



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:38 AM EDT

PDB ID : 2F2O / pdb_00002f2o
Title : Structure of calmodulin bound to a calcineurin peptide: a new way of making an old binding mode
Authors : Ye, Q.; Wong, A.; Jia, Z.
Deposited on : 2005-11-17
Resolution : 2.17 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
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

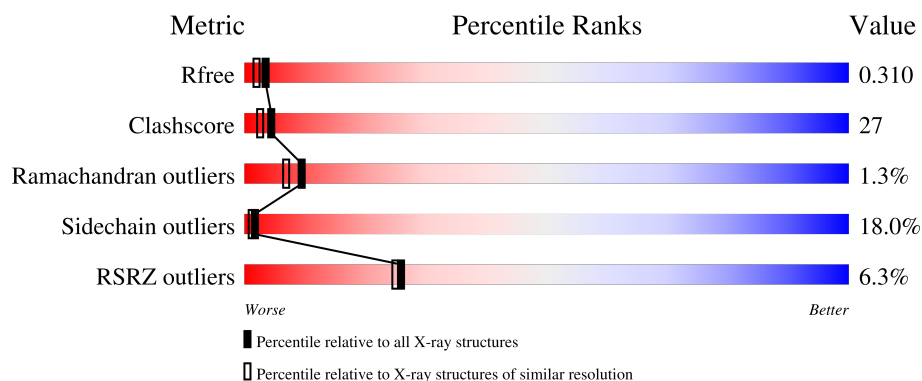
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	179	6% 34% 31% 19% • 13%
1	B	179	5% 31% 38% 18% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2676 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 fused with calmodulin-binding domain of calcineurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1236	762	206	258	10			
1	B	159	Total	C	N	O	S	0	0	0
			1254	773	212	259	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	GLY	-	linker	UNP P62157
A	150	GLY	-	linker	UNP P62157
A	151	GLY	-	linker	UNP P62157
A	152	GLY	-	linker	UNP P62157
A	153	GLY	-	linker	UNP P62157
B	149	GLY	-	linker	UNP P62157
B	150	GLY	-	linker	UNP P62157
B	151	GLY	-	linker	UNP P62157
B	152	GLY	-	linker	UNP P62157
B	153	GLY	-	linker	UNP P62157

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		
2	B	4	Total	Ca	0	0
			4	4		

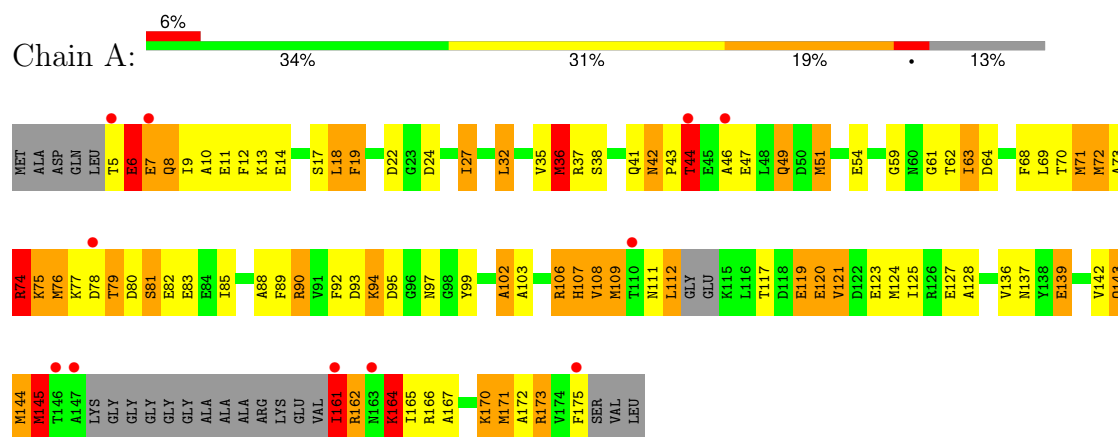
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total 85	O 85	0	0
3	B	93	Total 93	O 93	0	0

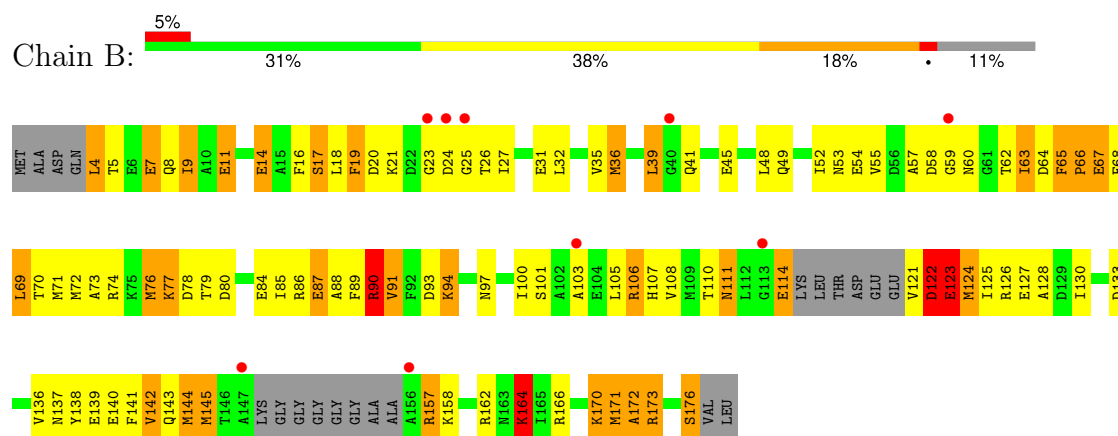
3 Residue-property plots [i](#)

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: Calmodulin fused with calmodulin-binding domain of calcineurin



- Molecule 1: Calmodulin fused with calmodulin-binding domain of calcineurin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.24Å 42.77Å 71.15Å 90.00° 110.39° 90.00°	Depositor
Resolution (Å)	67.42 – 2.17 66.69 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.9 (67.42-2.17) 97.9 (66.69-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.289 0.245 , 0.310	Depositor DCC
R_{free} test set	1790 reflections (9.75%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.8	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	0.91	EDS
Total number of atoms	2676	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.63	75/1247 (6.0%)	1.98	33/1668 (2.0%)
