



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 01:30 PM EDT

PDB ID : 3ODL  
Title : Crystal structure of cyclophilin A in complex with Voclosporin Z-ISA247  
Authors : Kuglstatter, A.; Stihle, M.; Benz, J.; Hennig, M.  
Deposited on : 2010-08-11  
Resolution : 2.31 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

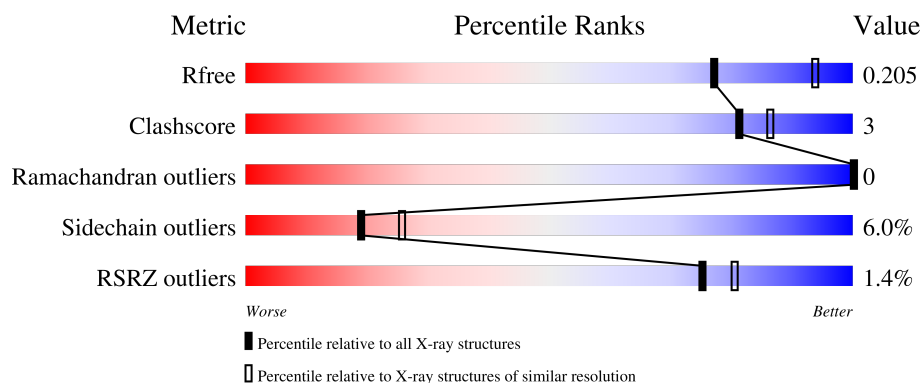
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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))
$R_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	<div> <div>93%</div> <div>6%</div> </div>
1	C	165	<div> <div>94%</div> <div>5%</div> </div>
1	E	165	<div> <div>94%</div> <div>6%</div> </div>
1	G	165	<div> <div>94%</div> <div>5%</div> </div>
1	I	165	<div> <div>95%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	165	 3% 92% 7%
1	M	165	 2% 92% 7%
1	O	165	 2% 93% 6%
1	Q	165	 % 93% 5%
1	S	165	 % 91% 9%
2	B	11	 18% 36% 45%
2	D	11	 18% 45% 36%
2	F	11	 18% 36% 45%
2	H	11	 18% 36% 45%
2	J	11	 27% 45% 27%
2	L	11	 18% 36% 45%
2	N	11	 18% 36% 45%
2	P	11	 18% 36% 45%
2	R	11	 18% 45% 36%
2	T	11	 18% 36% 45%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15246 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 Cyclophilin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	C	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	E	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	G	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	I	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	K	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	M	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	O	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	Q	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	S	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			

- Molecule 2 is a protein called Voclosporin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			86	63	11	12			
2	D	11	Total	C	N	O	0	0	0
			86	63	11	12			
2	F	11	Total	C	N	O	0	0	0
			86	63	11	12			
2	H	11	Total	C	N	O	0	0	0
			86	63	11	12			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	11	Total	C	N	O	0	0	0
			86	63	11	12			
2	L	11	Total	C	N	O	0	0	0
			86	63	11	12			
2	N	11	Total	C	N	O	0	0	0
			86	63	11	12			
2	P	11	Total	C	N	O	0	0	0
			86	63	11	12			
2	R	11	Total	C	N	O	0	0	0
			86	63	11	12			
2	T	11	Total	C	N	O	0	0	0
			86	63	11	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	YYA	BMT	engineered mutation	NOR NOR00033
D	5	YYA	BMT	engineered mutation	NOR NOR00033
F	5	YYA	BMT	engineered mutation	NOR NOR00033
H	5	YYA	BMT	engineered mutation	NOR NOR00033
J	5	YYA	BMT	engineered mutation	NOR NOR00033
L	5	YYA	BMT	engineered mutation	NOR NOR00033
N	5	YYA	BMT	engineered mutation	NOR NOR00033
P	5	YYA	BMT	engineered mutation	NOR NOR00033
R	5	YYA	BMT	engineered mutation	NOR NOR00033
T	5	YYA	BMT	engineered mutation	NOR NOR00033

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	4	Total	O	0	0
			4	4		
3	C	162	Total	O	0	0
			162	162		
3	D	3	Total	O	0	0
			3	3		
3	E	188	Total	O	0	0
			188	188		
3	F	6	Total	O	0	0
			6	6		

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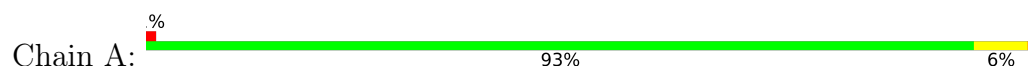
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	193	Total 193	O 193	0	0
3	H	4	Total 4	O 4	0	0
3	I	156	Total 156	O 156	0	0
3	J	5	Total 5	O 5	0	0
3	K	133	Total 133	O 133	0	0
3	L	4	Total 4	O 4	0	0
3	M	186	Total 186	O 186	0	0
3	N	2	Total 2	O 2	0	0
3	O	174	Total 174	O 174	0	0
3	P	5	Total 5	O 5	0	0
3	Q	180	Total 180	O 180	0	0
3	R	6	Total 6	O 6	0	0
3	S	163	Total 163	O 163	0	0
3	T	3	Total 3	O 3	0	0

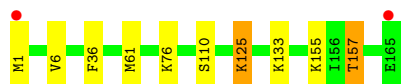
### 3 Residue-property plots [i](#)

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: Cyclophilin A



- Molecule 1: Cyclophilin A



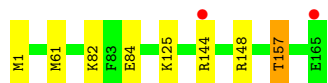
- Molecule 1: Cyclophilin A



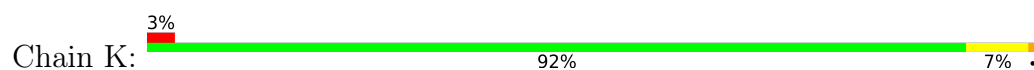
- Molecule 1: Cyclophilin A



- Molecule 1: Cyclophilin A



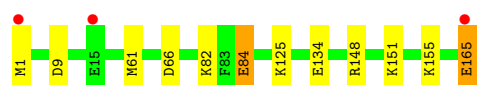
- Molecule 1: Cyclophilin A



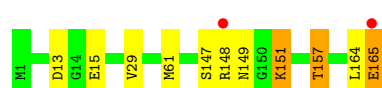
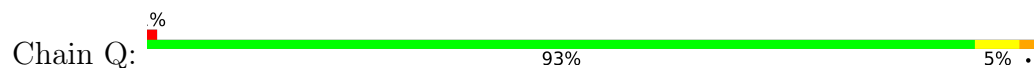
• Molecule 1: Cyclophilin A



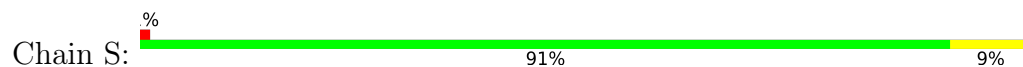
• Molecule 1: Cyclophilin A



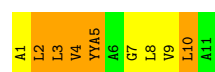
• Molecule 1: Cyclophilin A



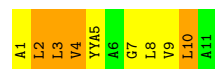
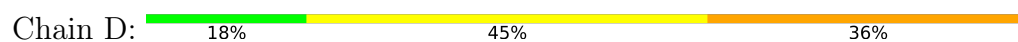
• Molecule 1: Cyclophilin A



