	0.76
1:C:25:ARG:HH21	1:C:58:LEU:HD23	1.50	0.76
1:B:95:ILE:HG22	1:C:71:ILE:HD13	1.69	0.75
1:D:50:ALA:HB3	1:D:55:LEU:HD21	1.68	0.74
1:B:47:GLU:HG3	1:B:55:LEU:HD21	1.70	0.74
1:C:72:ILE:O	1:C:76:GLU:HG2	1.88	0.74
1:A:75:GLN:HE21	1:D:92:LEU:HD11	1.51	0.73
1:C:64:GLU:O	1:C:68:ILE:HG12	1.90	0.71
1:B:95:ILE:HG22	1:C:71:ILE:CD1	2.21	0.70
1:D:79:LEU:HD23	1:D:83:ARG:HH12	1.54	0.70
1:C:44:LEU:C	1:C:44:LEU:HD23	2.18	0.69
1:B:75:GLN:O	1:B:79:LEU:HD23	1.93	0.69
1:D:93:ALA:O	1:D:94:GLN:OE1	2.11	0.68
1:A:43:GLY:C	1:A:44:LEU:HD12	2.19	0.67
1:B:2:VAL:CG1	1:B:3:LYS:N	2.58	0.66
1:A:69:ALA:O	1:A:72:ILE:HG13	1.95	0.66
1:D:79:LEU:HD23	1:D:83:ARG:NH1	2.10	0.66
1:A:32:PHE:CE1	1:A:45:VAL:HG13	2.32	0.65
1:D:31:VAL:HG22	1:D:44:LEU:HD12	1.79	0.65
1:B:44:LEU:HD12	1:B:44:LEU:N	2.12	0.65
1:C:4:VAL:CG2	1:C:17:THR:HG22	2.28	0.64
1:B:75:GLN:HG2	1:C:92:LEU:HD11	1.80	0.64
1:C:4:VAL:HG23	1:C:17:THR:HG22	1.81	0.63
1:C:17:THR:HA	1:C:20:ILE:HG13	1.81	0.61
1:C:25:ARG:HB2	1:C:58:LEU:HD21	1.83	0.61
1:D:94:GLN:OE1	1:D:94:GLN:HA	2.01	0.60
1:A:11:GLU:HA	1:A:11:GLU:OE1	2.01	0.60
1:D:17:THR:HB	1:D:57:MET:HE3	1.83	0.60
1:B:66:ALA:O	1:B:70:GLN:HG3	2.02	0.60
1:B:95:ILE:HG21	1:C:71:ILE:HD13	1.82	0.59
1:D:8:TYR:CD1	1:D:9:LYS:N	2.71	0.58
1:B:53:GLU:O	1:B:57:MET:HG3	2.04	0.58
1:D:50:ALA:HB3	1:D:55:LEU:HD23	1.86	0.58
1:B:22:HIS:CD2	1:B:24:PHE:HD1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLU:O	1:B:68:ILE:HG12	2.06	0.56
1:B:2:VAL:HG13	1:B:3:LYS:H	1.70	0.56
1:A:32:PHE:HE1	1:A:45:VAL:HG13	1.70	0.56
1:B:4:VAL:HG21	1:B:54:LEU:HD13	1.88	0.55
1:A:59:ALA:HA	1:A:62:GLU:OE1	2.05	0.55
1:A:81:LYS:HA	1:A:84:GLU:HG3	1.88	0.55
1:D:17:THR:HA	1:D:20:ILE:HG13	1.87	0.54
1:C:35:ASP:OD1	1:C:35:ASP:C	2.49	0.54
1:C:7:LYS:HD3	1:C:12:GLU:HA	1.89	0.54
1:A:80:ARG:O	1:A:84:GLU:HG3	2.09	0.53
1:B:82:GLU:HA	1:C:85:LEU:HD12	1.91	0.53
1:B:2:VAL:HG12	1:B:3:LYS:N	2.24	0.53
1:D:23:VAL:HG13	1:D:58:LEU:HD12	1.91	0.52
1:D:25:ARG:CB	1:D:58:LEU:HD21	2.38	0.52
1:D:23:VAL:HG13	1:D:23:VAL:O	2.10	0.52
1:D:6:PHE:N	1:D:6:PHE:CD2	2.78	0.52
