



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 02:57 PM EDT

PDB ID : 6YNS
Title : CaM-P458 complex (crystal form 2)
Authors : Mechaly, A.E.; Voegelé, A.; Haouz, A.; Chenal, A.
Deposited on : 2020-04-14
Resolution : 3.94 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

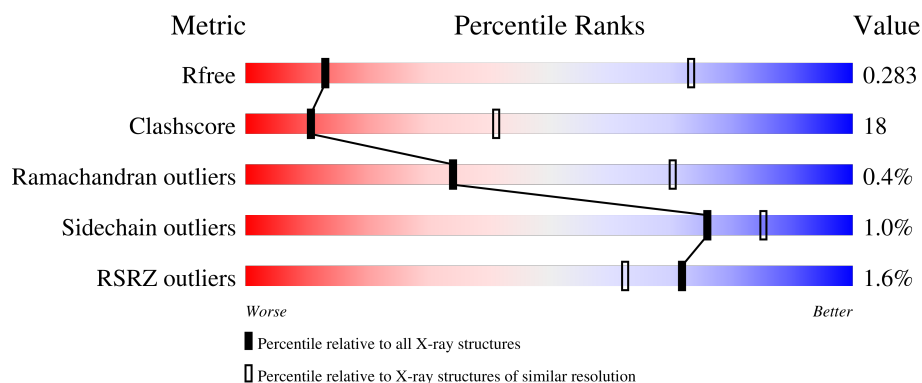
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.94 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	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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	148	 64% 28% 7%
1	B	148	 65% 28% 6%
1	C	148	 60% 31% 7%
1	D	148	 74% 20% 5%
1	E	148	 3% 63% 30% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	148	
1	G	148	
1	H	148	
1	I	148	
1	J	148	
1	K	148	
1	L	148	
2	N	24	
2	O	24	
2	Q	24	
2	R	24	
2	S	24	
2	T	24	
2	U	24	
2	V	24	
2	W	24	
2	X	24	
2	Y	24	
2	Z	24	
2	a	24	
2	b	24	
2	c	24	
2	d	24	
2	e	24	
2	f	24	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	g	24	<div><div></div><div>100%</div></div>
2	h	24	<div><div>4%</div><div></div><div>100%</div></div>
2	i	24	<div><div></div><div>96%</div><div></div><div>.</div></div>
2	j	24	<div><div></div><div>92%</div><div></div><div>8%</div></div>
2	k	24	<div><div>4%</div><div></div><div>96%</div><div></div><div>.</div></div>
2	l	24	<div><div></div><div>96%</div><div></div><div>.</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17084 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1088	669	176	235	8			
1	B	139	Total	C	N	O	S	0	0	0
			1095	674	178	234	9			
1	C	137	Total	C	N	O	S	0	0	0
			1081	664	174	235	8			
1	D	140	Total	C	N	O	S	0	0	0
			1103	678	178	238	9			
1	E	139	Total	C	N	O	S	0	0	0
			1095	673	177	237	8			
1	F	142	Total	C	N	O	S	0	0	0
			1118	686	180	243	9			
1	G	138	Total	C	N	O	S	0	0	0
			1088	669	176	235	8			
1	H	133	Total	C	N	O	S	0	0	0
			1048	645	170	225	8			
1	I	141	Total	C	N	O	S	0	0	0
			1112	684	180	239	9			
1	J	131	Total	C	N	O	S	0	0	0
			1028	633	164	223	8			
1	K	139	Total	C	N	O	S	0	0	0
			1095	673	177	237	8			
1	L	140	Total	C	N	O	S	0	0	0
			1104	678	178	239	9			

- Molecule 2 is a protein called Bifunctional adenylate cyclase toxin/hemolysin CyaA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	23	Total	C	N	O	0	0	0
			162	100	35	27			
2	O	24	Total	C	N	O	0	0	0
			176	111	37	28			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	21	Total	C	N	O	0	0	0
			155	96	34	25			
2	R	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	S	21	Total	C	N	O	0	0	0
			150	92	33	25			
2	T	21	Total	C	N	O	0	0	0
			149	91	33	25			
2	U	20	Total	C	N	O	0	0	0
			141	87	31	23			
2	V	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	W	22	Total	C	N	O	0	0	0
			154	94	34	26			
2	X	20	Total	C	N	O	0	0	0
			141	87	31	23			
2	Y	22	Total	C	N	O	0	0	0
			154	94	34	26			
2	Z	22	Total	C	N	O	0	0	0
			154	94	34	26			
2	a	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	b	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	c	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	d	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	e	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	f	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	g	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	h	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	i	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	j	24	Total	C	N	O	0	0	0
			176	111	37	28			
2	k	24	Total	C	N	O	0	0	0
			176	111	37	28			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	1	24	Total	C	N	O	0	0	0
			176	111	37	28			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