• Molecule 2: Voclosporin



• Molecule 2: Voclosporin



• Molecule 2: Voclosporin



Chain F:  18% 36% 45%



● Molecule 2: Voclosporin

Chain H:  18% 36% 45%



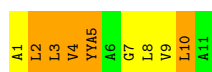
● Molecule 2: Voclosporin

Chain J:  27% 45% 27%



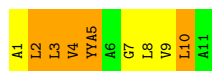
● Molecule 2: Voclosporin

Chain L:  18% 36% 45%



● Molecule 2: Voclosporin

Chain N:  18% 36% 45%




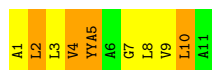
● Molecule 2: Voclosporin

Chain P:  18% 36% 45%



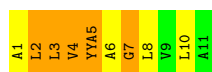
● Molecule 2: Voclosporin

Chain R:  18% 45% 36%



● Molecule 2: Voclosporin

Chain T:  18% 36% 45%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.42Å 141.12Å 149.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.31 39.78 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.31) 99.8 (39.78-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.95 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.169 , 0.207 0.169 , 0.205	Depositor DCC
$R_{free}$ test set	6176 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, MLE, SAR, YYA, MVA, ABA

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	0.38	0/1294	0.63	1/1733 (0.1%)
1	C	0.39	0/1294	0.63	0/1733
1	E	0.40	0/1294	0.64	3/1733 (0.2%)
1	G	0.40	0/1294	0.65	2/1733 (0.1%)
1	I	0.40	0/1294	0.64	0/1733
1	K	0.38	0/1294	0.63	1/1733 (0.1%)
1	M	0.42	0/1294	0.66	2/1733 (0.1%)
1	O	0.39	0/1294	0.64	2/1733 (0.1%)
1	Q	0.41	0/1294	0.65	1/1733 (0.1%)
1	S	0.40	0/1294	0.64	2/1733 (0.1%)
2	B	0.30	0/10	0.47	0/11
2	D	0.36	0/10	0.47	0/11
2	F	0.38	0/10	0.45	0/11
2	H	0.27	0/10	0.33	0/11
2	J	0.38	0/10	0.39	0/11
2	L	0.36	0/10	0.44	0/11
2	N	0.38	0/10	0.50	0/11
2	P	0.35	0/10	0.40	0/11
2	R	0.46	0/10	0.42	0/11
2	T	0.26	0/10	0.41	0/11
All	All	0.40	0/13040	0.64	14/17440 (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	M	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	9	ASP	CB-CG-OD2	5.83	123.55	118.30
1	S	66	ASP	CB-CG-OD2	5.68	123.41	118.30
1	G	13	ASP	CB-CG-OD2	5.56	123.31	118.30
1	M	66	ASP	CB-CG-OD2	5.53	123.28	118.30
1	M	9	ASP	CB-CG-OD2	5.30	123.07	118.30
1	Q	13	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	9	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	85	ASP	CB-CG-OD2	5.21	122.99	118.30
1	O	66	ASP	CB-CG-OD2	5.11	122.90	118.30
1	K	160	ASP	CB-CG-OD2	5.11	122.90	118.30
1	E	66	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	9	ASP	CB-CG-OD2	5.09	122.88	118.30
1	S	9	ASP	CB-CG-OD2	5.05	122.85	118.30
1	G	66	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	14	GLY	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	1266	0	1237	1	0
1	C	1266	0	1237	4	0
1	E	1266	0	1237	0	0
1	G	1266	0	1237	5	0
1	I	1266	0	1237	3	0
1	K	1266	0	1237	3	0
1	M	1266	0	1237	4	0
1	O	1266	0	1237	3	0
1	Q	1266	0	1237	6	0
1	S	1266	0	1237	2	0
2	B	86	0	109	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	86	0	109	4	0
2	F	86	0	109	5	0
2	H	86	0	109	5	0
2	J	86	0	109	2	0
2	L	86	0	109	4	0
2	N	86	0	109	4	0
2	P	86	0	109	4	0
2	R	86	0	109	3	0
2	T	86	0	109	5	0
3	A	149	0	0	0	0
3	B	4	0	0	0	0
3	C	162	0	0	1	0
3	D	3	0	0	0	0
3	E	188	0	0	0	0
3	F	6	0	0	0	0
3	G	193	0	0	4	0
3	H	4	0	0	0	0
3	I	156	0	0	2	0
3	J	5	0	0	0	0
3	K	133	0	0	0	0
3	L	4	0	0	0	0
3	M	186	0	0	1	0
3	N	2	0	0	0	0
3	O	174	0	0	2	0
3	P	5	0	0	0	0
3	Q	180	0	0	2	0
3	R	6	0	0	0	0
3	S	163	0	0	1	0
3	T	3	0	0	0	0
All	All	15246	0	13460	70	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 3.