1	B	2.64	73/1265 (5.8%)	1.93	33/1691 (2.0%)
All	All	2.64	148/2512 (5.9%)	1.95	66/3359 (2.0%)

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	1
All	All	0	3

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	MET	SD-CE	-15.13	1.41	1.79
1	B	71	MET	SD-CE	-14.65	1.43	1.79
1	B	145	MET	SD-CE	-14.63	1.43	1.79
1	B	171	MET	SD-CE	13.74	2.13	1.79
1	A	77	LYS	N-CA	12.26	1.60	1.46
1	B	68	PHE	CA-C	11.92	1.67	1.52
1	B	76	MET	SD-CE	-11.88	1.49	1.79
1	A	171	MET	SD-CE	11.68	2.08	1.79
1	A	51	MET	SD-CE	-11.59	1.50	1.79
1	B	106	ARG	C-O	11.31	1.37	1.24
1	B	68	PHE	N-CA	-11.20	1.32	1.46
1	A	77	LYS	C-O	-10.40	1.12	1.24
1	A	71	MET	SD-CE	-10.26	1.53	1.79
1	A	80	ASP	C-O	9.80	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	LEU	C-O	9.55	1.35	1.24
1	B	78	ASP	CA-CB	-9.49	1.38	1.53
1	A	102	ALA	CA-CB	9.26	1.68	1.53
1	A	27	ILE	CA-CB	-9.24	1.43	1.54
1	B	67	GLU	CD-OE1	9.23	1.42	1.25
1	A	80	ASP	CA-C	-9.13	1.41	1.52
1	A	83	GLU	CA-C	9.02	1.65	1.52
1	B	141	PHE	C-O	8.91	1.34	1.24
1	B	108	VAL	C-O	-8.88	1.14	1.24
1	A	93	ASP	C-O	-8.83	1.14	1.23
1	B	73	ALA	C-O	-8.66	1.14	1.24
1	A	109	MET	SD-CE	8.28	2.00	1.79
1	B	24	ASP	N-CA	8.23	1.56	1.46
1	A	121	VAL	CA-C	8.02	1.64	1.52
1	A	79	THR	C-O	-8.00	1.14	1.24
1	B	142	VAL	N-CA	7.74	1.55	1.46
1	A	72	MET	SD-CE	-7.68	1.60	1.79
1	B	19	PHE	CA-C	-7.64	1.43	1.52
1	B	60	ASN	CG-OD1	7.63	1.38	1.23
1	B	41	GLN	CA-CB	-7.59	1.41	1.53
1	B	103	ALA	CA-CB	-7.53	1.40	1.53
1	A	136	VAL	CA-C	-7.52	1.43	1.52
1	A	8	GLN	N-CA	-7.52	1.37	1.46
1	A	143	GLN	C-O	-7.51	1.14	1.24
1	B	53	ASN	CB-CG	7.44	1.70	1.52
1	B	31	GLU	C-O	-7.44	1.15	1.24
1	B	90	ARG	C-O	-7.38	1.15	1.24
1	A	85	ILE	N-CA	-7.34	1.38	1.46
1	A	36	MET	SD-CE	7.33	1.97	1.79
1	A	142	VAL	C-O	-7.08	1.15	1.24
1	A	128	ALA	CA-C	7.01	1.61	1.52
1	B	36	MET	C-O	-6.96	1.16	1.24
1	A	103	ALA	CA-CB	-6.96	1.42	1.53
1	A	108	VAL	CA-CB	-6.85	1.46	1.54
1	A	79	THR	CB-CG2	6.78	1.75	1.52
1	A	90	ARG	NE-CZ	6.73	1.40	1.33
1	A	127	GLU	C-O	-6.73	1.15	1.24
1	B	63	ILE	N-CA	6.72	1.54	1.46
1	B	79	THR	CA-C	6.69	1.61	1.52
1	B	69	LEU	C-O	-6.68	1.16	1.24
1	A	68	PHE	CA-CB	-6.68	1.42	1.53
1	B	67	GLU	CA-CB	-6.66	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	ALA	CA-CB	6.66	1.63	1.53
1	B	71	MET	CG-SD	6.66	1.97	1.80
1	A	78	ASP	CA-C	6.61	1.61	1.52
1	A	72	MET	CA-C	-6.60	1.44	1.52