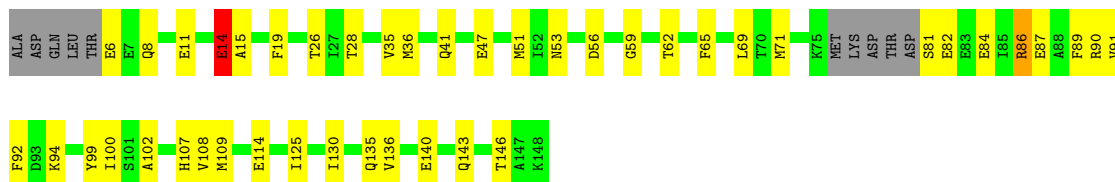
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	B	5	Total	Ca	0	0
			5	5		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		
3	G	2	Total	Ca	0	0
			2	2		
3	H	2	Total	Ca	0	0
			2	2		
3	I	2	Total	Ca	0	0
			2	2		
3	J	2	Total	Ca	0	0
			2	2		
3	K	3	Total	Ca	0	0
			3	3		
3	L	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

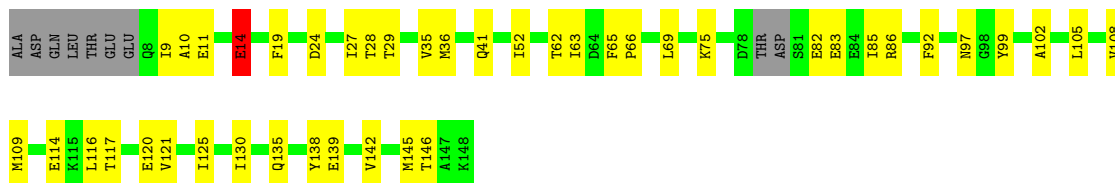
• Molecule 1: Calmodulin-1

Chain A: 



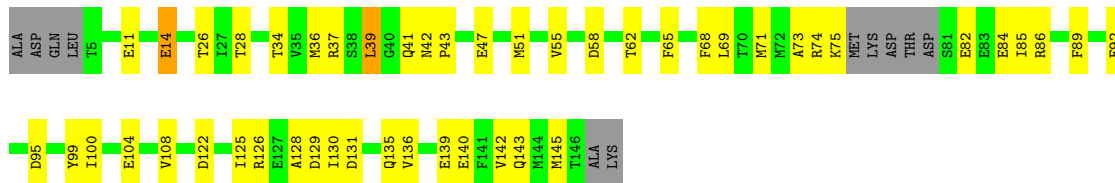
• Molecule 1: Calmodulin-1

Chain B: 



• Molecule 1: Calmodulin-1

Chain C: 



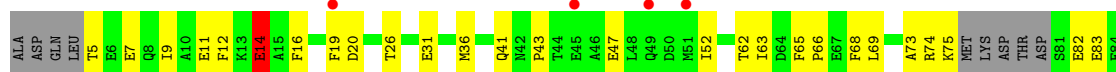
• Molecule 1: Calmodulin-1

Chain D: 

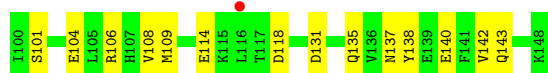




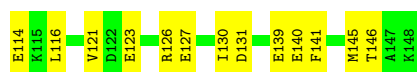
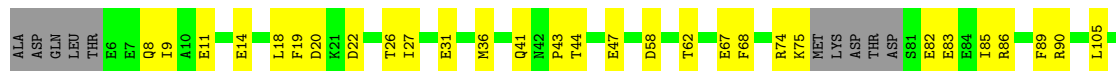
- Molecule 1: Calmodulin-1