All (70) 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:M:157:THR:HG21	3:M:178:HOH:O	1.79	0.81
1:G:157:THR:HG21	3:G:840:HOH:O	1.84	0.77
1:K:164:LEU:O	1:K:165:GLU:HB3	1.88	0.73
1:G:13:ASP:O	3:G:186:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:LYS:HD3	3:G:1526:HOH:O	1.98	0.62
1:M:165:GLU:HG2	1:M:165:GLU:O	2.02	0.60
1:Q:157:THR:HG21	3:Q:1066:HOH:O	2.03	0.59
1:G:157:THR:HB	3:G:186:HOH:O	2.04	0.57
1:C:157:THR:HG21	3:C:1478:HOH:O	2.05	0.56
1:I:157:THR:HG21	3:I:1221:HOH:O	2.08	0.53
1:O:84:GLU:H	1:O:84:GLU:CD	2.13	0.52
1:Q:164:LEU:O	1:Q:165:GLU:HB3	2.10	0.52
1:A:11:ALA:HB3	1:A:157:THR:HG22	1.91	0.51
1:Q:157:THR:HB	3:Q:181:HOH:O	2.11	0.50
1:Q:147:SER:OG	1:Q:151:LYS:HE3	2.12	0.50
1:S:76:LYS:HA	3:S:1629:HOH:O	2.12	0.49
2:B:4:MVA:HA	2:B:5:YYA:HN	1.70	0.47
2:R:9:VAL:HA	2:R:10:MLE:HN1	1.55	0.46
2:P:9:VAL:HA	2:P:10:MLE:HN1	1.53	0.46
2:H:4:MVA:HA	2:H:5:YYA:HN	1.76	0.46
2:J:4:MVA:HA	2:J:5:YYA:HN	1.78	0.46
1:Q:165:GLU:HG2	1:Q:165:GLU:O	2.15	0.46
2:T:1:DAL:HA	2:T:2:MLE:HN1	1.67	0.46
2:B:9:VAL:HA	2:B:10:MLE:HN1	1.54	0.46
2:D:1:DAL:HA	2:D:2:MLE:HN1	1.64	0.46
2:D:9:VAL:HA	2:D:10:MLE:HN1	1.56	0.45
2:J:1:DAL:HA	2:J:2:MLE:HN1	1.69	0.45
2:N:9:VAL:HA	2:N:10:MLE:HN1	1.54	0.45
1:I:144:ARG:HE	1:I:144:ARG:HB2	1.45	0.45
1:Q:151:LYS:HD2	1:Q:151:LYS:C	2.37	0.45
2:B:3:MLE:HA	2:B:4:MVA:HN1	1.82	0.44
2:P:1:DAL:HA	2:P:2:MLE:HN1	1.62	0.44
1:S:55:ARG:HH22	2:T:3:MLE:HN3	1.81	0.44
1:O:82:LYS:HE3	3:O:395:HOH:O	2.17	0.44
2:H:9:VAL:HA	2:H:10:MLE:HN1	1.59	0.44
2:R:4:MVA:HA	2:R:5:YYA:HN	1.79	0.44
2:D:4:MVA:HA	2:D:5:YYA:HN	1.69	0.44
2:N:4:MVA:HA	2:N:5:YYA:HN	1.73	0.44
2:L:9:VAL:HA	2:L:10:MLE:HN1	1.53	0.43
2:F:1:DAL:HA	2:F:2:MLE:HN1	1.62	0.43
1:I:144:ARG:HD3	3:I:534:HOH:O	2.18	0.43
2:B:1:DAL:HA	2:B:2:MLE:HN1	1.71	0.42
2:F:4:MVA:HA	2:F:5:YYA:HN	1.77	0.42
1:C:6:VAL:HG21	1:C:36:PHE:HE2	1.83	0.42
1:C:125:LYS:HE3	1:C:125:LYS:HB2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:GLU:H	1:K:84:GLU:CD	2.22	0.42
2:T:4:MVA:HA	2:T:5:YYA:HN	1.83	0.42
1:G:76:LYS:O	1:G:110:SER:HB3	2.20	0.42
2:N:1:DAL:HA	2:N:2:MLE:HN1	1.63	0.42
1:K:58:PRO:HA	1:K:143:GLU:HG2	2.02	0.42
1:M:99:SER:HB3	1:M:113:PHE:CZ	2.54	0.42
2:L:4:MVA:HA	2:L:5:YYA:HN	1.75	0.42
2:R:1:DAL:HA	2:R:2:MLE:HN1	1.63	0.42
1:M:55:ARG:HH22	2:N:3:MLE:HN3	1.85	0.42
2:H:2:MLE:HA	2:H:3:MLE:HN1	1.89	0.41
2:L:2:MLE:HA	2:L:3:MLE:HN1	1.82	0.41
2:H:1:DAL:HA	2:H:2:MLE:HN1	1.62	0.41
2:T:3:MLE:HA	2:T:4:MVA:HN1	1.84	0.41
2:D:2:MLE:HA	2:D:3:MLE:HN1	1.87	0.41
2:P:3:MLE:HA	2:P:4:MVA:HN1	1.90	0.41
2:T:6:ABA:HA	2:T:7:SAR:HN1	1.92	0.41
2:P:5:YYA:HD1B	2:P:5:YYA:HE	1.87	0.41
2:H:3:MLE:HA	2:H:4:MVA:HN1	1.88	0.41
2:B:2:MLE:HA	2:B:3:MLE:HN1	1.81	0.40
1:C:76:LYS:O	1:C:110:SER:HB3	2.21	0.40
2:F:9:VAL:HA	2:F:10:MLE:HN1	1.53	0.40
2:F:2:MLE:HA	2:F:3:MLE:HN1	1.83	0.40
2:F:5:YYA:HD1B	2:F:5:YYA:HE	1.90	0.40
2:L:1:DAL:HA	2:L:2:MLE:HN1	1.64	0.40
1:O:165:GLU:HB3	3:O:1598:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/165 (99%)	158 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
1	E	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
1	G	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
1	I	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
1	K	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
1	M	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
1	O	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
1	Q	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
1	S	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
2	B	1/11 (9%)	1 (100%)	0	0	100	100
2	D	1/11 (9%)	1 (100%)	0	0	100	100
2	F	1/11 (9%)	1 (100%)	0	0	100	100
2	H	1/11 (9%)	1 (100%)	0	0	100	100
2	J	1/11 (9%)	1 (100%)	0	0	100	100
2	L	1/11 (9%)	1 (100%)	0	0	100	100
2	N	1/11 (9%)	1 (100%)	0	0	100	100
2	P	1/11 (9%)	1 (100%)	0	0	100	100
2	R	1/11 (9%)	1 (100%)	0	0	100	100
2	T	1/11 (9%)	1 (100%)	0	0	100	100
All	All	1640/1760 (93%)	1578 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	133/133 (100%)	124 (93%)	9 (7%)	16	20
1	C	133/133 (100%)	127 (96%)	6 (4%)	27	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	133/133 (100%)	126 (95%)	7 (5%)	22	31
1	G	133/133 (100%)	128 (96%)	5 (4%)	33	46
1	I	133/133 (100%)	126 (95%)	7 (5%)	22	31
1	K	133/133 (100%)	123 (92%)	10 (8%)	13	16
1	M	133/133 (100%)	125 (94%)	8 (6%)	19	26
1	O	133/133 (100%)	124 (93%)	9 (7%)	16	20
1	Q	133/133 (100%)	125 (94%)	8 (6%)	19	26
1	S	133/133 (100%)	122 (92%)	11 (8%)	11	13
2	B	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
2	F	1/1 (100%)	1 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
2	J	1/1 (100%)	1 (100%)	0	100	100
2	L	1/1 (100%)	1 (100%)	0	100	100
2	N	1/1 (100%)	1 (100%)	0	100	100
2	P	1/1 (100%)	1 (100%)	0	100	100
2	R	1/1 (100%)	1 (100%)	0	100	100
2	T	1/1 (100%)	1 (100%)	0	100	100
All	All	1340/1340 (100%)	1260 (94%)	80 (6%)	19	26

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	61	MET
1	A	69	ARG
1	A	125	LYS
1	A	133	LYS
1	A	134	GLU
1	A	148	ARG
1	A	157	THR
1	A	165	GLU
1	C	1	MET
1	C	61	MET
1	C	125	LYS
1	C	133	LYS

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Mol	Chain	Res	Type
1	C	155	LYS
1	C	157	THR
1	E	13	ASP
1	E	15	GLU
1	E	61	MET
1	E	81	GLU
1	E	82	LYS
1	E	134	GLU
1	E	165	GLU
1	G	61	MET
1	G	148	ARG
1	G	151	LYS
1	G	157	THR
1	G	165	GLU
1	I	1	MET
1	I	61	MET
1	I	82	LYS
1	I	84	GLU
1	I	125	LYS
1	I	148	ARG
1	I	157	THR
1	K	29	VAL
1	K	44	LYS
1	K	61	MET
1	K	69	ARG
1	K	84	GLU
1	K	125	LYS
1	K	133	LYS
1	K	134	GLU
1	K	153	SER
1	K	165	GLU
1	M	1	MET
1	M	15	GLU
1	M	44	LYS
1	M	61	MET
1	M	82	LYS
1	M	151	LYS
1	M	157	THR
1	M	165	GLU
1	O	1	MET
1	O	61	MET
1	O	84	GLU