1:C:96:ARG:O	1:C:97:GLN:C	2.53	0.51
1:B:85:LEU:HG	1:B:89:ARG:HH21	1.76	0.51
1:D:68:ILE:HG23	1:D:72:ILE:HD13	1.92	0.51
1:A:20:ILE:HD12	1:A:54:LEU:HD12	1.87	0.50
1:D:29:LEU:CB	1:D:44:LEU:HD11	2.42	0.50
1:D:8:TYR:HB3	1:D:13:LYS:HD2	1.92	0.50
1:B:47:GLU:HG3	1:B:55:LEU:CD2	2.39	0.50
1:C:44:LEU:HD23	1:C:45:VAL:N	2.27	0.50
1:B:32:PHE:CD1	1:B:32:PHE:N	2.80	0.49
1:A:75:GLN:NE2	1:D:92:LEU:CD1	2.65	0.48
1:D:50:ALA:CB	1:D:55:LEU:CD2	2.84	0.48
1:B:47:GLU:CG	1:B:55:LEU:HD21	2.41	0.48
1:D:92:LEU:C	1:D:92:LEU:HD23	2.39	0.48
1:A:11:GLU:OE1	1:A:11:GLU:CA	2.63	0.47
1:C:87:GLU:HA	1:C:87:GLU:OE1	2.14	0.47
1:C:95:ILE:C	1:C:97:GLN:H	2.22	0.47
1:D:94:GLN:OE1	1:D:94:GLN:CA	2.63	0.47
1:D:23:VAL:O	1:D:23:VAL:CG1	2.63	0.47
1:C:25:ARG:NH2	1:C:58:LEU:HD23	2.26	0.46
1:D:64:GLU:HG3	1:D:65:LYS:N	2.31	0.46
1:D:81:LYS:HD2	1:D:84:GLU:OE1	2.15	0.46
1:A:22:HIS:ND1	1:A:23:VAL:N	2.63	0.46
1:A:20:ILE:HD12	1:A:54:LEU:HD13	1.93	0.46
1:D:35:ASP:OD1	1:D:35:ASP:C	2.59	0.46
1:D:64:GLU:O	1:D:68:ILE:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:C	1:C:44:LEU:CD2	2.89	0.45
1:B:43:GLY:C	1:B:44:LEU:HD12	2.41	0.45
1:D:64:GLU:O	1:D:65:LYS:C	2.60	0.45
1:B:58:LEU:HD12	1:B:58:LEU:O	2.17	0.45
1:C:45:VAL:O	1:C:45:VAL:HG23	2.17	0.45
1:D:65:LYS:HA	1:D:65:LYS:HD2	1.64	0.44
1:A:57:MET:HE2	1:A:57:MET:HB3	1.72	0.44
1:C:15:VAL:HG21	1:C:34:TYR:CG	2.52	0.44
1:A:52:LYS:HA	1:A:55:LEU:HB2	1.99	0.44
1:C:22:HIS:HB2	1:C:33:TYR:HB2	2.00	0.44
1:B:70:GLN:O	1:B:71:ILE:C	2.61	0.44
1:C:35:ASP:HA	1:C:39:LYS:O	2.18	0.44
1:D:32:PHE:HE1	1:D:45:VAL:HG23	1.83	0.44
1:A:90:LYS:O	1:A:91:LYS:C	2.61	0.44
1:C:26:HIS:HD2	1:C:31:VAL:CG2	2.30	0.44
1:D:23:VAL:HG13	1:D:58:LEU:CD1	2.47	0.44
1:D:34:TYR:CE1	1:D:41:GLY:C	2.96	0.44
1:B:22:HIS:O	1:B:32:PHE:HA	2.18	0.43
1:B:8:TYR:CE2	1:B:9:LYS:HG3	2.54	0.43
1:B:87:GLU:O	1:B:91:LYS:HG2	2.19	0.43
1:A:11:GLU:HG3	1:A:13:LYS:HG2	2.01	0.42
1:A:27:GLY:C	1:A:29:LEU:H	2.26	0.42
1:D:81:LYS:HD2	1:D:81:LYS:HA	1.75	0.42
1:A:10:GLY:O	1:A:11:GLU:C	2.61	0.42
1:D:92:LEU:O	1:D:95:ILE:HG22	2.20	0.42