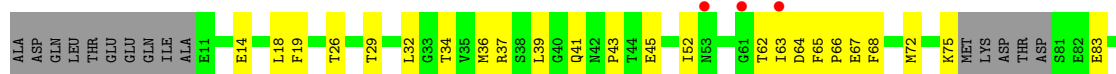
- Molecule 1: Calmodulin-1



- Molecule 1: Calmodulin-1

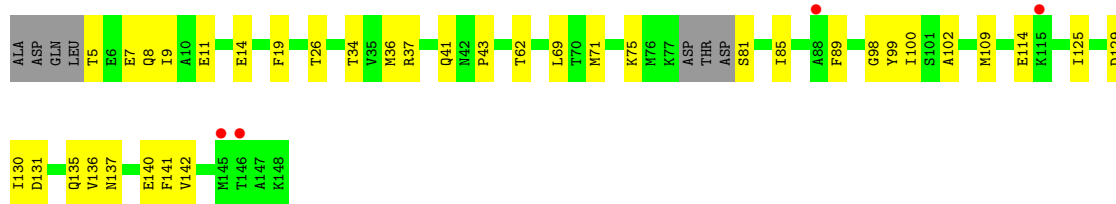


- Molecule 1: Calmodulin-1

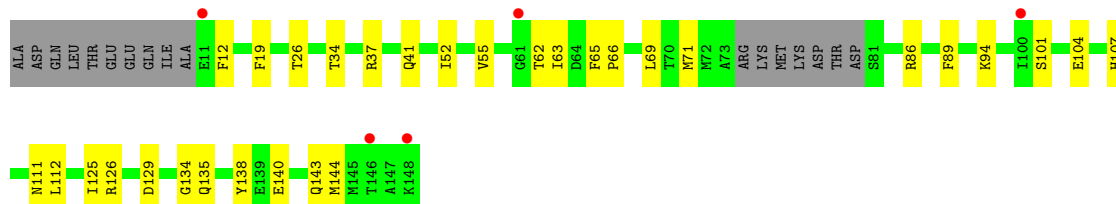


- Molecule 1: Calmodulin-1

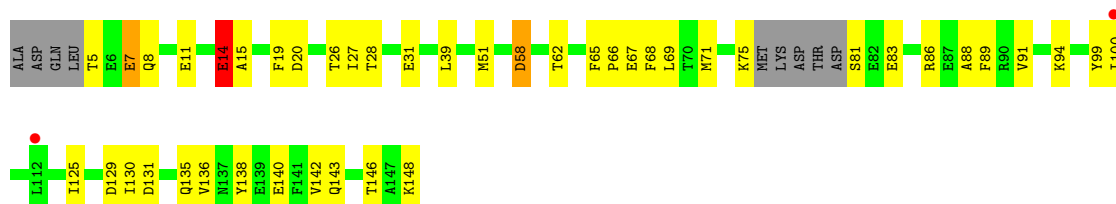




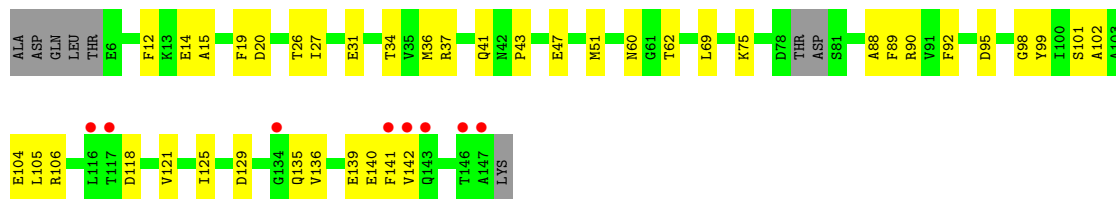
• Molecule 1: Calmodulin-1



• Molecule 1: Calmodulin-1



• Molecule 1: Calmodulin-1

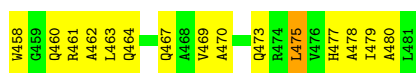


• Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



• Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

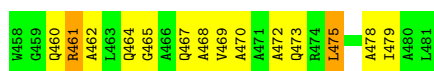




- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



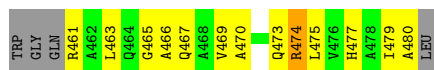
- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

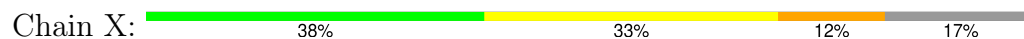


- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA





- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



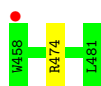
- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



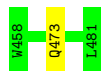
- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA





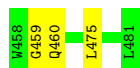
- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

Chain e: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

Chain f: 88% 12%



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

Chain g: 100%

There are no outlier residues recorded for this chain.