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Mol	Chain	Res	Type
1	O	125	LYS
1	O	134	GLU
1	O	148	ARG
1	O	151	LYS
1	O	155	LYS
1	O	165	GLU
1	Q	15	GLU
1	Q	29	VAL
1	Q	61	MET
1	Q	148	ARG
1	Q	149	ASN
1	Q	151	LYS
1	Q	157	THR
1	Q	165	GLU
1	S	1	MET
1	S	6	VAL
1	S	29	VAL
1	S	61	MET
1	S	82	LYS
1	S	84	GLU
1	S	134	GLU
1	S	151	LYS
1	S	154	LYS
1	S	155	LYS
1	S	157	THR

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 ⓘ

90 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	J	8	2	7,8,9	1.96	1 (14%)	6,9,11	0.96	0
2	MLE	B	3	2	7,8,9	2.02	1 (14%)	6,9,11	1.08	0
2	MVA	H	4	2	6,7,8	2.14	1 (16%)	7,8,10	1.65	2 (28%)
2	ABA	J	6	2	4,5,6	0.56	0	1,5,7	0.30	0
2	MLE	H	2	2	7,8,9	2.01	1 (14%)	6,9,11	1.08	1 (16%)
2	YYA	J	5	2	12,13,14	0.60	0	13,15,17	1.28	2 (15%)
2	SAR	T	7	2	4,4,5	1.88	1 (25%)	1,3,5	2.54	1 (100%)
2	YYA	D	5	2	12,13,14	0.55	0	13,15,17	1.08	0
2	YYA	F	5	2	12,13,14	0.57	0	13,15,17	1.21	1 (7%)
2	MLE	N	3	2	7,8,9	2.02	1 (14%)	6,9,11	1.16	1 (16%)
2	MLE	D	2	2	7,8,9	2.06	1 (14%)	6,9,11	1.04	1 (16%)
2	YYA	L	5	2	12,13,14	0.55	0	13,15,17	1.24	2 (15%)
2	MLE	F	2	2	7,8,9	2.06	1 (14%)	6,9,11	1.01	0
2	YYA	R	5	2	12,13,14	0.56	0	13,15,17	1.40	2 (15%)
2	SAR	B	7	2	4,4,5	1.89	1 (25%)	1,3,5	2.33	1 (100%)
2	ABA	N	6	2	4,5,6	0.54	0	1,5,7	0.32	0
2	MLE	L	10	2	7,8,9	2.01	1 (14%)	6,9,11	1.14	0
2	MLE	H	10	2	7,8,9	2.00	1 (14%)	6,9,11	1.04	0
2	MLE	D	8	2	7,8,9	2.02	1 (14%)	6,9,11	0.86	0
2	MLE	D	3	2	7,8,9	2.02	1 (14%)	6,9,11	1.08	1 (16%)
2	MLE	T	8	2	7,8,9	2.00	1 (14%)	6,9,11	0.95	0
2	MVA	L	4	2	6,7,8	2.16	1 (16%)	7,8,10	1.45	1 (14%)
2	MLE	F	8	2	7,8,9	1.97	1 (14%)	6,9,11	0.92	0
2	MLE	F	3	2	7,8,9	2.03	1 (14%)	6,9,11	1.03	1 (16%)
2	SAR	N	7	2	4,4,5	1.92	1 (25%)	1,3,5	2.48	1 (100%)
2	ABA	H	6	2	4,5,6	0.68	0	1,5,7	0.25	0
2	MLE	B	8	2	7,8,9	2.00	1 (14%)	6,9,11	0.88	0
2	MLE	J	3	2	7,8,9	2.05	1 (14%)	6,9,11	1.06	1 (16%)
2	MLE	N	10	2	7,8,9	2.01	1 (14%)	6,9,11	1.09	0
2	MLE	H	3	2	7,8,9	2.05	1 (14%)	6,9,11	1.11	1 (16%)
2	MLE	L	2	2	7,8,9	2.03	1 (14%)	6,9,11	0.92	0
2	MVA	D	4	2	6,7,8	2.19	1 (16%)	7,8,10	1.35	1 (14%)
2	SAR	D	7	2	4,4,5	1.92	1 (25%)	1,3,5	2.34	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLE	L	3	2	7,8,9	1.99	1 (14%)	6,9,11	1.06	1 (16%)
2	SAR	F	7	2	4,4,5	1.94	1 (25%)	1,3,5	2.27	1 (100%)
2	MLE	P	2	2	7,8,9	2.00	1 (14%)	6,9,11	1.04	0
2	MLE	R	3	2	7,8,9	1.95	1 (14%)	6,9,11	1.25	1 (16%)
2	YYA	P	5	2	12,13,14	0.52	0	13,15,17	1.28	2 (15%)
2	MLE	T	3	2	7,8,9	1.95	1 (14%)	6,9,11	1.23	1 (16%)
2	ABA	F	6	2	4,5,6	0.68	0	1,5,7	0.29	0
2	MVA	B	4	2	6,7,8	2.14	1 (16%)	7,8,10	1.55	1 (14%)
2	MVA	J	4	2	6,7,8	2.14	1 (16%)	7,8,10	1.62	3 (42%)
2	MLE	J	2	2	7,8,9	2.02	1 (14%)	6,9,11	0.93	0
2	MLE	N	8	2	7,8,9	2.00	1 (14%)	6,9,11	0.94	0
2	SAR	J	7	2	4,4,5	1.86	1 (25%)	1,3,5	2.46	1 (100%)
2	SAR	P	7	2	4,4,5	1.88	1 (25%)	1,3,5	2.32	1 (100%)
2	YYA	T	5	2	12,13,14	0.60	0	13,15,17	1.30	2 (15%)
2	MLE	P	3	2	7,8,9	1.98	1 (14%)	6,9,11	1.20	1 (16%)
2	MVA	R	4	2	6,7,8	2.14	1 (16%)	7,8,10	1.59	2 (28%)
2	MLE	R	2	2	7,8,9	2.03	1 (14%)	6,9,11	0.89	0
2	SAR	R	7	2	4,4,5	1.93	1 (25%)	1,3,5	2.50	1 (100%)
2	MLE	H	8	2	7,8,9	1.99	1 (14%)	6,9,11	0.82	0
2	ABA	L	6	2	4,5,6	0.54	0	1,5,7	0.27	0
2	YYA	B	5	2	12,13,14	0.54	0	13,15,17	1.31	2 (15%)
2	MVA	F	4	2	6,7,8	2.11	1 (16%)	7,8,10	1.60	2 (28%)
2	MLE	D	10	2	7,8,9	2.02	1 (14%)	6,9,11	1.01	0
2	MLE	N	2	2	7,8,9	2.02	1 (14%)	6,9,11	0.92	0
2	MLE	F	10	2	7,8,9	2.01	1 (14%)	6,9,11	0.99	0
2	ABA	R	6	2	4,5,6	0.64	0	1,5,7	0.30	0
2	ABA	T	6	2	4,5,6	0.61	0	1,5,7	0.25	0
2	ABA	D	6	2	4,5,6	0.67	0	1,5,7	0.20	0
2	YYA	H	5	2	12,13,14	0.53	0	13,15,17	1.37	1 (7%)
2	MVA	N	4	2	6,7,8	2.15	1 (16%)	7,8,10	1.13	0
2	SAR	L	7	2	4,4,5	1.88	1 (25%)	1,3,5	2.61	1 (100%)
2	MLE	B	2	2	7,8,9	2.01	1 (14%)	6,9,11	0.92	0
2	MLE	P	10	2	7,8,9	2.01	1 (14%)	6,9,11	1.10	0
2	MLE	P	8	2	7,8,9	1.99	1 (14%)	6,9,11	0.95	0
2	ABA	P	6	2	4,5,6	0.61	0	1,5,7	0.26	0
2	YYA	N	5	2	12,13,14	0.55	0	13,15,17	1.26	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLE	B	10	2	7,8,9	2.02	1 (14%)	6,9,11	1.15	0
2	MLE	L	8	2	7,8,9	2.00	1 (14%)	6,9,11	0.87	0
2	MLE	R	8	2	7,8,9	2.00	1 (14%)	6,9,11	0.90	0
2	MVA	T	4	2	6,7,8	2.15	1 (16%)	7,8,10	1.76	3 (42%)
2	MLE	T	10	2	7,8,9	1.98	1 (14%)	6,9,11	1.15	0
2	MVA	P	4	2	6,7,8	2.22	1 (16%)	7,8,10	1.38	1 (14%)
2	SAR	H	7	2	4,4,5	1.93	1 (25%)	1,3,5	2.46	1 (100%)