1:D:79:LEU:O	1:D:80:ARG:C	2.62	0.42
1:C:29:LEU:HD13	1:C:44:LEU:HD11	2.01	0.42
1:C:45:VAL:O	1:C:45:VAL:CG2	2.69	0.41
1:A:32:PHE:CD1	1:A:32:PHE:N	2.88	0.41
1:C:92:LEU:O	1:C:95:ILE:HG22	2.21	0.41
1:D:23:VAL:CG1	1:D:58:LEU:HA	2.51	0.41
1:B:28:LYS:C	1:B:29:LEU:HD23	2.46	0.40
1:D:86:GLU:OE2	1:D:89:ARG:NH1	2.54	0.40
1:D:63:ARG:O	1:D:64:GLU:C	2.64	0.40
1:B:80:ARG:O	1:B:84:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	93/100 (93%)	87 (94%)	6 (6%)	0	100	100
1	B	94/100 (94%)	89 (95%)	5 (5%)	0	100	100
1	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
1	D	93/100 (93%)	86 (92%)	7 (8%)	0	100	100
All	All	374/400 (94%)	352 (94%)	22 (6%)	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	55/84 (66%)	55 (100%)	0	100	100
1	B	65/84 (77%)	65 (100%)	0	100	100
1	C	57/84 (68%)	57 (100%)	0	100	100
1	D	51/84 (61%)	51 (100%)	0	100	100
All	All	228/336 (68%)	228 (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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	75	GLN
1	B	22	HIS
1	C	26	HIS
1	D	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	QUK	F	3	2	19,19,20	1.46	3 (15%)	22,25,27	1.33	2 (9%)
2	A1JAG	E	1	2	10,10,11	0.58	0	9,9,11	0.96	1 (11%)
2	QVS	E	4	2	15,15,16	1.59	3 (20%)	19,21,23	2.08	5 (26%)
2	QOL	F	5	2	21,21,22	1.38	3 (14%)	23,28,30	1.08	1 (4%)
2	V53	F	2	2	20,20,21	2.00	7 (35%)	25,29,31	1.58	6 (24%)
2	A1JAG	F	1	2	10,10,11	0.59	0	9,9,11	0.95	1 (11%)
2	QVS	F	4	2	15,15,16	1.56	5 (33%)	19,21,23	1.42	5 (26%)
2	V53	E	6	2	21,21,21	1.87	6 (28%)	29,31,31	1.42	6 (20%)
2	V53	E	2	2	20,20,21	2.01	9 (45%)	25,29,31	1.52	5 (20%)
2	QOL	E	5	2	21,21,22	1.40	3 (14%)	23,28,30	1.21	2 (8%)
2	V53	F	6	2	21,21,21	1.87	6 (28%)	29,31,31	1.58	6 (20%)
2	QUK	E	3	2	19,19,20	1.50	4 (21%)	22,25,27	1.14	1 (4%)

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	QUK	F	3	2	-	3/7/7/9	0/2/2/2
2	A1JAG	E	1	2	-	6/7/8/9	-
2	QVS	E	4	2	-	0/2/2/4	0/2/2/2
2	QOL	F	5	2	-	5/11/11/13	0/2/2/2
2	V53	F	2	2	-	2/8/8/10	0/2/2/2
2	A1JAG	F	1	2	-	4/7/8/9	-
2	QVS	F	4	2	-	0/2/2/4	0/2/2/2