1	B	76	MET	CG-SD	6.60	1.97	1.80
1	A	12	PHE	C-O	-6.43	1.16	1.24
1	A	139	GLU	C-O	-6.41	1.16	1.24
1	B	133	ASP	N-CA	6.40	1.54	1.46
1	B	58	ASP	CB-CG	6.36	1.68	1.52
1	A	107	HIS	C-O	6.36	1.31	1.24
1	A	144	MET	CG-SD	-6.31	1.65	1.80
1	B	77	LYS	CA-C	6.31	1.60	1.52
1	B	62	THR	CA-C	6.29	1.60	1.52
1	B	157	ARG	CA-C	6.29	1.60	1.52
1	A	19	PHE	C-O	-6.29	1.16	1.24
1	A	88	ALA	CA-CB	-6.27	1.42	1.53
1	B	137	ASN	CA-C	6.26	1.61	1.53
1	B	89	PHE	C-O	6.19	1.31	1.24
1	B	110	THR	CA-CB	6.16	1.63	1.53
1	B	17	SER	C-O	-6.13	1.16	1.24
1	B	63	ILE	CA-CB	-6.11	1.46	1.53
1	A	38	SER	C-O	-6.10	1.16	1.24
1	B	93	ASP	C-O	-6.07	1.16	1.23
1	B	142	VAL	CB-CG1	6.06	1.72	1.52
1	A	46	ALA	N-CA	6.05	1.53	1.46
1	B	136	VAL	C-O	6.04	1.30	1.24
1	B	66	PRO	CA-C	6.04	1.60	1.52
1	B	114	GLU	CA-C	6.00	1.65	1.52
1	A	108	VAL	C-O	-5.89	1.17	1.24
1	A	68	PHE	C-O	-5.82	1.17	1.24
1	A	136	VAL	C-O	5.78	1.30	1.24
1	B	90	ARG	CA-CB	5.72	1.62	1.53
1	A	74	ARG	CA-C	5.70	1.60	1.52
1	A	13	LYS	CE-NZ	5.70	1.66	1.49
1	B	111	ASN	C-O	-5.68	1.17	1.24
1	A	124	MET	CB-CG	-5.59	1.35	1.52
1	B	70	THR	C-O	-5.58	1.17	1.24
1	A	90	ARG	CB-CG	5.57	1.69	1.52
1	B	110	THR	C-O	5.57	1.30	1.24
1	B	67	GLU	CA-C	5.57	1.60	1.52
1	B	164	LYS	CA-C	5.53	1.59	1.52
1	B	72	MET	C-O	5.53	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	LEU	N-CA	-5.53	1.39	1.46
1	A	59	GLY	C-O	-5.53	1.17	1.24
1	B	100	ILE	CA-CB	5.52	1.60	1.54
1	A	164	LYS	C-O	-5.51	1.17	1.24
1	B	65	PHE	CA-C	5.51	1.58	1.52
1	A	171	MET	C-O	-5.50	1.17	1.24
1	B	57	ALA	C-O	5.47	1.30	1.24
1	A	9	ILE	CB-CG2	5.45	1.70	1.52
1	A	68	PHE	CD2-CE2	5.44	1.54	1.38
1	B	17	SER	N-CA	5.41	1.53	1.46
1	B	27	ILE	CA-CB	5.38	1.60	1.54
1	A	119	GLU	CA-C	5.37	1.59	1.52
1	B	58	ASP	C-O	-5.35	1.17	1.24
1	B	124	MET	CG-SD	5.35	1.94	1.80
1	B	93	ASP	CA-C	-5.35	1.46	1.53
1	B	70	THR	CA-C	5.33	1.59	1.52
1	A	62	THR	C-O	-5.33	1.17	1.23
1	B	170	LYS	CD-CE	5.32	1.68	1.52
1	A	70	THR	CA-CB	5.31	1.61	1.53
1	A	79	THR	CB-OG1	-5.31	1.35	1.43
1	B	63	ILE	C-O	5.31	1.29	1.24
1	A	103	ALA	N-CA	-5.28	1.39	1.46
1	B	23	GLY	C-O	5.28	1.31	1.23
1	A	72	MET	C-O	-5.28	1.18	1.24
1	A	171	MET	CA-C	-5.27	1.46	1.52
1	B	11	GLU	CA-CB	5.27	1.61	1.53
1	A	94	LYS	CD-CE	5.26	1.68	1.52
1	A	165	ILE	CA-CB	-5.25	1.48	1.54
1	A	63	ILE	C-O	5.23	1.29	1.24
1	A	24	ASP	CG-OD1	5.21	1.35	1.25
1	A	78	ASP	C-O	-5.21	1.17	1.24
1	A	123	GLU	CA-C	5.21	1.59	1.52