2	ABA	B	6	2	4,5,6	0.56	0	1,5,7	0.27	0
2	MLE	R	10	2	7,8,9	2.01	1 (14%)	6,9,11	1.06	0
2	MLE	T	2	2	7,8,9	2.01	1 (14%)	6,9,11	1.01	1 (16%)
2	MLE	J	10	2	7,8,9	2.01	1 (14%)	6,9,11	0.98	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	J	8	2	-	2/5/8/10	-
2	MLE	B	3	2	-	0/5/8/10	-
2	MVA	H	4	2	-	1/6/8/10	-
2	ABA	J	6	2	-	0/3/4/6	-
2	MLE	H	2	2	-	0/5/8/10	-
2	YYA	J	5	2	-	1/14/17/19	-
2	SAR	T	7	2	-	1/1/2/3	-
2	YYA	D	5	2	-	1/14/17/19	-
2	YYA	F	5	2	-	1/14/17/19	-
2	MLE	N	3	2	-	0/5/8/10	-
2	MLE	D	2	2	-	0/5/8/10	-
2	YYA	L	5	2	-	1/14/17/19	-
2	MLE	F	2	2	-	0/5/8/10	-
2	YYA	R	5	2	-	1/14/17/19	-
2	SAR	B	7	2	-	1/1/2/3	-
2	ABA	N	6	2	-	0/3/4/6	-
2	MLE	L	10	2	-	0/5/8/10	-
2	MLE	H	10	2	-	0/5/8/10	-
2	MLE	D	8	2	-	1/5/8/10	-
2	MLE	D	3	2	-	0/5/8/10	-
2	MLE	T	8	2	-	1/5/8/10	-
2	MVA	L	4	2	-	3/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	F	8	2	-	1/5/8/10	-
2	MLE	F	3	2	-	0/5/8/10	-
2	SAR	N	7	2	-	1/1/2/3	-
2	ABA	H	6	2	-	0/3/4/6	-
2	MLE	B	8	2	-	1/5/8/10	-
2	MLE	J	3	2	-	0/5/8/10	-
2	MLE	N	10	2	-	0/5/8/10	-
2	MLE	H	3	2	-	0/5/8/10	-
2	MLE	L	2	2	-	0/5/8/10	-
2	MVA	D	4	2	-	3/6/8/10	-
2	SAR	D	7	2	-	1/1/2/3	-
2	MLE	L	3	2	-	0/5/8/10	-
2	SAR	F	7	2	-	1/1/2/3	-
2	MLE	P	2	2	-	0/5/8/10	-
2	MLE	R	3	2	-	0/5/8/10	-
2	YYA	P	5	2	-	2/14/17/19	-
2	MLE	T	3	2	-	0/5/8/10	-
2	ABA	F	6	2	-	0/3/4/6	-
2	MVA	B	4	2	-	3/6/8/10	-
2	MVA	J	4	2	-	1/6/8/10	-
2	MLE	J	2	2	-	0/5/8/10	-
2	MLE	N	8	2	-	1/5/8/10	-
2	SAR	J	7	2	-	1/1/2/3	-
2	SAR	P	7	2	-	1/1/2/3	-
2	YYA	T	5	2	-	1/14/17/19	-
2	MLE	P	3	2	-	0/5/8/10	-
2	MVA	R	4	2	-	2/6/8/10	-
2	MLE	R	2	2	-	0/5/8/10	-
2	SAR	R	7	2	-	1/1/2/3	-
2	MLE	H	8	2	-	0/5/8/10	-
2	ABA	L	6	2	-	0/3/4/6	-
2	YYA	B	5	2	-	1/14/17/19	-
2	MVA	F	4	2	-	2/6/8/10	-
2	MLE	D	10	2	-	0/5/8/10	-
2	MLE	N	2	2	-	0/5/8/10	-
2	MLE	F	10	2	-	0/5/8/10	-
2	ABA	R	6	2	-	0/3/4/6	-
2	ABA	T	6	2	-	0/3/4/6	-
2	ABA	D	6	2	-	0/3/4/6	-
2	YYA	H	5	2	-	1/14/17/19	-
2	MVA	N	4	2	-	3/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAR	L	7	2	-	1/1/2/3	-
2	MLE	B	2	2	-	0/5/8/10	-
2	MLE	P	10	2	-	0/5/8/10	-
2	MLE	P	8	2	-	1/5/8/10	-
2	ABA	P	6	2	-	0/3/4/6	-
2	YYA	N	5	2	-	2/14/17/19	-
2	MLE	B	10	2	-	0/5/8/10	-
2	MLE	L	8	2	-	1/5/8/10	-
2	MLE	R	8	2	-	2/5/8/10	-
2	MVA	T	4	2	-	2/6/8/10	-
2	MLE	T	10	2	-	0/5/8/10	-
2	MVA	P	4	2	-	2/6/8/10	-
2	SAR	H	7	2	-	1/1/2/3	-
2	ABA	B	6	2	-	0/3/4/6	-
2	MLE	R	10	2	-	0/5/8/10	-
2	MLE	T	2	2	-	0/5/8/10	-
2	MLE	J	10	2	-	0/5/8/10	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	MLE	O-C	5.43	1.41	1.19
2	P	4	MVA	O-C	5.42	1.41	1.19
2	D	2	MLE	O-C	5.41	1.41	1.19
2	J	3	MLE	O-C	5.38	1.41	1.19
2	H	3	MLE	O-C	5.36	1.41	1.19
2	D	4	MVA	O-C	5.34	1.41	1.19
2	L	2	MLE	O-C	5.34	1.41	1.19
2	R	2	MLE	O-C	5.34	1.41	1.19
2	J	2	MLE	O-C	5.34	1.41	1.19
2	N	2	MLE	O-C	5.33	1.41	1.19
2	D	3	MLE	O-C	5.31	1.41	1.19
2	D	10	MLE	O-C	5.31	1.41	1.19
2	P	10	MLE	O-C	5.31	1.41	1.19
2	B	2	MLE	O-C	5.30	1.41	1.19
2	B	10	MLE	O-C	5.30	1.41	1.19
2	R	10	MLE	O-C	5.30	1.41	1.19
2	H	2	MLE	O-C	5.29	1.41	1.19
2	L	10	MLE	O-C	5.29	1.41	1.19
2	F	3	MLE	O-C	5.29	1.41	1.19
2	N	3	MLE	O-C	5.29	1.41	1.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4	MVA	O-C	5.29	1.41	1.19
2	J	10	MLE	O-C	5.29	1.41	1.19
2	B	3	MLE	O-C	5.29	1.41	1.19
2	N	10	MLE	O-C	5.28	1.41	1.19
2	T	2	MLE	O-C	5.28	1.41	1.19
2	H	10	MLE	O-C	5.27	1.40	1.19
2	N	8	MLE	O-C	5.26	1.40	1.19
2	F	10	MLE	O-C	5.26	1.40	1.19
2	D	8	MLE	O-C	5.26	1.40	1.19
2	P	2	MLE	O-C	5.26	1.40	1.19
2	L	8	MLE	O-C	5.25	1.40	1.19
2	N	4	MVA	O-C	5.25	1.40	1.19
2	T	8	MLE	O-C	5.25	1.40	1.19
2	B	8	MLE	O-C	5.24	1.40	1.19
2	T	4	MVA	O-C	5.23	1.40	1.19
2	B	4	MVA	O-C	5.23	1.40	1.19
2	J	4	MVA	O-C	5.21	1.40	1.19
2	R	8	MLE	O-C	5.21	1.40	1.19
2	R	4	MVA	O-C	5.21	1.40	1.19
2	H	4	MVA	O-C	5.21	1.40	1.19
2	L	3	MLE	O-C	5.21	1.40	1.19
2	P	8	MLE	O-C	5.20	1.40	1.19
2	T	10	MLE	O-C	5.20	1.40	1.19
2	P	3	MLE	O-C	5.19	1.40	1.19
2	H	8	MLE	O-C	5.17	1.40	1.19
2	F	4	MVA	O-C	5.16	1.40	1.19
2	F	8	MLE	O-C	5.13	1.40	1.19
2	J	8	MLE	O-C	5.13	1.40	1.19
2	T	3	MLE	O-C	5.11	1.40	1.19
2	R	3	MLE	O-C	5.10	1.40	1.19
2	F	7	SAR	O-C	3.74	1.41	1.19
2	N	7	SAR	O-C	3.72	1.41	1.19
2	R	7	SAR	O-C	3.71	1.41	1.19
2	D	7	SAR	O-C	3.68	1.40	1.19
2	H	7	SAR	O-C	3.67	1.40	1.19
2	P	7	SAR	O-C	3.66	1.40	1.19
2	B	7	SAR	O-C	3.65	1.40	1.19
2	L	7	SAR	O-C	3.64	1.40	1.19
2	T	7	SAR	O-C	3.64	1.40	1.19
2	J	7	SAR	O-C	3.59	1.40	1.19