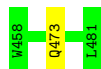
- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

Chain h: 4% 100%



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

Chain i: 96% .



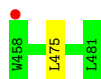
- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

Chain j: 92% 8%



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

Chain k: 4% 96% .



- Molecule 2: Bifunctional adenylate cyclase toxin/hemolysin CyaA

Chain 1:  96% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.00Å 106.97Å 221.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.86 – 3.94 110.82 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (88.86-3.94) 99.9 (110.82-3.94)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.89Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.14_3260	Depositor
R, R_{free}	0.222 , 0.284 0.225 , 0.283	Depositor DCC
R_{free} test set	1081 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	112.9	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17084	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2693e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA

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	0.94	2/1099 (0.2%)	0.98	2/1473 (0.1%)
1	B	0.91	2/1106 (0.2%)	0.95	0/1481
1	C	0.78	2/1092 (0.2%)	0.88	1/1465 (0.1%)
1	D	0.75	0/1114	0.87	1/1493 (0.1%)
1	E	0.87	4/1106 (0.4%)	0.94	0/1483
1	F	0.69	2/1129 (0.2%)	0.85	2/1514 (0.1%)
1	G	0.74	1/1099 (0.1%)	0.91	1/1473 (0.1%)
1	H	0.70	1/1059 (0.1%)	0.81	0/1419
1	I	0.66	0/1123	0.83	1/1504 (0.1%)
1	J	0.68	0/1039	0.85	0/1394
1	K	0.80	2/1106 (0.2%)	0.92	2/1483 (0.1%)
1	L	0.78	2/1115 (0.2%)	0.86	0/1494
2	N	0.69	0/162	1.14	1/218 (0.5%)
2	O	0.78	0/178	1.05	1/241 (0.4%)
2	Q	1.00	0/157	1.14	2/212 (0.9%)
2	R	0.83	0/178	1.20	2/241 (0.8%)
2	S	0.80	0/150	1.09	2/202 (1.0%)
2	T	0.84	0/149	1.23	3/200 (1.5%)
2	U	0.85	0/141	1.12	1/190 (0.5%)
2	V	1.11	2/178 (1.1%)	1.11	2/241 (0.8%)
2	W	0.71	0/154	0.89	0/207
2	X	1.21	2/141 (1.4%)	1.33	1/190 (0.5%)
2	Y	0.96	0/154	1.42	1/207 (0.5%)
2	Z	0.80	0/154	1.01	1/207 (0.5%)
2	a	0.65	0/178	1.07	1/241 (0.4%)
2	b	0.65	0/178	0.93	0/241
2	c	0.78	0/178	0.98	1/241 (0.4%)
2	d	0.78	0/178	1.10	1/241 (0.4%)
2	e	0.78	0/178	1.00	0/241
2	f	0.62	0/178	0.95	1/241 (0.4%)
2	g	0.91	0/178	0.96	0/241
2	h	0.75	0/178	0.93	0/241

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	i	0.73	0/178	1.01	1/241 (0.4%)
2	j	0.60	0/178	0.92	1/241 (0.4%)
2	k	0.72	0/178	1.02	1/241 (0.4%)
2	l	0.59	0/178	0.90	0/241
All	All	0.79	22/17219 (0.1%)	0.94	34/23124 (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	K	0	1
2	b	0	1
All	All	0	2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	GLU	CG-CD	10.44	1.67	1.51
1	A	14	GLU	CB-CG	9.97	1.71	1.52
1	B	14	GLU	CG-CD	9.81	1.66	1.51
1	K	14	GLU	CG-CD	7.94	1.63	1.51
1	C	14	GLU	CG-CD	7.69	1.63	1.51

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	463	LEU	CB-CG-CD1	-13.58	87.91	111.00
2	d	475	LEU	CB-CG-CD1	-7.52	98.21	111.00
2	R	461	ARG	CG-CD-NE	-7.07	96.95	111.80
2	O	475	LEU	CA-CB-CG	6.95	131.29	115.30
2	k	475	LEU	CB-CG-CD2	-6.94	99.20	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	7	GLU	Peptide
2	b	473	GLN	Mainchain