1	A	99	TYR	CA-C	5.17	1.58	1.52
1	A	137	ASN	CA-C	5.17	1.60	1.53
1	A	71	MET	N-CA	5.16	1.52	1.46
1	B	20	ASP	CA-C	5.13	1.59	1.53
1	A	121	VAL	C-O	-5.12	1.17	1.24
1	B	58	ASP	N-CA	5.12	1.52	1.46
1	A	90	ARG	CD-NE	5.11	1.53	1.46
1	B	72	MET	CB-CG	-5.11	1.37	1.52
1	B	55	VAL	N-CA	5.11	1.51	1.46
1	B	76	MET	N-CA	-5.11	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	VAL	C-O	-5.09	1.18	1.24
1	A	10	ALA	CA-CB	5.09	1.61	1.53
1	A	108	VAL	CB-CG2	5.05	1.69	1.52
1	B	90	ARG	CG-CD	5.05	1.67	1.52
1	B	57	ALA	CA-CB	5.04	1.61	1.53
1	A	161	ILE	CA-CB	5.02	1.68	1.54
1	A	6	GLU	C-O	-5.02	1.17	1.24
1	B	140	GLU	CA-C	5.01	1.59	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	THR	CA-C-O	-9.32	110.67	120.55
1	A	36	MET	CG-SD-CE	-9.23	80.59	100.90
1	B	71	MET	CG-SD-CE	-8.74	81.67	100.90
1	A	124	MET	CG-SD-CE	-8.12	83.03	100.90
1	B	110	THR	N-CA-C	-7.71	102.95	111.36
1	B	101	SER	N-CA-C	-7.67	99.11	110.46
1	A	175	PHE	CA-C-O	7.39	133.36	120.80
1	B	173	ARG	N-CA-C	-7.37	103.18	111.14
1	B	36	MET	CG-SD-CE	-7.03	85.43	100.90
1	B	164	LYS	N-CA-C	-7.02	103.56	111.14
1	B	55	VAL	CB-CA-C	-6.96	102.82	112.36
1	A	143	GLN	N-CA-C	-6.86	102.91	112.45
1	B	59	GLY	N-CA-C	6.81	123.42	113.48
1	B	108	VAL	N-CA-C	-6.76	104.26	110.82
1	A	49	GLN	CB-CA-C	-6.75	99.59	110.79
1	A	19	PHE	N-CA-C	6.40	118.34	111.36
1	A	42	ASN	N-CA-C	-6.40	94.53	108.81
1	A	76	MET	CG-SD-CE	6.39	114.97	100.90
1	B	80	ASP	N-CA-C	-6.38	104.24	111.07
1	B	172	ALA	O-C-N	6.36	128.62	122.07
1	B	128	ALA	N-CA-C	6.36	120.77	112.89
1	A	103	ALA	N-CA-C	-6.31	104.48	111.36
1	A	73	ALA	N-CA-C	6.27	117.78	111.07
1	B	172	ALA	CA-C-N	6.22	128.90	120.44
1	B	172	ALA	C-N-CA	6.22	128.90	120.44
1	B	25	GLY	CA-C-N	-6.18	112.88	122.59
1	B	25	GLY	C-N-CA	-6.18	112.88	122.59
1	A	68	PHE	N-CA-C	-6.15	104.66	111.36
1	A	125	ILE	N-CA-C	-6.09	104.80	110.53
1	A	6	GLU	CA-C-N	6.02	132.24	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	GLU	C-N-CA	6.02	132.24	122.67
1	A	79	THR	O-C-N	6.01	128.49	122.12
1	B	45	GLU	N-CA-C	5.97	117.79	111.28
1	B	85	ILE	N-CA-C	5.95	116.13	110.42
1	A	8	GLN	N-CA-C	-5.95	104.14	111.33
1	B	16	PHE	N-CA-C	-5.94	104.80	111.28
1	B	74	ARG	N-CA-CB	-5.91	101.43	110.12
1	B	9	ILE	CA-C-O	-5.79	115.09	121.29
1	A	22	ASP	N-CA-C	5.66	120.05	113.20
1	A	89	PHE	CA-C-N	5.62	127.82	120.28