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	YYA	CG2-CD2-CE	-3.36	108.82	113.98
2	T	4	MVA	CB-CA-N	3.14	115.26	111.17
2	R	5	YYA	CG2-CD2-CE	-3.13	109.18	113.98
2	B	4	MVA	CB-CA-N	3.07	115.16	111.17
2	H	4	MVA	CB-CA-N	2.96	115.02	111.17
2	R	4	MVA	CB-CA-N	2.81	114.83	111.17
2	F	5	YYA	CG2-CD2-CE	-2.72	109.81	113.98
2	N	5	YYA	CG2-CD2-CE	-2.71	109.82	113.98
2	L	4	MVA	CB-CA-N	2.70	114.68	111.17
2	R	5	YYA	CB-CA-N	2.69	116.76	111.41
2	J	5	YYA	CB-CA-N	2.68	116.74	111.41
2	L	7	SAR	O-C-CA	-2.61	117.86	125.42
2	T	5	YYA	CG2-CD2-CE	-2.60	109.99	113.98
2	P	5	YYA	CG2-CD2-CE	-2.59	110.00	113.98
2	B	5	YYA	CG2-CD2-CE	-2.58	110.03	113.98
2	L	5	YYA	CG2-CD2-CE	-2.58	110.03	113.98
2	F	4	MVA	CB-CA-N	2.55	114.50	111.17
2	T	7	SAR	O-C-CA	-2.54	118.07	125.42
2	R	3	MLE	O-C-CA	-2.52	118.17	124.78
2	P	5	YYA	CB-CA-N	2.52	116.41	111.41
2	R	7	SAR	O-C-CA	-2.50	118.18	125.42
2	N	7	SAR	O-C-CA	-2.48	118.23	125.42
2	J	7	SAR	O-C-CA	-2.46	118.29	125.42
2	H	7	SAR	O-C-CA	-2.46	118.30	125.42
2	P	4	MVA	CB-CA-N	2.46	114.37	111.17
2	P	3	MLE	O-C-CA	-2.40	118.48	124.78
2	D	7	SAR	O-C-CA	-2.34	118.63	125.42
2	D	4	MVA	CB-CA-N	2.34	114.22	111.17
2	B	7	SAR	O-C-CA	-2.33	118.66	125.42
2	T	3	MLE	O-C-CA	-2.33	118.68	124.78
2	P	7	SAR	O-C-CA	-2.32	118.69	125.42
2	T	4	MVA	CG2-CB-CA	2.32	114.76	111.21
2	J	4	MVA	CG2-CB-CA	2.29	114.72	111.21
2	F	7	SAR	O-C-CA	-2.27	118.84	125.42
2	F	4	MVA	CG2-CB-CA	2.22	114.61	111.21
2	J	4	MVA	CB-CA-N	2.21	114.05	111.17
2	J	4	MVA	O-C-CA	-2.19	118.73	124.83
2	N	3	MLE	O-C-CA	-2.19	119.04	124.78
2	H	3	MLE	O-C-CA	-2.18	119.06	124.78
2	D	2	MLE	O-C-CA	-2.17	119.09	124.78
2	B	5	YYA	CB-CA-N	2.16	115.70	111.41
2	H	4	MVA	CG2-CB-CA	2.15	114.50	111.21
2	D	3	MLE	O-C-CA	-2.12	119.21	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3	MLE	O-C-CA	-2.12	119.23	124.78
2	L	5	YYA	CB-CA-N	2.11	115.61	111.41
2	R	4	MVA	O-C-CA	-2.10	118.97	124.83
2	H	2	MLE	O-C-CA	-2.09	119.29	124.78
2	F	3	MLE	O-C-CA	-2.09	119.29	124.78
2	J	5	YYA	CG2-CD2-CE	-2.07	110.81	113.98
2	J	3	MLE	O-C-CA	-2.06	119.37	124.78
2	T	5	YYA	CB-CA-N	2.04	115.46	111.41
2	T	4	MVA	O-C-CA	-2.01	119.23	124.83
2	T	2	MLE	O-C-CA	-2.01	119.52	124.78