2	V53	E	6	2	-	3/10/10/10	0/2/2/2
2	V53	E	2	2	-	5/8/8/10	0/2/2/2
2	QOL	E	5	2	-	6/11/11/13	0/2/2/2
2	V53	F	6	2	-	3/10/10/10	0/2/2/2
2	QUK	E	3	2	-	1/7/7/9	0/2/2/2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	V53	P-O2	-4.01	1.45	1.54
2	F	2	V53	P-O2	-3.99	1.45	1.54
2	E	2	V53	P-O3	-3.97	1.45	1.54
2	F	2	V53	P-O3	-3.97	1.45	1.54
2	F	6	V53	P-O3	-3.97	1.45	1.54
2	E	6	V53	P-O3	-3.94	1.45	1.54
2	E	6	V53	P-O2	-3.90	1.46	1.54
2	F	6	V53	P-O2	-3.86	1.46	1.54
2	E	3	QUK	C10-C	3.70	1.52	1.48
2	E	5	QOL	C10-C	3.09	1.51	1.48
2	F	5	QOL	C10-C	3.04	1.51	1.48
2	F	2	V53	CAJ-C	2.99	1.51	1.48
2	E	4	QVS	CA-C	2.74	1.51	1.48
2	E	2	V53	CAJ-C	2.67	1.51	1.48
2	F	3	QUK	C10-C	2.64	1.51	1.48
2	F	3	QUK	C7-N11	-2.61	1.32	1.37
2	F	3	QUK	CA-C7	-2.59	1.38	1.42
2	E	4	QVS	C8-C6	-2.58	1.37	1.42
2	E	6	V53	CA-CAM	-2.54	1.38	1.42
2	F	6	V53	CA-CAM	-2.48	1.38	1.42
2	E	3	QUK	CA-C7	-2.44	1.38	1.42
2	E	4	QVS	C2-C7	-2.44	1.38	1.42
2	E	2	V53	CA-CAM	-2.43	1.38	1.42
2	E	6	V53	O01-C01	-2.40	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	QVS	C8-C6	-2.38	1.37	1.42
2	F	4	QVS	C7-N11	-2.36	1.32	1.37
2	F	4	QVS	CA-C	2.34	1.51	1.48
2	F	2	V53	CA-N	2.31	1.45	1.38
2	E	2	V53	O01-C01	-2.27	1.40	1.43
2	F	6	V53	P-C01	2.27	1.86	1.80
2	F	2	V53	O01-C01	-2.27	1.40	1.43
2	F	6	V53	O01-C01	-2.26	1.40	1.43
2	E	5	QOL	C7-N11	-2.24	1.32	1.37
2	F	5	QOL	C7-N11	-2.24	1.32	1.37
2	F	2	V53	CA-CAM	-2.24	1.38	1.42
2	E	6	V53	P-C01	2.18	1.85	1.80
2	E	2	V53	CA-N	2.17	1.45	1.38
2	F	4	QVS	C2-C7	-2.15	1.38	1.42
2	E	5	QOL	CA-N	2.14	1.45	1.38
2	F	4	QVS	C2-N	2.14	1.45	1.38
2	E	3	QUK	C7-N11	-2.13	1.33	1.37
2	E	3	QUK	C8-C6	-2.13	1.36	1.42
2	F	6	V53	CA-N	2.10	1.45	1.38
2	E	6	V53	CA-N	2.09	1.45	1.38
2	F	5	QOL	CA-C7	-2.09	1.38	1.42
2	E	2	V53	P-C01	2.05	1.85	1.80
2	E	2	V53	P-O1	-2.05	1.45	1.50
2	E	2	V53	CAM-NAH	-2.03	1.33	1.37
2	F	2	V53	P-C01	2.02	1.85	1.80

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	QVS	O-C-CA	-4.73	119.74	124.22
2	F	6	V53	C01-O01-CAF	-4.67	111.88	118.19
2	E	4	QVS	C7-C2-N	-3.99	110.46	118.07
2	F	2	V53	C01-O01-CAF	-3.60	113.33	118.19