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	1088	0	1020	35	0
1	B	1095	0	1034	44	0
1	C	1081	0	1009	36	0
1	D	1103	0	1036	33	0
1	E	1095	0	1027	37	0
1	F	1118	0	1047	33	0
1	G	1088	0	1020	34	0
1	H	1048	0	984	37	0
1	I	1112	0	1049	26	0
1	J	1028	0	958	26	0
1	K	1095	0	1027	40	0
1	L	1104	0	1033	35	0
2	N	162	0	172	25	0
2	O	176	0	182	26	0
2	Q	155	0	155	13	0
2	R	176	0	182	17	0
2	S	150	0	158	22	0
2	T	149	0	156	21	0
2	U	141	0	150	24	0
2	V	176	0	182	15	0
2	W	154	0	161	20	0
2	X	141	0	150	10	0
2	Y	154	0	161	32	0
2	Z	154	0	161	16	0
2	a	176	0	182	0	0
2	b	176	0	182	0	0
2	c	176	0	182	0	0
2	d	176	0	182	0	0
2	e	176	0	182	0	0
2	f	176	0	182	0	0
2	g	176	0	182	0	0
2	h	176	0	182	0	0
2	i	176	0	182	0	0
2	j	176	0	182	0	0
2	k	176	0	182	0	0
2	l	176	0	182	0	0
3	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	3	0	0	0	0
3	L	1	0	0	0	0
All	All	17084	0	16398	503	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 503 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:J:143:GLN:HB2	2:Z:463:LEU:HD12	1.41	1.03
2:O:462:ALA:HB1	2:Y:480:ALA:HB1	1.43	1.01
1:F:90:ARG:NH2	2:U:474:ARG:HH12	1.60	0.99
1:D:83:GLU:HG2	1:E:83:GLU:HG2	1.43	0.99
1:I:75:LYS:HG3	2:W:478:ALA:HA	1.43	0.97

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	134/148 (90%)	130 (97%)	4 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	135/148 (91%)	131 (97%)	3 (2%)	1 (1%)	22	60
1	C	133/148 (90%)	130 (98%)	3 (2%)	0	100	100
1	D	136/148 (92%)	133 (98%)	3 (2%)	0	100	100
1	E	135/148 (91%)	133 (98%)	1 (1%)	1 (1%)	22	60
1	F	138/148 (93%)	136 (99%)	2 (1%)	0	100	100
1	G	134/148 (90%)	133 (99%)	1 (1%)	0	100	100
1	H	129/148 (87%)	122 (95%)	6 (5%)	1 (1%)	19	57
1	I	137/148 (93%)	129 (94%)	8 (6%)	0	100	100
1	J	127/148 (86%)	123 (97%)	4 (3%)	0	100	100
1	K	135/148 (91%)	135 (100%)	0	0	100	100
1	L	136/148 (92%)	135 (99%)	1 (1%)	0	100	100
2	N	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
2	O	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
2	Q	19/24 (79%)	18 (95%)	1 (5%)	0	100	100
2	R	22/24 (92%)	22 (100%)	0	0	100	100
2	S	19/24 (79%)	19 (100%)	0	0	100	100
2	T	19/24 (79%)	17 (90%)	1 (5%)	1 (5%)	2	21
2	U	18/24 (75%)	18 (100%)	0	0	100	100
2	V	22/24 (92%)	22 (100%)	0	0	100	100
2	W	20/24 (83%)	19 (95%)	1 (5%)	0	100	100
2	X	18/24 (75%)	15 (83%)	1 (6%)	2 (11%)	0	7
2	Y	20/24 (83%)	18 (90%)	1 (5%)	1 (5%)	2	22
2	Z	20/24 (83%)	20 (100%)	0	0	100	100
2	a	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
2	b	22/24 (92%)	22 (100%)	0	0	100	100
2	c	22/24 (92%)	22 (100%)	0	0	100	100
2	d	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
2	e	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
2	f	22/24 (92%)	20 (91%)	1 (4%)	1 (4%)	2	24
2	g	22/24 (92%)	22 (100%)	0	0	100	100
2	h	22/24 (92%)	20 (91%)	2 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	i	22/24 (92%)	22 (100%)	0	0	100	100
2	j	22/24 (92%)	21 (96%)	0	1 (4%)	2	24
2	k	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
2	l	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
All	All	2113/2352 (90%)	2051 (97%)	53 (2%)	9 (0%)	34	70

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	ALA
1	E	74	ARG
2	X	462	ALA
1	H	132	GLY
2	f	459	GLY