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MVA	N-CA-CB-CG2
2	D	4	MVA	N-CA-CB-CG2
2	F	4	MVA	N-CA-CB-CG2
2	T	4	MVA	N-CA-CB-CG2
2	B	8	MLE	O-C-CA-CB
2	D	8	MLE	O-C-CA-CB
2	F	8	MLE	O-C-CA-CB
2	J	8	MLE	O-C-CA-CB
2	L	8	MLE	O-C-CA-CB
2	N	8	MLE	O-C-CA-CB
2	P	8	MLE	O-C-CA-CB
2	R	8	MLE	O-C-CA-CB
2	T	8	MLE	O-C-CA-CB
2	L	4	MVA	N-CA-CB-CG2
2	R	4	MVA	N-CA-CB-CG2
2	N	5	YYA	CE-CD2-CG2-CB
2	P	5	YYA	CE-CD2-CG2-CB
2	B	5	YYA	CB-CA-N-CN
2	D	5	YYA	CB-CA-N-CN
2	F	5	YYA	CB-CA-N-CN
2	H	5	YYA	CB-CA-N-CN
2	J	5	YYA	CB-CA-N-CN
2	L	5	YYA	CB-CA-N-CN
2	N	5	YYA	CB-CA-N-CN
2	P	5	YYA	CB-CA-N-CN
2	R	5	YYA	CB-CA-N-CN
2	T	5	YYA	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
2	J	8	MLE	N-CA-CB-CG
2	B	4	MVA	CB-CA-N-CN
2	D	4	MVA	CB-CA-N-CN
2	F	4	MVA	CB-CA-N-CN
2	H	4	MVA	CB-CA-N-CN
2	J	4	MVA	CB-CA-N-CN
2	L	4	MVA	CB-CA-N-CN
2	N	4	MVA	CB-CA-N-CN
2	P	4	MVA	CB-CA-N-CN
2	R	4	MVA	CB-CA-N-CN
2	T	4	MVA	CB-CA-N-CN
2	B	4	MVA	O-C-CA-CB
2	D	4	MVA	O-C-CA-CB
2	L	4	MVA	O-C-CA-CB
2	N	4	MVA	O-C-CA-CB
2	B	7	SAR	C-CA-N-CN
2	D	7	SAR	C-CA-N-CN
2	F	7	SAR	C-CA-N-CN
2	H	7	SAR	C-CA-N-CN
2	J	7	SAR	C-CA-N-CN
2	L	7	SAR	C-CA-N-CN
2	N	7	SAR	C-CA-N-CN
2	P	7	SAR	C-CA-N-CN
2	R	7	SAR	C-CA-N-CN
2	T	7	SAR	C-CA-N-CN
2	N	4	MVA	N-CA-CB-CG2
2	P	4	MVA	N-CA-CB-CG2
2	R	8	MLE	N-CA-CB-CG

There are no ring outliers.