2	E	4	QVS	C3-C2-N	3.34	127.04	120.36
2	E	2	V53	C01-O01-CAF	-3.32	113.70	118.19
2	F	2	V53	O2-P-O1	-3.24	103.83	112.39
2	E	6	V53	O2-P-O1	-3.20	103.94	112.39
2	F	6	V53	O3-P-O1	-3.11	104.16	112.39
2	F	4	QVS	O-C-CA	-3.06	121.33	124.22
2	E	6	V53	C01-O01-CAF	-3.02	114.11	118.19
2	E	2	V53	O2-P-O1	-3.02	104.41	112.39
2	F	3	QUK	C3-CA-N	2.97	126.30	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	QUK	CA-C7-N11	-2.93	115.74	118.64
2	E	6	V53	O3-P-O1	-2.93	104.63	112.39
2	E	2	V53	O3-P-O1	-2.82	104.94	112.39
2	F	6	V53	O2-P-O1	-2.82	104.94	112.39
2	F	2	V53	O3-P-O1	-2.80	104.98	112.39
2	E	4	QVS	OB-C8-C6	2.75	119.74	116.31
2	F	1	A1JAG	O-C-C50	-2.62	118.49	126.39
2	F	4	QVS	OB-C8-C6	2.61	119.57	116.31
2	E	2	V53	O2-P-C01	2.60	114.67	106.68
2	E	4	QVS	C-CA-N11	2.60	117.21	114.66
2	E	3	QUK	C3-CA-N	2.55	125.46	120.36
2	E	1	A1JAG	O-C-C50	-2.54	118.73	126.39
2	E	6	V53	OXT-C-CAJ	2.52	120.43	114.69
2	F	2	V53	O3-P-C01	2.50	114.36	106.68
2	F	6	V53	O3-P-C01	2.49	114.32	106.68
2	E	6	V53	O2-P-C01	2.47	114.26	106.68
2	F	6	V53	O2-P-C01	2.40	114.05	106.68
2	E	2	V53	O3-P-C01	2.38	113.99	106.68
2	F	6	V53	OXT-C-CAJ	2.36	120.05	114.69
2	F	4	QVS	C8-C9-CA	-2.34	116.78	119.05
2	F	4	QVS	C3-C2-N	2.33	125.03	120.36
2	E	6	V53	O3-P-C01	2.17	113.33	106.68
2	F	2	V53	O2-P-C01	2.15	113.27	106.68
2	F	2	V53	O-C-CAJ	-2.08	122.25	124.22
2	E	5	QOL	C3-CA-N	2.05	124.45	120.36
2	F	5	QOL	O-C-C10	-2.04	122.29	124.22
2	E	5	QOL	CG-OB-C8	-2.03	111.61	118.25
2	F	4	QVS	C7-C2-N	-2.00	114.25	118.07

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	V53	O-C-CAJ-CAD
2	E	2	V53	O-C-CAJ-NAH
2	E	2	V53	O01-C01-P-O1
2	E	2	V53	O01-C01-P-O2
2	E	2	V53	O01-C01-P-O3
2	F	2	V53	O-C-CAJ-CAD
2	F	2	V53	O-C-CAJ-NAH
2	F	3	QUK	O-C-C10-N11
2	F	3	QUK	O-C-C10-C9

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Mol	Chain	Res	Type	Atoms
2	E	5	QOL	CG-CD-CE1-OZ1
2	E	5	QOL	CE2-CD-CG-OB
2	F	5	QOL	CE2-CD-CG-OB
2	F	6	V53	O01-C01-P-O1
2	F	6	V53	O01-C01-P-O2
2	F	6	V53	O01-C01-P-O3
2	F	1	A1JAG	C54-C53-O14-C52