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	117/126 (93%)	116 (99%)	1 (1%)	78	87
1	B	118/126 (94%)	116 (98%)	2 (2%)	60	78
1	C	117/126 (93%)	117 (100%)	0	100	100
1	D	119/126 (94%)	119 (100%)	0	100	100
1	E	118/126 (94%)	116 (98%)	2 (2%)	60	78
1	F	121/126 (96%)	121 (100%)	0	100	100
1	G	117/126 (93%)	117 (100%)	0	100	100
1	H	113/126 (90%)	113 (100%)	0	100	100
1	I	120/126 (95%)	118 (98%)	2 (2%)	60	78
1	J	111/126 (88%)	110 (99%)	1 (1%)	78	87
1	K	118/126 (94%)	117 (99%)	1 (1%)	81	88
1	L	119/126 (94%)	119 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	13/14 (93%)	12 (92%)	1 (8%)	13	41
2	O	14/14 (100%)	14 (100%)	0	100	100
2	Q	12/14 (86%)	11 (92%)	1 (8%)	11	38
2	R	14/14 (100%)	14 (100%)	0	100	100
2	S	12/14 (86%)	12 (100%)	0	100	100
2	T	12/14 (86%)	12 (100%)	0	100	100
2	U	11/14 (79%)	10 (91%)	1 (9%)	9	33
2	V	14/14 (100%)	14 (100%)	0	100	100
2	W	12/14 (86%)	12 (100%)	0	100	100
2	X	11/14 (79%)	10 (91%)	1 (9%)	9	33
2	Y	12/14 (86%)	11 (92%)	1 (8%)	11	38
2	Z	12/14 (86%)	11 (92%)	1 (8%)	11	38
2	a	14/14 (100%)	14 (100%)	0	100	100
2	b	14/14 (100%)	14 (100%)	0	100	100
2	c	14/14 (100%)	14 (100%)	0	100	100
2	d	14/14 (100%)	14 (100%)	0	100	100
2	e	14/14 (100%)	14 (100%)	0	100	100
2	f	14/14 (100%)	13 (93%)	1 (7%)	14	43
2	g	14/14 (100%)	14 (100%)	0	100	100
2	h	14/14 (100%)	14 (100%)	0	100	100
2	i	14/14 (100%)	14 (100%)	0	100	100
2	j	14/14 (100%)	14 (100%)	0	100	100
2	k	14/14 (100%)	14 (100%)	0	100	100
2	l	14/14 (100%)	13 (93%)	1 (7%)	14	43
All	All	1725/1848 (93%)	1708 (99%)	17 (1%)	76	85