1	A	89	PHE	C-N-CA	5.62	127.82	120.28
1	A	120	GLU	N-CA-C	5.62	117.40	111.28
1	A	89	PHE	O-C-N	5.61	127.84	122.07
1	A	9	ILE	CB-CA-C	-5.60	104.69	112.02
1	A	106	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	B	69	LEU	CB-CA-C	-5.53	101.56	110.74
1	B	74	ARG	N-CA-C	5.53	117.31	111.28
1	B	32	LEU	N-CA-C	-5.52	105.34	111.36
1	B	100	ILE	CB-CA-C	-5.51	104.29	110.96
1	A	44	THR	N-CA-CB	-5.50	102.40	110.26
1	B	84	GLU	CA-C-N	5.47	127.45	120.56
1	B	84	GLU	C-N-CA	5.47	127.45	120.56
1	B	88	ALA	N-CA-C	-5.39	105.40	111.28
1	A	139	GLU	CB-CG-CD	5.36	121.72	112.60
1	B	141	PHE	N-CA-C	-5.26	105.46	111.14
1	A	51	MET	N-CA-C	-5.21	105.78	111.82
1	A	81	SER	CA-C-N	-5.17	112.95	120.29
1	A	81	SER	C-N-CA	-5.17	112.95	120.29
1	A	18	LEU	CA-CB-CG	5.16	134.36	116.30
1	B	123	GLU	CA-CB-CG	5.12	124.34	114.10
1	A	72	MET	N-CA-C	5.11	116.54	111.07
1	B	91	VAL	CB-CA-C	-5.11	105.24	112.14
1	B	72	MET	CB-CA-C	-5.06	102.90	110.90
1	B	130	ILE	CB-CG1-CD1	5.04	124.39	113.80
1	A	61	GLY	CA-C-O	5.01	124.57	119.01
1	A	90	ARG	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	A	7	GLU	Peptide
1	B	122	ASP	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	1236	0	1185	69	0
1	B	1254	0	1209	63	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	85	0	0	23	0
3	B	93	0	0	23	0
All	All	2676	0	2394	130	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 27.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:CB	1:A:79:THR:CG2	1.74	1.56
1:A:171:MET:CE	1:A:171:MET:SD	2.08	1.42
1:B:171:MET:SD	1:B:171:MET:CE	2.13	1.35
1:B:76:MET:SD	3:B:1091:HOH:O	2.15	1.05
1:B:121:VAL:O	1:B:122:ASP:C	2.00	1.01
1:B:4:LEU:O	1:B:8:GLN:HG3	1.61	0.98
1:B:7:GLU:O	1:B:11:GLU:HG3	1.69	0.92
1:A:106:ARG:HB3	3:A:1078:HOH:O	1.72	0.89
1:A:95:ASP:HA	3:A:1043:HOH:O	1.73	0.88
1:B:121:VAL:HG23	1:B:124:MET:HE3	1.57	0.86
1:A:117:THR:HG21	3:A:1061:HOH:O	1.76	0.85
1:A:64:ASP:HB2	3:A:1073:HOH:O	1.78	0.83
1:B:4:LEU:HD23	1:B:4:LEU:N	1.94	0.80
1:A:108:VAL:HG22	3:B:1017:HOH:O	1.85	0.76
1:A:172:ALA:HB2	1:B:39:LEU:HD22	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:MET:HA	1:B:145:MET:HE2	1.68	0.74
1:A:117:THR:CG2	1:A:120:GLU:H	2.00	0.74
1:A:117:THR:HG22	1:A:120:GLU:H	1.52	0.73
1:A:139:GLU:CG	3:A:1010:HOH:O	2.36	0.72
1:B:176:SER:CB	3:B:1095:HOH:O	2.38	0.72
1:B:144:MET:SD	1:B:145:MET:HE3	2.31	0.70