2	E	3	QUK	CE-CD-CG-OB
2	F	3	QUK	CE-CD-CG-OB
2	E	5	QOL	C6-C8-OB-CG
2	E	5	QOL	C9-C8-OB-CG
2	E	1	A1JAG	C53-C54-O15-C55
2	E	1	A1JAG	O14-C53-C54-O15
2	F	1	A1JAG	O14-C53-C54-O15
2	F	5	QOL	C6-C8-OB-CG
2	F	5	QOL	C9-C8-OB-CG
2	E	1	A1JAG	O13-C51-C52-O14
2	E	6	V53	CAL-CAF-O01-C01
2	E	5	QOL	CE1-CD-CG-OB
2	F	5	QOL	CE1-CD-CG-OB
2	E	1	A1JAG	C51-C52-O14-C53
2	F	1	A1JAG	C-C50-O13-C51
2	E	1	A1JAG	C52-C51-O13-C50
2	E	1	A1JAG	C54-C53-O14-C52
2	E	5	QOL	CE2-CD-CE1-OZ1
2	F	5	QOL	CD-CG-OB-C8
2	E	6	V53	CAD-CAF-O01-C01
2	F	1	A1JAG	C52-C51-O13-C50
2	E	6	V53	P-C01-O01-CAF

There are no ring outliers.

No monomer is involved in short contacts.

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	95/100 (95%)	0.53	6 (6%) 26 19	50, 65, 94, 105	0
1	B	96/100 (96%)	0.30	4 (4%) 40 32	44, 59, 83, 99	0
1	C	96/100 (96%)	0.35	3 (3%) 51 41	49, 65, 84, 98	0
1	D	95/100 (95%)	0.66	10 (10%) 11 8	45, 73, 99, 112	0
2	E	0/6	-	-	-	-
2	F	0/6	-	-	-	-
All	All	382/412 (92%)	0.46	23 (6%) 27 21	44, 65, 92, 112	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	32	PHE	3.9
1	A	97	GLN	3.8
1	D	4	VAL	3.6
1	D	64	GLU	3.4
1	B	97	GLN	3.4
1	C	32	PHE	3.4
1	B	44	LEU	2.8
1	A	38	GLY	2.6
1	D	97	GLN	2.6
1	D	45	VAL	2.5
1	B	54	LEU	2.4
1	D	3	LYS	2.4
1	A	44	LEU	2.4
1	D	34	TYR	2.3
1	C	54	LEU	2.3
1	D	56	ASP	2.2
1	D	30	VAL	2.2
1	B	43	GLY	2.2
1	C	4	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	36	ASP	2.1
1	A	18	SER	2.1
1	A	30	VAL	2.1
1	D	15	VAL	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1JAG	F	1	11/12	0.81	0.15	52,60,64,65	0
2	QOL	F	5	20/21	0.88	0.12	46,50,67,70	0
2	A1JAG	E	1	11/12	0.89	0.13	39,52,60,62	0
2	QVS	E	4	14/15	0.90	0.10	50,56,63,69	0
2	QOL	E	5	20/21	0.90	0.11	44,50,67,69	0
2	QUK	F	3	18/19	0.90	0.09	44,56,67,68	0
2	V53	F	2	19/20	0.91	0.08	44,52,82,82	0
2	QUK	E	3	18/19	0.91	0.10	36,49,70,70	0
2	V53	E	2	19/20	0.91	0.11	47,59,73,78	0
2	V53	E	6	20/20	0.91	0.10	42,58,89,93	0
2	V53	F	6	20/20	0.92	0.09	46,55,91,95	0
2	QVS	F	4	14/15	0.93	0.07	42,49,57,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.