48 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	MLE	2	0
2	H	4	MVA	2	0
2	H	2	MLE	2	0
2	J	5	YYA	1	0
2	T	7	SAR	1	0
2	D	5	YYA	1	0
2	F	5	YYA	2	0
2	N	3	MLE	1	0
2	D	2	MLE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	5	YYA	1	0
2	F	2	MLE	2	0
2	R	5	YYA	1	0
2	L	10	MLE	1	0
2	H	10	MLE	1	0
2	D	3	MLE	1	0
2	L	4	MVA	1	0
2	F	3	MLE	1	0
2	N	10	MLE	1	0
2	H	3	MLE	2	0
2	L	2	MLE	2	0
2	D	4	MVA	1	0
2	L	3	MLE	1	0
2	P	2	MLE	1	0
2	P	5	YYA	1	0
2	T	3	MLE	2	0
2	B	4	MVA	2	0
2	J	4	MVA	1	0
2	J	2	MLE	1	0
2	T	5	YYA	1	0
2	P	3	MLE	1	0
2	R	4	MVA	1	0
2	R	2	MLE	1	0
2	B	5	YYA	1	0
2	F	4	MVA	1	0
2	D	10	MLE	1	0
2	N	2	MLE	1	0
2	F	10	MLE	1	0
2	T	6	ABA	1	0
2	H	5	YYA	1	0
2	N	4	MVA	1	0
2	B	2	MLE	2	0
2	P	10	MLE	1	0
2	N	5	YYA	1	0
2	B	10	MLE	1	0
2	T	4	MVA	2	0
2	P	4	MVA	1	0
2	R	10	MLE	1	0
2	T	2	MLE	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	165/165 (100%)	-0.27	2 (1%) 79 83	18, 26, 39, 47	0
1	C	165/165 (100%)	-0.55	2 (1%) 79 83	17, 24, 35, 40	0
1	E	165/165 (100%)	-0.57	1 (0%) 89 92	14, 20, 29, 38	0
1	G	165/165 (100%)	-0.55	3 (1%) 68 75	12, 18, 29, 35	0
1	I	165/165 (100%)	-0.44	2 (1%) 79 83	15, 22, 36, 42	0
1	K	165/165 (100%)	-0.14	5 (3%) 50 57	17, 28, 44, 49	0
1	M	165/165 (100%)	-0.65	3 (1%) 68 75	15, 19, 28, 37	0
1	O	165/165 (100%)	-0.49	3 (1%) 68 75	13, 20, 33, 40	0
1	Q	165/165 (100%)	-0.52	2 (1%) 79 83	13, 22, 32, 42	0
1	S	165/165 (100%)	-0.53	1 (0%) 89 92	15, 21, 35, 41	0
2	B	2/11 (18%)	-0.50	0 100 100	21, 21, 21, 22	0
2	D	2/11 (18%)	-0.22	0 100 100	24, 24, 24, 26	0
2	F	2/11 (18%)	-0.70	0 100 100	19, 19, 19, 21	0
2	H	2/11 (18%)	-0.48	0 100 100	18, 18, 18, 20	0
2	J	2/11 (18%)	-0.53	0 100 100	18, 18, 18, 20	0
2	L	2/11 (18%)	-0.20	0 100 100	22, 22, 22, 23	0
2	N	2/11 (18%)	-0.99	0 100 100	21, 21, 21, 23	0
2	P	2/11 (18%)	-0.64	0 100 100	18, 18, 18, 20	0
2	R	2/11 (18%)	-0.70	0 100 100	17, 17, 17, 19	0
2	T	2/11 (18%)	-0.11	0 100 100	18, 18, 18, 21	0
All	All	1670/1760 (94%)	-0.47	24 (1%) 75 80	12, 22, 37, 49	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	165	GLU	4.4
1	K	165	GLU	4.3
1	A	165	GLU	4.3
1	O	165	GLU	4.1
1	I	165	GLU	4.1
1	E	165	GLU	4.0
1	C	1	MET	3.9
1	M	165	GLU	3.7
1	G	165	GLU	3.6
1	M	1	MET	3.6
1	O	1	MET	3.2
1	S	165	GLU	3.2
1	O	15	GLU	2.7
1	G	1	MET	2.6
1	G	13	ASP	2.6
1	K	1	MET	2.6
1	A	15	GLU	2.5
1	M	14	GLY	2.4
1	K	13	ASP	2.2
1	C	165	GLU	2.2
1	Q	148	ARG	2.2
1	K	148	ARG	2.1
1	I	144	ARG	2.1
1	K	15	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	DAL	D	1	5/6	0.89	0.13	25,25,25,26	0
2	MLE	T	2	9/10	0.91	0.17	18,19,19,20	0
2	DAL	B	1	5/6	0.92	0.12	22,22,22,23	0
2	DAL	J	1	5/6	0.93	0.13	20,20,20,20	0
2	DAL	P	1	5/6	0.93	0.10	19,20,20,20	0
2	MLE	B	2	9/10	0.93	0.17	21,21,22,22	0
2	MLE	D	2	9/10	0.93	0.12	23,23,24,24	0
2	MLE	P	2	9/10	0.93	0.14	17,18,18,19	0
2	DAL	H	1	5/6	0.93	0.10	19,19,19,19	0
2	MLE	F	2	9/10	0.94	0.13	17,18,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DAL	L	1	5/6	0.94	0.13	22,23,23,23	0
2	MLE	R	2	9/10	0.94	0.12	17,17,18,18	0
2	DAL	T	1	5/6	0.94	0.11	20,20,20,20	0
2	SAR	L	7	5/6	0.94	0.13	21,21,21,21	0
2	MLE	B	8	9/10	0.94	0.12	20,20,21,22	0
2	DAL	N	1	5/6	0.95	0.10	22,22,22,22	0
2	DAL	R	1	5/6	0.95	0.12	19,19,19,19	0
2	MLE	H	2	9/10	0.95	0.16	15,16,17,18	0
2	MVA	L	4	8/9	0.95	0.18	19,20,20,20	0
2	MLE	J	2	9/10	0.95	0.10	18,19,19,19	0
2	MLE	L	2	9/10	0.95	0.14	21,21,21,22	0
2	MVA	D	4	8/9	0.96	0.12	20,21,21,21	0
2	MVA	J	4	8/9	0.96	0.13	16,16,17,17	0
2	DAL	F	1	5/6	0.96	0.11	20,20,20,21	0
2	YYA	B	5	14/15	0.96	0.13	18,18,24,25	0
2	YYA	H	5	14/15	0.96	0.14	13,14,21,23	0
2	YYA	N	5	14/15	0.96	0.10	16,17,24,25	0
2	YYA	P	5	14/15	0.96	0.13	15,16,24,25	0
2	ABA	D	6	6/7	0.96	0.13	20,21,21,21	0
2	ABA	T	6	6/7	0.96	0.13	15,15,16,16	0
2	SAR	D	7	5/6	0.96	0.13	21,21,22,22	0
2	SAR	F	7	5/6	0.96	0.11	16,16,16,17	0
2	MLE	D	3	9/10	0.96	0.14	21,21,22,22	0
2	SAR	R	7	5/6	0.96	0.09	15,16,16,16	0
2	MVA	B	4	8/9	0.96	0.18	17,18,18,18	0
2	MLE	D	8	9/10	0.96	0.17	22,23,24,25	0
2	MLE	H	8	9/10	0.96	0.14	16,16,17,17	0
2	MLE	L	8	9/10	0.96	0.12	21,21,22,23	0
2	MLE	N	8	9/10	0.96	0.11	19,20,22,24	0
2	MLE	R	8	9/10	0.96	0.13	16,16,17,18	0
2	MLE	F	10	9/10	0.96	0.11	19,20,20,20	0
2	YYA	T	5	14/15	0.97	0.11	15,16,20,21	0
2	ABA	B	6	6/7	0.97	0.12	18,18,18,18	0
2	MLE	J	3	9/10	0.97	0.08	17,17,18,18	0
2	ABA	F	6	6/7	0.97	0.12	15,16,16,16	0
2	ABA	J	6	6/7	0.97	0.18	16,16,16,17	0
2	ABA	L	6	6/7	0.97	0.16	20,20,20,20	0
2	ABA	N	6	6/7	0.97	0.08	17,17,18,18	0
2	MLE	N	3	9/10	0.97	0.10	17,18,18,19	0
2	MVA	N	4	8/9	0.97	0.09	15,16,17,17	0
2	MVA	P	4	8/9	0.97	0.13	14,15,15,16	0
2	SAR	J	7	5/6	0.97	0.18	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MVA	T	4	8/9	0.97	0.14	15,16,16,16	0
2	SAR	N	7	5/6	0.97	0.10	18,18,19,20	0
2	SAR	P	7	5/6	0.97	0.13	16,16,17,17	0
2	MLE	N	2	9/10	0.97	0.09	19,20,20,21	0
2	SAR	T	7	5/6	0.97	0.11	15,16,16,17	0
2	YYA	D	5	14/15	0.97	0.16	19,20,24,25	0
2	MLE	F	3	9/10	0.97	0.11	16,17,17,17	0
2	MLE	F	8	9/10	0.97	0.13	17,18,20,21	0
2	YYA	J	5	14/15	0.97	0.12	14,16,22,22	0
2	MLE	J	8	9/10	0.97	0.14	17,17,18,20	0
2	YYA	L	5	14/15	0.97	0.16	19,20,23,23	0
2	MVA	F	4	8/9	0.97	0.12	14,15,15,16	0
2	MVA	H	4	8/9	0.97	0.15	13,14,14,14	0
2	MLE	D	10	9/10	0.97	0.15	24,24,25,26	0
2	YYA	R	5	14/15	0.97	0.11	15,15,20,21	0
2	MLE	H	10	9/10	0.97	0.11	18,19,19,20	0
2	MLE	J	10	9/10	0.97	0.11	18,18,19,19	0
2	MLE	L	10	9/10	0.97	0.11	22,22,23,23	0
2	MLE	N	10	9/10	0.97	0.10	21,21,23,23	0
2	MLE	P	10	9/10	0.97	0.10	18,19,20,21	0
2	MLE	T	10	9/10	0.97	0.12	19,19,20,20	0
2	MLE	H	3	9/10	0.98	0.14	12,14,15,15	0
2	SAR	H	7	5/6	0.98	0.10	15,15,15,15	0
2	MVA	R	4	8/9	0.98	0.13	14,14,14,14	0
2	MLE	P	8	9/10	0.98	0.15	17,17,17,17	0
2	ABA	H	6	6/7	0.98	0.10	14,15,15,15	0
2	MLE	T	8	9/10	0.98	0.13	16,17,18,18	0
2	MLE	B	10	9/10	0.98	0.09	21,21,23,23	0
2	MLE	R	3	9/10	0.98	0.10	15,15,16,16	0
2	MLE	T	3	9/10	0.98	0.11	17,17,18,18	0
2	MLE	B	3	9/10	0.98	0.15	19,19,20,20	0
2	ABA	P	6	6/7	0.98	0.11	16,16,16,16	0
2	ABA	R	6	6/7	0.98	0.08	15,15,15,15	0
2	YYA	F	5	14/15	0.98	0.11	14,15,20,21	0
2	SAR	B	7	5/6	0.98	0.08	19,19,19,20	0
2	MLE	R	10	9/10	0.98	0.09	17,18,18,18	0
2	MLE	L	3	9/10	0.98	0.13	21,21,21,21	0
2	MLE	P	3	9/10	0.99	0.10	15,16,17,17	0

## 6.3 Carbohydrates ⓘ

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.