1:B:121:VAL:O	1:B:123:GLU:N	2.24	0.70
1:B:14:GLU:HG3	3:B:1060:HOH:O	1.92	0.69
1:B:19:PHE:HA	1:B:35:VAL:HG21	1.74	0.69
1:B:123:GLU:HA	3:B:1073:HOH:O	1.94	0.68
1:B:106:ARG:NH1	3:B:1049:HOH:O	2.26	0.68
1:B:4:LEU:CD2	1:B:9:ILE:HD11	2.25	0.66
1:A:107:HIS:O	1:A:111:ASN:ND2	2.28	0.66
1:B:176:SER:HB2	3:B:1095:HOH:O	1.96	0.64
1:B:4:LEU:N	1:B:4:LEU:CD2	2.60	0.64
1:A:5:THR:O	1:A:6:GLU:CG	2.46	0.64
1:A:112:LEU:HB2	3:A:1047:HOH:O	1.97	0.64
1:B:76:MET:HB3	3:B:1033:HOH:O	1.97	0.63
1:B:4:LEU:HD21	1:B:9:ILE:HD11	1.79	0.63
1:B:139:GLU:OE1	3:B:1029:HOH:O	2.15	0.63
1:A:161:ILE:C	3:A:1022:HOH:O	2.41	0.62
1:B:121:VAL:HG23	1:B:124:MET:CE	2.29	0.62
1:B:124:MET:HB2	3:B:1020:HOH:O	1.97	0.62
1:B:121:VAL:C	1:B:123:GLU:N	2.58	0.62
1:A:139:GLU:HG3	3:A:1010:HOH:O	1.96	0.62
1:A:7:GLU:HG3	3:A:1040:HOH:O	2.00	0.61
1:A:79:THR:CG2	1:A:79:THR:CA	2.73	0.60
1:B:106:ARG:CZ	3:B:1049:HOH:O	2.49	0.60
1:A:121:VAL:HG23	3:A:1066:HOH:O	2.02	0.60
1:A:79:THR:CG2	1:A:79:THR:OG1	2.45	0.59
1:A:121:VAL:C	3:A:1066:HOH:O	2.46	0.58
1:A:42:ASN:CG	3:A:1068:HOH:O	2.47	0.56
1:A:112:LEU:CB	3:A:1047:HOH:O	2.53	0.56
1:A:36:MET:HG2	1:A:43:PRO:HG3	1.85	0.56
1:A:42:ASN:ND2	3:A:1068:HOH:O	2.40	0.55
1:B:138:TYR:O	1:B:142:VAL:HG23	2.07	0.55
1:A:109:MET:HA	1:A:109:MET:HE2	1.88	0.54
1:B:173:ARG:HD2	3:B:1057:HOH:O	2.07	0.54
1:A:6:GLU:CG	1:A:8:GLN:HG3	2.37	0.54
1:B:4:LEU:O	1:B:5:THR:OG1	2.26	0.54
1:B:124:MET:HG3	3:B:1054:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:OD1	1:B:111:ASN:C	2.52	0.53
1:A:139:GLU:HG2	3:A:1010:HOH:O	2.04	0.52
1:A:5:THR:N	3:A:1025:HOH:O	2.43	0.52
1:A:7:GLU:O	1:A:11:GLU:HG3	2.09	0.51
1:A:121:VAL:HB	3:A:1066:HOH:O	2.09	0.51
1:A:167:ALA:O	1:A:171:MET:HG2	2.10	0.51
1:A:121:VAL:CB	3:A:1066:HOH:O	2.58	0.51
1:B:121:VAL:N	1:B:124:MET:HB3	2.26	0.51
1:B:21:LYS:HD3	3:B:1035:HOH:O	2.10	0.51
1:B:87:GLU:HG3	1:B:172:ALA:HB1	1.93	0.51
1:B:87:GLU:HG3	1:B:90:ARG:HH11	1.76	0.51
1:A:75:LYS:HD3	3:A:1021:HOH:O	2.11	0.50
1:A:112:LEU:HD21	1:A:164:LYS:HE3	1.93	0.50
1:A:117:THR:HG23	1:A:119:GLU:N	2.27	0.50
1:A:161:ILE:N	1:A:161:ILE:HD13	2.27	0.49
1:A:121:VAL:CG2	3:A:1066:HOH:O	2.59	0.49
1:A:5:THR:O	1:A:6:GLU:HG3	2.12	0.49
1:A:37:ARG:HA	1:A:41:GLN:O	2.12	0.49
1:A:44:THR:CG2	1:A:47:GLU:H	2.25	0.49
1:A:170:LYS:O	1:A:173:ARG:HB3	2.13	0.49
1:B:65:PHE:HB2	3:B:1064:HOH:O	2.13	0.48