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	477	HIS
2	l	460	GLN
1	J	112	LEU
1	K	14	GLU
2	N	477	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	473	GLN
2	Y	467	GLN
2	k	473	GLN
2	h	473	GLN
1	H	135	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 29 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	138/148 (93%)	-0.42	0	100	100	61, 80, 111, 123	0
1	B	139/148 (93%)	-0.39	0	100	100	55, 82, 111, 138	0
1	C	137/148 (92%)	-0.36	0	100	100	67, 111, 162, 180	0
1	D	140/148 (94%)	-0.28	0	100	100	79, 115, 139, 173	0
1	E	139/148 (93%)	-0.08	4 (2%)	51	41	58, 108, 150, 163	0
1	F	142/148 (95%)	-0.15	3 (2%)	63	54	96, 128, 152, 162	0
1	G	138/148 (93%)	-0.14	0	100	100	58, 110, 142, 151	0
1	H	133/148 (89%)	0.12	5 (3%)	40	32	96, 133, 167, 188	0
1	I	141/148 (95%)	0.08	4 (2%)	53	42	84, 142, 209, 220	0
1	J	131/148 (88%)	0.06	5 (3%)	40	32	90, 129, 166, 178	0
1	K	139/148 (93%)	-0.25	2 (1%)	75	66	73, 111, 167, 189	0
1	L	140/148 (94%)	0.08	8 (5%)	23	20	94, 143, 189, 213	0
2	N	23/24 (95%)	-0.40	0	100	100	77, 94, 118, 120	0
2	O	24/24 (100%)	-0.51	0	100	100	61, 91, 127, 138	0
2	Q	21/24 (87%)	-0.28	0	100	100	57, 78, 104, 111	0
2	R	24/24 (100%)	-0.08	0	100	100	83, 107, 148, 156	0
2	S	21/24 (87%)	-0.21	0	100	100	79, 96, 124, 135	0
2	T	21/24 (87%)	-0.14	0	100	100	74, 99, 116, 130	0
2	U	20/24 (83%)	-0.41	0	100	100	60, 91, 124, 125	0
2	V	24/24 (100%)	-0.02	1 (4%)	36	30	115, 135, 158, 162	0
2	W	22/24 (91%)	-0.43	0	100	100	84, 116, 159, 162	0
2	X	20/24 (83%)	-0.20	0	100	100	115, 131, 156, 166	0
2	Y	22/24 (91%)	0.06	0	100	100	56, 82, 102, 112	0
2	Z	22/24 (91%)	-0.34	0	100	100	93, 112, 129, 140	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	a	24/24 (100%)	-0.17	1 (4%) 36 30	52, 80, 119, 122	0
2	b	24/24 (100%)	-0.17	0 100 100	51, 70, 103, 121	0
2	c	24/24 (100%)	-0.16	0 100 100	69, 97, 123, 145	0
2	d	24/24 (100%)	-0.27	0 100 100	64, 87, 111, 119	0
2	e	24/24 (100%)	-0.37	0 100 100	47, 65, 94, 109	0
2	f	24/24 (100%)	-0.28	0 100 100	53, 82, 129, 143	0
2	g	24/24 (100%)	-0.31	0 100 100	56, 72, 112, 115	0
2	h	24/24 (100%)	-0.18	1 (4%) 36 30	84, 107, 145, 157	0
2	i	24/24 (100%)	-0.24	0 100 100	82, 103, 131, 145	0
2	j	24/24 (100%)	-0.30	0 100 100	76, 102, 132, 157	0
2	k	24/24 (100%)	-0.06	1 (4%) 36 30	73, 97, 127, 133	0
2	l	24/24 (100%)	-0.08	0 100 100	70, 109, 164, 170	0
All	All	2209/2352 (93%)	-0.17	35 (1%) 72 62	47, 111, 168, 220	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	49	GLN	4.5
1	L	117	THR	3.6
1	I	145	MET	3.5
1	L	146	THR	3.4
1	L	116	LEU	3.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	CA	E	202	1/1	0.83	0.21	116,116,116,116	0
3	CA	B	203	1/1	0.84	0.06	70,70,70,70	0
3	CA	C	202	1/1	0.88	0.10	79,79,79,79	0
3	CA	F	202	1/1	0.88	0.04	93,93,93,93	0
3	CA	F	201	1/1	0.92	0.11	115,115,115,115	0
3	CA	C	201	1/1	0.92	0.05	64,64,64,64	0
3	CA	I	202	1/1	0.93	0.05	80,80,80,80	0
3	CA	H	202	1/1	0.94	0.08	83,83,83,83	0
3	CA	H	201	1/1	0.94	0.05	67,67,67,67	0
3	CA	K	203	1/1	0.94	0.19	190,190,190,190	0
3	CA	I	201	1/1	0.95	0.03	97,97,97,97	0
3	CA	G	202	1/1	0.96	0.10	53,53,53,53	0
3	CA	B	204	1/1	0.96	0.07	76,76,76,76	0
3	CA	G	201	1/1	0.97	0.06	42,42,42,42	0
3	CA	A	201	1/1	0.97	0.06	43,43,43,43	0
3	CA	D	201	1/1	0.97	0.09	105,105,105,105	0
3	CA	D	202	1/1	0.97	0.07	194,194,194,194	0
3	CA	A	204	1/1	0.97	0.04	44,44,44,44	0
3	CA	B	205	1/1	0.97	0.08	71,71,71,71	0
3	CA	J	202	1/1	0.97	0.09	104,104,104,104	0
3	CA	K	202	1/1	0.97	0.08	88,88,88,88	0
3	CA	B	202	1/1	0.97	0.09	74,74,74,74	0
3	CA	K	201	1/1	0.98	0.06	53,53,53,53	0
3	CA	J	201	1/1	0.98	0.03	62,62,62,62	0
3	CA	A	202	1/1	0.98	0.10	79,79,79,79	0
3	CA	E	201	1/1	0.99	0.07	54,54,54,54	0
3	CA	A	203	1/1	0.99	0.08	66,66,66,66	0
3	CA	B	201	1/1	0.99	0.06	60,60,60,60	0
3	CA	L	201	1/1	0.99	0.06	102,102,102,102	0

6.5 Other polymers ⓘ

There are no such residues in this entry.