1:A:14:GLU:OE1	1:B:164:LYS:HD3	2.14	0.47
1:B:162:ARG:HE	1:B:166:ARG:NH2	2.12	0.47
1:B:124:MET:HE2	3:B:1020:HOH:O	2.13	0.47
1:A:27:ILE:HB	1:A:63:ILE:HB	1.95	0.47
1:B:17:SER:HB2	3:B:1094:HOH:O	2.15	0.47
1:B:91:VAL:O	1:B:94:LYS:NZ	2.46	0.46
1:A:44:THR:HG22	1:A:47:GLU:HB2	1.98	0.46
1:B:121:VAL:N	1:B:124:MET:H	2.14	0.46
1:A:92:PHE:CE1	1:A:108:VAL:HG11	2.51	0.45
1:A:145:MET:HA	1:A:145:MET:HE2	1.97	0.45
1:A:64:ASP:OD1	1:A:64:ASP:C	2.59	0.45
1:B:65:PHE:N	1:B:66:PRO:HD2	2.31	0.45
1:A:6:GLU:HG3	1:A:8:GLN:H	1.82	0.45
1:A:145:MET:CE	1:A:162:ARG:HG3	2.46	0.45
1:B:121:VAL:C	1:B:123:GLU:H	2.25	0.44
1:A:54:GLU:O	1:A:74:ARG:NH1	2.51	0.44
1:B:52:ILE:HG12	1:B:63:ILE:CD1	2.47	0.44
1:B:52:ILE:HG12	1:B:63:ILE:HG13	2.00	0.44
1:A:92:PHE:CE1	1:A:108:VAL:CG1	3.01	0.44
1:A:49:GLN:HG3	3:A:1081:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD22	1:A:112:LEU:O	2.18	0.44
1:A:63:ILE:HD13	1:A:63:ILE:HG21	1.75	0.43
1:B:107:HIS:CD2	3:B:1043:HOH:O	2.69	0.43
1:B:64:ASP:OD1	1:B:67:GLU:HG3	2.19	0.43
1:A:5:THR:O	1:A:6:GLU:CB	2.66	0.43
1:A:51:MET:HB3	1:A:71:MET:HE2	2.00	0.43
1:B:123:GLU:O	1:B:127:GLU:HG3	2.19	0.42
1:A:117:THR:HG23	1:A:119:GLU:H	1.84	0.42
1:A:139:GLU:CD	1:A:139:GLU:H	2.27	0.42
1:B:7:GLU:HG3	1:B:11:GLU:OE1	2.20	0.42
1:B:4:LEU:HG	1:B:9:ILE:HD13	2.01	0.42
1:B:63:ILE:HA	1:B:67:GLU:OE2	2.19	0.42
1:B:105:LEU:HD22	1:B:125:ILE:HD11	2.01	0.42
1:B:76:MET:HG2	3:B:1033:HOH:O	2.20	0.42
1:B:144:MET:HE2	3:B:1054:HOH:O	2.19	0.42
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.94	0.42
1:A:94:LYS:HG3	3:A:1008:HOH:O	2.19	0.42
1:B:4:LEU:HG	1:B:9:ILE:CD1	2.50	0.41
1:A:6:GLU:CD	1:A:8:GLN:H	2.28	0.41
1:B:106:ARG:HB2	3:B:1050:HOH:O	2.20	0.41
1:A:72:MET:HA	1:A:72:MET:HE2	2.03	0.41
1:B:125:ILE:O	1:B:126:ARG:C	2.62	0.41
1:A:173:ARG:HD2	1:A:173:ARG:C	2.45	0.41
1:A:19:PHE:HA	1:A:35:VAL:HG21	2.03	0.41
1:A:112:LEU:C	1:A:112:LEU:CD2	2.94	0.41
1:B:76:MET:CG	3:B:1033:HOH:O	2.68	0.40
1:A:102:ALA:HB1	3:A:1066:HOH:O	2.20	0.40
1:B:76:MET:CB	3:B:1033:HOH:O	2.61	0.40
1:B:114:GLU:OE2	1:B:164:LYS:CE	2.70	0.40
1:A:143:GLN:HE21	1:A:143:GLN:HB3	1.59	0.40
1:A:117:THR:HG23	1:A:120:GLU:H	1.82	0.40
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.90	0.40
1:B:106:ARG:HG3	1:B:121:VAL:CG1	2.52	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	150/179 (84%)	142 (95%)	6 (4%)	2 (1%)	9	7
1	B	153/179 (86%)	144 (94%)	7 (5%)	2 (1%)	9	7
All	All	303/358 (85%)	286 (94%)	13 (4%)	4 (1%)	9	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	145	MET
1	B	122	ASP
1	B	123	GLU

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	133/146 (91%)	110 (83%)	23 (17%)	2	1
1	B	134/146 (92%)	109 (81%)	25 (19%)	1	1
All	All	267/292 (91%)	219 (82%)	48 (18%)	2	1

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	17	SER

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Mol	Chain	Res	Type
1	A	18	LEU
1	A	32	LEU
1	A	36	MET
1	A	44	THR
1	A	69	LEU
1	A	74	ARG
1	A	75	LYS
1	A	76	MET
1	A	81	SER
1	A	82	GLU
1	A	90	ARG
1	A	97	ASN
1	A	112	LEU
1	A	144	MET
1	A	145	MET
1	A	161	ILE
1	A	162	ARG
1	A	164	LYS
1	A	166	ARG
1	A	170	LYS
1	A	173	ARG
1	B	4	LEU
1	B	7	GLU
1	B	14	GLU
1	B	18	LEU
1	B	26	THR
1	B	36	MET
1	B	39	LEU
1	B	49	GLN
1	B	54	GLU
1	B	69	LEU
1	B	77	LYS
1	B	86	ARG
1	B	87	GLU
1	B	90	ARG
1	B	94	LYS
1	B	97	ASN
1	B	122	ASP
1	B	123	GLU
1	B	143	GLN
1	B	144	MET
1	B	157	ARG

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Mol	Chain	Res	Type
1	B	158	LYS
1	B	164	LYS
1	B	170	LYS
1	B	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	49	GLN
1	A	111	ASN
1	A	143	GLN
1	B	49	GLN
1	B	53	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [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	156/179 (87%)	0.78	11 (7%) 22 21	27, 32, 43, 50	0
1	B	159/179 (88%)	0.70	9 (5%) 29 28	21, 33, 45, 62	0
All	All	315/358 (87%)	0.74	20 (6%) 26 25	21, 33, 44, 62	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	ALA	4.5
1	A	46	ALA	4.0
1	A	161	ILE	3.7
1	B	25	GLY	3.6
1	B	156	ALA	3.3
1	A	163	ASN	3.2
1	B	103	ALA	2.8
1	B	40	GLY	2.8
1	B	147	ALA	2.7
1	A	78	ASP	2.5
1	A	175	PHE	2.5
1	B	24	ASP	2.4
1	A	110	THR	2.4
1	A	5	THR	2.3
1	B	113	GLY	2.3
1	B	23	GLY	2.1
1	B	59	GLY	2.1
1	A	44	THR	2.1
1	A	146	THR	2.1
1	A	7	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
2	CA	B	1002	1/1	0.90	0.13	48,48,48,48	0
2	CA	B	1001	1/1	0.93	0.20	62,62,62,62	0
2	CA	A	1003	1/1	0.99	0.08	32,32,32,32	0
2	CA	A	1004	1/1	0.99	0.16	33,33,33,33	0
2	CA	A	1001	1/1	0.99	0.12	36,36,36,36	0
2	CA	A	1002	1/1	0.99	0.10	44,44,44,44	0
2	CA	B	1003	1/1	0.99	0.10	39,39,39,39	0
2	CA	B	1004	1/1	0.99	0.10	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.